Chapter 1: Essential Ideas

Key Concepts

1.1 Chemistry as a Science: Introduction of the History of Chemistry

1.2 Description of Matter

1.3 Physical and Chemical Properties

1.4 Measurements and Significant Figures

1.5 SI Units

1.6 Dimensional Analysis

I. Chemistry as a Science: Introduction of the History of Chemistry

Ancient Chemistry

In the era of the ancient Greeks, people tried to explain the chemical changes they observed. At that time, natural objects were thought to consist of only four basic elements: earth, air, fire, and water. Then, in the fourth century BC, two Greek philosophers, **Democritus** and **Leucippus**, suggested that matter was not infinitely divisible into smaller particles but instead consisted of fundamental, indivisible particles called **atoms**. Unfortunately, these early philosophers did not have the technology to test their hypothesis. They would have been unlikely to do so in any case because the ancient Greeks did not conduct experiments or use the scientific method. They believed that the nature of the universe could be discovered by rational thought alone. In the Middle Ages and Renaissance, two millennia after the ancient Greeks, **alchemists**, who engaged in a form of chemistry and speculative philosophy achieved many advances in chemistry. Their major goal was to convert certain elements into others by a process they called transmutation. In particular, alchemists wanted to find a way to transform cheaper metals into gold. Although most alchemists did not approach chemistry systematically and many appear to have been outright frauds, alchemists in China, the Arab kingdoms, and medieval Europe made major contributions, including the discovery of elements such as quicksilver (mercury) and the preparation of several strong acids.

Figure 1.1 Alchemist, the chemists of the Middle Ages and Renaissance, achieved many advances in science.

Ref: commons.wikimedia.org/

Modern Chemistry

Modern chemistry beginnings are centered in the 16th and 17th centuries. During this period, great advances were made in metallurgy, the extraction of metals from ores, and the first systematic quantitative experiments were carried out. In 1661, the Englishman **Robert Boyle** (1627–91) published The Sceptical Chymist, which described the relationship between the pressure and the volume of air. More important, Boyle defined an element as a substance that cannot be broken down into two or more simpler substances by chemical means. This led to the identification of a large number of elements, many of which were metals. Ironically, Boyle himself never thought that metals were elements.

In the 18th century, the English clergyman **Joseph Priestley** (1733–1804) discovered oxygen gas and found that many carbon-containing materials burn vigorously in an oxygen atmosphere, a process called **combustion**. Priestley also discovered that the gas produced by fermenting beer, which we now know to be carbon dioxide, is the same as one of the gaseous products of combustion. Although Priestley did not understand its identity, he found that carbon dioxide dissolved in water to produce seltzer water. In essence, he may be considered the founder of the multibillion-dollar carbonated soft drink industry.

Chemistry as a Central Science

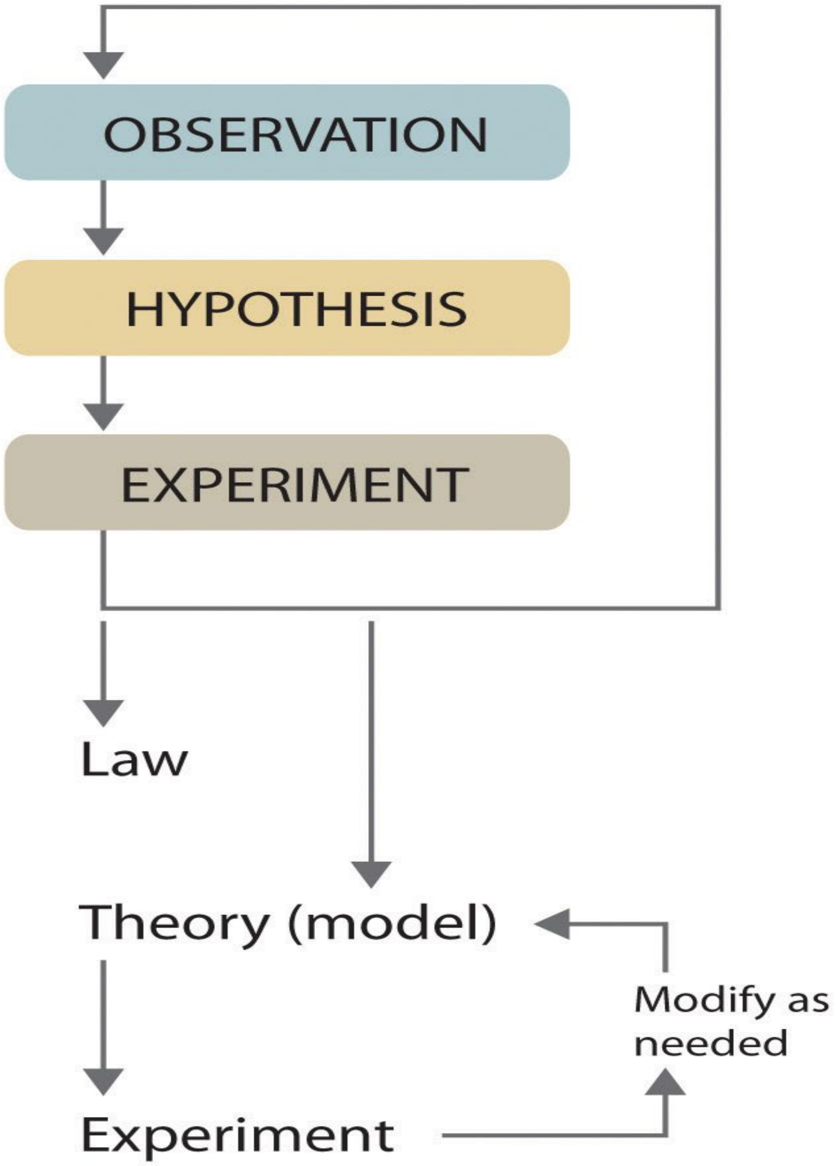
Chemistry is the study of matter and the changes that material substances undergo. Of all the scientific disciplines, it is perhaps the most extensively connected to other fields of study. Chemistry is a central science! **Geologists** who want to locate new mineral or oil deposits use chemical techniques to analyze and identify rock samples. **Oceanographers** use chemistry to track ocean currents, determine the flux of nutrients into the sea, and measure the rate of exchange of nutrients between ocean layers. **Engineers** consider the relationships between the structures and the properties of substances when they specify materials for various uses. **Physicists** take advantage of the properties of substances to detect new subatomic particles. **Astronomers** use chemical signatures to determine the age and distance of stars and thus answer questions about how stars form and how old the universe is. The entire subject of **environmental science** depends on chemistry to explain the origin and impacts of phenomena such as air pollution, ozone layer depletion, and global warming.

The disciplines that focus on living organisms and their interactions with the physical world rely heavily on **biochemistry**, the application of chemistry to the study of biological processes. A living cell contains a large collection of complex molecules that carry out thousands of chemical reactions, including those that are necessary for the cell to reproduce. Biological phenomena such as vision, taste, smell, and movement result from numerous chemical reactions. Fields such as medicine, pharmacology, nutrition, and toxicology focus specifically on how the chemical substances that enter our bodies interact with the chemical components of the body to maintain our health and well-being. For example, in the specialized area of sports medicine, a knowledge of chemistry is needed to understand why muscles get sore after exercise as well as how prolonged exercise produces the euphoric feeling known as "runner's high."

Although law is not normally considered a field related to chemistry, forensic scientists use chemical methods to analyze blood, fibers, and other evidence as they investigate crimes. In particular, DNA matching—comparing biological samples of genetic material to see whether they could have come from the same person—has been used to solve many high-profile criminal cases as well as clear innocent people who have been wrongly accused or convicted. Forensics is a rapidly growing area of applied chemistry. In addition, the proliferation of chemical and biochemical innovations in industry is producing rapid growth in the area of patent law. Therefore, chemistry is the study of matter and the changes material substances undergo. It is essential for understanding much of the natural world and central to many other scientific disciplines, including astronomy, geology, paleontology, biology, and medicine.

The Scientific Method

Scientists search for answers to questions and solutions to problems by using a procedure called the **scientific method**. This procedure consists of making observations, formulating hypotheses, and designing experiments, which in turn lead to additional observations, hypotheses, and experiments in repeated cycles (Figure 1.2).



Ref: commons.wikimedia.org/

As depicted in this flowchart, the scientific method consists of making observations, formulating hypotheses, and designing experiments. A scientist may enter the cycle at any point.

Observations can be qualitative or quantitative. **Qualitative observations** describe properties or occurrences in ways that do not rely on numbers. Examples of qualitative observations include the following: the outside air temperature is cooler during the winter season, table salt is a crystalline solid, sulfur crystals are yellow, and dissolving a penny in dilute nitric acid forms a blue solution and a brown gas. **Quantitative observations** are measurements, which by definition consist of both a number and a unit. Examples of quantitative observations include the following: the melting point of crystalline sulfur is 115.21 degrees Celsius, and 35.9 grams of table salt—whose chemical name is sodium chloride—dissolve in 100 grams of water at 20 degrees Celsius.

After deciding to learn more about an observation or a set of observations, scientists generally begin an investigation by forming a **hypothesis**, a tentative explanation for the observation(s). The hypothesis may not be correct, but it puts the scientist's understanding of the system being studied into a form that can be tested. For example, the observation that we experience alternating periods of light and darkness corresponding to observed movements of the sun, moon, clouds, and shadows is consistent with either of two hypotheses: (1) Earth rotates on its axis every 24 hours, alternately exposing one side to the sun, or (2) the sun revolves around Earth every 24 hours. Suitable experiments can be designed to choose between these two alternatives. After a hypothesis has been formed, scientists conduct experiments to test its validity. **Experiments** are systematic observations or measurements, preferably made under controlled conditions—that is, under conditions in which a single variable changes. A properly designed and executed experiment enables a scientist to determine whether the original hypothesis is valid. Experiments often demonstrate that the hypothesis is incorrect or that it must be modified. More experimental data are then collected and analyzed, at which point a scientist may begin to think that the results are sufficiently reproducible (i.e., dependable) to merit being summarized in a **law**, a verbal or mathematical description of a phenomenon that allows for general predictions. A law simply says what happens; it does not address the question of why. One example of a law, the law of definite proportions, which was discovered by the French scientist Joseph Proust (1754–1826), states that a chemical substance always contains the same proportions of elements by mass. Thus, sodium chloride (table salt) always contains the same proportion by mass of sodium to chlorine, in this case 39.34% sodium and 60.66% chlorine by mass, and sucrose (table sugar) is always 42.11% carbon, 6.48% hydrogen, and 51.41% oxygen by mass. Whereas a law states only what happens, a **theory** attempts to explain why nature behaves as it does. Laws are unlikely to change greatly over time unless a major experimental error is discovered. In contrast, a theory, by definition, is incomplete and imperfect, evolving with time to explain new facts as they are discovered.

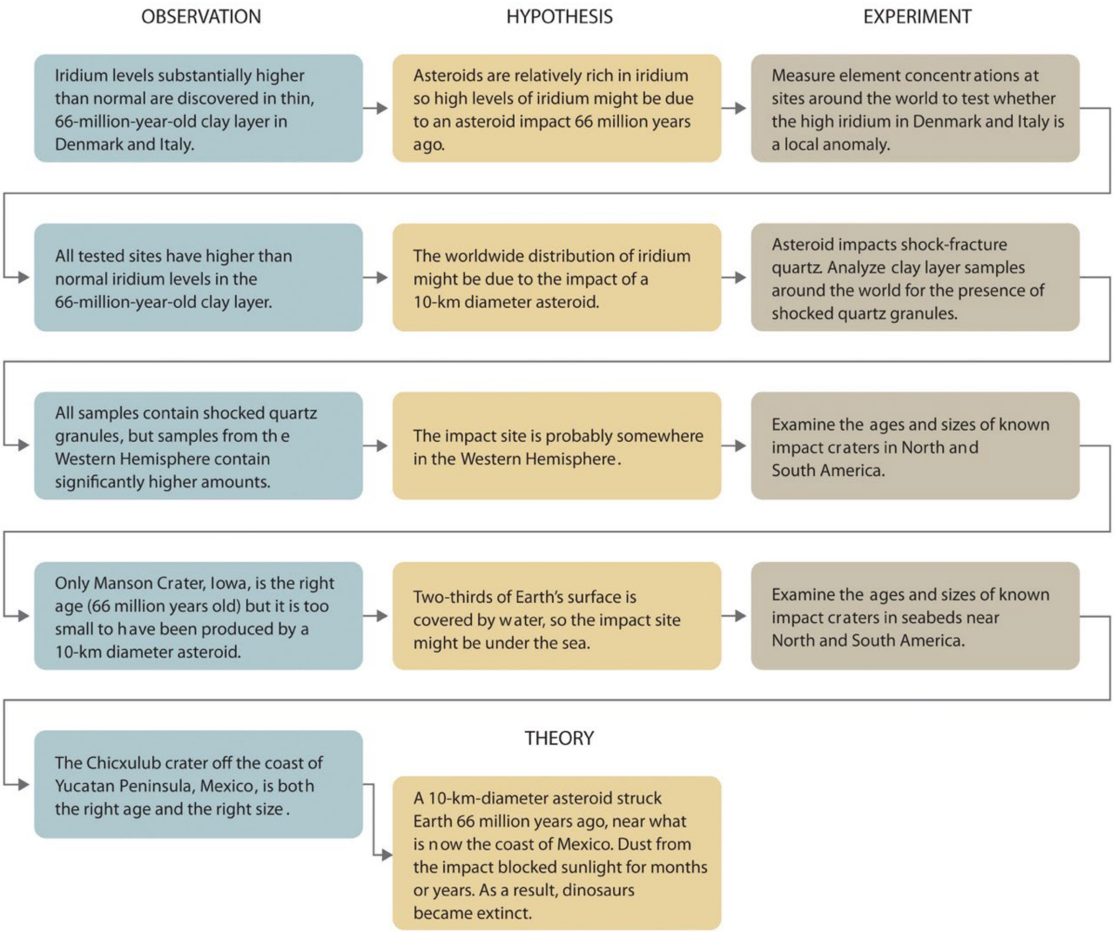


Figure 1.3 The scientific method

Ref: commons.wikimedia.org/

EXAMPLE 1

Classify each statement as a law, a theory, an experiment, a hypothesis, a qualitative observation, or a quantitative observation.

1. Ice always floats on liquid water.
2. Birds evolved from dinosaurs.
3. Hot air is less dense than cold air, probably because the components of hot air are moving more rapidly.
4. When 10 g of ice were added to 100 mL of water at 25°C, the temperature of the water decreased to 15.5°C after the ice melted.
5. The ingredients of Ivory soap were analyzed to see whether it really is 99.44% pure, as advertised.

Solution:

Given: components of the scientific method

Asked for: statement classification

Strategy:

Refer to the definitions in this section to determine which category best describes each statement.

Answers:

1. This is a general statement of a relationship between the properties of liquid and solid water, so it is a law.
2. This is a possible explanation for the origin of birds, so it is a hypothesis.
3. This is a statement that tries to explain the relationship between the temperature and the density of air based on fundamental principles, so it is a theory.
4. The temperature is measured before and after a change is made in a system, so these are quantitative observations.
5. This is an analysis designed to test a hypothesis (in this case, the manufacturer's claim of purity), so it is an experiment.

Because scientists can enter the scientific method cycle at any point, the actual application of the scientific method to different topics can take many different forms. For example, a scientist may start with a hypothesis formed by reading about work done by others in the field, rather than by making direct observations. In summary, chemists expand their knowledge by observing, carrying out experiments, and testing hypotheses to develop laws to summarize their results and theories to explain them. In doing so, they are using the scientific method. Therefore, chemists expand their knowledge by using the scientific method.

Math skills required in this course:

As a freshman chemistry student, it is your responsibility to ensure that you can do the basic types of math discussed in this letter. Your grade depends on being familiar with the math requirements in the course. This math is nothing new—you have been taught this over the years. This instruction should only be a review of what you already know.

1) Algebra: Algebra is used to solve equations by un-doing whatever is being done to an unknown variable. For example, if an equation has “x+2” then you would subtract “2” to solve for “x”. Everything that is done to one side must be done to the other side of the equation as well.

Visit the following websites and observe how algebraic equations are manipulated.

https://www.youtube.com/watch?v=dM3UQrx91ms

https://www.youtube.com/watch?v=BpLHHTY_umM

https://www.youtube.com/watch?v=chmHzxfM3L0

On the Khan Academy website make sure you solve the practice problems

https://www.khanacademy.org/math/algebra2/modeling-with-algebra#manipulating-formulas

Simplify the following:

1. X+ b= c

X?

Subtract b from both sides

X+b-b= c-b

X= c-b

2. X/A= B

   X=?

   X= A.B

3. F/X= G

X=?

X= F/G

$X= \frac{A/B}{R/S}$ =?? Ans: AS/BR [Explanation:[(A/B)*(S/R)]

$\frac{12}{4/3}$ = Ans is 9 not 1

2) Review on Exponentials

Practice:

Express in nonexponential form.

1. 10^3 = 10 x 10 x 10 = 1000 (The exponent tells you how many zeroes)

2. 10^7 = 10,000,000

3. 10^1 = 10 (Exponent of 1 tells you there is one zero)

4. 10^0 = 1 (Exponent of zero tells you there is no zero.

Also, remember that anything to the power of zero equals to 1.)

5. 10^{-3} = ? (There are two ways to look at this.) A negative exponent means it is the inverse, or reciprocal. 10–3 = 1/103 = 1/1000 = 0.001 (one thousandth) Or, you can consider 10–3 = 1 x 10–3. To convert to the nonexponential form, the exponent must increase by 3, from –3 to 0. This means the decimal point must move 3 places to the left of 1. Thus, 10–3 = 0.001

6. 10–6 = 0.000001 (Decimal is 6 places to the left of 1).

7. When you raise an exponent to a power, you multiply the exponents. (10a) b = 10a x b

1. $(10^3\ )\ 4 = 10^{3x4} = 10^{12}$ = 1,000,000,000,000

2. $(10–1)\ ^3 = 10^{-3}$ = 0.001

3. $(2 \text{ x } 10^{-2})\ ^3 = 23 \text{ x } 10^{-6} = 8 \text{ x } 10^{-6}$ = 0.000008

4. $(2 + 102\ )\ ^2 = (2 + 100)^2 = 102^2$ = 10404 $(2 + 102\ )\ ^2$ is NOT (22 + 104) which would give you the wrong answer of 10004! The distributive pr^{2}operty in question 3 above does not apply when you are doing an addition or subtraction within the parenthesis.

3) Calculator tips: Ask your instructor on how to operate your calculator

4) Order of Operation: Even though your calculator may know some of the rules below and do it correctly, you need to know the rules yourself so that you enter the numbers in the right order. This is the order:

1. Do operations inside the parenthesis first.

2. Do logarithms, and powers next.

3. Do multiplication and divisions next.

4. Do addition and subtraction last.

Given the problem: 4 + 9 ÷ 3 − 2 x 3 + (3 + 1) x 4 First think about which operation must be done FIRST. First you do 9 ÷ 3 = 3 and 2 x 3 = 6 and (3+1) = 4 and so (3+1) x 4 becomes 4 x 4 = 16. Then you do 4 + 3 − 6 + 16 = 17 So 4 + 9 ÷ 3 − 2 x 3 + (3 + 1) x 4 = 4 + 3 − 6 + 16 = 17 (The correct answer is 17.)

Now try it with your calculator. Try entering in exactly the same order as written: 4 + 9 ÷ 3 – 2 x 3 + (3+1) x 4 You should be getting the same answer of 17. Unless you have an ancient calculator, your calculator should know to do the operations inside a parenthesis, and the multiplication and division first before addition and subtraction. What you don’t want to do is to press ENTER after 4+9 before pressing ÷ 3. If you did, you are telling the calculator to do 4+9 before dividing by 3, but the problem does not tell you to add first. You are supposed to do 9 ÷3 before adding 4 to it. Now, using your calculator, do the following calculation without writing down intermediate answers. In other words, use “chain operation” to do the following computations: 5.7 x 2.8 3.1 x 4.2 The answer should be 0.815789474… If you calculator shows 6.395789473… you have entered the operations incorrectly into your calculator. You must have entered the steps in this order: 3.1 x 4.2 ÷ (5.7 x 2.8) which is incorrect. The correct way to enter the operations is to either put parenthesis around the terms in the numerator and denominator ( ) ( ) = 5.7 x 2.8 3.1 x 4.2 or remember that 2.8 is in the denominator, so you need to press ÷ not X: 3.1 X 4.2 ÷ 5.7 ÷ 2.8

It is important you understand this sequence of operations because you will OFTEN be needing to do this type of calculations this semester..

Practice with this problem, using your calculator: $$\frac{3.2 \times 10^{32} \times 5.1 \times 10^{-12}}{7.4 \times 10^{12}}$$

answer 2.205405×10^{-9}

Units can be handled just like algebraic terms.

$\frac{\text{gallon}}{\text{gallon/mile}}$ = gallon* mile/gallon= mile

*** **A short math review worksheet is provided for practice**

Section 1.2 Description of Matter: Classification of Matter

Chemists study the structures, physical properties, and chemical properties of material substances. These consist of **matter**, which is anything that occupies space and has mass. Gold and iridium are matter, as are peanuts, people, and postage stamps. Smoke, smog, and laughing gas are matter. Energy, light, and sound, however, are not matter; ideas and emotions are also not matter. The **mass** of an object is the quantity of matter it contains. Do not confuse an object's mass with its weight, which is a force caused by the gravitational attraction that operates on the object. Mass is a fundamental property of an object that does not depend on its location. In physical terms, the mass of an object is directly proportional to the force required to change its speed or direction. Weight, on the other hand, depends on the location of an object. An astronaut whose mass is 95 kg weighs about 210 lb on Earth, but only about 35 lb on the moon because the gravitational force he or she experiences on the moon is approximately one-sixth the force experienced on Earth. For practical purposes, weight and mass are often used interchangeably in laboratories.

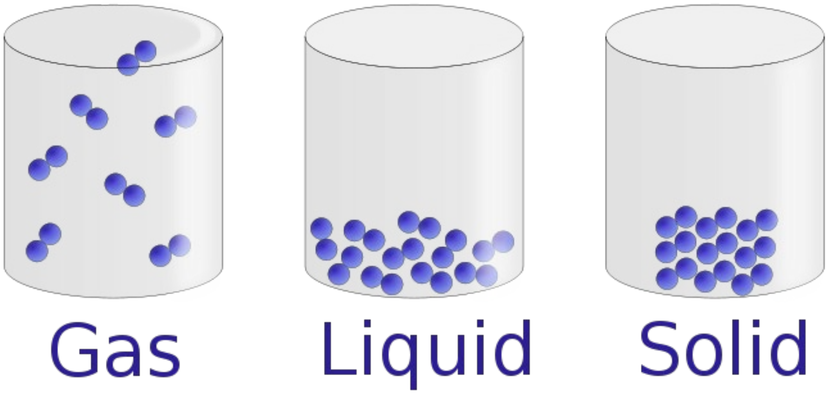


Fig. 1.4 Molecular view of State of Matter

Ref: commons.wikimedia.org/

Under normal conditions, there are three distinct states of matter: **solids, liquids, and gases** (Figure 1.4). **Solids** are relatively rigid and have fixed shapes and volumes. A rock, for example, is a solid. In contrast, **liquids** have fixed volumes but flow to assume the shape of their containers, such as a beverage in a can. **Gases**, such as air in an automobile tire, have neither fixed shapes nor fixed volumes and expand to completely fill their containers. Whereas the volume of gases strongly depends on their temperature and pressure (the amount of force exerted on a given area), the volumes of liquids and solids are virtually independent of temperature and pressure.

Solid iodine $I_2(s)$

Liquid bromine $Br_2(l)$

Gaseous chlorine $Cl_2(g)$

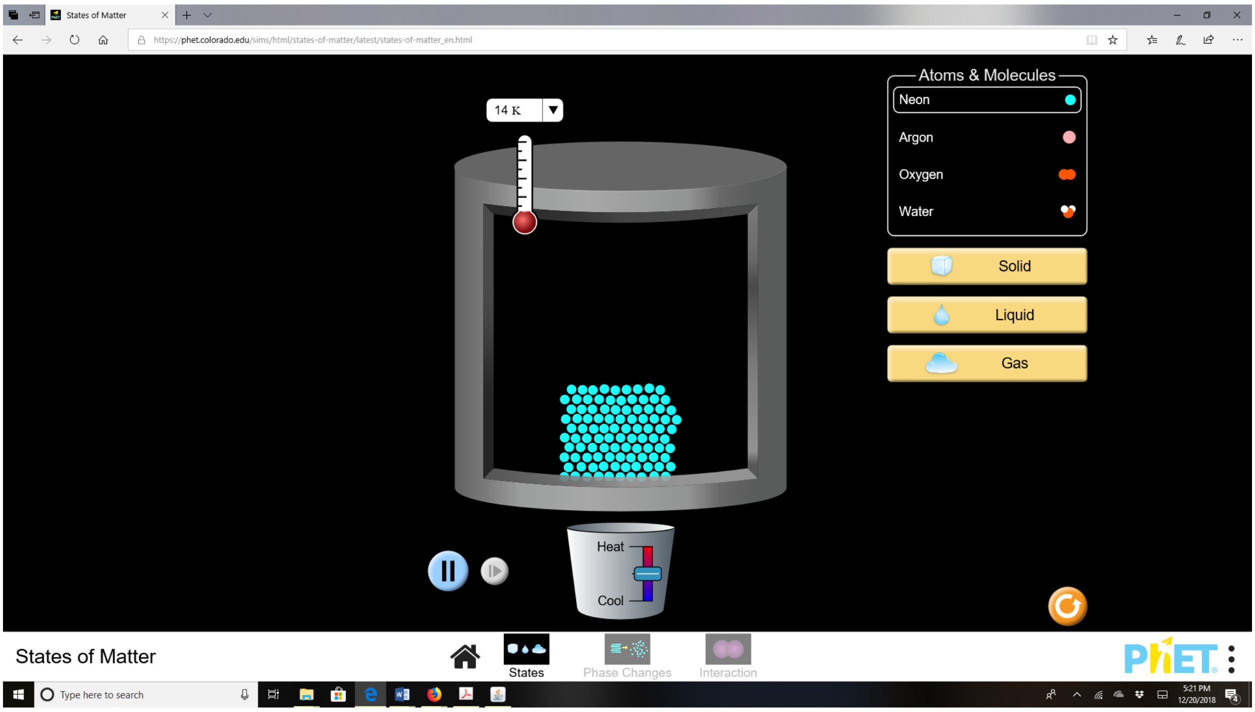
Figure 1.5 The States of Matter

Ref: commons.wikimedia.org/

Solids have a defined shape and volume. **Liquids** have a fixed volume but flow to assume the shape of their containers. **Gases** completely fill their containers, regardless of volume.

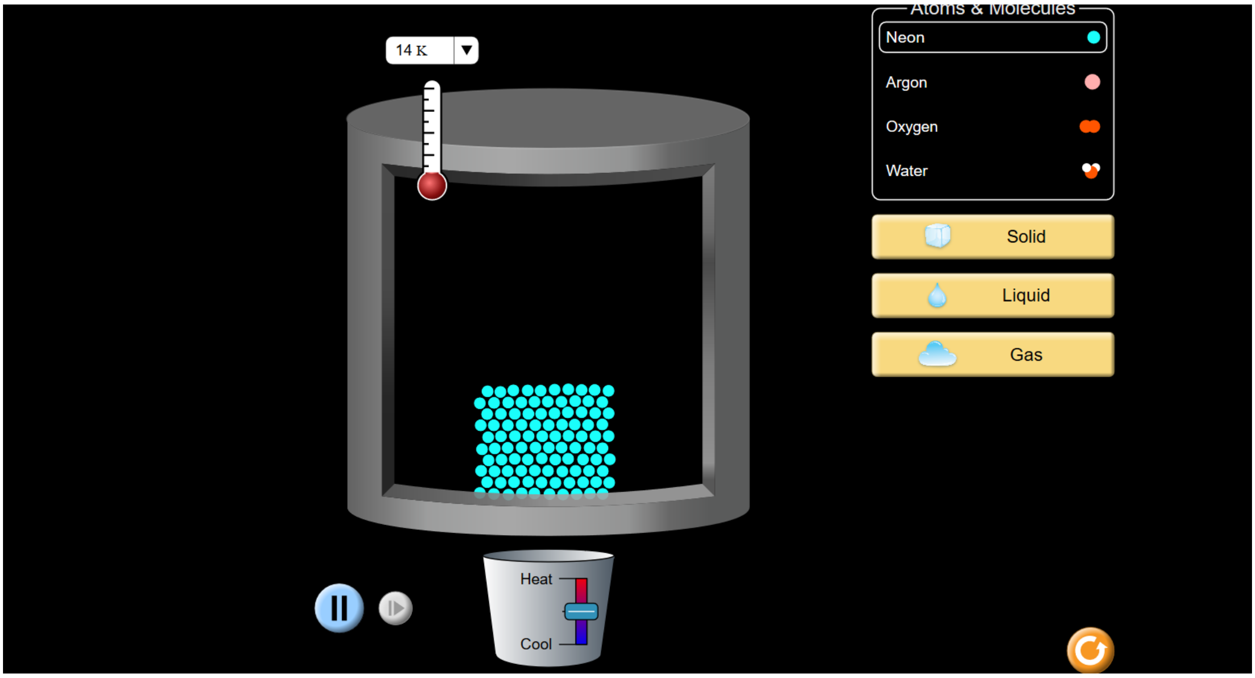
Try this out!

https://phet.colorado.edu/sims/html/states-of-matter/latest/states-of-matter_en.html



Go to the above PHET simulation activity of states of matter.

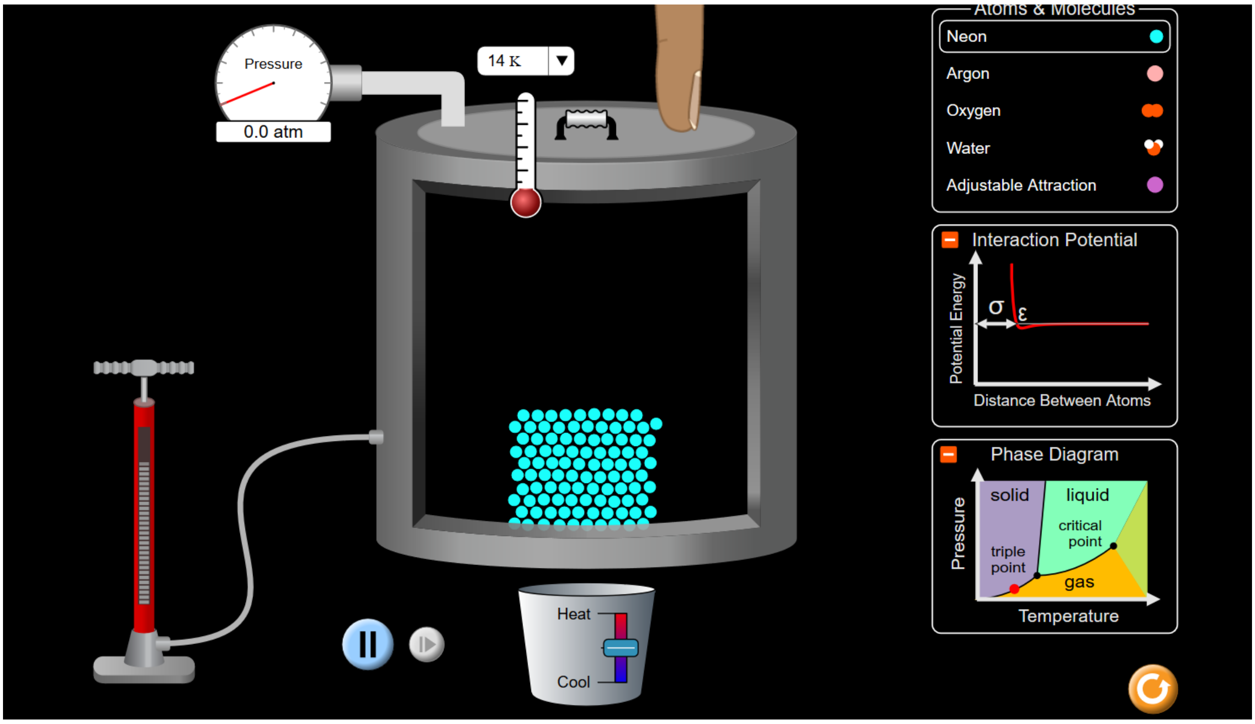
1) Click on Neon and observe the motion as solid liquid and gas. What do you notice?
2) Change the substance from Neon to Argon and click on solid, liquid and gas respectively. Both are atoms. What do you observe?
3) Now change to molecules like oxygen and water. What do you observe?
4) What do you observe when you increase or decrease the temperature of solid, liquid and gas?



Now Click on the phase change tab and press the finger to increase the pressure for solid, liquid and gas.

5) Which states of matter can be mostly compressed?

6) What do you conclude about volume and shape of three states of matter from this experiment?



Ans: 1) Solid particles are rigid with little vibration, liquid particles are slightly mobile, gas particles are moving with high speed, colliding with each other.

2) same

3) same

4) kinetic energy decreases with decreasing temp and increases with increasing with temperature

5) Gas

6) With increasing motion

Observable properties of matter

The science of chemistry developed from observations made about the nature and behavior of different kinds of matter, which we refer to collectively as the ***properties*** of matter.

The properties we refer to in this lesson are all ***macroscopic*** properties: those that can be observed in bulk matter. At the ***microscopic*** level, matter is of course characterized by its *structure*: the spatial arrangement of the individual atoms in a molecular unit or an extended solid.

The study of matter begins with the study of its *properties*

By observing a sample of matter and measuring its various properties, we gradually acquire enough information to *characterize* it; to distinguish it from other kinds of matter. This is the first step in the development of chemical science, in which interest is focussed on specific kinds of matter and the transformations between them.

Extensive and intensive properties

If you think about the various observable properties of matter, it will become apparent that these fall into two classes. Some properties, such as mass and volume, depend on the *quantity* of matter in the sample we are studying. Clearly, these properties, as important as they may be, cannot by themselves be used to characterize a kind of matter; to say that "water has a mass of 2 kg" is nonsense, although it may be quite true in a particular instance. Properties of this kind are called ***extensive properties*** of matter.

This definition of the density illustrates an important general rule: the **ratio of two extensive properties is always an *intensive* property**.

Suppose we make further measurements, and find that the same quantity of water whose mass is 2.0 kg also occupies a volume of 2.0 liters. We have measured two extensive properties (mass and volume) of the same sample of matter. This allows us to define a new quantity, the quotient m/V which defines another property of water which we call the ***density***. Unlike the mass and the volume, which by themselves refer only to individual samples of water, the density (mass per unit volume) is a property of *all* samples of pure water at the same temperature. Density is an example of an ***intensive property*** of matter.

Intensive properties are extremely important, because every possible kind of matter possesses a unique set of intensive properties that distinguishes it from every other kind of matter. Some intensive properties can be determined by simple observations: color (absorption spectrum), melting point, density, solubility, acidic or alkaline nature, and density are common examples. Even more fundamental, but less directly observable, is chemical composition.

The more intensive properties we know, the more precisely we can characterize a sample of matter.

Intensive properties are extremely important, because every possible kind of matter possesses a unique set of intensive properties that distinguishes it from every other kind of matter. In other words, **intensive properties serve to characterize matter**. Many of the intensive properties depend on such variables as the temperature and pressure, but the ways in which these properties change with such variables can themselves be regarded as intensive properties.

Problem Example:

Classify each of the following as an extensive or intensive property.

The volume of beer in a mug	ext; depends on size of the mug.
The percentage of alcohol in the beer	int; same for any same-sized sample.
The number of calories of energy you derive from eating a banana	ext; depends on size and sugar content of the banana.
The number of calories of energy made available to your body when you consume 10.0 g of sugar	int; same for any 10-g portion of sugar.
The mass of iron present in your blood	ext; depends on volume of blood in the body.
The mass of iron present in 5 mL of your blood	int; the same for any 5-mL sample.
The electrical resistance of a piece of 22-gauge copper wire.	ext; depends on length of the wire.
The electrical resistance of a 1-km length of 22-gauge copper wire	int; same for any 1-km length of the same wire.
The pressure of air in a bicycle tire	pressure itself is intensive, but is also dependent on the quantity of air in the tire.

The last example shows that not everything is black or white!

But we often encounter matter that is not uniform throughout, whose different parts exhibit different sets of intensive properties. This brings up another distinction that we address immediately below.

Pure Substances and Mixtures

A **pure chemical substance** is any matter that has a fixed chemical composition and characteristic properties. Oxygen, for example, is a pure chemical substance that is a colorless, odorless gas at 25°C. Very few samples of matter consist of pure substances; instead, most are **mixtures**, which are combinations of two or more pure substances in variable proportions in which the individual substances retain their identity. Air, tap water, milk, blue cheese, bread, and dirt are all mixtures. If all portions of a material are in the same state, have no visible boundaries, and are uniform throughout, then the material is **homogeneous**. Examples of homogeneous mixtures are the air we breathe and the tap water we drink. **Homogeneous mixtures are also called solutions.** Thus, air is a solution of nitrogen, oxygen, water vapor, carbon dioxide, and several other gases; tap water is a solution of small amounts of several substances in water. Although most solutions we encounter are liquid, solutions can also be solid. The gray substance still used by some dentists to fill tooth cavities is a complex solid solution that contains 50% mercury and 50% of a powder that contains mostly silver, tin, and copper, with small amounts of zinc and mercury. Solid solutions of two or more metals are commonly called **alloys**.

If the composition of a material is not completely uniform, then it is **heterogeneous** (e.g., chocolate chip cookie dough, blue cheese, and dirt). Mixtures that appear to be homogeneous are often found to be heterogeneous after microscopic examination. Milk, for example, appears to be homogeneous, but when examined under a microscope, it clearly consists of tiny globules of fat and protein dispersed in water (Figure 1.5). Milk is actually a colloidal solution (see below).

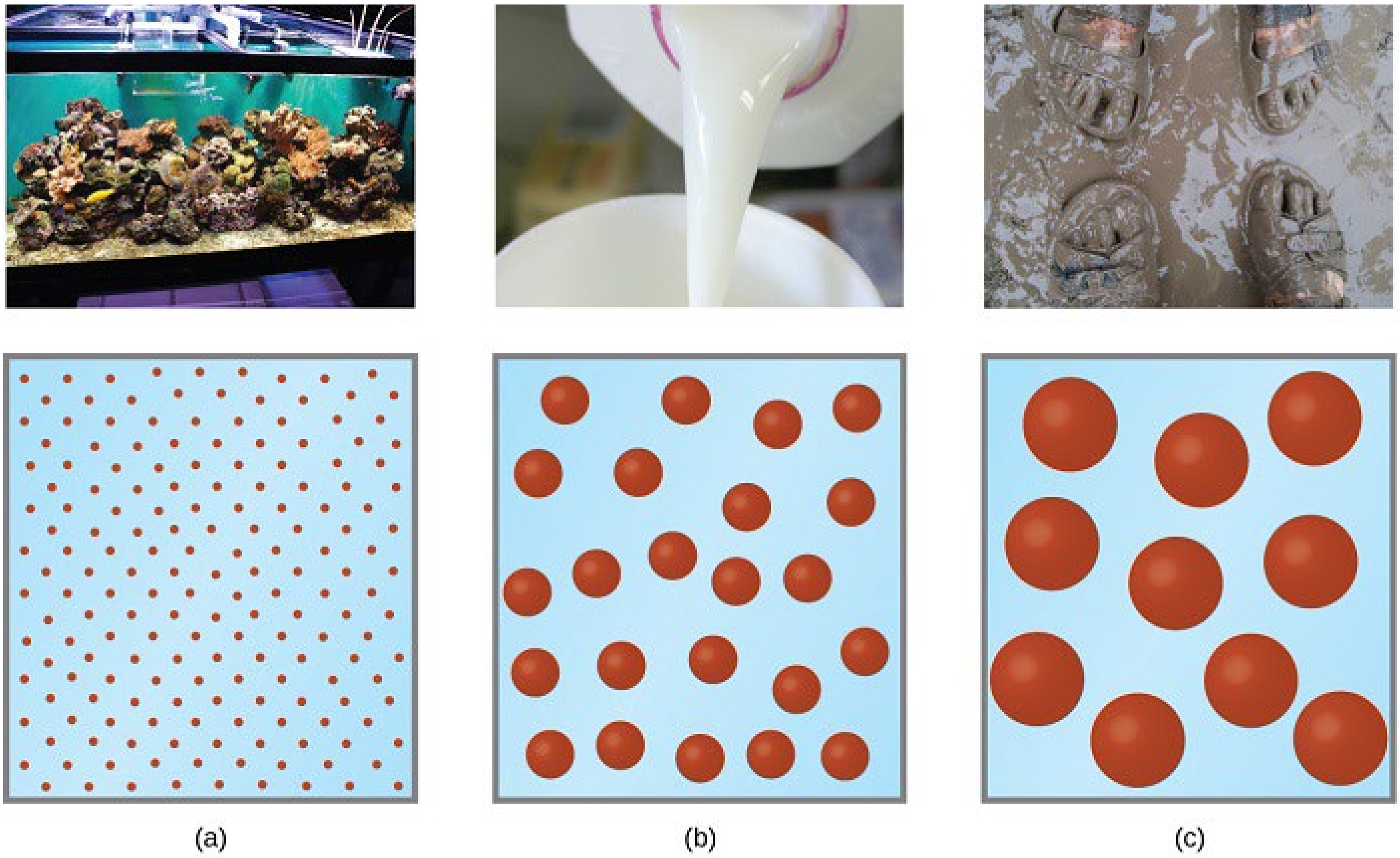


Figure 1.6 (a) A solution is a homogeneous mixture that appears clear, such as the saltwater in this aquarium. (b) In a colloid, such as milk, the particles are much larger but remain dispersed and do not settle. (c) A suspension, such as mud, is a heterogeneous mixture of suspended particles that appears cloudy and in which the particles can settle. (credit a photo: modification of work by Adam Wimsatt; credit b photo: modification of work by Melissa Wiese; credit c photo: modification of work by Peter Burgess)

Ref:

https://chem.libretexts.org/Bookshelves/General_Chemistry/Chemistry_(OpenSTAX)/11%3A_Solutions_and_Colloids/11.5%3A_Colloids

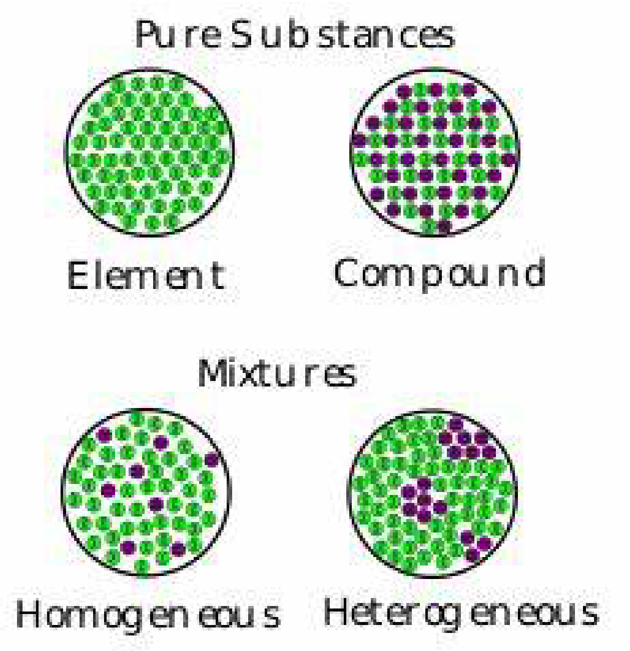
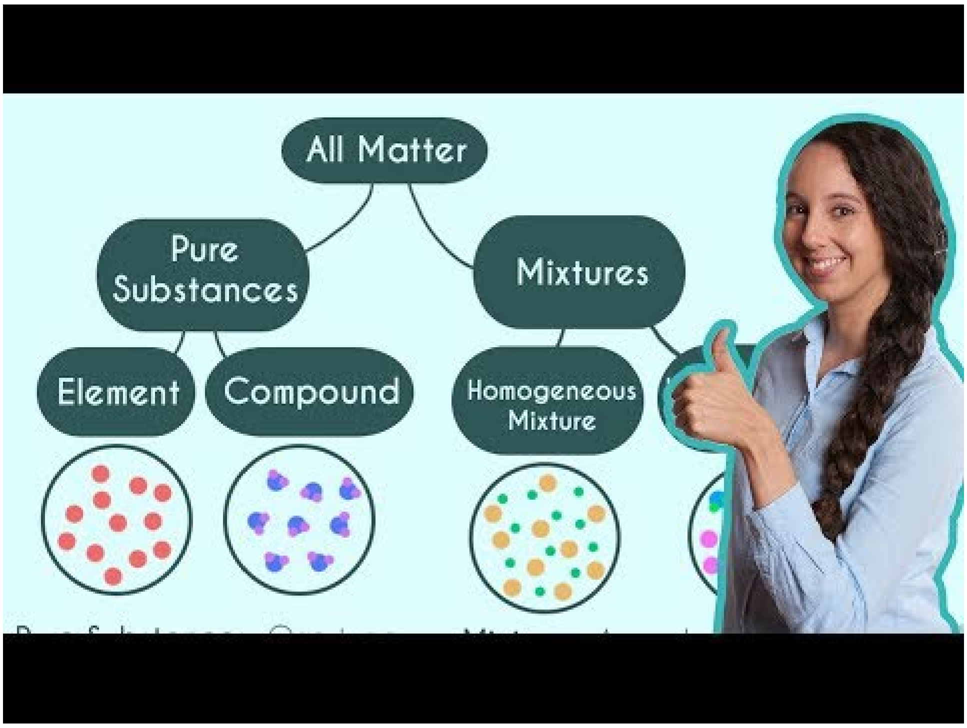


Fig. 1.7 Pure substances vs. Mixtures

Ref: commons.wikimedia.org/



The components of heterogeneous mixtures can usually be separated by simple means. Solid-liquid mixtures such as sand in water or tea leaves in tea are readily separated by filtration, which consists of passing the mixture through a barrier, such as a strainer, with holes or pores that are smaller than the solid particles. In principle, mixtures of two or more solids, such as sugar and salt, can be separated by microscopic inspection and sorting. More complex operations are usually necessary, though, such as when separating gold nuggets from river gravel by panning. First solid material is filtered from river water; then the solids are separated by inspection. If gold is embedded in rock, it may have to be isolated using chemical methods. **Homogeneous mixtures (solutions)** can be separated into their component substances by physical processes that rely on differences in some physical property, such as differences in their boiling points. Two of these separation methods are distillation and crystallization. **Distillation** makes use of differences in volatility, a measure of how easily a substance is converted to a gas at a given temperature. Figure 1.6 shows a simple distillation apparatus for separating a mixture of substances, at least one of which is a liquid. The most volatile component boils first and is condensed back to a liquid in the water-cooled condenser, from which it flows into the receiving flask. If a solution of salt and water is distilled, for example, the more volatile component, pure water, collects in the receiving flask, while the salt remains in the distillation flask. The solution

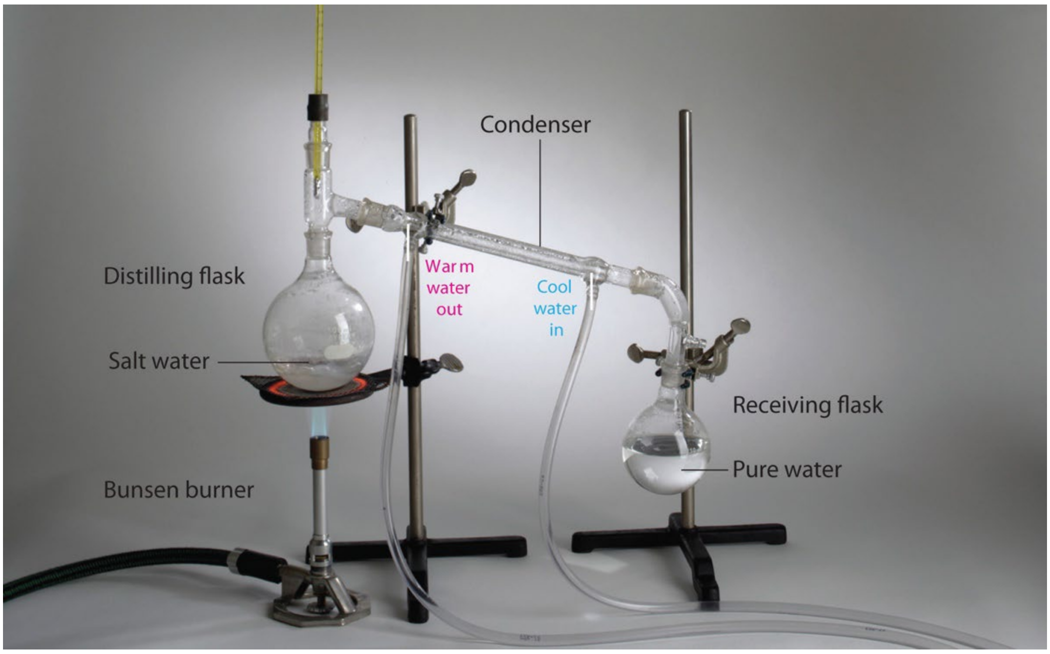


Figure 1.8. The distillation of a solution of table salt in water.

of salt in water is heated in the distilling flask until it boils. The resulting vapor is enriched in the more volatile component (water), which condenses to a liquid in the cold condenser and is then collected in the receiving flask. Mixtures of two or more liquids with different boiling points can be separated with a more complex distillation apparatus. One example is the refining of crude petroleum into a range of useful products: aviation fuel, gasoline, kerosene, diesel fuel, and lubricating oil (in the approximate order of decreasing volatility). Another example is the distillation of alcoholic spirits such as brandy or whiskey. This relatively simple procedure caused more than a few headaches for federal authorities in the 1920s during the era of Prohibition, when illegal stills proliferated in remote regions of the United States.

Crystallization separates mixtures based on differences in solubility, a measure of how much solid substance remains dissolved in a given amount of a specified liquid. Most substances are more soluble at higher temperatures, so a mixture of two or more substances can be dissolved at an elevated temperature and then allowed to cool slowly (Figure 1.7).

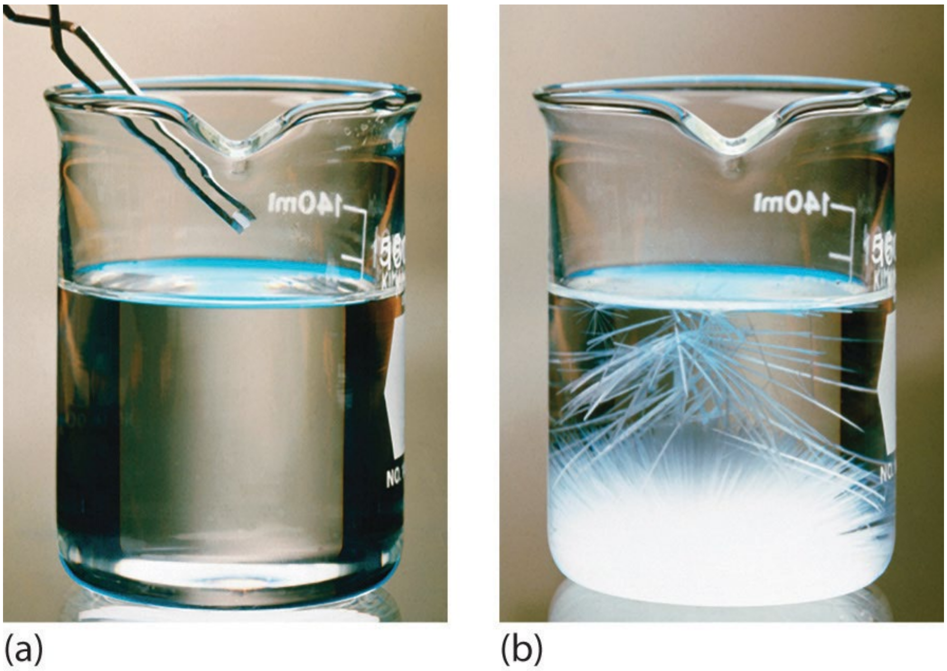


Figure 1.9. The crystallization of sodium acetate from a concentrated solution of sodium acetate in water.

Most mixtures can be separated into pure substances, which may be either elements or compounds. An **element**, such as gray, metallic sodium, is a substance that cannot be broken down into simpler ones by chemical changes; a **compound**, such as white, crystalline sodium chloride, contains two or more elements and has chemical and physical properties that are usually different from those of the elements of which it is composed. With only a few exceptions, a particular compound has the same elemental composition (the same elements in the same proportions) regardless of its source or history. The chemical composition of a substance is altered in a process called a chemical change. The conversion of two or more elements, such as sodium and chlorine, to a chemical compound, sodium chloride, is an example of a chemical change, often called a chemical reaction.

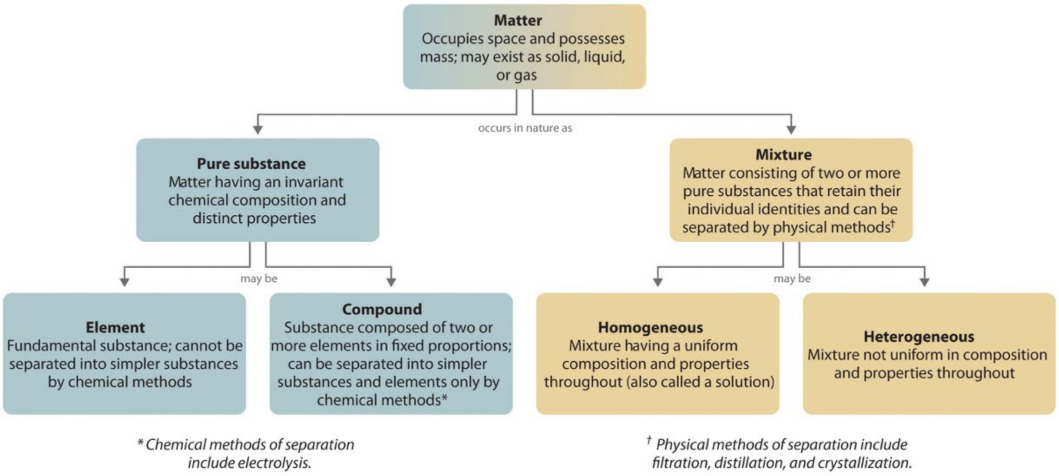


Figure 1.10 Classification of matter.

Example 2

Identify each substance as a compound, an element, a heterogeneous mixture, or a homogeneous mixture (solution).

1. filtered tea
2. freshly squeezed orange juice
3. a compact disc
4. aluminum oxide, a white powder that contains a 2:3 ratio of aluminum and oxygen atoms

2. selenium

Solution

Given: a chemical substance

Asked for: its classification

Strategy:

A. Decide whether a substance is chemically pure. If it is pure, the substance is either an element or a compound. If a substance can be separated into its elements, it is a compound.

B. If a substance is not chemically pure, it is either a heterogeneous mixture or a homogeneous mixture. If its composition is uniform throughout, it is a homogeneous mixture.

Solution:

1. A Tea is a solution of compounds in water, so it is not chemically pure. It is usually separated from tea leaves by filtration. B Because the composition of the solution is uniform throughout, it is a homogeneous mixture.
2. A Orange juice contains particles of solid (pulp) as well as liquid; it is not chemically pure. B Because its composition is not uniform throughout, orange juice is a heterogeneous mixture.
3. A compact disc is a solid material that contains more than one element, with regions of different compositions visible along its edge. Hence a compact disc is not chemically pure. B The regions of different composition indicate that a compact disc is a heterogeneous mixture.
4. Aluminum oxide is a single, chemically pure compound.
5. Selenium is one of the known elements.

Section 1.3. Physical and Chemical Properties

All matter has physical and chemical properties. **Physical properties** are characteristics that scientists can measure without changing the composition of the sample under study, such as mass, color, and volume (the amount of space occupied by a sample). **Chemical properties** describe the characteristic ability of a substance to react to form new substances; they include its flammability and susceptibility to corrosion. All samples of a pure substance have the same chemical and physical properties. For example, pure copper is always a reddish-brown solid (a physical property) and always dissolves in dilute nitric acid to produce a blue solution and a brown gas (a chemical property). Physical properties can be extensive or intensive. **Extensive properties** vary with the amount of the substance and include mass, weight, and volume. **Intensive properties**, in contrast, do not depend on the amount of the substance; they include color, melting point, boiling point, electrical conductivity, and physical state at a given temperature. For example, elemental sulfur is a yellow crystalline solid that does not conduct electricity and has a melting point of 115.2°C, no matter what amount is examined. Scientists commonly measure intensive properties to determine a substance's identity, whereas extensive properties convey information about the amount of the substance in a sample.

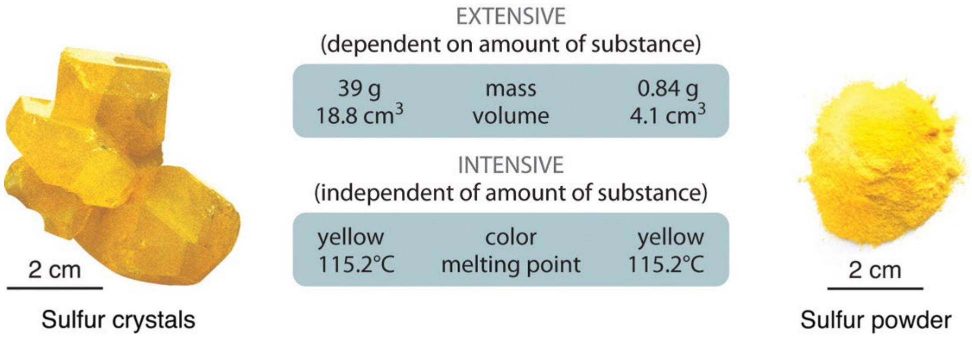


Figure 1.11 The difference between extensive and intensive properties of matter.

Because they differ in size, the two samples of sulfur have different extensive properties, such as mass and volume. In contrast, their intensive properties, including color, melting point, and electrical conductivity, are identical.

Although mass and volume are both extensive properties, their ratio is an important intensive property called density (d). **Density** is defined as mass per unit volume and is usually expressed in grams per cubic centimeter (g/mL). As mass increases in a given volume, density also increases. For example, lead, with its greater mass, has a far greater density than the same volume of air, just as a brick has a greater density than the same volume of Styrofoam. At a given temperature and pressure, the density of a pure substance is a constant:

density = mass/volume

Density is a physical property that relates the mass of a substance to its volume. Density is defined as mass per unit volume of a substance. Density is reported as g/ml or g/cc. The mathematical form of density $d = m/v$.
Physical meaning of density refers to the compactness of the substance.

Density of a substance depends on temperature. Specially for liquids and gases, when temperature increases, volume expands and therefore density decreases. For most substances solid state is denser than liquid and liquid is more dense than gas. Water is an exception. Ice is less dense than liquid water. A less dense substance floats on a denser liquid.

Density also depends on pressure. An allotrope of carbon Diamond can be converted to graphite at a very high pressure. Although they contain the same atoms of carbon but they do not share the same density.

If two liquids are mixed together and they are immiscible, liquid with lower density is always on top of liquid with higher density. In other words, substance with higher density always sinks in substance with lower density and vice versa.

There are two different ways density can be determined in Lab. 1) dimensional method and 2) displacement method.

In dimensional method, volume of the regularly shaped object is determined applying the standard formula. Mass of the object is determined using analytical balance. Then mass is divided by volume to determine the density.

Example: Determine the density of a unknown metal cube that has side length 3.00cmand mass is 310.672g.

Volume of the metal cube 3.00*3.00*3.00= 27.0 cm^3

Density of the metal= 310.671/27.0= 11.5 g/cm^3

In displacement method some water is taken in the graduated cylinder and then the irregular shaped object is dropped in the cylinder. Volume of water in the cylinder rises. The difference in volume between initial and final volume of graduated cylinder is the volume of the cylinder.

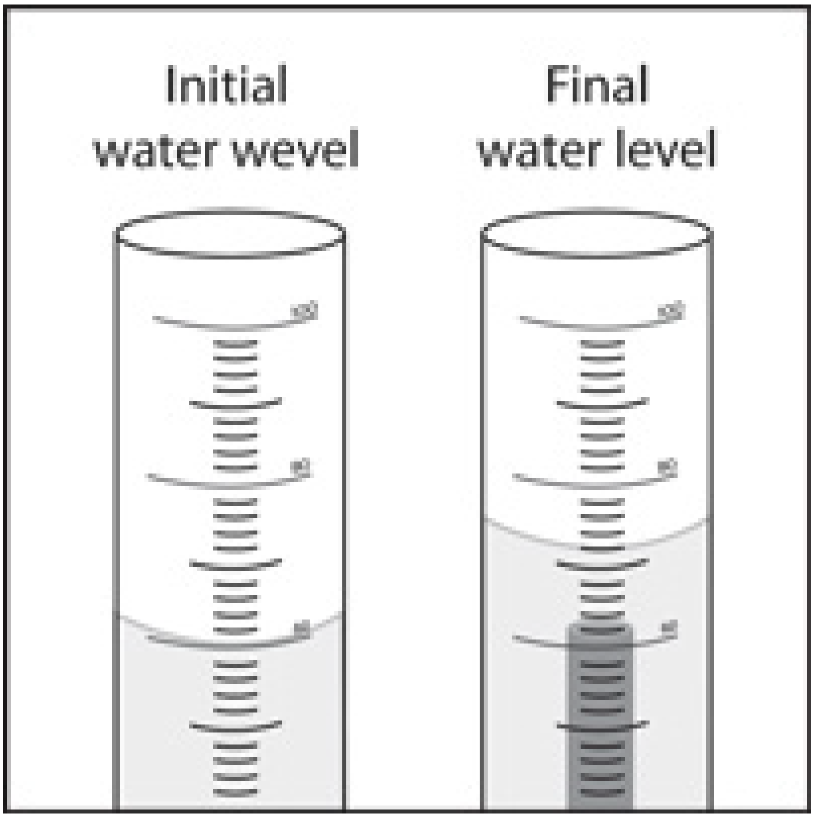
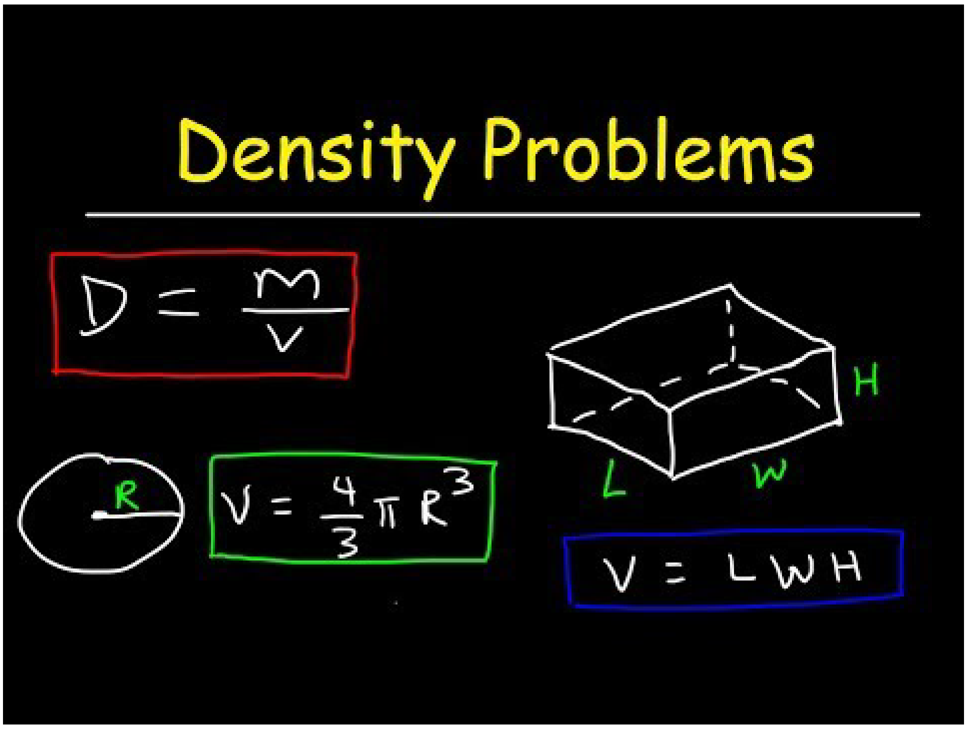


Figure. 1.12 Determination of Density using displacement method

In the above example, volume of the liquid (96.0-90.0)ml =6.0 ml.

If the mass of the sample 16.9050g, the density of the sample = 16.9050/6.0 ml= 2.8 g/ml.

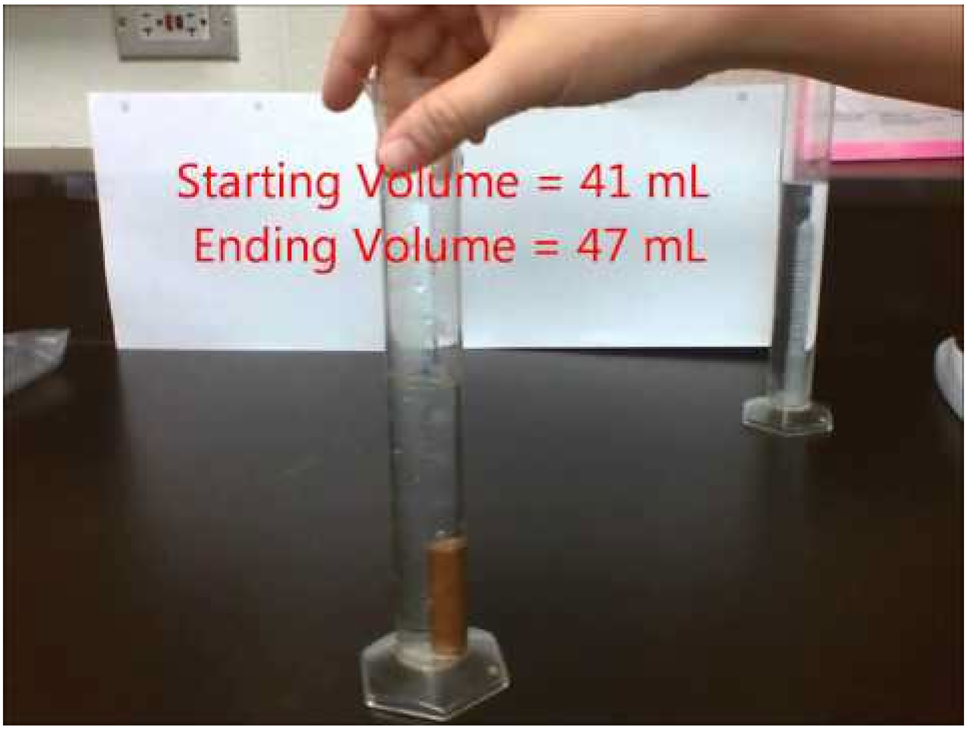


Density Problems

$D = \frac{M}{V}$

$V = \frac{4}{3}\pi R^3$

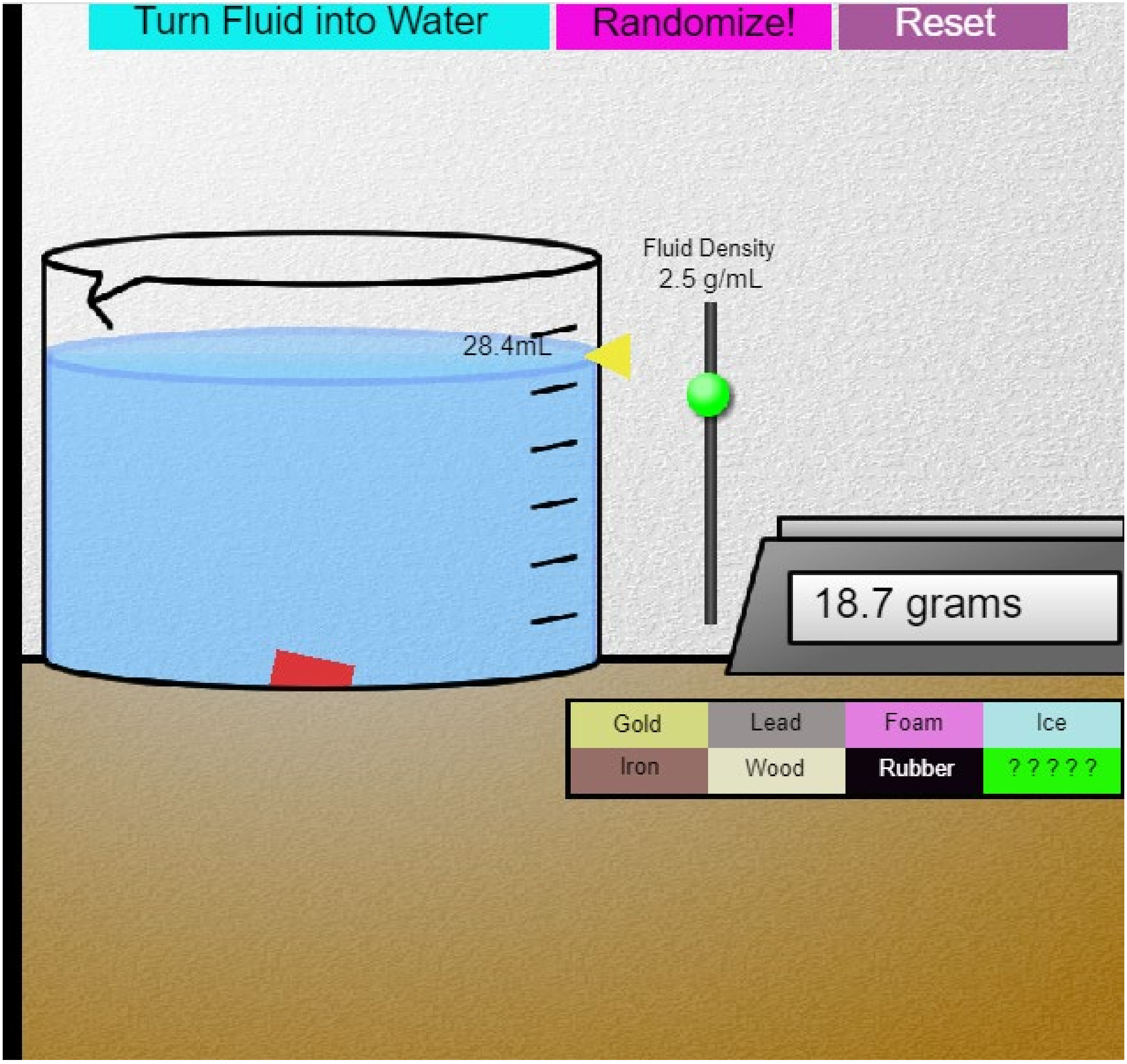
$V = LWH$



Starting Volume = 41 mL
Ending Volume = 47 mL

Go to the following site and check out the simulation

https://pba.pbslearningmedia.org/resource/arct15-sci-densitylab/density-lab/



Play with different substances including “Gold, lead, Foam and find the density of unknown.

First 1) put the object on balance,

2) read the volume level in the beaker

3) drop the object in beaker

4) read the new volume in beaker

5) determine the difference in volume , equal to the volume of the substance.

6) determine density

Objects	Mass on object	Initial Volume of the liquid	Final volume of the liquid	Volume of the object	Density
Gold					

Table 1.1 lists the density of common substances. Pure water, for example, has a density of 0.998 g/mL at 25°C. Notice that corn oil has a lower mass to volume ratio than water. This means that when added to water, corn oil will “float.” Example 3 shows how density measurements can be used to identify pure substances.

Substance	Density at 25°C (g/cm3)
blood	1.035
body fat	0.918
whole milk	1.030
corn oil	0.922
mayonnaise	0.910
honey	1.420

Table 1.1 Densities of Common Substances

EXAMPLE 3

The densities of liquids in example 3 are listed in Table 1.2. Imagine you have five bottles containing colorless liquids (labeled A–E). You must identify them by measuring the density of each. Using a pipette, a laboratory instrument for accurately measuring and transferring liquids, you carefully measure 25.00 mL of each liquid into five beakers of known mass (1 mL = 1 mL). You then weigh each sample on a laboratory balance. Use the tabulated data to calculate the density of each sample. Based solely on your results, can you unambiguously identify all five liquids?

Masses of samples: (1) 17.72 g; (2) 19.75 g; (3) 24.91 g; (4) 19.65 g; (5) 27.80 g

Substance	Density at 25°C (g/mL)
water	0.998
ethanol (the alcohol in beverages)	0.789
methanol (wood alcohol)	0.792
ethylene glycol (used in antifreeze)	1.113
diethyl ether (“ether”; once widely used as an anesthetic)	0.708
isopropanol (rubbing alcohol)	0.785

Table 1.2 Densities of liquids in example 3

Solution:

Given: volume and mass

Asked for: density

Strategy:

1. Calculate the density of each liquid from the volumes and masses given.
2. Check to make sure that your answer makes sense.
3. Compare each calculated density with those given in Table 1. 2. If the calculated density of a liquid is not significantly different from that of one of the liquids given in the table, then the unknown liquid is most likely the corresponding liquid.
4. If none of the reported densities corresponds to the calculated density, then the liquid cannot be unambiguously identified.

Solution:

1. Density is mass per unit volume and is usually reported in grams per cubic centimeter (or grams per milliliter because 1 mL = 1 mL). The masses of the samples are given in grams, and the volume of all the samples is 25.00 mL. The density of each sample is calculated by dividing the mass by its volume. The density of sample 1, for example, is

density = 17.72 g/25.00 mL=0.7088 g/mL

Both the volume and the mass are given to four significant figures, so four significant figures are permitted in the result. The densities of the other samples (in grams per cubic centimeter) are as follows: (2) 0.7900; (3) 0.9964; (4) 0.7860; and (5) 1.112.

(2) Except for sample E, the calculated densities are slightly less than 1 g/cm3. This makes sense because the masses (in grams) of samples A–D are all slightly less than the volume of the samples, 25.00 mL. In contrast, the mass of sample E is slightly greater than 25 g, so its density must be somewhat greater than 1 g/cm3.

(3) Comparing these results with the data given in shows that sample 1 is probably diethyl ether (0.708 g/mL and 0.7088 g/mL are not substantially different), sample C is probably water (0.998 g/mL in the table versus 0.9964 g/mL measured), and sample E is probably ethylene glycol (1.113 g/mL in the table versus 1.112 g/mL measured).

(4) Samples 2 and 4 are more difficult to identify for two reasons: (1) Both have similar densities (0.7900 and 0.7860 g/mL), so they may or may not be chemically identical. (2) Within experimental error, the measured densities of 2 and 4 are indistinguishable from the densities of ethanol (0.789 g/mL), methanol (0.792 g/mL), and isopropanol (0.785 g/mL). Thus, some property other than density must be used to identify each sample.

Physical and Chemical Changes

Just as chemists have classified elements and compounds, they have also classified types of changes. Changes are either classified as physical or chemical changes. Chemists learn a lot about the nature of matter by studying the changes that matter can undergo. Chemists make a distinction between two different types of changes that they study - physical changes and chemical changes.

Physical Change

Physical changes are changes in which no bonds are broken or formed. This means that the same types of compounds or elements that were there at the beginning of the change are there at the end of the change. Because the ending materials are the same as the beginning materials, the properties (such as color, boiling point, etc) will also be the same. Physical changes involve moving molecules around, but not changing them. Some types of physical changes include:

- Changes of state (changes from a solid to a liquid or a gas and vice versa)
- Separation of a mixture
- Physical deformation (cutting, denting, stretching)
- Making solutions (special kinds of mixtures)

As an ice cube melts, its shape changes as it acquires the ability to flow. However, its composition does not change. Melting is an example of a physical change (Figure 1.10). A physical change is a change to a sample of matter in which some properties of the material change, but the identity of the matter does not. When we heat the liquid water, it changes to water vapor. But even though the physical properties have changed, the molecules are exactly the same as before. We still have each water molecule containing two hydrogen atoms and one oxygen atom covalently bonded. When you have a jar containing a mixture of pennies and nickels and you sort the mixture so that you have one pile of pennies and another pile of nickels, you have not altered the identity of either the pennies or the nickels - you've merely separated them into two groups. This would be an example of a physical change. Similarly, if you have a piece of paper, you don't change it into something other than a piece of paper by ripping it up. What was paper before you started tearing is still paper when you're done. Again, this is an example of a physical change.

Figure 1.13. Ice Melting is a physical change.

When solid water (ice) melts into liquid water, it appears changed; however, this change is only physical as the composition of the constituent molecules is the same: 11.19% hydrogen and 88.81% oxygen by mass.

Physical changes can further be classified as reversible or irreversible. The melted ice cube may be refrozen, so melting is a reversible physical change. Physical changes that involve a change of state are all reversible. Other changes of state include **vaporization** (liquid to gas), **freezing** (liquid to solid), and **condensation** (gas to liquid). Dissolving is also a reversible physical change. When salt is dissolved into water, the salt is said to have entered the aqueous state. The salt may be regained by boiling off the water, leaving the salt behind.

Chemical Change

Chemical changes occur when bonds are broken and/or formed between molecules or atoms. This means that one substance with a certain set of properties (such as melting point, color, taste, etc) is turned into a different substance with different properties. Chemical changes are frequently harder to reverse than physical changes.

One good example of a chemical change is burning a candle (Figure 1.11). The act of burning paper actually results in the formation of new chemicals (carbon dioxide and water, to be exact) from the burning of the wax. Another example of a chemical change is what occurs when natural gas is burned in your furnace. In chemical terms this can be described as a molecule of methane, CH_4, and two molecules of oxygen, O_2, react in a combustion type of chemical reaction to form two molecules of water, H_2O, and one molecule of carbon dioxide, CO_2. In this case, not only has the appearance changed, but the structure of the molecules has also changed. The new substances do not have the same chemical properties as the original ones. Therefore, this is a chemical change.

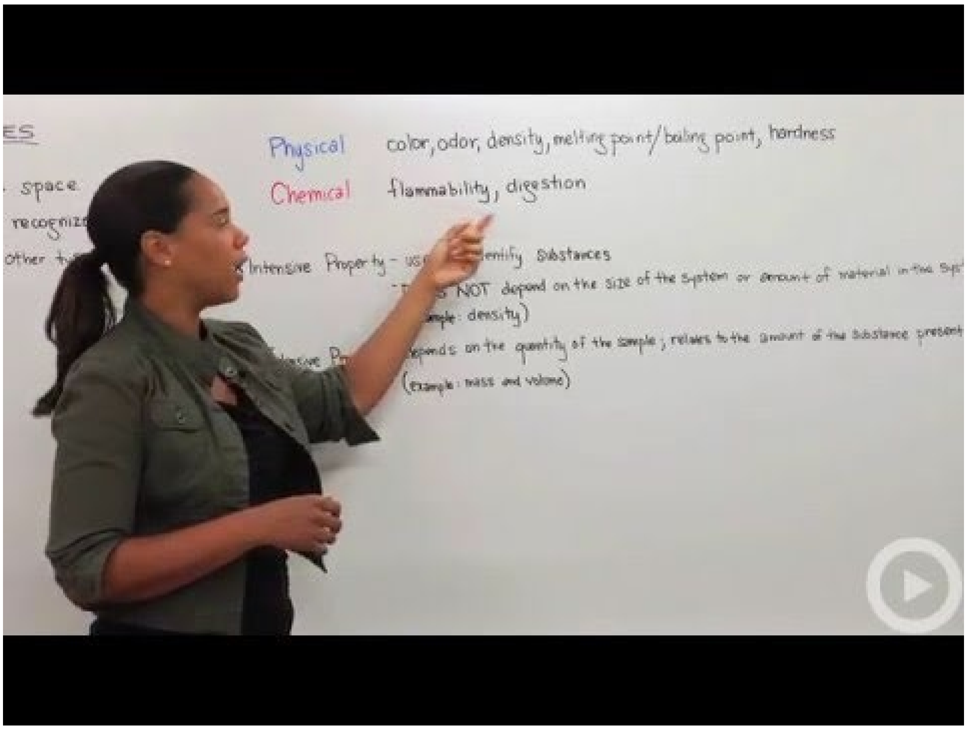
Figure 1.14 Burning of a candle is a type of chemical change.

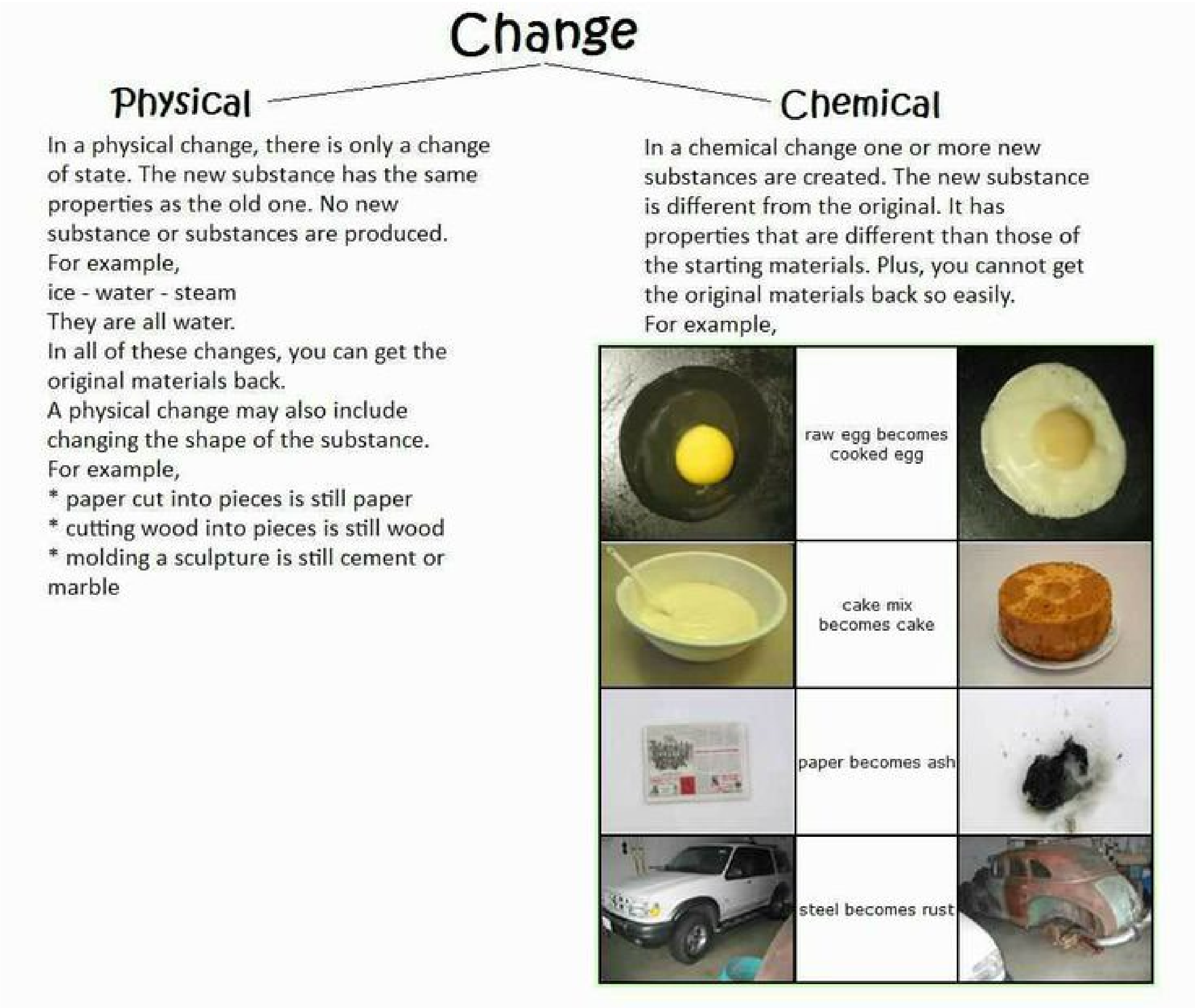
We cannot actually see molecules breaking and forming bonds, although that's what defines chemical changes. We have to make other observations to indicate that a chemical change has happened. Some of the evidence for chemical change will involve the energy changes that occur in chemical changes, but some evidence involves the fact that new substances with different properties are formed in a chemical change.

Observations that help to indicate chemical change include:

- Temperature changes (either the temperature increases or decreases)

- Light is given off
- Unexpected color changes (a substance with a different color is made, rather than just mixing the original colors together)
- Bubbles are formed (but the substance is not boiling - you made a substance that is a gas at the temperature of the beginning materials, instead of a liquid)
- Different smell or taste (do not taste your chemistry experiments, though!)
- Formation of a solid, if two clear liquids are mixed.





Change

Physical

In a physical change, there is only a change of state. The new substance has the same properties as the old one. No new substance or substances are produced.
For example,
ice - water - steam
They are all water.
In all of these changes, you can get the original materials back.
A physical change may also include changing the shape of the substance.
For example,
* paper cut into pieces is still paper
* cutting wood into pieces is still wood
* molding a sculpture is still cement or marble

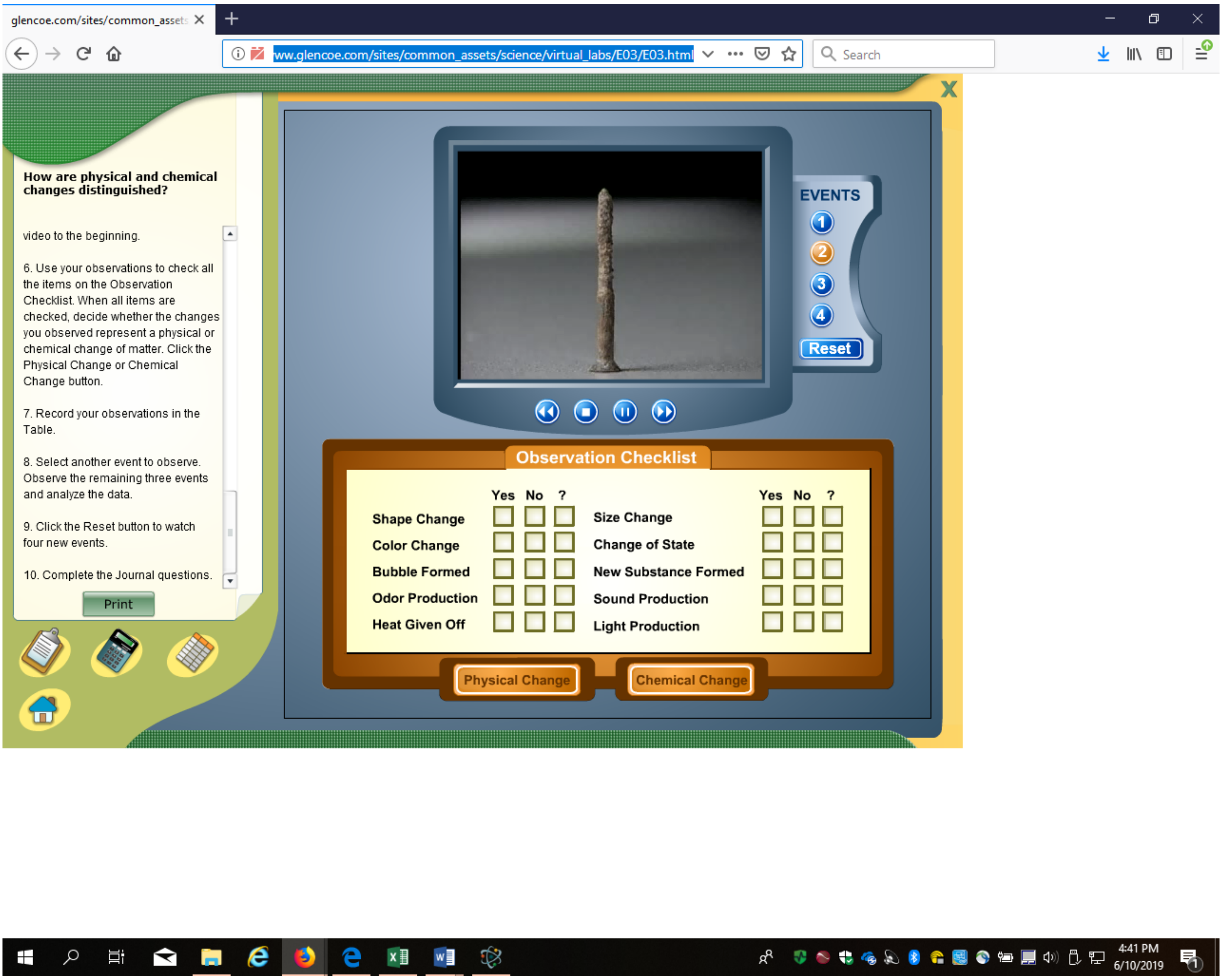
Chemical

In a chemical change one or more new substances are created. The new substance is different from the original. It has properties that are different than those of the starting materials. Plus, you cannot get the original materials back so easily.
For example,

Figure 1.15: Physical & Chemical Change

Go to the following activity and complete the activity:

http://www.glencoe.com/sites/common_assets/science/virtual_labs/E03/E03.html



How are physical and chemical changes distinguished?

video to the beginning.

6. Use your observations to check all the items on the Observation Checklist. When all items are checked, decide whether the changes you observed represent a physical or chemical change of matter. Click the Physical Change or Chemical Change button.

7. Record your observations in the Table.

8. Select another event to observe. Observe the remaining three events and analyze the data.

9. Click the Reset button to watch four new events.

10. Complete the Journal questions.

Observation Checklist

	Yes	No	?		Yes	No	?
Shape Change	☐	☐	☐	Size Change	☐	☐	☐
Color Change	☐	☐	☐	Change of State	☐	☐	☐
Bubble Formed	☐	☐	☐	New Substance Formed	☐	☐	☐
Odor Production	☐	☐	☐	Sound Production	☐	☐	☐
Heat Given Off	☐	☐	☐	Light Production	☐	☐	☐

Example 4

Label each of the following changes as a physical or chemical change. Give evidence to support your answer.

a. Boiling water

b. A nail rusting

c. A green solution and colorless solution are mixed. The resulting mixture is a solution with a pale green color.

d. Two colorless solutions are mixed. The resulting mixture has a yellow precipitate.

Solution

a. Physical: boiling and melting are physical changes. When water boils no bonds are broken or formed. The change could be written: $H_2O(l) \rightarrow H_2O(g)$ $H_2O(l) \rightarrow H_2O(g)$

b. Chemical: The dark grey nail changes color to form an orange flaky substance (the rust); this must be a chemical change. Color changes indicate chemical change. The following reaction occurs: $Fe + O_2 \rightarrow Fe_2O_3$ $Fe + O_2 \rightarrow Fe_2O_3$

c. Physical: because none of the properties changed, this is a physical change. The green mixture is still green and the colorless solution is still colorless. They have just been spread together. No color change occurred or other evidence of chemical change.

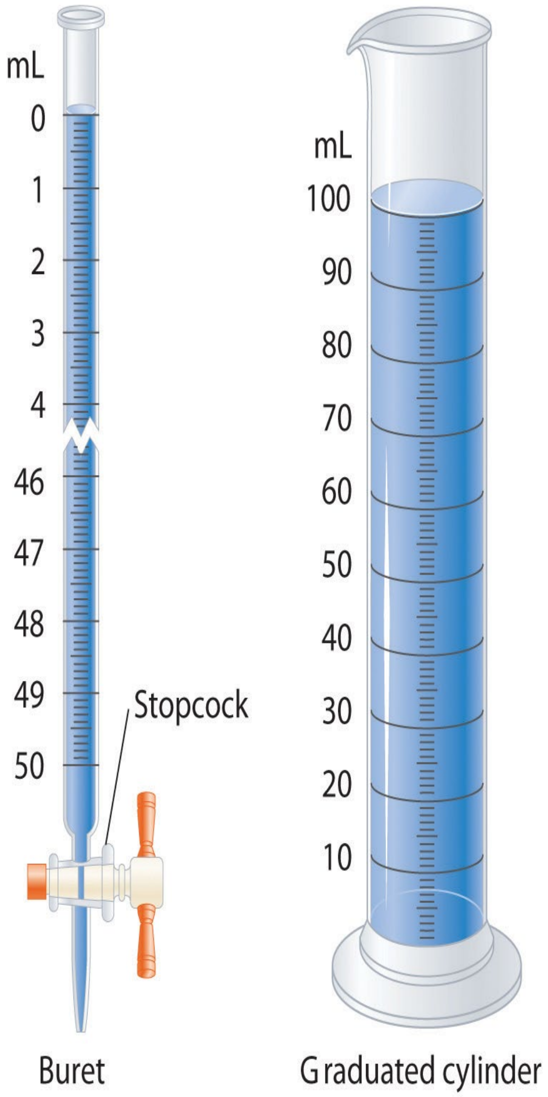
d. Chemical: the formation of a precipitate and the color change from colorless to yellow indicate a chemical change.

Section 1.4. Measurements and Significant Figures

This section describes some of the fundamental laboratory and mathematical skills you will need to be successful in your chemistry course. For some of you, this discussion will serve as a review, whereas others may be encountering at least some of the ideas and techniques for the first time.

Measurement

Instruments of Measurement



Buret

Graduated cylinder

Figure 1.16 Graduated glassware is used to deliver variable volumes of liquid.

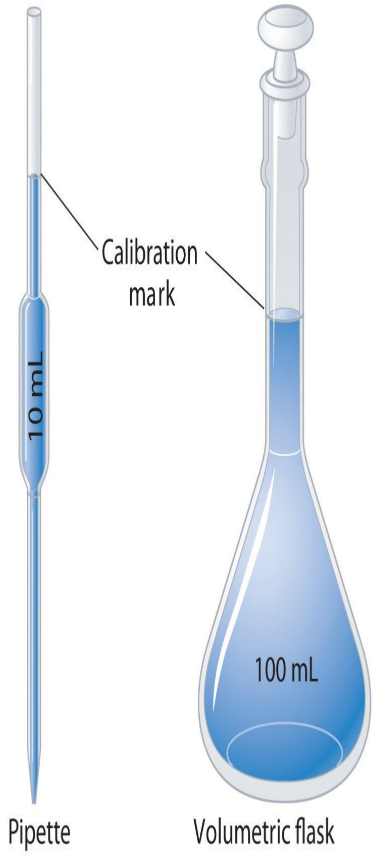


Figure 1.17. Volumetric glassware is used to deliver (pipette) or contain (volumetric flask) a single volume accurately when filled to the calibration mark.

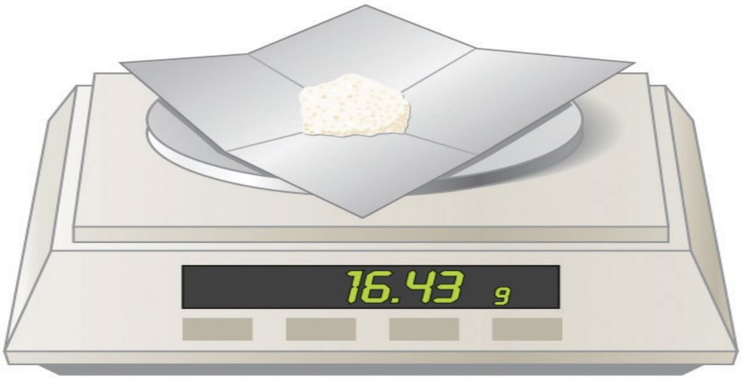


Figure 1.18. A balance is used to measure mass.

A variety of instruments are available for making direct measurements of the macroscopic properties of a chemical substance. For example, we usually measure the volume of a liquid sample with pipettes, burets, graduated cylinders, and volumetric flasks, whereas we usually measure the mass of a solid or liquid substance with a balance. Measurements on an atomic or molecular scale, in contrast, require specialized instrumentation, such as the mass spectrometer.

Exact number and Measured number

An exact number results from counting objects or is a part of a definition. For example, 30 students present in class. 30 is the exact number. There are 60 minutes in 1 hour. 60 is the exact number. A measured number results from a measurement or observation and contains some uncertainty also called Inexact number. Limitation of the measuring device and limited powers of the observation of the individual making the measurement involving a degree of uncertainty or error. That is why measured number are sometimes called approximate number.

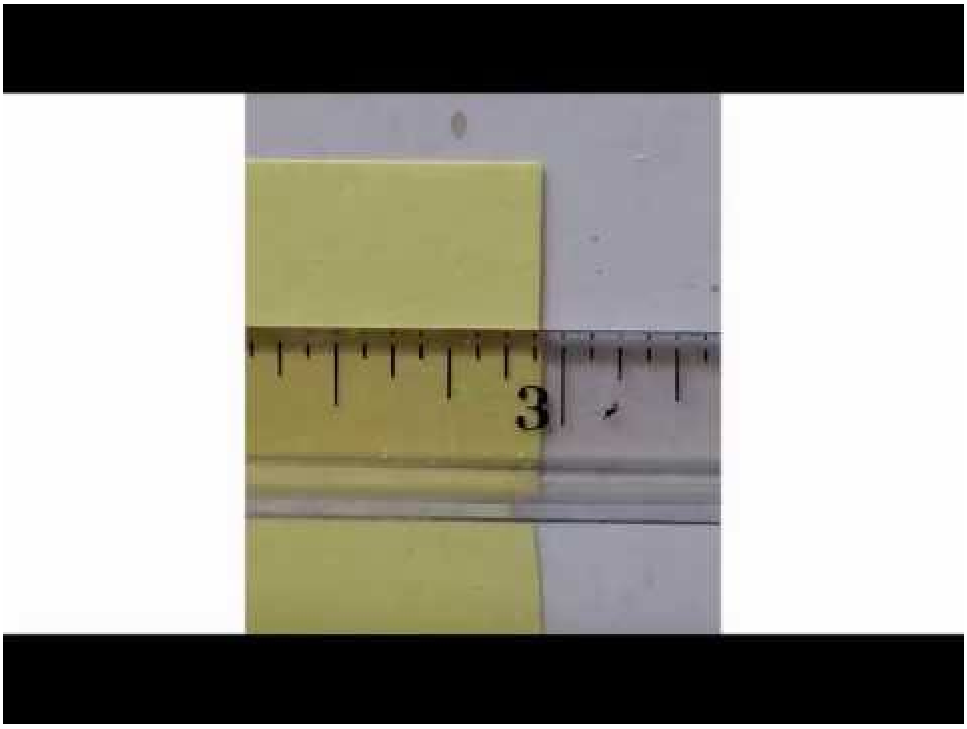
Example of exact number: 30 students in class, 12 oranges. Example of measured number: the child weights 30.5 lbs, The height of Mount Everest is 8,848 meters.

Any exact doesn't have any uncertainty in it. In case of measured number always, the last digit is uncertain. The uncertain number depends on the calibration of the device.

In a measured number always, all digits are certain except the last one. The last digit in a measured number of based on instrumental precision and human eye estimation. It is called uncertain digit or estimated digit. Certain and uncertain digits together make significant figures.

Watch the following video about certain and uncertain digits.

https://www.youtube.com/watch?v=TKoskMGAmSo



Following tutorial may help you to understand the concept.

https://www.sophia.org/tutorials/identifying-certain-and-uncertain-digits

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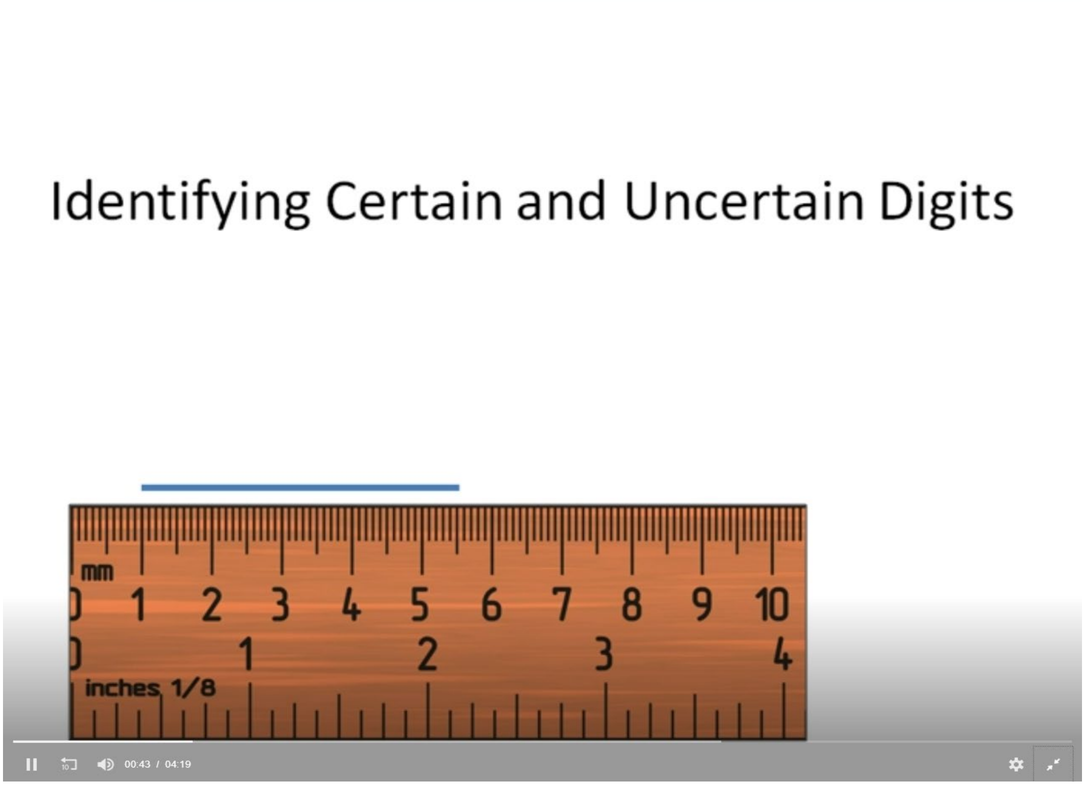
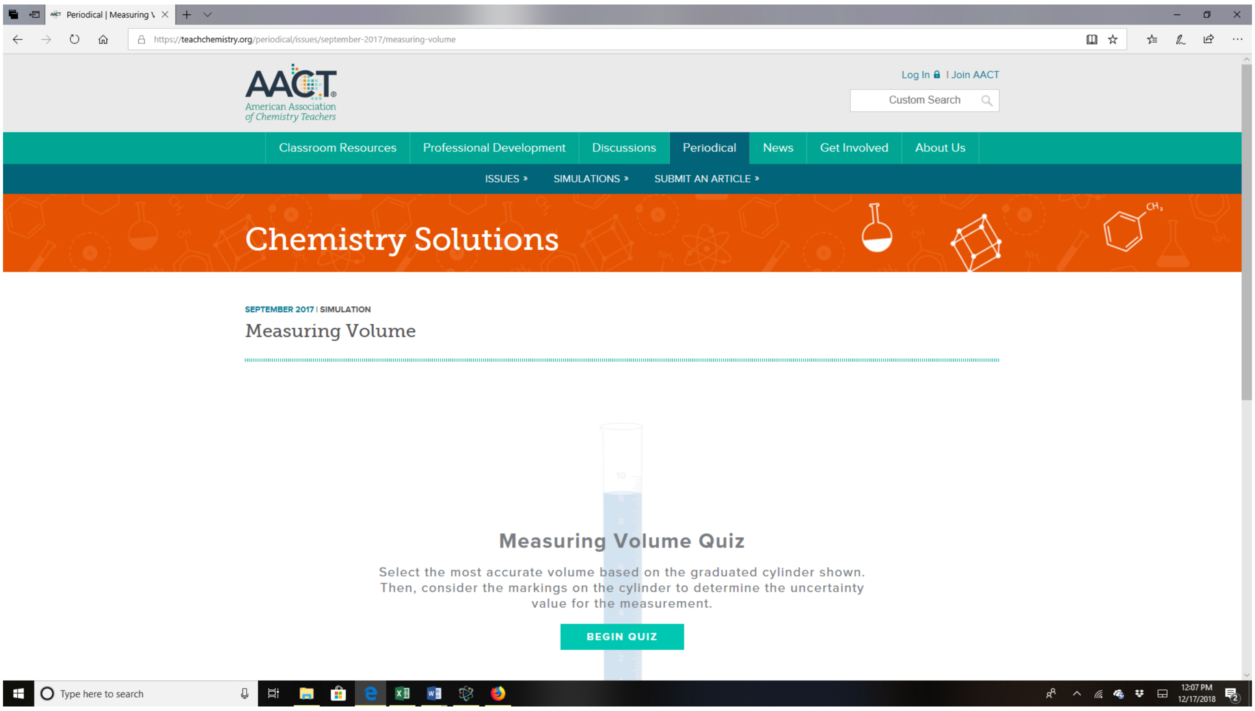


Identifying Certain and Uncertain Digits

Questions:

1. Indicate whether the following numbers are exact or inexact?
   a) The length of a river
   b) Conference attendees
2. Go to the following link Take the quiz:

https://teachchemistry.org/periodical/issues/september-2017/measuring-volume



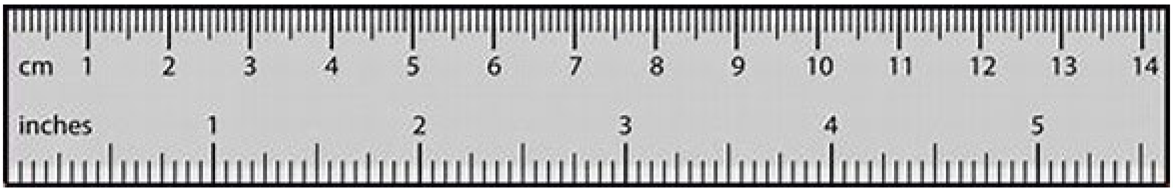
SEPTEMBER 2017 | SIMULATION

Measuring Volume

Measuring Volume Quiz

Select the most accurate volume based on the graduated cylinder shown. Then, consider the markings on the cylinder to determine the uncertainty value for the measurement.

3. What measurement can be shown with following ruler?



Ans:

1. a) measured

b)exact

2. Quiz
3. 14.30 cm

Scientific Notation

Chemists often work with numbers that are exceedingly large or small. For example, entering the mass in grams of a hydrogen atom into a calculator requires a display with at least 24 decimal places. A system called scientific notation avoids much of the tedium and awkwardness of manipulating numbers with large or small magnitudes. In scientific notation, these numbers are expressed in the form

$N \times 10^n$

where N is greater than or equal to 1 and less than 10 ($1 \leq N < 10$), and n is a positive or negative integer ($10^0 = 1$). The number 10 is called the base because it is this number that is raised to the power n. Although a base number may have values other than 10, the base number in scientific notation is always 10.

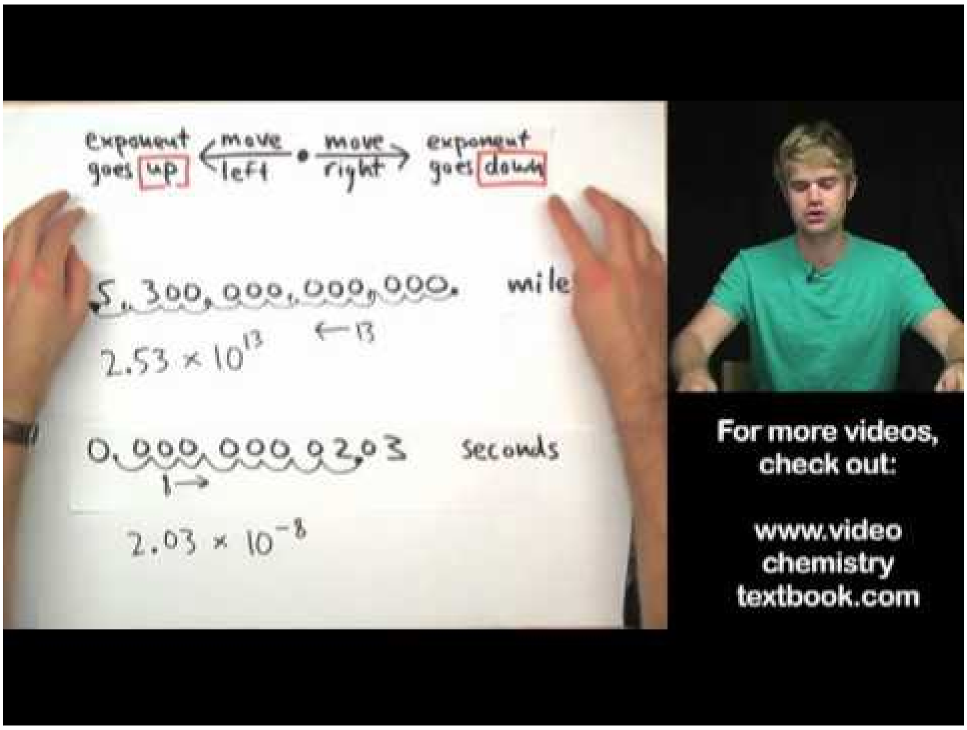
A simple way to convert numbers to scientific notation is to move the decimal point as many places to the left or right as needed to give a number from 1 to 10 (N). The magnitude of n is then determined as follows:

- If the decimal point is moved to the left n places, n is positive.
- If the decimal point is moved to the right n places, n is negative.

Another way to remember this is to recognize that as the number N decreases in magnitude, the exponent increases and vice versa.

Watch this out!

https://www.youtube.com/watch?v=Dme-G4rc6NI&t=136s



For more videos, check out:

www.videochemistrytextbook.com

Example 5

Convert each number to scientific notation.

a. 637.8

b. 0.0479

c. 7.86

d. 12,378

Solution

a. To convert 637.8 to a number from 1 to 10, we move the decimal point two places to the left: 6.378. Because the decimal point was moved two places to the left, n = 2. In scientific notation, 637.8 = 6.378×10^2.

b. To convert 0.0479 to a number from 1 to 10, we move the decimal point two places to the right:4.79. Because the decimal point was moved two places to the right, n = −2. In scientific notation, 0.0479 = 4.79×10^{-2}.

c. 7.86×10^0: this is usually expressed simply as 7.86. (Recall that 100 = 1.)

d. 1.2378×10^4; because the decimal point was moved four places to the left, n = 4.

Significant Figures

No measurement is free from error. Error is introduced by (1) the limitations of instruments and measuring devices (such as the size of the divisions on a graduated cylinder) and (2) the imperfection of human senses. Although errors in calculations can be enormous, they do not contribute to uncertainty in measurements. Chemists describe the estimated degree of error in a measurement as the uncertainty of the measurement, and they are careful to report all measured values using only significant figures, numbers that describe the value without exaggerating the degree to which it is known to be accurate. Chemists report as significant all numbers known with absolute certainty, plus one more digit that is understood to contain some uncertainty. The uncertainty in the final digit is usually assumed to be ±1, unless otherwise stated.

The following rules, **Significant Figures Rules**, have been developed for counting the number of significant figures in a measurement or calculation:

1. Any nonzero digit is significant.
2. Any zeros between nonzero digits are significant. The number 2005, for example, has four significant figures.
3. Any zeros used as a placeholder preceding the first nonzero digit are not significant. So, 0.05 has one significant figure because the zeros are used to indicate the placement of the digit 5. In contrast, 0.050 has two significant figures because the last two digits correspond to the number 50; the last zero is not a placeholder. As an additional example, 5.0 has two significant figures because the zero is used not to place the 5 but to indicate 5.0.
4. When a number does not contain a decimal point, zeros added after a nonzero number may or may not be significant. An example is the number 100, which may be interpreted as having one, two, or three significant figures. (Note: treat all trailing zeros in exercises and problems in this text as significant unless you are specifically told otherwise.)
5. Integers obtained either by counting objects or from definitions are exact numbers, which are considered to have infinitely many significant figures. If we have counted four objects, for example, then the number

4 has an infinite number of significant figures (i.e., it represents 4.000…). Similarly, 1 foot (ft) is defined to contain 12 inches (in), so the number 12 in the following equation has infinitely many significant figures:

1 ft = 12 in

An effective method for determining the number of significant figures is to convert the measured or calculated value to scientific notation because any zero used as a placeholder is eliminated in the conversion. When 0.0800 is expressed in scientific notation as 8.00×10^{-2}, it is more readily apparent that the number has three significant figures rather than five; in scientific notation, the number preceding the exponential (i.e., N) determines the number of significant figures.

Example 8

Give the number of significant figures in each. Identify the rule for each.

a. 5.87

b. 0.031

c. 52.90

d. 00.2001

Solution

a. three (rule 1)
b. two (rule 3); in scientific notation, this number is represented as 3.1×10^{-2}, showing that it has two significant figures.
c. four (rule 3)
d. four (rule 2); this number is 2.001×10^{-1} in scientific notation, showing that it has four significant figures.

Example 9

Which measuring apparatus would you use to deliver 9.7 mL of water as accurately as possible? To how many significant figures can you measure that volume of water with the apparatus you selected?

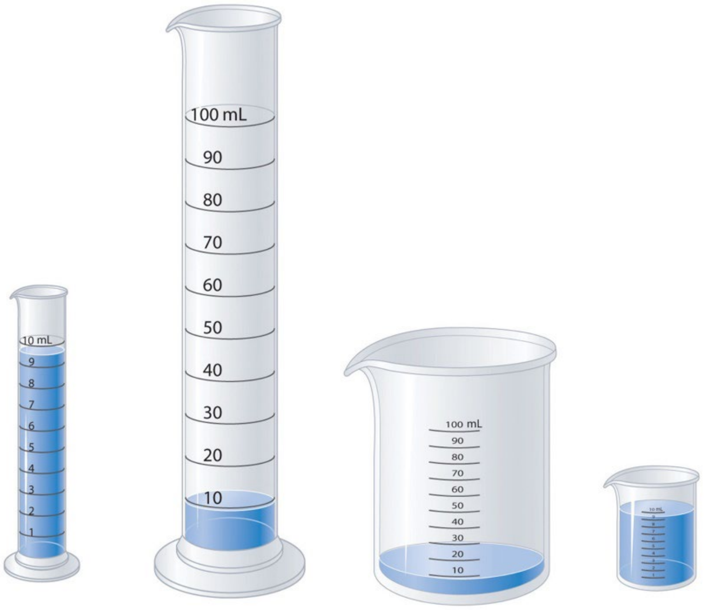


Fig. 1.19 Calibration in different Equipment

Ref: commons.wikimedia.org/

Solution

Use the 10 mL graduated cylinder, which will be accurate to two significant figures.

Mathematical operations are carried out using all the digits given and then rounding the final result to the correct number of significant figures to obtain a reasonable answer. This method avoids compounding inaccuracies by successively rounding intermediate calculations. After you complete a calculation, you may have to round the last significant figure up or down depending on the value of the digit that follows it. If the digit is 5 or greater, then the number is rounded up. For example, when rounded to three significant figures, 5.215 is 5.22, whereas 5.213 is 5.21. Similarly, to three significant figures, 5.005 kg becomes 5.01 kg, whereas 5.004 kg becomes 5.00 kg. The procedures for dealing with significant figures are different for addition and subtraction versus multiplication and division.

When we add or subtract measured values, the value with the fewest significant figures to the right of the decimal point determines the number of significant figures to the right of the decimal point in the answer. Drawing a vertical line to the right of the column corresponding to the smallest number of significant figures is a simple method of determining the proper number of significant figures for the answer:

$$3240.7 + 21.236 = 3261.9\underline{36}$$

The line indicates that the digits 3 and 6 are not significant in the answer. These digits are not significant because the values for the corresponding places in the other measurement are unknown (3240.7??). Consequently, the answer is expressed as 3261.9, with five significant figures. Again, numbers greater than or equal to 5 are rounded up. If our second number in the calculation had been 21.256, then we would have rounded 3261.956 to 3262.0 to complete our calculation.

When we multiply or divide measured values, the answer is limited to the smallest number of significant figures in the calculation; thus, $42.9 \times 8.323 = 357.057 = 357$. Although the second number in the calculation has four significant figures, we are justified in reporting the answer to only three significant figures because the first number in the calculation has only three significant figures. An exception to this rule occurs when multiplying a number by an integer, as in 12.793×12. In this case, the number of significant figures in the answer is determined by the number 12.973, because we are in essence adding 12.973 to itself 12 times. The correct answer is therefore 155.516, an increase of one significant figure, not 155.52.

When you use a calculator, it is important to remember that the number shown in the calculator display often shows more digits than can be reported as significant in your answer. When a measurement reported as 5.0 kg is divided by 3.0 L, for example, the display may show 1.666666667 as the answer. We are justified in reporting the answer to only two significant figures, giving 1.7 kg/L as the answer, with the last digit understood to have some uncertainty.

In calculations involving several steps, slightly different answers can be obtained depending on how rounding is handled, specifically whether rounding is performed on intermediate results or postponed until the last step. Rounding to the correct number of significant figures should always be performed at the end of a series of calculations because rounding of intermediate results can sometimes cause the final answer to be significantly in error.

In practice, chemists generally work with a calculator and carry all digits forward through subsequent calculations. The final answer is then rounded to the correct number of significant figures at the very end.

Example 10

SKILL BUILDER

Complete the calculations and report your answers using the correct number of significant figures.

a. 87.25 mL + 3.0201 mL

b. 26.843 g + 12.23 g

c. 6 × 12.011

d. 2(1.008) g + 15.99 g

e. 137.3 + 2(35.45)

Solution

a. 90.27 mL

b. 39.07 g

c. 72.066 (See rule 5 under "Significant Figures.")

d. 2(1.008) g + 15.99 g = 2.016 g + 15.99 g = 18.01 g

e. 137.3 + 2(35.45) = 137.3 + 70.90 = 208.2

Addition and Subtraction

Before numbers expressed in scientific notation can be added or subtracted, they must be converted to a form in which all the exponents have the same value. The appropriate operation is then carried out on the values of N.

Example 6

Carry out the appropriate operation on each number and then express the answer in scientific notation.

a. $(1.36 \times 10^2) + (4.73 \times 10^3)$

b. $(6.923 \times 10^{-3}) - (8.756 \times 10^{-4})$

Solution

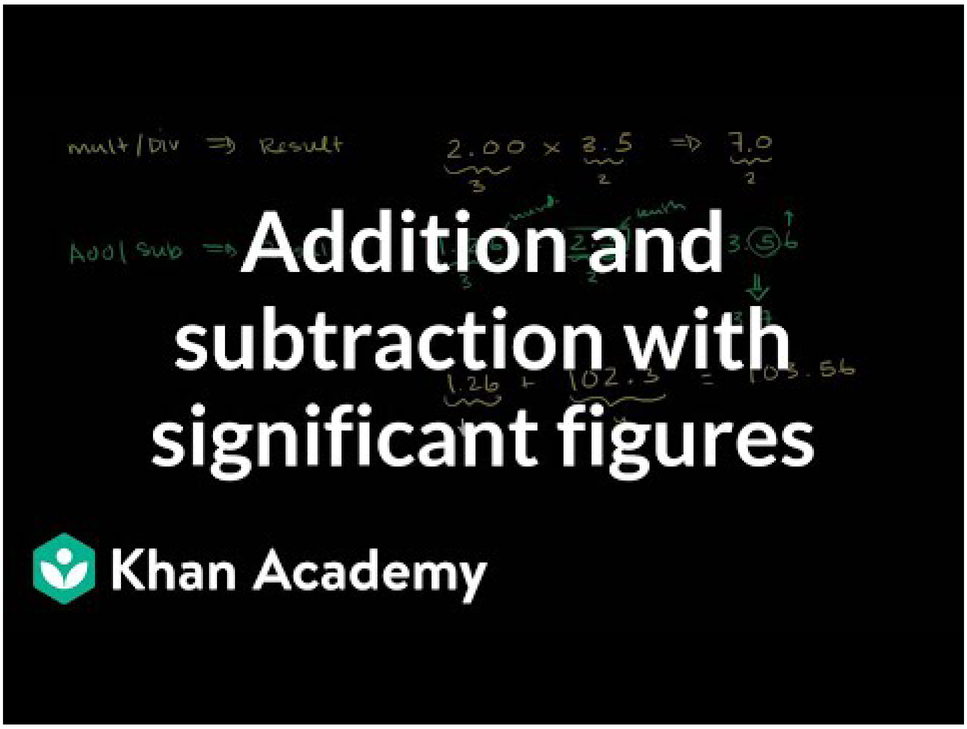
a. Both exponents must have the same value, so these numbers are converted to either $(1.36 \times 10^2) + (47.3 \times 10^2)$ or $(0.136 \times 10^3) + (4.73 \times 10^3)$. Choosing either alternative gives the same answer, reported to two decimal places:

$(1.36 \times 10^2) + (47.3 \times 10^2) = (1.36 + 47.3) \times 10^2 = 48.66 \times 10^2 = 4.87 \times 10^3 (0.136 \times 10^3) + (4.73 \times 10^3) = (0.136 + 4.73) \times 10^3 = 4.87 \times 10^3$

In converting 48.66×10^2 to scientific notation, n has become more positive by 1 because the value of N has decreased.

b. Converting the exponents to the same value gives either $(6.923 \times 10^{-3}) - (0.8756 \times 10^{-3})$ or $(69.23 \times 10^{-4}) - (8.756 \times 10^{-4})$. Completing the calculations gives the same answer, expressed to three decimal places:

$(6.923 \times 10^{-3}) - (0.8756 \times 10^{-3}) = (6.923 - 0.8756) \times 10^{-3} = 6.047 \times 10^{-3} (69.23 \times 10^{-4}) - (8.756 \times 10^{-4}) = (69.23 - 8.756) \times 10^{-4} = 60.474 \times 10^{-4} = 6.047 \times 10^{-3}$



https://www.youtube.com/watch?v=iorZdz4dsBU&t=2s

Multiplication and Division

When multiplying numbers expressed in scientific notation, we multiply the values of N and add together the values of n. Conversely, when dividing, we divide N in the dividend (the number being divided) by N in the divisor (the number by which we are dividing) and then subtract n in the divisor from n in the dividend. In contrast to addition and subtraction, the exponents do not have to be the same in multiplication and division.

Example 7

Perform the appropriate operation on each expression and express your answer in scientific notation.

a. $(6.022 \times 10^{23})(6.42 \times 10^{-2})$

b. $1.67\times10^{-24}/9.12\times10^{-28}$

Solution

a. In multiplication, we add the exponents:

$(6.022 \times 10^{23})(6.42 \times 10^{-2}) = (6.022)(6.42) \times 10^{[23 + (-2)]} = 38.7 \times 10^{21} = 3.87 \times 10^{22}$

b. In division, we subtract the exponents:

$1.67 \times 10^{-24}/9.12 \times 10^{-28} = 1.67/9.12 \times 10^{[-24 - (-28)]} = 0.183 \times 10^{4} = 1.83 \times 10^{3}$

Accuracy and Precision

Measurements may be accurate, meaning that the measured value is the same as the true value; they may be precise, meaning that multiple measurements give nearly identical values (i.e., reproducible results); they may be both accurate and precise; or they may be neither accurate nor precise. The goal of scientists is to obtain measured values that are both accurate and precise.

Suppose, for example, that the mass of a sample of gold was measured on one balance and found to be 1.896 g. On a different balance, the same sample was found to have a mass of 1.125 g. Which was correct? Careful and repeated measurements, including measurements on a calibrated third balance, showed the sample to have a mass of 1.895 g. The masses obtained from the three balances are in the following table:

Balance 1	**Balance 2**	**Balance 3**
1.896 g	1.125 g	1.893 g
1.895 g	1.158 g	1.895 g
1.894 g	1.067 g	1.895 g

Whereas the measurements obtained from balances 1 and 3 are reproducible (**precise**) and are close to the accepted value (**accurate**), those obtained from balance 2 are neither. Even if the measurements obtained from balance 2 had been precise (if, for example, they had been 1.125, 1.124, and 1.125), they still would not have been accurate. We can assess the precision of a set of measurements by calculating the average deviation of the measurements as follows:

1. Calculate the average value of all the measurements:

   average = sum of measurements number of measurements

2. Calculate the deviation of each measurement, which is the absolute value of the difference between each measurement and the average value:

   deviation = |measurement − average|

   where | | means absolute value (i.e., convert any negative number to a positive number).
3. Add all the deviations and divide by the number of measurements to obtain the average deviation:

   average = sum of deviations number of measurements

Then we can express the precision as a percentage by dividing the average deviation by the average value of the measurements and multiplying the result by 100. In the case of balance 2, the average value is

1.125 g + 1.158 + 1.067 g3= 1.117 g

The deviations are 1.125 g − 1.117 g = 0.008 g, 1.158 g − 1.117 g = 0.041 g, and |1.067 g − 1.117 g| = 0.050 g. So, the average deviation is

0.008 g + 0.041 g + 0.050 g = 0.033 g

The precision of this set of measurements is therefore

0.033g1.117g×100 = 3.0%

When a series of measurements is precise but not accurate, the error is usually systematic. Systematic errors can be caused by faulty instrumentation or faulty technique. The difference between accuracy and precision is demonstrated in Skill Builder ES7.

Example 11

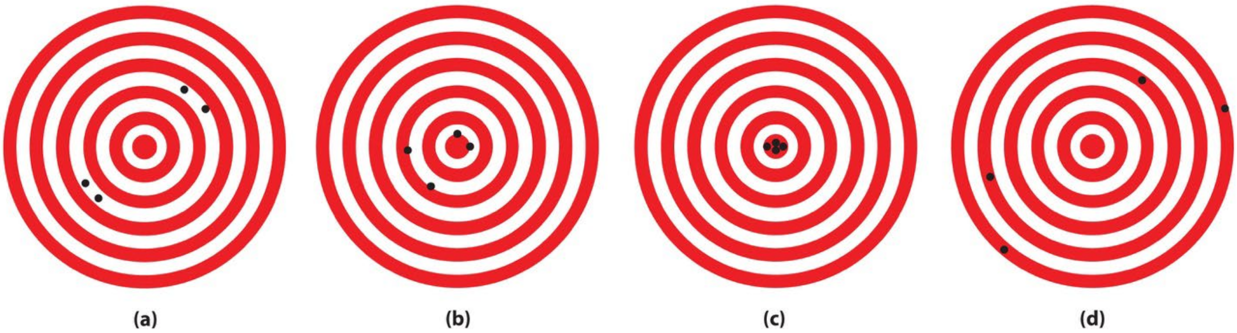
The following archery targets show marks that represent the results of four sets of measurements. Which target shows

a. a precise but inaccurate set of measurements?

b. an accurate but imprecise set of measurements?

c. a set of measurements that is both precise and accurate?

d. a set of measurements that is neither precise nor accurate?



Solution

(c), (a), (b), and (d)

Example 12

A 1-carat diamond has a mass of 200.0 mg. When a jeweler repeatedly weighed a 2-carat diamond, he obtained measurements of 450.0 mg, 459.0 mg, and 463.0 mg. Were the jeweler's measurements accurate? Were they precise?

Solution

The expected mass of a 2-carat diamond is 2 × 200.0 mg = 400.0 mg. The average of the three measurements is 457.3 mg, about 13% greater than the true mass. These measurements are not particularly accurate. The deviations of the measurements are 7.3 mg, 1.7 mg, and 5.7 mg, respectively, which give an average deviation of 4.9 mg and a precision of 4.9mg457.3mg×100 = 1.1%. These measurements are rather precise.

Example 13

A single copper penny was tested three times to determine its composition. The first analysis gave a composition of 93.2% zinc and 2.8% copper, the second gave 92.9% zinc and 3.1% copper, and the third gave 93.5% zinc and 2.5% copper. The actual composition of the penny was 97.6% zinc and 2.4% copper. Were the results accurate? Were they precise?

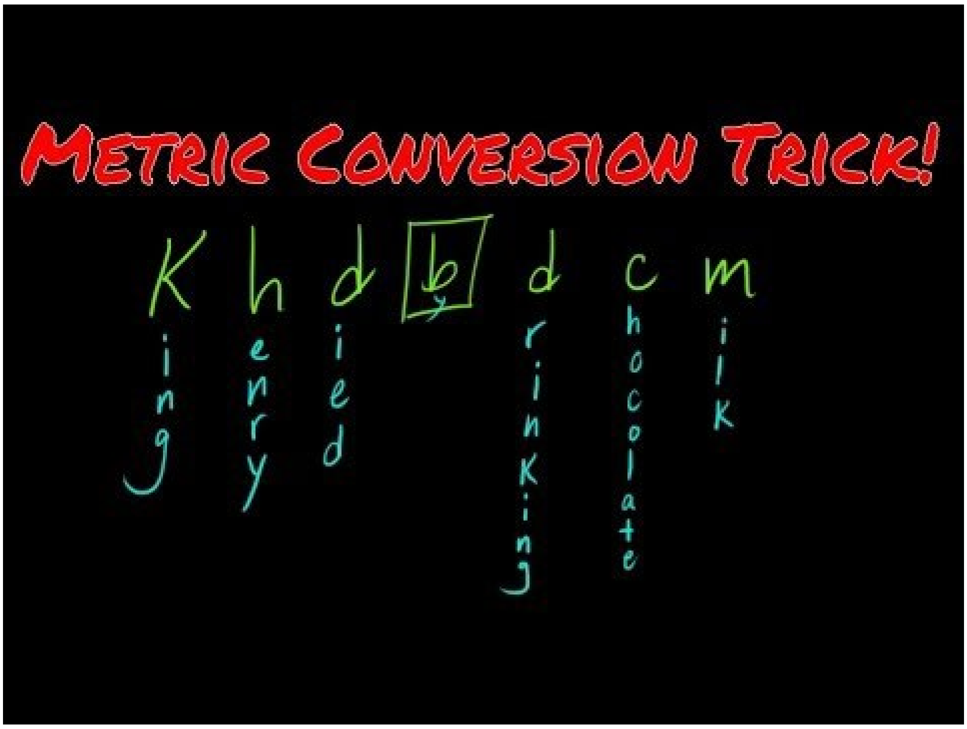
Solution

The average values of the measurements are 93.2% zinc and 2.8% copper versus the true values of 97.6% zinc and 2.4% copper. Thus, these measurements are not very accurate, with errors of −4.5% and + 17% for zinc and copper, respectively. The sum of the measured zinc and copper contents is only 96.0% rather than 100%, which tells us that either there is a significant error in one or both measurements or some other element is present. The deviations of the measurements are 0.0%, 0.3%, and 0.3% for both zinc and copper, which give an average deviation of 0.2% for both metals. We might therefore conclude that the measurements are equally precise, but that is not the case. Recall that precision is the average deviation divided by the average value times 100. Because the average value of the zinc measurements is much greater than the average value of the copper measurements (93.2% versus 2.8%), the copper measurements are much less precise.

precision (Zn) =0.2%93.2%×100 = 0.2%

precision (Cu) =0.2%2.8%×100 = 7%

Section 1.5. SI Units



SI Units

Metric system is the oldest method of measurement. In each type of measurement, there is a base unit. The other units are related to the base unit by power of 10. These are called metric prefixes. The prefix of the unit name indicates if the unit is larger or smaller than the base unit.

Length is measured by determining the distance between two points. Mass is determined by the amount of matter in an object. Volume is determined by the amount of space occupied by a three -dimensional object.

Metric Base Units

The metric system uses the following base units:

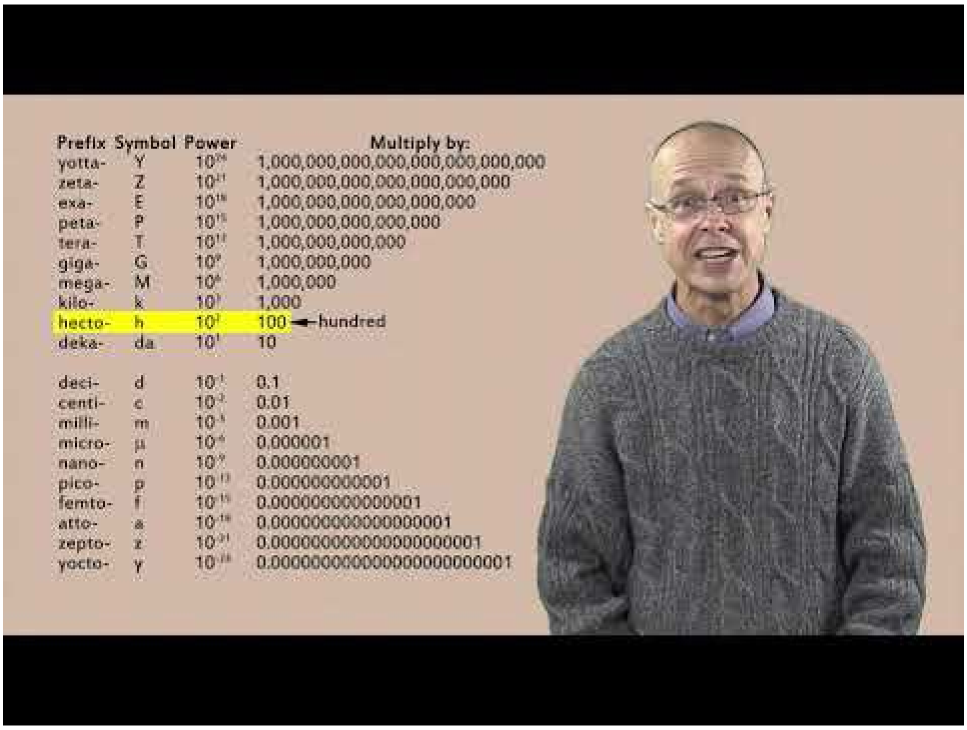
Unit of Measurement	Name of Unit	Abbreviation
Length	Meter	m or cm
Mass	Gram	g
Volume	Liter	L

Find below common metric prefixes.

Table 1.3.

Prefix	Symbol	Value	Power of 10	Meaning
tera	T	1,000,000,000,000	10^{12}	trillion
giga	G	1,000,000,000	10^{9}	billion
mega	M	1,000,000	10^{6}	million
kilo	k	1000	10^{3}	thousand
hecto	h	100	10^{2}	hundred
deca	da	10	10^{1}	ten
—	—	1	10^{0}	one
deci	d	0.1	10^{-1}	tenth
centi	c	0.01	10^{-2}	hundredth
milli	m	0.001	10^{-3}	thousandth
micro	µ	0.000001	10^{-6}	millionth
nano	n	0.000000001	10^{-9}	billionth
pico	p	0.000000000001	10^{-12}	trillionth

Prefix	Symbol	Value	Power of 10	Meaning
femto	f	0.000000000000001	10^{-15}	quadrillionth



Prefix	Symbol	Power	Multiply by:
yotta-	Y	10^{24}	1,000,000,000,000,000,000,000,000
zeta-	Z	10^{21}	1,000,000,000,000,000,000,000
exa-	E	10^{18}	1,000,000,000,000,000,000
peta-	P	10^{15}	1,000,000,000,000,000
tera-	T	10^{12}	1,000,000,000,000
giga-	G	10^{9}	1,000,000,000
mega-	M	10^{6}	1,000,000
kilo-	k	10^{3}	1,000
hecto-	h	10^{2}	100 ←hundred
deka-	da	10^{1}	10
deci-	d	10^{-1}	0.1
centi-	c	10^{-2}	0.01
milli-	m	10^{-3}	0.001
micro-	µ	10^{-6}	0.000001
nano-	n	10^{-9}	0.000000001
pico-	p	10^{-12}	0.000000000001
femto-	f	10^{-15}	0.000000000000001
atto-	a	10^{-18}	0.000000000000000001
zepto-	z	10^{-21}	0.000000000000000000001
yocto-	y	10^{-24}	0.000000000000000000000001

All reported measurements must include an appropriate unit of measurement because to say that a substance has "a mass of 10," for example, does not tell whether the mass was measured in grams, pounds, tons, or some other unit. To establish worldwide standards for the consistent measurement of important physical and chemical properties, an international body called the General Conference on Weights and Measures devised the **Système internationale d'unités** (or SI). The International System of Units is based on metric units and requires that measurements be expressed in decimal form. Table 1.7 "SI Base Units" lists the seven base units of the SI system; all other SI units of measurement are derived from them.

By attaching prefixes to the base unit, the magnitude of the unit is indicated; each prefix indicates that the base unit is multiplied by a specified power of 10. The prefixes, their symbols, and their numerical significance are given below. To study chemistry, you need to know the information presented in tables 1.3 and 1.4 containing the SI base units and the prefixes to be used with the SI units, respectively.

Base Quantity	**Unit Name**	**Abbreviation**
mass	kilogram	kg
length	meter	m
time	second	s
temperature	kelvin	K
electric current	ampere	A
amount of substance	mole	mol
luminous intensity	candela	cd

Table 1.4 Prefixes used with SI units of mass, volume, and length

The units of measurement you will encounter most frequently in chemistry are those for mass, volume, and length. The basic SI unit for mass is the **kilogram (kg)**, but in the laboratory, mass is usually expressed in either grams (g) or milligrams (mg): 1000 g = 1 kg, 1000 mg = 1 g, and 1,000,000 mg = 1 kg. Units for volume are derived from the cube of the SI unit for length, which is the meter (m). Thus, the basic SI unit for volume is **cubic meters** (length × width × height = m^3). In chemistry, however, volumes are usually reported in cubic centimeters (cm^3) and cubic decimeters (dm^3) or milliliters (mL) and liters (L), although the liter is not an SI unit of measurement. The relationships between these units are as follows:

$1\ L = 1000\ mL = 1\ dm^3 1\ mL = 1\ cm^3 1000\ cm^3 = 1\ L$

Liter: It is a nonstandard metric unit. Liter is defined as volume of 0.1 m cube or 1 decimeter cube. A smaller non SI unit is often used to measure volume which is 1 milliliter. Since 1000ml = 1L and 1 L contains 1000 cm3, therefore 1 cm3= 1ml. Usually 1 cm3 is used for solid substances and 1 ml is used liquid substances.

Mass	Kilogram	kg
Temperature	Kelvin	K
Time	Second	s
Amount of Substance	Mole	mol
Electric Current	Ampere	I
		I_v
Luminous Intensity	Lumen	

Table 1.5 SI Units & Symbols

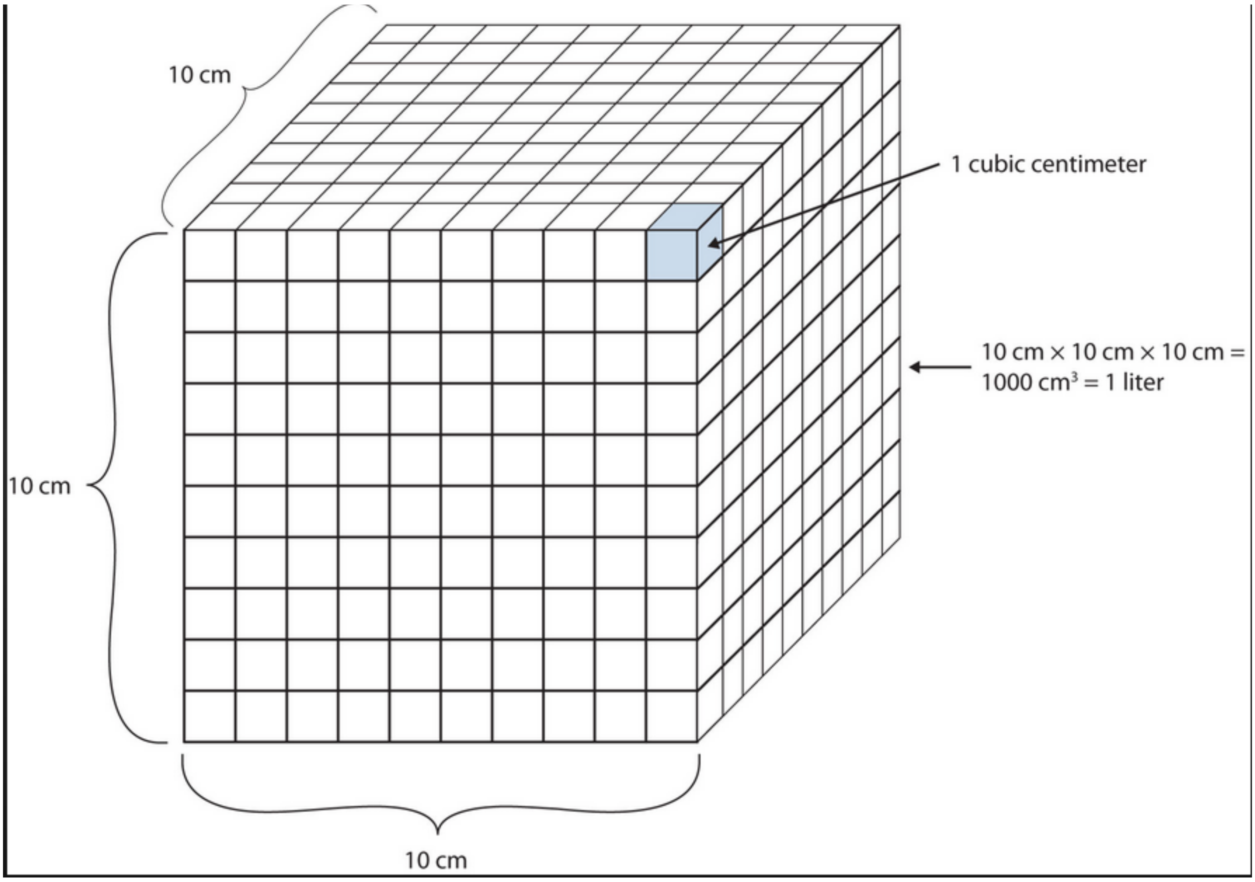


Figure 1.20 Definition of 1 Liter

*****The new definition of the kilogram sets it equal to the mass of 1.4755214 x 10^{40} photons from a cesium atom.**

Kelvin is defined in terms of Boltzman constant

Mol is defined in terms of Avogadro number 6.02214076 × 10^{23} mol^{-1}.

Section 1.6. Dimensional Analysis

Dimensional analysis (also called factor label method or unit analysis) is used to convert from one set of units to another. This method is used for both simple (feet to inches) and complex (g/cm^3 to kg / gallon) conversions and uses relationships or conversion factors between different sets of units. While the terms are frequently used interchangeably, conversion factors and relationships are different. Conversion factors are quantities that are equal to one another, such as 100 cm = 1m, 100 cm = 1m, in which both values describe a length. Relationships are between two values that are not necessarily a measure of the same quantity. For example, the density of water is 1.00 g / mL. Grams are a measure of mass while milliliters measure volume so this is considered a relationship rather than a conversion factor. Either way, we depend on units to help set up and solve the calculation. We will see additional examples of relationships as we explore other details about chemical substance.

Conversion Factors

Many quantities can be expressed in several different ways. The English system measurement of 4 cups is also equal to 2 pints, 1 quart, and 1414of a gallon. Notice that the numerical component of each quantity is different, while the actual amount of material that it represents is the same. That is because the units are different. We can establish the same set of equalities for the metric system:

1meter = 10 decimeters = 100 centimeters = 1000 millimeters 1 meter = 10 decimeters = 100 centimeters = 1000 millimeters.

The metric system's use of powers of 10 for all conversions makes this quite simple. We can write conversion factors between any pair of equivalent quantities. In each conversion factor, the numerator and denominator represent equal quantities so they are all valid conversion factors. Additionally, these conversion factors can be inverted or used in combination with other conversion factors in a dimensional analysis problem.

1 meter = 10 decimeters = 100 centimeters = 1000 milimeters

Case1: Conversion factor can be used within a system of units or between different units of system. (defined relationship)

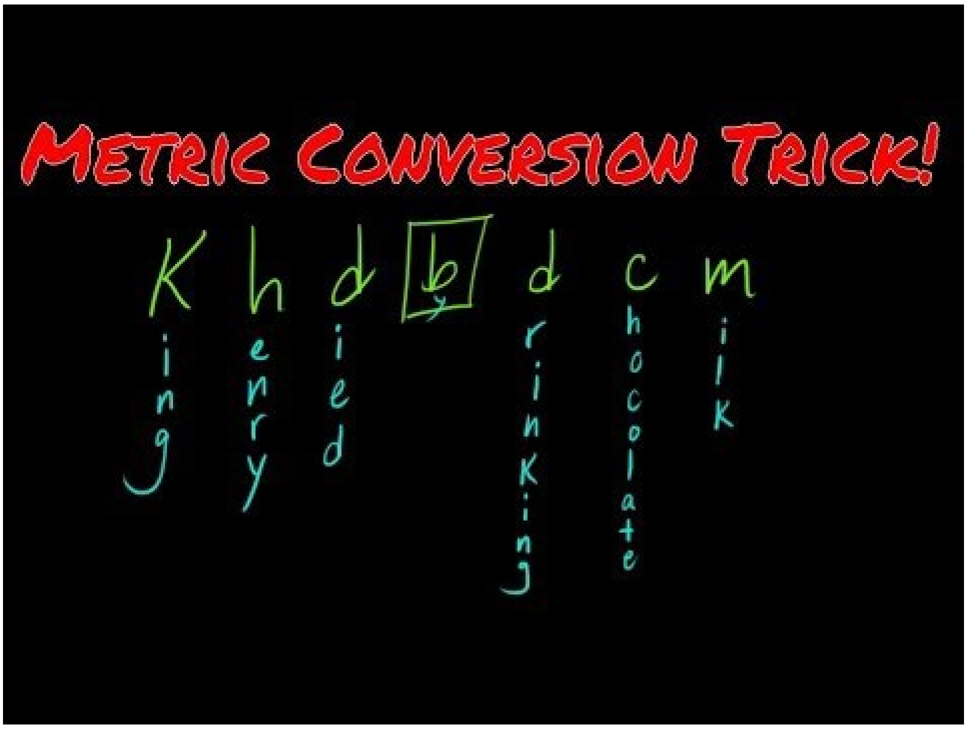
Example problem: A lab test showed an individual's cholesterol level to be 186 mg/dL. Convert this quantity into g/dL

given 1g= 1000mg

$$\frac{186mg}{1dL} \times \frac{1\,g}{1000mg} = 0.186\,g/dL$$

In order to obtain metric to metric conversion factor, the meaning of metric prefixes and their values must be known.

For more information watch:



https://www.youtube.com/watch?v=5tHpDzXP-lg

Metric conversion: ladder method

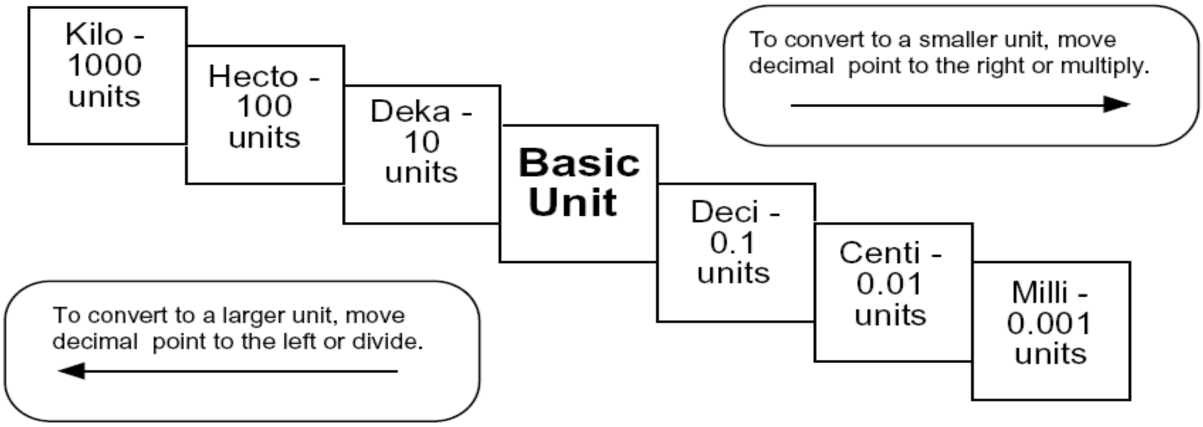


Figure 1.21: Ladder method of Metric System

Ref: commons.wikimedia.org/

How do you use ladder method?

1st – Determine your starting point.

2nd – Count the "jumps" to your ending point.

3rd – Move the decimal the same number of jumps in the same direction.

Example: 4km =__________m

↑start ↑End

4. 0 0 0 = 4000m

Write the abbreviation of following Metric Conversions:

1) Kilogram ______

2) Meter ______

3) Gram ______

4) Milliliter ______

5) Millimeter ______

6) Liter ______

7) Kilometer ______

8) Centimeter ______

9) Milligram ______

Try these conversions, using the ladder method.

10) 2000 mg = ________ g

11) 104 km = ________ m

12) 480 cm = ______ m

13) 5.6 kg = ______ g

14) 8 mm = ______ cm

15) 5 L = ________ mL

16) 198 g = ________ kg

17) 75 mL = ______ L

18) 50 cm = ______ m

19) 5.6 m = ______ cm

20) 16 cm = ________ mm

21) 2500 m = ________ km

22) 65 g = ______ mg

23) 6.3 cm = ______ mm

24) 120 mg = ______ g

Compare using <, >, or =.

56 cm 6 m

7 g 698 mg

5 g 508 mg

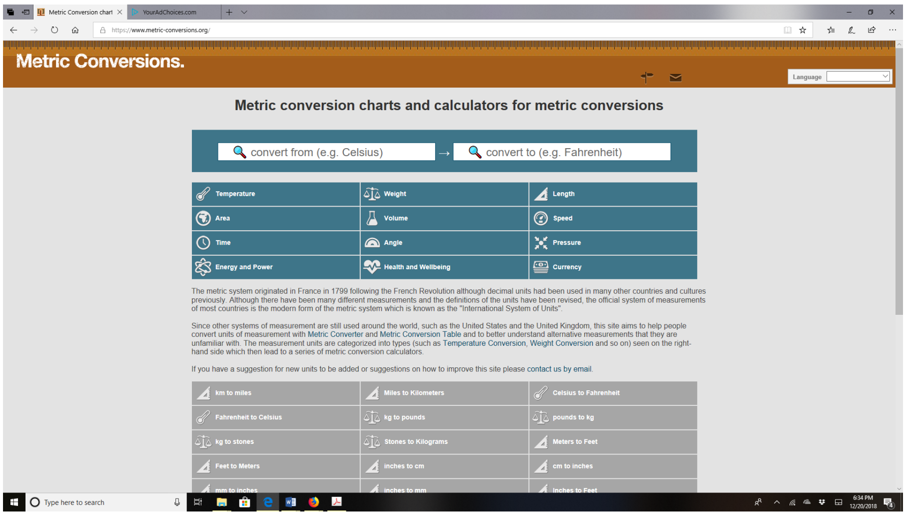
1,500 mL 1.5 L

536 cm 53.6 dm

43 mg 5 g

3.6 m 36 cm

For more information visit:



https://www.metric-conversions.org/

Metric conversion charts and calculators for metric conversions

The metric system originated in France in 1799 following the French Revolution although decimal units had been used in many other countries and cultures previously. Although there have been many different measurements and the definitions of the units have been revised, the official system of measurements of most countries is the modern form of the metric system which is known as the "International System of Units".

Since other systems of measurement are still used around the world, such as the United States and the United Kingdom, this site aims to help people convert units of measurement with Metric Converter and Metric Conversion Table and to better understand alternative measurements that they are unfamiliar with. The measurement units are categorized into types (such as Temperature Conversion, Weight Conversion and so on) seen on the right-hand side which then lead to a series of metric conversion calculators.

If you have a suggestion for new units to be added or suggestions on how to improve this site please contact us by email.

https://www.metric-conversions.org/

Questions:

1. Convert each of the following measurements into meters?

a. 2.5×10^3 mm

b. 25 µm

Case 2: Metric to English conversion factors are specified with different number of significant figures. (measured relationship). They are called equalities. For example: 1 mile= 1.61 km. mile is the English unit and kilometer (km) in the metric unit.

Example #1 : Capillaries, the microscopic vessels that carry the blood from small arteries to small veins, are on the average only 0.1cm long. What is the average length of a capillary in inches?

Given 1 inch= 2.54 cm

$$0.1 \text{ cm} \times \frac{1 \text{ inch}}{2.54 \text{ cm}} = 0.0393 \text{ in} = 0.04 \text{ in}$$ (lowest 1 sig fig used in calc)

Here is the table of most common metric to metric and metric to English conversion factors:

Example #2: Convert 10.8 ft to meters

Given that 12 in = 1ft, 2.54 cm= 1 inch and 100 cm = 1meter

$$\text{Pathway: ft} * \frac{\text{12 in} \quad * \text{ 2.54 cm} \quad * \text{ 1 m}}{\text{1 ft} \qquad \text{1 in} \qquad \text{100 cm}} = \text{meter}$$

Now plug in the numbers in tis problem:

$$\frac{\text{10.8 ft} * \text{12 in} * \text{2.54 cm} * \text{1m}}{\text{1ft} * \text{1 in} * \text{100cm}} = \text{3.28 m (ans)}$$

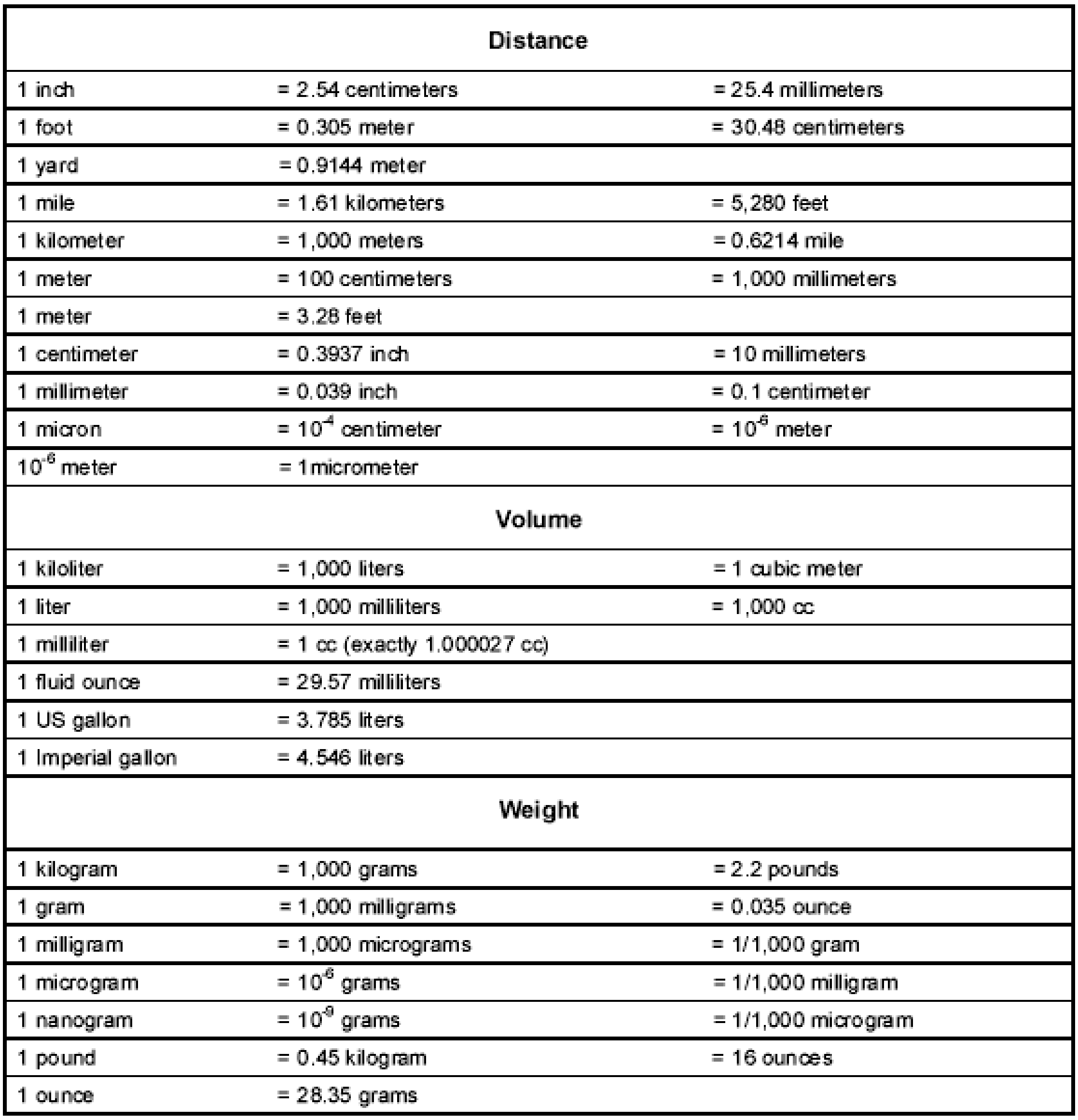
Example#3: Convert 58.8 lbs to kg.

Given : 58.8 lbs, needed kg. conversion factor: 2.205 lbs= 1 kg

$$\text{pathway: lbs} * \frac{\text{1kg}}{\text{1.205 lbs}}$$

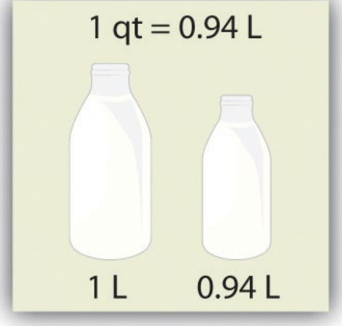
now use the values given in the problem,

$$\frac{\text{58.8 lbs} * \text{1 kg}}{2.205} = \text{26.7 kg}$$

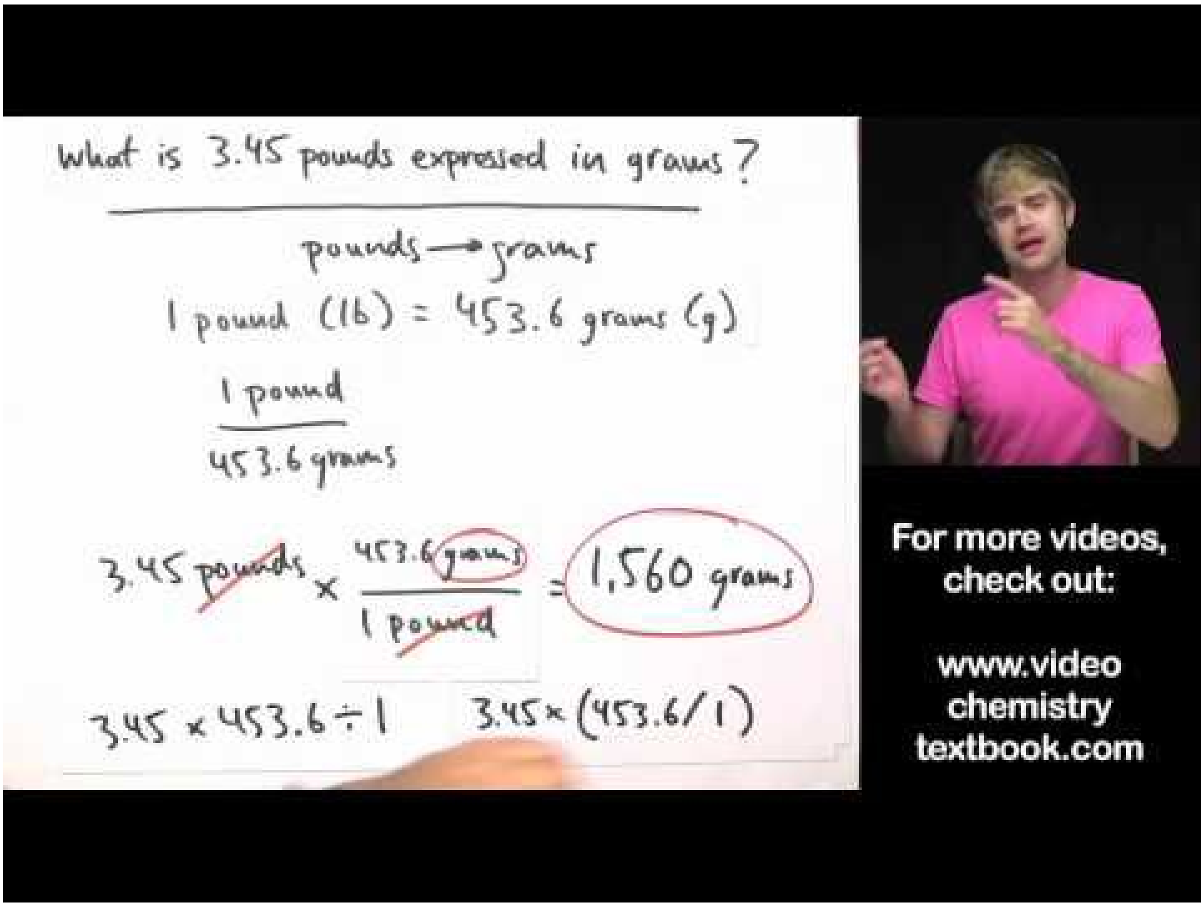


Distance		
1 inch	= 2.54 centimeters	= 25.4 millimeters
1 foot	= 0.305 meter	= 30.48 centimeters
1 yard	= 0.9144 meter	
1 mile	= 1.61 kilometers	= 5,280 feet
1 kilometer	= 1,000 meters	= 0.6214 mile
1 meter	= 100 centimeters	= 1,000 millimeters
1 meter	= 3.28 feet	
1 centimeter	= 0.3937 inch	= 10 millimeters
1 millimeter	= 0.039 inch	= 0.1 centimeter
1 micron	= 10^{-4} centimeter	= 10^{-6} meter
10^{-6} meter	= 1micrometer	
Volume		
1 kiloliter	= 1,000 liters	= 1 cubic meter
1 liter	= 1,000 milliliters	= 1,000 cc
1 milliliter	= 1 cc (exactly 1.000027 cc)	
1 fluid ounce	= 29.57 milliliters	
1 US gallon	= 3.785 liters	
1 Imperial gallon	= 4.546 liters	
Weight		
1 kilogram	= 1,000 grams	= 2.2 pounds
1 gram	= 1,000 milligrams	= 0.035 ounce
1 milligram	= 1,000 micrograms	= 1/1,000 gram
1 microgram	= 10^{-6} grams	= 1/1,000 milligram
1 nanogram	= 10^{-9} grams	= 1/1,000 microgram
1 pound	= 0.45 kilogram	= 16 ounces
1 ounce	= 28.35 grams	

Table 1.6 Unit Conversion factors between Metric & English



For more information watch:



What is 3.45 pounds expressed in grams?

pounds → grams

1 pound (lb) = 453.6 grams (g)

$$\frac{1\ \text{pound}}{453.6\ \text{grams}}$$

$$3.45\ \cancel{\text{pounds}} \times \frac{453.6\ \cancel{\text{grams}}}{1\ \cancel{\text{pound}}} = \boxed{1{,}560\ \text{grams}}$$

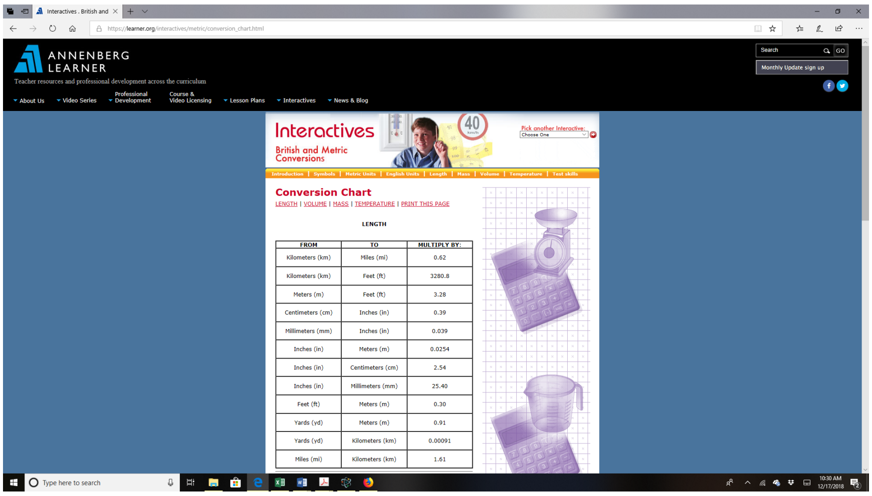
$3.45 \times 453.6 \div 1$ $3.45 \times (453.6/1)$

For more videos, check out:

www.videochemistrytextbook.com

https://www.youtube.com/watch?v=7N0lRJLwpPI

For more information visit:



Conversion Chart

LENGTH | VOLUME | MASS | TEMPERATURE | PRINT THIS PAGE

LENGTH

FROM	TO	MULTIPLY BY:
Kilometers (km)	Miles (mi)	0.62
Kilometers (km)	Feet (ft)	3280.8
Meters (m)	Feet (ft)	3.28
Centimeters (cm)	Inches (in)	0.39
Millimeters (mm)	Inches (in)	0.039
Inches (in)	Meters (m)	0.0254
Inches (in)	Centimeters (cm)	2.54
Inches (in)	Millimeters (mm)	25.40
Feet (ft)	Meters (m)	0.30
Yards (yd)	Meters (m)	0.91
Yards (yd)	Kilometers (km)	0.00091
Miles (mi)	Kilometers (km)	1.61

https://learner.org/interactives/metric/conversion_chart.html

Practice Questions:

1. A chemistry student weighs 83.1 kg and 1.93 m tall. What are the person's equivalent measurements in pounds and feet?
2. What volume of water in gallons would be required to fill a 30.ml of container?

Example 14

How many centimeters are in 3.4m?

Solution

This problem requires the conversion from one unit to another so we can use dimensional analysis to solve the problem. We need to identify the units that are given (m), the units for the answer (cm), and any relationships that relate the units of the known and unknown values. In this case, we will use the relationship of 1 m = 100 cm. Start with the known value and its unit.

3.4 m× ? = ___ cm

Then, we look at the units of our relationship to see which value goes in the numerator and which value goes in the denominator. Remember, we are trying to find the value in centimeters. Since our known value is in units of meters, we need meters to be in the denominator so that it will cancel. As a result, centimeters will be in the numerator.

3.4 m × 100 cm / 1 m

Note that the numbers stay with the appropriate unit (100 with centimeters and 1 with meters). Now, the meters will cancel out and we are left with units of centimeters. Always check that your problem is set up completely and that your units cancel correctly before you do the actual calculation.

3.4 m × 100 cm / 1 m = 340 cm = 3.4×10^2 cm

We find the answer to be 340 cm or 3.4×10^2 cm.

Derived Units

Using dimensional analysis with derived units requires special care. When units are squared or cubed as with area or volume, the conversion factors themselves must also be squared or cubed. Two convenient volume units are the liter, which is equal to a cubic decimeter, and the milliliters, which is equal to a cubic centimeter. There are thus 1000 cm^3 in $1dm^3$, which is the same thing as saying there are 1000 mL in 1L. The conversion factor of $1cm^3$ = 1 mL is a very useful conversion.

Example 15

Convert 3.6 mm^3 to mL.

Solution

Determine the units of the known value, mm^3 and the units of the unknown value, mL. The starting and ending units will help guide the setup of the problem. Next, list any known conversion factors that might be helpful.

1 m = 1000 mm

1 mL = $1cm^3$

1 m = 100 cm

Now, we can set up the problem to find the value in units of mL. Once we know the starting units, we can then use the conversion factors to find the answer.

3.6 mm^3 × (??)

Continue to use the conversion factors between the units to set up the rest of the problem. Note that all of the units cancel except mL, which are the requested units for the answer. Since the values in these conversion factors are exact numbers, they will not affect the number of significant figures in the answer. Only the original value (3.6) will be considered in determining significant figures.

3.6 mm^3 × (1m / 1000 mm)^3 × (??)

Once you have solved the problem, always ask if the answer seems reasonable. Remember, a millimeter is very small and a cubic millimeter is also very small. Therefore, we would expect a small volume which means 0.0036mL0.0036mL is reasonable.

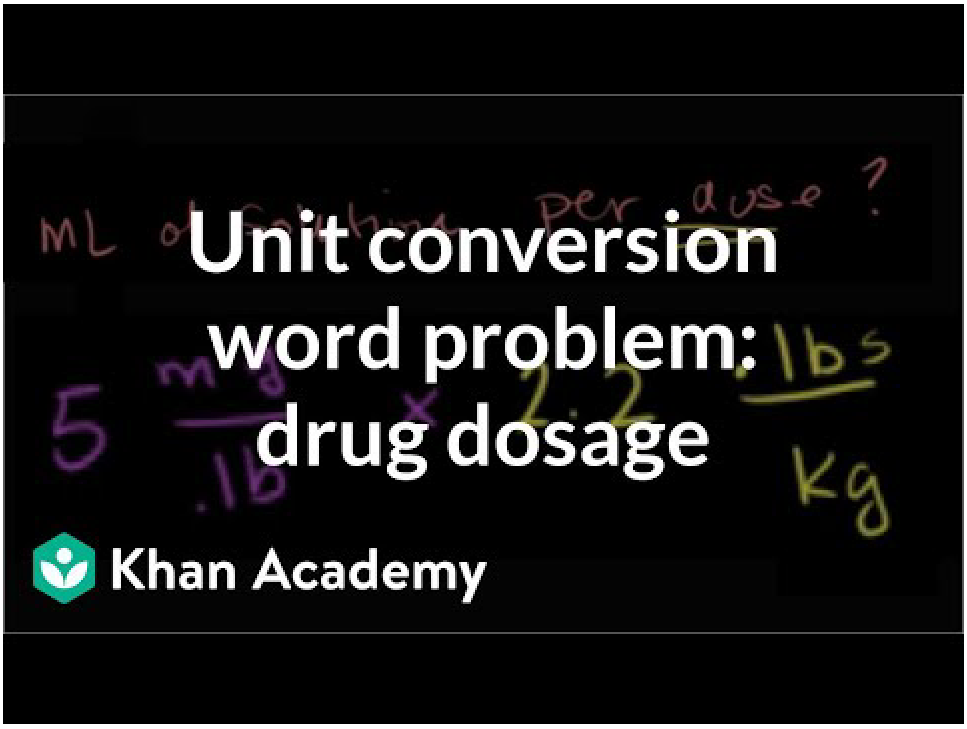
If you find that you forgot to cube numbers as well as units, you can setup the problem in an expanded form which is the equivalent to the previous method to cube the numerical values.

Step#1: Identify the units of known or given quantity and the units of target quantity

Step#2: Figure out the conversion factors required from given unit to target unit.

Step#3: Multiply the given quantity by one or more conversion factors in such a manner that the original units are canceled leaving only the desired unit.

Watch this out to solve drug dosage related problems that require conversion factors.



Example Problem:

(A) A dose of 250 mg of acetaminophen is prescribed for a 20-kg child. How many ml of Children's Tynenol (100. mg of acetaminophen per 2.5 ml) are needed?

Step#1: Identify given and target quantity and numbers:

Given: 250mg target: ml

Step#2: Write the conversion factors:

Provided in the problem: $\frac{2.5 \text{ ml}}{100 \text{ mg}}$

Step#3. Multiply the given quantity by the conversion factor.

$$250 \text{ mg} \times \frac{2.5 \text{ ml}}{100 \text{ mg}} = 6.3\text{ml (lowest 2 sig fig)}$$

Check: the answer is reasonable. Since the required dose is larger than standard dose, volume would be larger than standard.

Nurses Conversion units for drugs

Drug Calculations

Drug calculations vary depending on whether you are dealing with liquid or solid medications, or if the dose is to be given over a period of time. In this section I will go over each of these situations in turn.

It is very important that you know how drug dosages are worked out, because it is good practise to always check calculations before giving medication, no matter who worked out the original amount. It is far better to point out a mistake on paper than overdose a patient.

a) Tablets

Working out dosage from tablets is simple.

Formula for dosage:

$$\frac{\textbf{Total dosage required}}{\textbf{Dosage per tablet}} = \textbf{Number of tablets required}$$

Note-If your answer involves small fractions of tablets, it would be more sensible to try to find tablets of a different strength rather than try to make $\frac{2}{3}$ of a tablet for example.

Examples

1. A patient needs 500mg of X per day. X comes in 125mg tablets. How many tablets per day does he need to take?

Total dosage required is 500mg,
Dosage per tablet is 125mg

So our calculation is $\frac{500}{12} = 4$
He needs 4 tablets a day

b) Liquid Medicines

Liquid medicines are a little trickier to deal with as they will contain a certain dose within a certain amount of liquid, such as 250mg in 50ml, for example.

To work out the dosage, we use the formula:

What you want × What it's in What
you've got

Note: In order to use this formula, the units of measurement must be the same for 'What you want' and 'What you've got'; i.e. both mg or both mcg etc.

Examples

2. We need a dose of 500mg of Y. Y is available in a solution of 250mg per 50ml.

In this case,

What we want = 500 What
we've got = 250 What it's
in = 50

So our calculation is $\frac{500}{250} \times 50 = 100$

We need 100ml of solution.

3. We need a dose of 250mg of Z. Z is available in a solution of 400mg per 200ml. In this

case,

What we want = 250 What
we've got = 400 What it's
in = 200

So our calculation is $\frac{250}{400} \times 200 = 125$

We need 125ml of solution.

c) Medicine over Time

1) Tablets/liquids

This differs from the normal calculations in that we have to split our answer for the total dosage into 2 or more smaller doses.

Look at Example 1 again. If the patient needed the 500mg dose to last the day, and tablets were taken four times a day, then our total of 4 tablets would have to be split over 4 doses.

$\frac{\text{Total amount of liquid/tablets for day}}{\text{Number of doses per day}} = \text{Amount to be given per dose}$

We would perform the calculation: 4÷4=1 So he would need 1 tablet 4 times a day.

2) Drugs delivered via infusion

For calculations involving infusion, we need the following information:

- The total dosage required
- The period of time over which medication is to be given
- How much medication there is in the solution

Example

4. A patient is receiving 500mg of medicine X over a 20 hour period. X is delivered in a solution of 10mg per 50ml.

What rate should the infusion be set to? Here

our total dosage required is 500mg

Period of time is 20 hours

There are 10mg of X per 50ml of solution

Firstly we need to know the total volume of solution that the patient is to receive. Using the formula for liquid dosage we have:

$\frac{500}{1} \times 50 = 2500$ So the patient needs to receive 2500mls.

We now divide the amount to be given by the time to be taken: $\frac{25}{2} = 125$

$\underline{00}$

The patient needs 2500mls to be given at a rate of 125mls per hour

Note: Working out medicines over time can appear daunting, but all you do is work out how much medicine is needed in total, and then divide it by the amount of hours/doses needed

d) Drugs labelled as a percentage

Some drugs may be labelled in different ways to those used earlier.

V/V and W/V

Some drugs may have V/V or W/V on the label.

V/V means that the percentage on the bottle corresponds to volume of drug per volume of solution

i.e 15% V/V means for every 100ml of solution, 15ml is the drug.

W/V means that the percentage on the bottle corresponds to the weight of drug **per volume** of solution. Normally this is of the form ‘number of grams per number of millilitres’. So in this case 15% W/V means that for every 100ml of solution there are 15 grams of the drug.

If we are converting between solution strengths, such as diluting a 20% solution to make it a 10% solution, we do not need to know whether the solution is V/V or W/V.

Examples

5. We need to make up 1 litre of a 5% solution of A. We have stock solution of 10%. How much of the stock solution do we need? How much water do we need?

We can adapt the formula for liquid medicines here:

What we want × **What we want it to be in**
What we've got

We want a 5% solution. This is the same

10

5/101/20

1

We've got a 10% solution. This is the same as 10/100 or 10 .

We want our finished solution to have a volume of 1000ml. Our formula becomes: (1/20) * 1000

(1/10)

(using the rule for dividing fractions)

= 1/2×1000 = 500 .

We need 500mls of the A solution.

Which means we need 1000 - 500 = 500mls of water.

(Alternatively you can use the fact that a 5% solution is half the strength of a 10% solution to see that you need 500ml of solution and 500ml of water)

6. You have a 20% V/V solution of drug F. The patient requires 30ml of the drug. How much of the solution is required?

20% V/V means that for every 100ml of solution we have 20ml of drug F. Using our formula:

What you want ×
What it's in

What you've got

This becomes
2
30 ×100 = 150

We need

150mls of

solution.

7. Drug G comes in a W/V solution of 5%. The patient requires 15 grams of G. How many mls of solution are needed?

5% W/V means that for every 100mls of solution, there are 5 grams of G. Using the formula gives us

$$\frac{15}{5}\times 100 = 300$$

300mls of solution are required.

Other Dimensional analysis problem example:

(B) A person is driving a car with a speed of 229.8 km/h. What is the speed in

1) Miles per hour

2) Feet per second

Given 1 km= 0.6214 mile 1000m= 1km, 1 m= 3.28 ft, 60 sec=1min and 60 min= 1 hr

1) Step#1: Identify given and target quantity and numbers:

Given: 229.8km/hr target: mi/hr

Step#2: Write the conversion factors:

Provided in the problem: $\frac{0.6214\ \text{mi}}{1\ \text{km}}$

Step#3. Multiply the given quantity by the conversion factor.

$$229.8\ \text{km} \times \frac{0.6214\ \text{mi}}{1\ \text{km}} = 143.4\text{mi/hr}$$ (lowest 4 sig fig used in problem)

2) Step#1: Identify given and target quantity and numbers:

Given: 229.8km/hr target: ft/s

Step#2: Write the conversion factors:

Provided in the problem: $\frac{3.28\ \text{ft}}{1\ \text{m}}$ & $\frac{0.6214\ \text{mi}}{1\ \text{km}}$

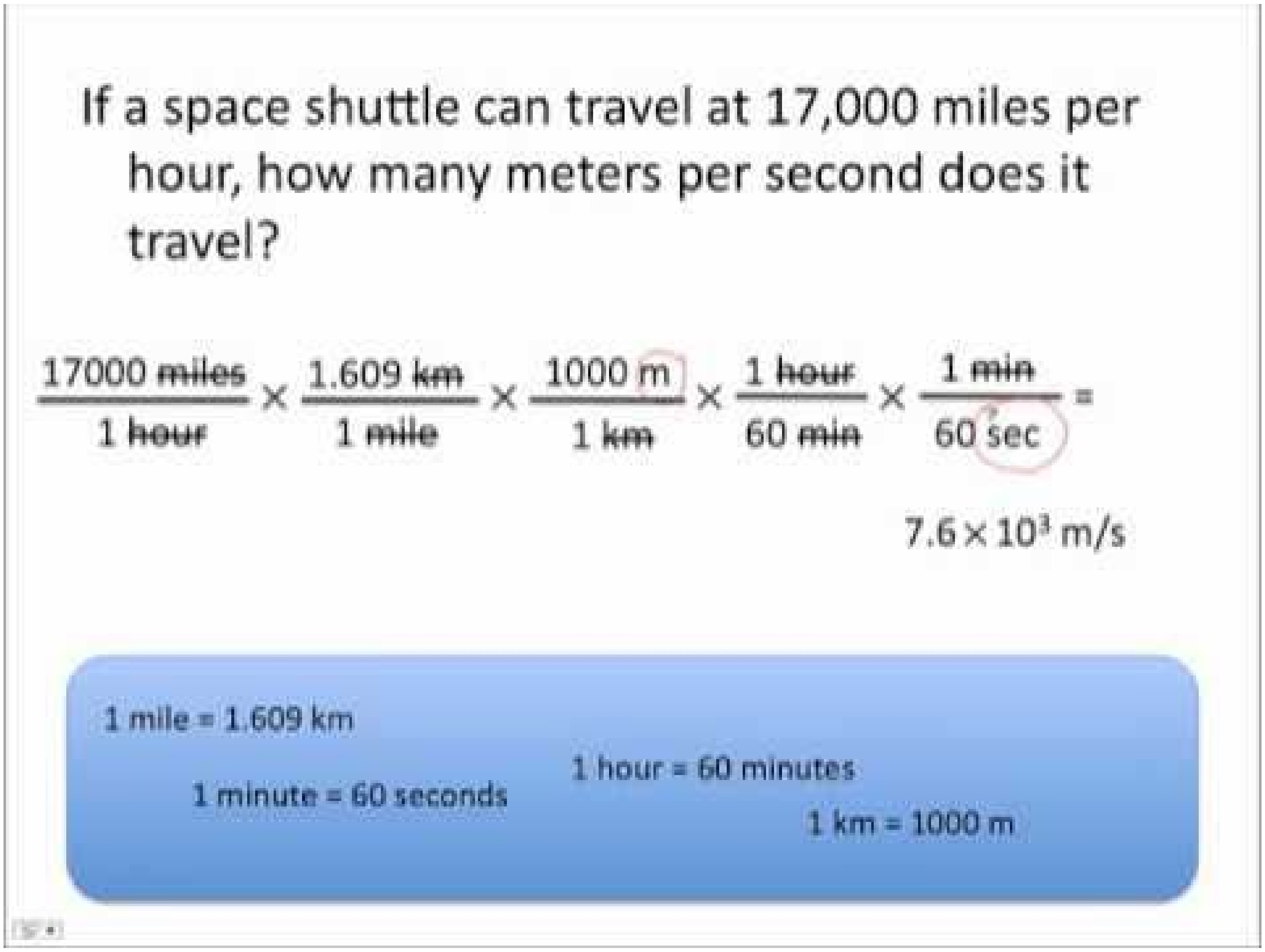
$\frac{1\ \text{hr}}{60\ \text{min}}$, $\frac{1\ \text{min}}{60\ \text{sec}}$

Step#3. Multiply the given quantity by the conversion factor.

$$\frac{229.8\ \text{km}}{1\ \text{hr}} \times \frac{1000\text{m}}{1\ \text{km}} \times \frac{3.28\ \text{ft}}{1\ \text{m}} \times \frac{1\ \text{hr}}{60\ \text{min}} \times \frac{1\ \text{min}}{60\ \text{sec}}$$

= 209 ft/s (lowest 3 sig fig used in calc).

For more information watch this out:



If a space shuttle can travel at 17,000 miles per hour, how many meters per second does it travel?

$$\frac{17000\ \cancel{\text{miles}}}{1\ \cancel{\text{hour}}} \times \frac{1.609\ \cancel{\text{km}}}{1\ \cancel{\text{mile}}} \times \frac{1000\ \boxed{\text{m}}}{1\ \cancel{\text{km}}} \times \frac{1\ \cancel{\text{hour}}}{60\ \cancel{\text{min}}} \times \frac{1\ \cancel{\text{min}}}{60\ \boxed{\text{sec}}} =$$

7.6×10^3 m/s

1 mile = 1.609 km

1 minute = 60 seconds

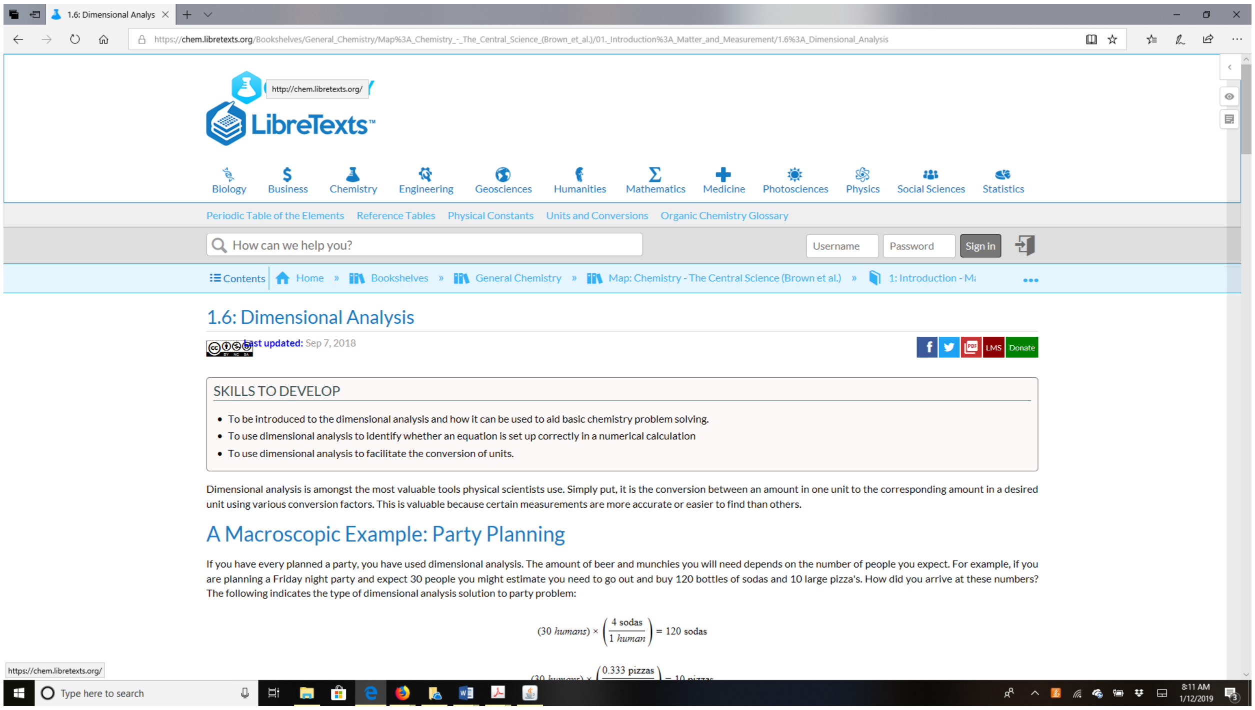
1 hour = 60 minutes

1 km = 1000 m

https://www.youtube.com/watch?v=DsTg1CeWchc

For more practice visit:

https://chem.libretexts.org/Bookshelves/General_Chemistry/Map%3A_Chemistry_-_The_Central_Science_(Brown_et_al.)/01._Introduction%3A_Matter_and_Measurement/1.6%3A_Dimensional_Analysis



1.6: Dimensional Analysis

Last updated: Sep 7, 2018

SKILLS TO DEVELOP

- To be introduced to the dimensional analysis and how it can be used to aid basic chemistry problem solving.
- To use dimensional analysis to identify whether an equation is set up correctly in a numerical calculation
- To use dimensional analysis to facilitate the conversion of units.

Dimensional analysis is amongst the most valuable tools physical scientists use. Simply put, it is the conversion between an amount in one unit to the corresponding amount in a desired unit using various conversion factors. This is valuable because certain measurements are more accurate or easier to find than others.

A Macroscopic Example: Party Planning

If you have every planned a party, you have used dimensional analysis. The amount of beer and munchies you will need depends on the number of people you expect. For example, if you are planning a Friday night party and expect 30 people you might estimate you need to go out and buy 120 bottles of sodas and 10 large pizza's. How did you arrive at these numbers? The following indicates the type of dimensional analysis solution to party problem:

$$(30\ humans) \times \left(\frac{4\text{ sodas}}{1\ human}\right) = 120\text{ sodas}$$

Questions:

1. If one teaspoon contains 5.0 ml, how many teaspoons of Children Tylenol (100. mg of acetaminophen per 2.5 ml) are needed for a child with a dose of 240 mg?
2. A patient is prescribed 0.150mg of a drug that is available in 25 µg tablets. How many tablets are needed?
3. How many milliliters of Children's Mortin (100 mg of ibuprofen per 5 ml) are needed to give a child a dose of 180 mg?

The following classroom resources has been taken from AACT.

Cupcake Conversions, from Bench to Bakery

Background

All consumer products start as a small batch to formulate ideal qualities but are scaled up to mass production for consumer purchase. In this process troubleshooting is essential to maintain quality and consistency of product.

You will take on the role of a successful baker who has an award winning recipe for cupcakes which is going to be scaled up to commercial baking. To achieve this end goal you will look at conversions from English units to Metric units and then standardize all units to grams regardless of ingredients. Finally you will look at issues on a microscale of production and see how they would affect macroscale baking of the product.

Objectives

- Convert measurements from English to the International Units of Measurement (Metric).
- Scale up measurements for a standard recipe to a larger quantity.
- Trouble shoot problems encountered with scaling up a product from bench to bakery (small to larger quantities).

Activity 1

1. Read the recipe for a vanilla cupcake below:

Vanilla Cupcakes

The following recipe yields 20-25 cupcakes.

Ingredients:

- 2 cups of flour
- ½ teaspoon of salt
- 2 teaspoons of baking powder
- ½ cup of unsalted butter, softened
- ¾ cup of sugar
- 2 eggs
- 1 cup of whole milk
- 1 teaspoon vanilla extract (optional)

Directions for baking:

- Preheat oven to 375°F; line muffin cups with papers.
- Beat and mix butter and sugar until it becomes a light and fluffy homogenous mixture. Beat in eggs one at a time.
- Mix baking powder, salt and flour.
- Add the flour mixture alternating with milk; beat well.
- Stir in the vanilla.
- Divide evenly among pans and bake for 18 minutes.
- Let cool in pans.

2. You live in a global society and you realize that this recipe should be out there for the rest of the world. Unfortunately, the rest of the world (except for the United States, Liberia and Myanmar) doesn't use the English Standard of measurement. They all use the International System of Measurement, or the Metric scale. Please convert each of the measurements below from English Standard to Metric.

   a. How many grams are in 2 cups of wheat flour if 1 cup is 120.00 grams? Remember to use dimensional analysis to solve this problem.

      Example:

      Starting unit x Conversion = Answer

$$2.00\ \cancel{\text{Cups of Flour}} \times \frac{120.00\ \text{grams}}{1.00\ \cancel{\text{Cup of Flour}}} = 240.\ g$$

Note that the units are cancelled because anything divided by itself is the value of 1.00.

b. How many grams are in ½ teaspoon of salt if 5.00 grams of salt are in 1.00 teaspoon?

c. How many grams are in 2 teaspoons of baking powder if 4.60 grams of baking powder are in 1.00 teaspoon?

d. How many grams are in ½ cup of unsalted butter if there are 227.00 grams of butter in 1.00 cup?

e. How many grams of sugar are in ¾ cup of sugar if there are 200.00 grams of sugar in 1.00 cup?

f. What is the mass of 2 eggs if the mass of an average egg is 2.00 ounces? There are 28.50 grams per ounce. You must first convert from the number of eggs to ounces and then the number of ounces to grams.

g. How many grams of milk are in 1 cup of milk if there are 473.176 mL of milk in 2.00 cups and the density of milk is 1.027 grams/mL? You must first convert the cups of milk to milliliters and then convert milliliters to grams using the density. Remember use dimensional analysis.

h. How many grams of vanilla extract are in 1 teaspoon vanilla extract if 1.00 teaspoon is 0.15 fluid ounces and 1.00 fluid ounce is 28.35 grams? You must first convert the teaspoon to fluid ounces and then the fluid ounces to grams. Remember to use dimensional analysis.

i. Convert the baking temperature of 375 °F to Celsius.
   a. Why Celsius? Watch the Temperature Guys video to understand the difference between the two scales.
   b. Use the following formula for the conversion:

   $T_{(°C)} = (T_{(F)} - 32) \times 5/9$

j. Successful bakeries don't just make one batch of anything. In order to be competitive this recipe must be scaled up. How much of each ingredient would be required to make 200 cupcakes? Fill in the table below with your scale up information.

Ingredients	Amount Calculated (g) for Single Batch or 24 Cupcakes	Amount Calculated (g) for 8.33 Batches or 200 Cupcakes
Flour		
Salt		

Baking Powder		
Unsalted Butter		
Sugar		
Eggs		
Milk		
Vanilla Extract		

Activity 2

Scaling up is not as simple as taking the basic ingredients and then multiplying by a factor to get the total quantity. So many variables can affect the outcome.

1. Using the graphic organizer below, brainstorm at least three issues that could arise when baking cupcakes (i.e. what could go wrong) at the micro-level (home/test kitchen).

Heating	Ingredients	Mixing	Pan Selection

2. Using the graphic organizer below, brainstorm at least three issues that could arise when baking cupcakes (i.e. what could go wrong) at the macro-level (commercial bakery).

Heating	Ingredients	Mixing	Pan Selection

3. Share your thoughts with at least one other person in class. Fill in ideas that you didn't have in your graphic organizer.

4. Be prepared to share your ideas during the teacher lead discussion.

5. Answer the following questions:

a. After listening to other students and watching the slide show summarize your findings in a concise set of directives to the bakery manager to:

    i. Ensure that the final product (the 200 cupcakes) maintains its quality and consistency.

    ii. Provide the final recipe, in grams, to the bakery manager.

b. Putting yourself in the role of the bakery manager explain why you will still need to do testing to ensure quality control.

Answer Key: Cupcake Conversions, from Bench to Bakery

**Note that not all answers are calculated using significant digits.*

Activity 1

3. Read the recipe for a vanilla cupcake below:

Vanilla Cupcakes

The following recipe yields 20-25 cupcakes.

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- 2 cups of flour
- ½ teaspoon of salt
- 2 teaspoons of baking powder

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- Mix baking powder, salt and flour.
- Add the flour mixture alternating with milk; beat well.
- Stir in the vanilla.
- Divide evenly among pans and bake for 18 minutes.
- Let cool in pans.

4. You live in a global society and you realize that this recipe should be out there for the rest of the world. Unfortunately, the rest of the world (except for the United States, Liberia and Myanmar) doesn't use the English Standard of measurement. They all use the International System of Measurement, or the Metric scale. Please convert each of the measurements below from English Standard to Metric.

k. How many grams are in 2 cups of wheat flour if 1 cup is 120.00 grams?

Remember to use dimensional analysis to solve this problem.

Example:

Starting unit x Conversion = Answer

$$2.00\ \cancel{\text{Cups of Flour}} \times \frac{120.00\ \text{grams}}{1.00\ \cancel{\text{Cup of Flour}}} = 240.\ \text{g}$$

Note that the units are cancelled because anything divided by itself is the value of 1.00.

l. How many grams are in ½ teaspoon of salt if 5.00 grams of salt are in 1.00 teaspoon?

$$0.5\ \cancel{\text{teaspoons of salt}} \times \frac{5.00\ \text{grams}}{1.00\ \cancel{\text{teaspoons of salt}}} = 2.50\ \text{g}$$

m. How many grams are in 2 teaspoons of baking powder if 4.60 grams of baking powder are in 1.00 teaspoon?

$$2.00\ \cancel{\text{teaspoons of baking powder}} \times \frac{4.60\ \text{grams}}{1.00\ \cancel{\text{teaspoons of baking powder}}} = 9.20\ \text{g}$$

n. How many grams are in ½ cup of unsalted butter if there are 227.00 grams of butter in 1.00 cup?

$$0.50\ \cancel{\text{Cups of butter}} \quad \times \quad \frac{227.00\ \text{grams}}{1.00\ \cancel{\text{Cup of butter}}} = \quad 113.5\ g$$

o. How many grams of sugar are in ¾ cup of sugar if there are 200.00 grams of sugar in 1.00 cup?

$$.75\ \cancel{\text{Cups of sugar}} \quad \times \quad \frac{200.00\ \text{grams}}{1.00\ \cancel{\text{Cup of sugar}}} = \quad 150.00\ g$$

p. What is the mass of 2 eggs if the mass of an average egg is 2.00 ounces? There are 28.50 grams per ounce. You must first convert from the number of eggs to ounces and then the number of ounces to grams.

$$2\ \cancel{\text{eggs}} \times \quad \frac{2.00\ \cancel{\text{ounce}}}{1\ \cancel{\text{egg}}} \quad \times \quad \frac{28.50\ \text{grams}}{1\ \cancel{\text{ounce}}} \quad = \quad 114\ g$$

q. How many grams of milk are in 1 cup of milk if there are 473.176 mL of milk in 2.00 cups and the density of milk is 1.027 grams/mL? You must first convert the cups of milk to milliliters and then convert milliliters to grams using the density. Remember use dimensional analysis.

$$1\ \cancel{\text{cup of milk}} \quad \times \quad \underline{473.176\ \cancel{\text{mL}}} \quad \times \quad \underline{1.027\ \text{grams}} \quad = \quad 242.98$$

g

2 ~~cups of milk~~ 1 ~~mL~~

r. How many grams of vanilla extract are in 1 teaspoon vanilla extract if 1.00 teaspoon is 0.15 fluid ounces and 1.00 fluid ounce is 28.35 grams? You must first convert the teaspoon to fluid ounces and then the fluid ounces to grams. Remember to use dimensional analysis.

$$1\ \cancel{\text{tsp vanilla}} \times \frac{0.15\ \cancel{\text{fl. ounce}}}{1\ \cancel{\text{tsp}}} \times \frac{28.35\ \text{grams}}{1\ \cancel{\text{fl. ounce}}} = 4.25\ \text{g}$$

s. Convert the baking temperature of 375 ^{o}F to Celsius.

   a. Why Celsius? Watch the [Temperature Guys video]() to understand the difference between the two scales.

   b. Use the following formula for the conversion:

   $T_{(°C)} = (T_{(F)} - 32) \times 5/9$

   190.5 °C

t. Successful bakeries don't just make one batch of anything. In order to be competitive this recipe must be scaled up. How much of each ingredient would be required to make 200 cupcakes? Fill in the table below with your scale up information.

Ingredients	Amount Calculated (g) for Single Batch or 24 Cupcakes	Amount Calculated (g) for 8.33 Batches or 200 Cupcakes
Flour	240	2000
Salt	2.50	20.83
Baking Powder	9.20	76.67
Unsalted Butter	113.5	945.83
Sugar	150.00	1250
Eggs	114	950
Milk	242.98	2024.83
Vanilla Extract	4.25	35.42

Activity 2

Scaling up is not as simple as taking the basic ingredients and then multiplying by a factor to get the total quantity. So many variables can affect the outcome.

6. Using the graphic organizer below, brainstorm at least three issues that could arise when baking cupcakes (i.e. what could go wrong) at the micro-level (home/test kitchen).

   Answers will vary.

Heating	Ingredients	Mixing	Pan Selection

7. Using the graphic organizer below, brainstorm at least three issues that could arise when baking cupcakes (i.e. what could go wrong) at the macro-level (commercial bakery).

   Answers will vary.

Heating	Ingredients	Mixing	Pan Selection

8. Share your thoughts with at least one other person in class. Fill in ideas that you didn't have in your graphic organizer.

9. Be prepared to share your ideas during the teacher lead discussion.

10. Answer the following questions:
    c. After listening to other students and watching the slide show summarize your findings in a concise set of directives to the bakery manager to:
        i. Ensure that the final product (the 200 cupcakes) maintains its quality and consistency.
        ii. Provide the final recipe, in grams, to the bakery manager.

    Answers will vary, some possibilities inclue:

    - Production baker needs to calibrate ovens.
    - Production baker might have different equipment so it will be different at larger scales so he/she will still need to trouble shoot batches of cupcakes.
    - He/she should change variables, collect data, and send the results back to the original baker so that trouble shooting can occur back at the micro level. This is what happens in industry with product development.

    d. Putting yourself in the role of the bakery manager explain why you will still need to do testing to ensure quality control.

Temperature

Temperature is a measure of how hot or cold object is. It is defined as measure of average kinetic energy of the particle. In scientific world,

three Temperature scales are used. Fahrenheit, Celcius and Kelvin.

T_f= 1.8Tc + 32 Tk= Tc + 273

-273.15 degree celcius is defined as absolute zero temperature. This is the lowest possible temperature theoretically possible in this universe. As temperature decreases, all energy of matter decreases as degrees of molecular and atomic motion decreases. A matter is expected to have all motion frozen at absolute zero temperature.

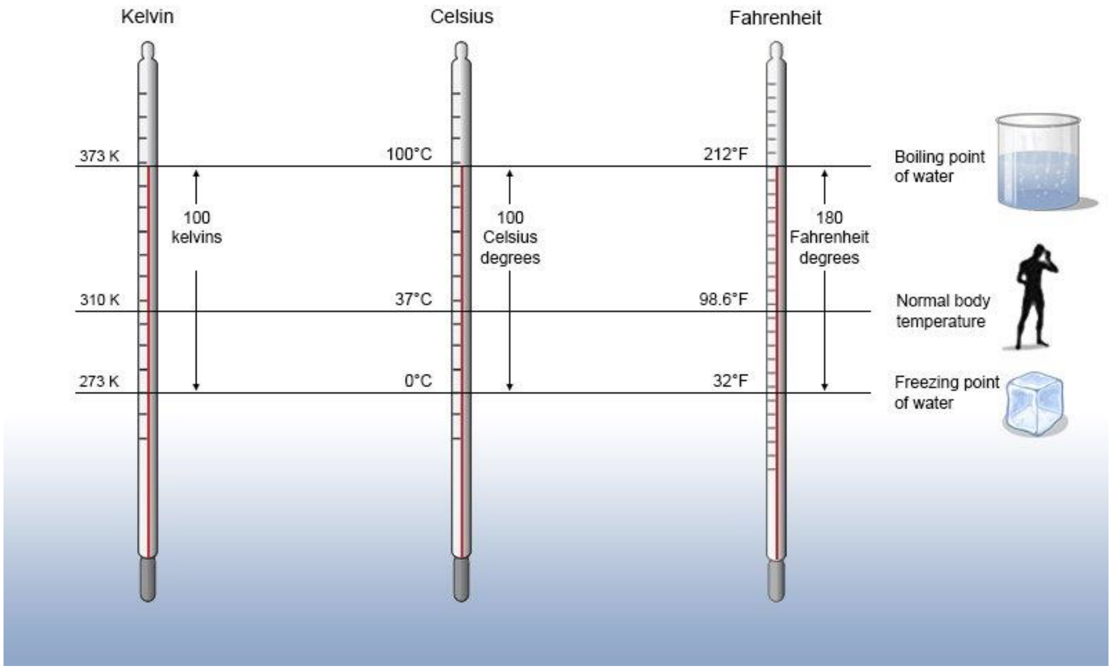
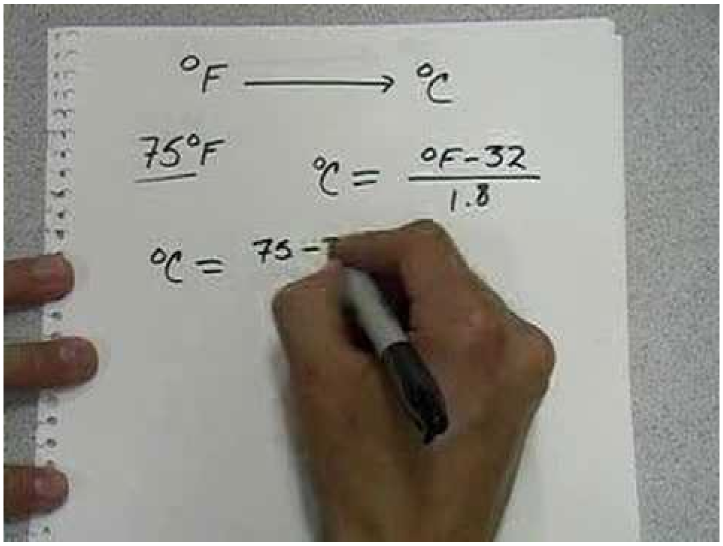


Figure: 1.21 Different Scales of Temperature

Watch the following video:

https://www.youtube.com/watch?v=9sEnXM3WeZk



Example Problem:

State the Temperature on the Celcius Thermometer and convert into Fahrenheit scale.

Celcius: 61.5^{o}C

Applying the formula: Tf= 1.8Tc+ 32

1.8*61.5 +32= 142.7= 143^{o}F

Applying the formula: Tf= 1.8Tc+ 32

155=1.8Tc +32

155-32= 1.8Tc,

1.8Tc=123

Tc= 68.3 oC

Tk= Tc+273= 341.3K

Questions:

1. Why is the number 1.8 (and not some other value) used in the formula for converting between Celsius and Fahrenheit temperatures?

2. Convert the following Farenheit temperature into celcius and kelvin
   a. 12^{0}F
   b. 32^{0}F
   c. 40^{0}F
   d. 212^{0}F

End of the Chapter Questions and Problems

1. Define combustion and discuss the contributions made by Priestley and Lavoisier toward understanding a combustion reaction.

2. Chemical engineers frequently use the concept of "mass balance" in their calculations, in which the mass of the reactants must equal the mass of the products. What law supports this practice? Why does it support the concept of "mass balance."

3. Does the law of multiple proportions apply to both mass ratios and atomic ratios? Why or why not?

4. What are the four hypotheses of the atomic theory of matter?

5. One of the minerals found in soil has an Al:Si:O atomic ratio of 0.2:0.2:0.5. Is this consistent with the law of multiple proportions? Why or why not? Is the ratio of elements consistent with Dalton's atomic theory of matter?

6. Nitrogen and oxygen react to form three different compounds that contain 0.571 g, 1.143 g, and 2.285 g of oxygen/gram of nitrogen, respectively. Is this consistent with the law of multiple proportions? Explain your answer.

7. Three binary compounds of vanadium and oxygen are known. The following table gives the masses of oxygen that combine with 10.00 g of vanadium to form each compound.

Compound	Mass of Oxygen (g)
A	4.71
B	6.27
C	

Determine the ratio of the masses of oxygen that combine with 3.14 g of vanadium in compounds A and B. Predict the mass of oxygen that would combine with 3.14 g of vanadium to form the third compound in the series.

8. Classify each statement as a law, a theory, an experiment, a hypothesis, a qualitative observation, or a quantitative observation.

a. Measured amounts of acid were added to a Rolaids tablet to see whether it really "consumes 47 times its weight in excess stomach acid."

b. Heat always flows from hot objects to cooler ones, not in the opposite direction.

c. The universe was formed by a massive explosion that propelled matter into a vacuum.

d. Michael Jordan is the greatest pure shooter ever to play professional basketball.

e. Limestone is relatively insoluble in water but dissolves readily in dilute acid with the evolution of a gas.

f. Gas mixtures that contain more than 4% hydrogen in air are potentially explosive.

9. What are the three components of the scientific method?

10, Is it necessary for an individual to conduct experiments to follow the scientific method?

11. Identify each statement as a theory or a law and explain your reasoning.

a. The ratio of elements in a pure substance is constant.

b. An object appears black because it absorbs all the visible light that strikes it.

c. Energy is neither created nor destroyed.

d. Metals conduct electricity because their electrons are not tightly bound to a particular nucleus and are therefore free to migrate.

12. Identify each statement as a theory or a law and explain your reasoning.

a. A pure chemical substance contains the same proportion of elements by mass.

b. The universe is expanding.

c. Oppositely charged particles attract each other.

d. Life exists on other planets.

13. Classify each statement as a qualitative observation or a quantitative observation.

a. Mercury and bromine are the only elements that are liquids at room temperature.

b. An element is both malleable and ductile.

c. The density of iron is 7.87 g/cm3.

d. Lead absorbs sound very effectively.

14. Classify each statement as a quantitative observation or a qualitative observation.

a. Nickel deficiency in rats is associated with retarded growth.

b. Boron is a good conductor of electricity at high temperatures.

c. There are 1.4–2.3 g of zinc in an average 70 kg adult.

d. Certain osmium compounds found in air in concentrations as low as 10.7 μg/m3 can cause lung cancer.

15. Given the volumes and masses of five samples of compounds used in blending gasoline, together with the densities of several chemically pure liquids, identify as many of the samples as possible.

Sample	Volume (mL)	Mass (g)
A	337	250.0
B	972	678.1
C	243	190.9
D	119	103.2
E	499	438.7

Substance	Density (g/cm3)
benzene	0.8787

Sample	Volume (mL)	Mass (g)
toluene	0.8669	
m-xylene	0.8684	
isooctane	0.6979	
methyl t-butyl ether	0.7405	
t-butyl alcohol	0.7856	

16. What is the difference between mass and weight? Is the mass of an object on Earth the same as the mass of the same object on Jupiter? Why or why not?

17. Is it accurate to say that a substance with a mass of 1 kg weighs 2.2 lb? Why or why not?

18. Construct a table with the headings “Solid,” “Liquid,” and “Gas.” For any given substance, state what you expect for each of the following: the relative densities of the three phases, the physical shapes of the three phases, the volumes for the same mass of compound, the sensitivity of the volume of each phase to changes in temperature, the sensitivity of the volume to changes in pressure.

19. Classify each substance as homogeneous or heterogeneous and explain your reasoning: platinum, a carbonated beverage, bronze, wood, natural gas, Styrofoam

20. Classify each substance as homogeneous or heterogeneous and explain your reasoning: snowflakes, gasoline, black tea, plastic wrap, blood, water containing ice cubes

21. Classify each substance as a pure substance or a mixture and explain your reasoning: seawater, coffee, 14-karat gold, diamond, distilled water

22. Classify each substance as a pure substance or a mixture: cardboard, caffeine, tin, a vitamin tablet, helium gas.

23. Classify each substance as an element or a compound: sugar, silver, rust, rubbing alcohol, copper.

24. Classify each substance as an element or a compound: water, iron, hydrogen gas, glass, nylon

25. What techniques could be used to separate each of the following? Sugar and water from an aqueous solution of sugar, a mixture of sugar and sand, a heterogeneous mixture of solids with different solubilities.

26. What techniques could be used to separate each of the following? Solid calcium chloride from a solution of calcium chloride in water, the components of a solution of vinegar in water, particulates from water in a fish tank.

27. Classify each statement as an extensive property or an intensive property: carbon, in the form of diamond, is one of the hardest known materials. A sample of crystalline silicon, a grayish solid, has a mass of 14.3 g. Germanium has a density of 5.32 g/cm3. Gray tin converts to white tin at 13.2°C. Lead is a bluish-white metal.

28. Classify each statement as a physical property or a chemical property: fluorine etches glass, chlorine interacts with moisture in the lungs to produce a respiratory irritant, bromine is a reddish-brown liquid.

29. If a person weighs 176 lb on Earth, what is his or her mass on Mars, where the force of gravity is 37% of that on Earth?

30, If a person weighs 135 lb on Earth, what is his or her mass on Jupiter, where the force of gravity is 236% of that on Earth?

31. Calculate the volume of 10.00 g of each element and then arrange the elements in order of decreasing volume. The numbers in parentheses are densities.

copper (8.92 g/cm3)

calcium (1.54 g/cm3)

titanium (4.51 g/cm3)

iridium (22.85 g/cm3)

32. Given 15.00 g of each element, calculate the volume of each and then arrange the elements in order of increasing volume. The numbers in parentheses are densities.

gold (19.32 g/cm^3)

lead (11.34 g/cm^3)

iron (7.87 g/cm^3)

sulfur (2.07 g/cm^3)

33. A silver bar has dimensions of 10.00 cm × 4.00 cm × 1.50 cm, and the density of silver is 10.49 g/cm^3. What is the mass of the bar?

34. Platinum has a density of 21.45 g/cm^3. What is the mass of a platinum bar measuring 3.00 cm × 1.50 cm × 0.500 cm?

35. Complete the following table.

Density (g/cm^3)	Mass (g)	Volume (cm^3)	Element
3.14	79.904		Br
3.51		3.42	C
	39.1	45.5	K
11.34	207.2		Pb
	107.868	10.28	Ag
6.51		14.0	Zr

36. Gold has a density of 19.30 g/cm^3. If a person who weighs 85.00 kg (1 kg = 1000 g) were given his or her weight in gold, what volume (in cm^3) would the gold occupy? Are we justified in using the SI unit of mass for the person's weight in this case?

An irregularly shaped piece of magnesium with a mass of 11.81 g was dropped into a graduated cylinder partially filled with water. The magnesium displaced 6.80 mL of water. What is the density of magnesium?

37. The density of copper is 8.92 g/cm^3. If a 10.00 g sample is placed in a graduated cylinder that contains 15.0 mL of water, what is the total volume that would be occupied?

At 20°C, the density of fresh water is 0.9982 kg/m3, and the density of seawater is 1.025 kg/m3.

38. Will a ship float higher in fresh water or in seawater? Explain your reasoning.

39. Label each of the following changes as a physical or chemical change. Give evidence to support your answer.

   a. Boiling water
   b. A nail rusting
   c. A green solution and colorless solution are mixed. The resulting mixture is a solution with a pale green color.
   d. Two colorless solutions are mixed. The resulting mixture has a yellow precipitate.

40. Convert each number to scientific notation.

   a. 637.8

   b. 0.0479

   c. 7.86

   d. 12,378

   e. 0.00032

   f. 61.06700

   g. 2002.080

   h. 0.01020

41. Carry out the appropriate operation and then express the answer in scientific notation.

a. $(1.36 \times 10^2) + (4.73 \times 10^3)$ $(1.36 \times 10^2) + (4.73 \times 10^3)$

b. $(6.923 \times 10^{-3}) - (8.756 \times 10^{-4})$ $(6.923 \times 10^{-3}) - (8.756 \times 10^{-4})$

42. Perform the appropriate operation and express your answer in scientific notation.

a. $[(6.022 \times 10^{23})\ (6.42 \times 10^{-2})$ $[(6.022 \times 10^{23})\ (6.42 \times 10^{-2})$

43. Use the dimensional analysis (unit conversion, factor label) problem-solving method to answer the following questions.

a. How many nickels would you get for a twenty dollar bill?

b. How many hours are in a week?

c. How many revolutions does the hour hand on a clock make in a year?

44. Find the number of centimeters in 1.00×10^2 yards.

45. Determine the number of meters in 1.00 mile.

46. The speed of light is 1.86×10^5 miles per second. How many meters will light travel in 1.0 second?

47. Calculate the number of seconds in a year.

48. A light year is the distance that light travels in one year. Determine the number of miles, meters, and kilometers in one light year.

49. A single layer of gold atoms forms a surface whose dimensions are 1.0×10^3 angstroms by 1.0×10^3 angstroms. 1 angstrom = 10^{-10} meter. a) What is the area of this surface in square angstroms? b) What is the surface area in square centimeters?

50. The units of the chain system of measure, used by surveyors, are as follows:

- 7.92 inches = 1 link
- 100 links = 1 chain
- 10 chains = 1 furlong
- 80 chains = 1 mile

The distance of the Kentucky Derby, a classic horse race, is 1.25 miles. How is this distance expressed in furlongs?

51. A cube that has a length of 1 cm on each side has a volume of 1 cm^3. How many cubic centimeters are in 1 cubic meter? (Hint: The answer is not 100.)

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Chapter 2: Atoms, Molecules and Ions

Key Concepts

2.1 Early Ideas in Atomic Theory

2.2 Evolution of Atomic Theory

2.3 Atomic Structure and Symbolism

2.4 The Periodic Table

2.5 Chemical Formulas

2.6 Molecular and Ionic Compounds

2.7 Chemical Nomenclature

Section 2.1: Early Ideas in Atomic Theory

Atomic Theory through the Nineteenth Century

The earliest recorded discussion of the basic structure of matter comes from ancient Greek philosophers, the scientists of their day. In the fifth century BC, Leucippus and Democritus argued that all matter was composed of small, finite particles that they called *atomos*, a term derived from the Greek word for "indivisible." They thought of atoms as moving particles that differed in shape and size, and which could join together. Later, Aristotle and others came to the conclusion that matter consisted of various combinations of the four "elements"—fire, earth, air, and water—and could be infinitely divided. Interestingly, these philosophers thought about atoms and "elements" as philosophical concepts, but apparently never considered performing experiments to test their ideas.

The Aristotelian view of the composition of matter held sway for over two thousand years, until English school teacher John Dalton helped to revolutionize chemistry with his hypothesis that the behavior of matter could be explained using an atomic theory. First published in 1807, many of Dalton's hypotheses about the microscopic features of matter are still valid in modern atomic theory. Here are the postulates of Dalton's atomic theory.

1. Matter is composed of exceedingly small particles called atoms. An atom is the smallest unit of an element that can participate in a chemical change.
2. An element consists of only one type of atom, which has a mass that is characteristic of the element and is the same for all atoms of that element (Figure 1). A macroscopic sample of an element contains an incredibly large number of atoms, all of which have identical chemical properties.
3. Atoms of one element differ in properties from atoms of all other elements.
4. A compound consists of atoms of two or more elements combined in a small, whole-number ratio. In a given compound, the numbers of atoms of each of its elements are always present in the same ratio (Figure 2).
5. Atoms are neither created nor destroyed during a chemical change, but are instead rearranged to yield substances that are different from those present before the change (Figure 3).

Watch the following video:

https://www.youtube.com/watch?v=OUoV--CuLDA&t=18s

Figure 2.1. A pre-1982 copper penny (left) contains approximately 3×10^{22} copper atoms (some of them are represented as brown spheres at the right), each of which has the same chemical properties.

Ref: commons.wikimedia.org/

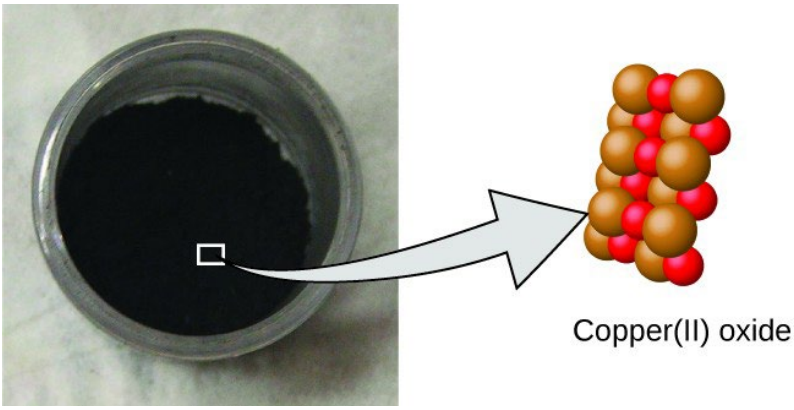


Figure 2.2 Copper (II) oxide, a powdery, black compound, results from the combination of two types of atoms—copper (brown spheres) and oxygen (red spheres)—in a 1:1 ratio.

Ref: commons.wikimedia.org/

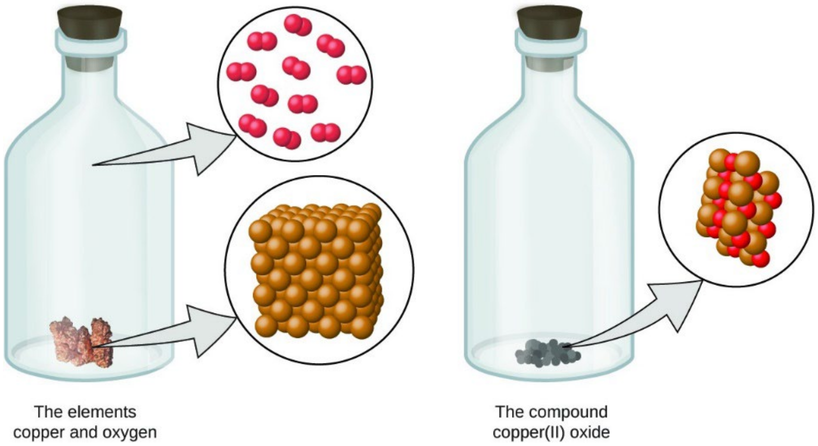
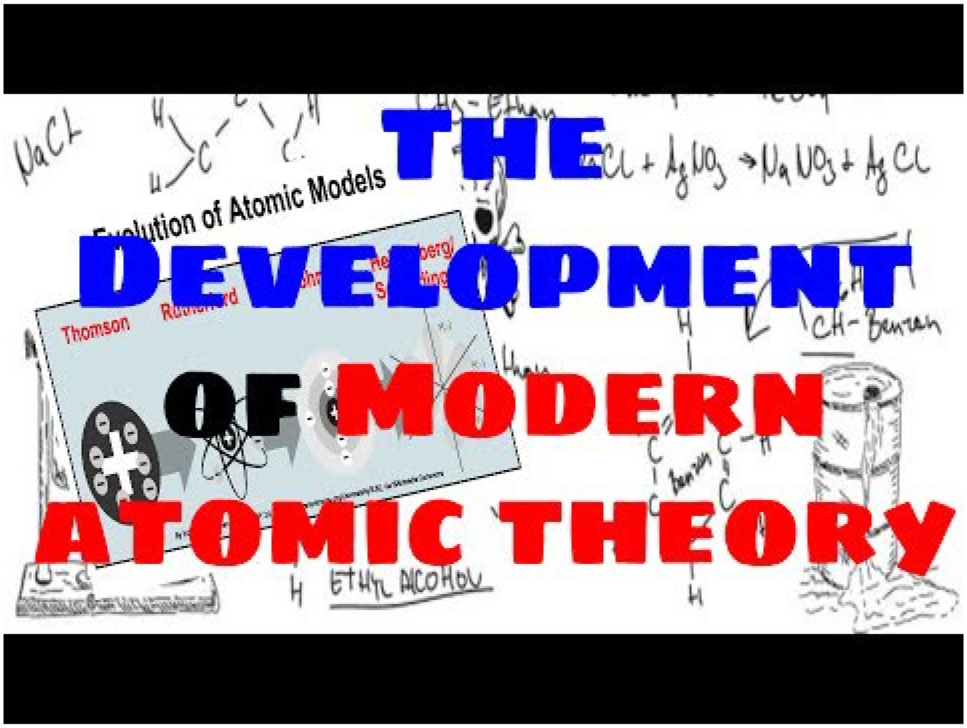


Figure 2.3 When the elements copper (a shiny, red-brown solid, shown here as brown spheres) and oxygen (a clear and colorless gas, shown here as red spheres) react, their atoms rearrange to form a compound containing copper and oxygen (a powdery, black solid).

Ref: www.openstax.org/

Dalton’s atomic theory provides a microscopic explanation of the many macroscopic properties of matter that you’ve learned about. For example, if an element such as copper consists of only one kind of atom, then it cannot be broken down into simpler substances, that is, into substances composed of fewer types of atoms. And if atoms are neither created nor destroyed during a chemical change, then the total mass of matter present when matter changes from one type to another will remain constant (the law of conservation of matter).



EXAMPLE 1: Testing Dalton’s Atomic Theory

In the following drawing, the green spheres represent atoms of a certain element. The purple spheres represent atoms of another element. If the spheres touch, they are part of a single unit of a compound. Does the following chemical change represented by these symbols violate any of the ideas of Dalton’s atomic theory? If so, which one?

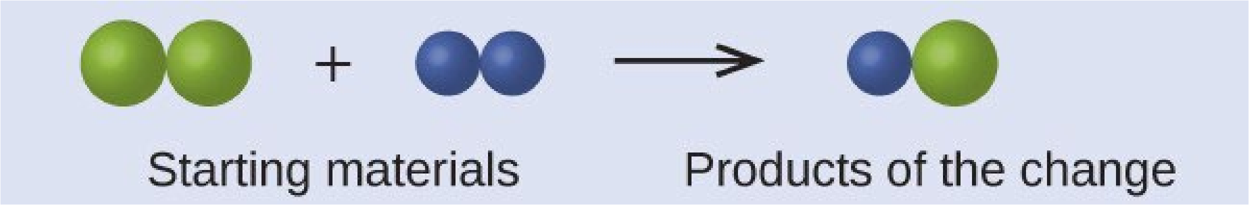


Figure 2.4 Dalton’s Postulates

Ref: www.openstax.org/

Solution

The starting materials consist of two green spheres and two purple spheres. The products consist of only one green sphere and one purple sphere. This violates Dalton’s postulate that atoms are neither created nor destroyed during a chemical change, but are merely redistributed. (In this case, atoms appear to have been destroyed.)

Dalton knew of the experiments of French chemist Joseph Proust, who demonstrated that *all samples of a pure compound contain the same elements in the same proportion by mass*. This statement is known as the law of definite proportions or the law of constant composition. The suggestion that the numbers of atoms of the elements in a given compound always exist in the same ratio is consistent with these observations. For example, when different samples of carbon dioxide, CO_2, are analyzed, they are found to have a carbon-to-oxygen mass ratio of 1:2.

It is worth noting that although all samples of a particular compound have the same mass ratio, the converse is not true in general. That is, samples that have the same mass ratio are not necessarily the same substance. For example, there are many compounds other than carbon dioxide that also have a carbon-to-oxygen mass ratio of 1:2.

Dalton also used data from Proust, as well as results from his own experiments, to formulate another interesting law. The law of multiple proportions states that *when two elements react to form more than one compound, a fixed mass of one element will react with masses of the other element in a ratio of small, whole numbers*. For example, copper and chlorine can form a green, crystalline solid with a mass ratio of 0.558 g chlorine to 1 g copper, as well as a brown crystalline solid with a mass ratio of 1.116 g chlorine to 1 g copper. These ratios by themselves may not seem particularly interesting or informative; however, if we take a ratio of these ratios, we obtain a useful and possibly surprising result: a small, whole-number ratio.

1.116 g Cl1 g Cu0.558 g Cl1 g Cu=211.116 g Cl1 g Cu0.558 g Cl1 g Cu=21

This 2-to-1 ratio means that the brown compound has twice the amount of chlorine per amount of copper as the green compound.

This can be explained by atomic theory if the copper-to-chlorine ratio in the brown compound is 1 copper atom to 2 chlorine atoms, and the ratio in the green compound is 1 copper atom to 1 chlorine atom. The ratio of chlorine atoms (and thus the ratio of their masses) is therefore 2 to 1 (Figure 4).

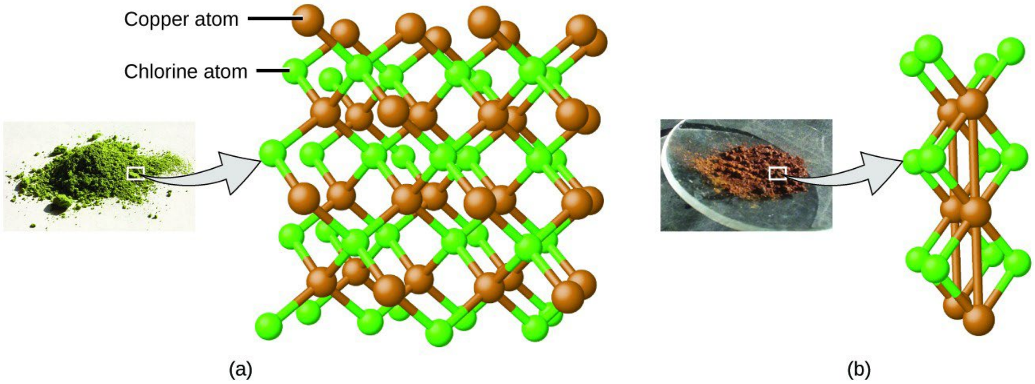


Figure 2.4. Compared to the copper chlorine compound in (a), where copper is represented by brown spheres and chlorine by green spheres, the copper chlorine compound in (b) has twice as many chlorine atoms per copper atom.
Ref: www.openstax.org/

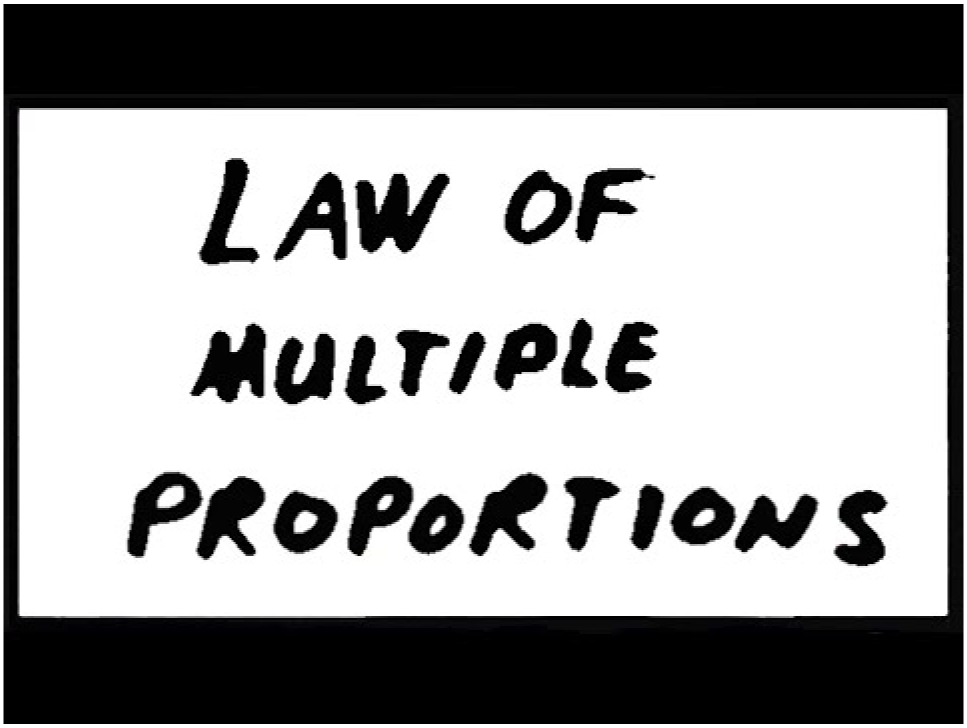
Example 2: Law of definite and multiple proportions

A sample of compound A (a clear, colorless gas) is analyzed and found to contain 4.27 g carbon and 5.69 g oxygen. A sample of compound B (also a clear, colorless gas) is analyzed and found to contain 5.19 g carbon and 13.84 g oxygen. Are these data an example of the law of definite proportions, the law of multiple proportions, or neither? What do these data tell you about substances A and B?

Solution

In compound A, the mass ratio of carbon to oxygen is 1.33 g / O1 g C
In compound B, the mass ratio of carbon to oxygen is 2.67 g / O1 g C
The ratio of these ratios is (1.33 g O / 1 g C) / (2.67 g O / 1 g C) = 1/2

This supports the law of multiple proportions. This means that A and B are different compounds, with A having one-half as much carbon per amount of oxygen (or twice as much oxygen per amount of carbon) as B. A possible pair of compounds that would fit this relationship would be A = CO_2 and B = CO.



Section 2.2: Evolution of Atomic Theory

In the two centuries since Dalton developed his ideas, scientists have made significant progress in furthering our understanding of atomic theory. Much of this came from the results of several seminal experiments that revealed the details of the internal structure of atoms. Here, we will discuss some of those key developments, with an emphasis on application of the scientific method, as well as understanding how the experimental evidence was analyzed. While the historical persons and dates behind these experiments can be quite interesting, it is most important to understand the concepts resulting from their work.

Atomic Theory after the Nineteenth Century

If matter were composed of atoms, what were atoms composed of? Were they the smallest particles, or was there something smaller? In the late 1800s, a number of scientists interested in questions like these investigated the electrical discharges that could be produced in low-pressure gases, with the most significant discovery made by English physicist J. J. Thomson using a cathode ray tube. This apparatus consisted of a sealed glass tube from which almost all the air had been removed; the tube contained two metal electrodes. When high voltage was applied across the electrodes, a visible beam called a cathode ray appeared between them. This beam was deflected toward the positive charge and away from the negative charge, and was produced in the same way with identical properties when different metals were used for the electrodes. In similar experiments, the ray was simultaneously deflected by an applied magnetic field, and measurements of the extent of deflection and the magnetic field strength allowed Thomson to calculate the charge-to-mass ratio of the cathode ray particles. The results of these measurements indicated that these particles were much lighter than atoms.

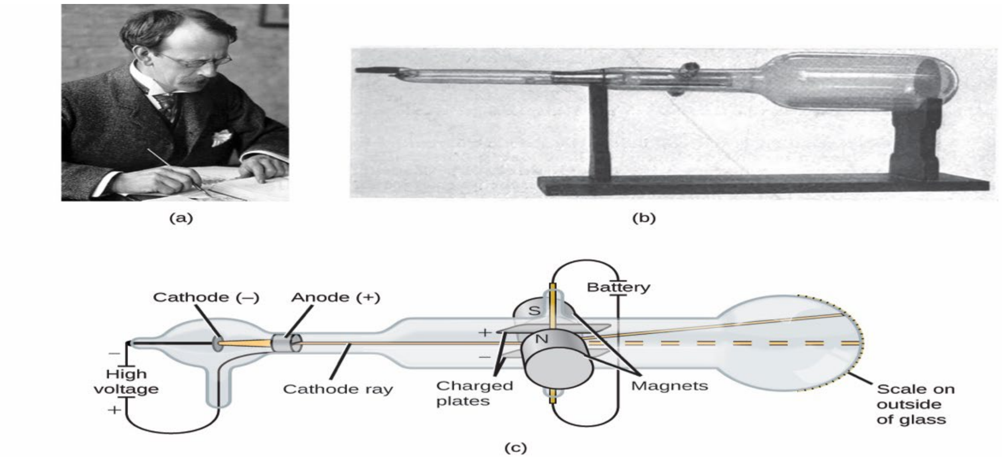
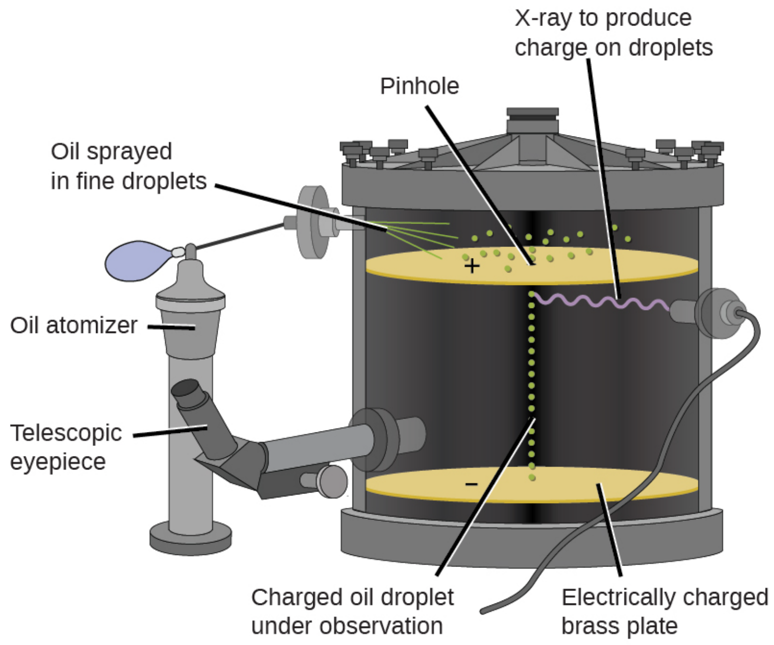


Figure 2.5. (a) J. J. Thomson produced a visible beam in a cathode ray tube. (b) This is an early cathode ray tube, invented in 1897 by Ferdinand Braun. (c) In the cathode ray, the beam (shown in yellow) comes from the cathode and is accelerated past the anode toward a fluorescent scale at the end of the tube. Simultaneous deflections by applied electric and magnetic fields permitted Thomson to calculate the mass-to-charge ratio of the particles composing the cathode ray.

Ref: www.openstax.org/

Based on his observations, here is what Thomson proposed and why: The particles are attracted by positive (+) charges and repelled by negative (−) charges, so they must be negatively charged (like charges repel and unlike charges attract); they are less massive than atoms and indistinguishable, regardless of the source material, so they must be fundamental, subatomic constituents of all atoms. Although controversial at the time, Thomson’s idea was gradually accepted, and his cathode ray particle is what we now call an electron, a negatively charged, subatomic particle with a mass more than one thousand-times less that of an atom. The term “electron” was coined in 1891 by Irish physicist George Stoney, from “*electr*ic *ion*.”

In 1909, more information about the electron was uncovered by American physicist Robert A. Millikan via his “oil drop” experiments. Millikan created microscopic oil droplets, which could be electrically charged by friction as they formed or by using X-rays. These droplets initially fell due to gravity, but their downward progress could be slowed or even reversed by an electric field lower in the apparatus. By adjusting the electric field strength and making careful measurements and appropriate calculations, Millikan was able to determine the charge on individual drops.



Oil drop	Charge in coulombs (C)
A	4.8×10^{-19} C
B	3.2×10^{-19} C
C	6.4×10^{-19} C
D	1.6×10^{-19} C
E	4.8×10^{-19} C

Figure 2.6. Millikan’s experiment measured the charge of individual oil drops. The tabulated data are examples of a few possible values.
Ref: www.openstax.org/

Looking at the charge data that Millikan gathered, you may have recognized that the charge of an oil droplet is always a multiple of a specific charge, 1.6×10^{-19} C. Millikan concluded that this value must therefore be a fundamental charge—the charge of a single electron—with his measured charges due to an excess of one electron (1 times 1.6×10^{-19} C, two electrons (2 times 1.6×10^{-19} C), three electrons (3 times 1.6×10^{-19} C, and so on, on a given oil droplet. Since the charge of an electron was now known due to Millikan's research, and the charge-to-mass ratio was already known due to Thomson's research (1.759×10^{11} C/kg), it only required a simple calculation to determine the mass of the electron as well.

Scientists had now established that the atom was not indivisible as Dalton had believed, and due to the work of Thomson, Millikan, and others, the charge and mass of the negative, subatomic particles—the electrons—were known. However, the positively charged part of an atom was not yet well understood. In 1904, Thomson proposed the "plum pudding" model of atoms, which described a positively charged mass with an equal amount of negative charge in the form of electrons embedded in it, since all atoms are electrically neutral. A competing model had been proposed in 1903 by Hantaro Nagaoka, who postulated a Saturn-like atom, consisting of a positively charged sphere surrounded by a halo of electrons.

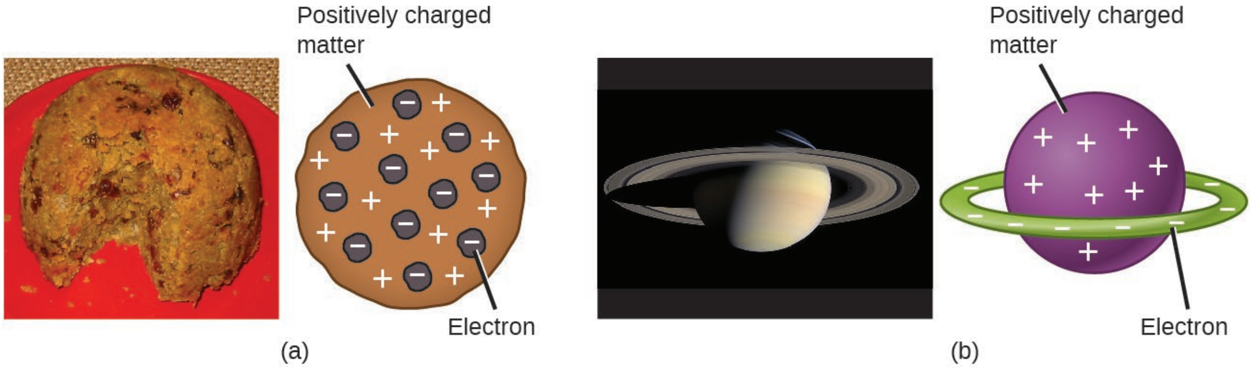


Figure 2.7. (a) Thomson suggested that atoms resembled plum pudding, an English dessert consisting of moist cake with embedded raisins ("plums"). (b) Nagaoka proposed that atoms resembled the planet Saturn, with a ring of electrons surrounding a positive "planet."

Ref: www.openstax.org/

The next major development in understanding the atom came from Ernest Rutherford, a physicist from New Zealand who largely spent his scientific career in Canada and England. He performed a series of experiments using a beam of high-speed, positively charged alpha particles (α particles) that were produced by the radioactive decay of radium; α particles consist of two protons and two neutrons. Rutherford and his colleagues Hans Geiger (later famous for the Geiger counter) and Ernest Marsden aimed a beam of α particles, the source of which was embedded in a lead block to absorb most of the radiation, at a very thin piece of gold foil and examined the resultant scattering of the α particles using a luminescent screen that glowed briefly where hit by an α particle.

What did they discover? Most particles passed right through the foil without being deflected at all. However, some were diverted slightly, and a very small number were deflected almost straight back toward the source. Rutherford described finding these results: "It was quite the most incredible event that has ever happened to me in my life. It was almost as incredible as if you fired a 15-inch shell at a piece of tissue paper and it came back and hit you".

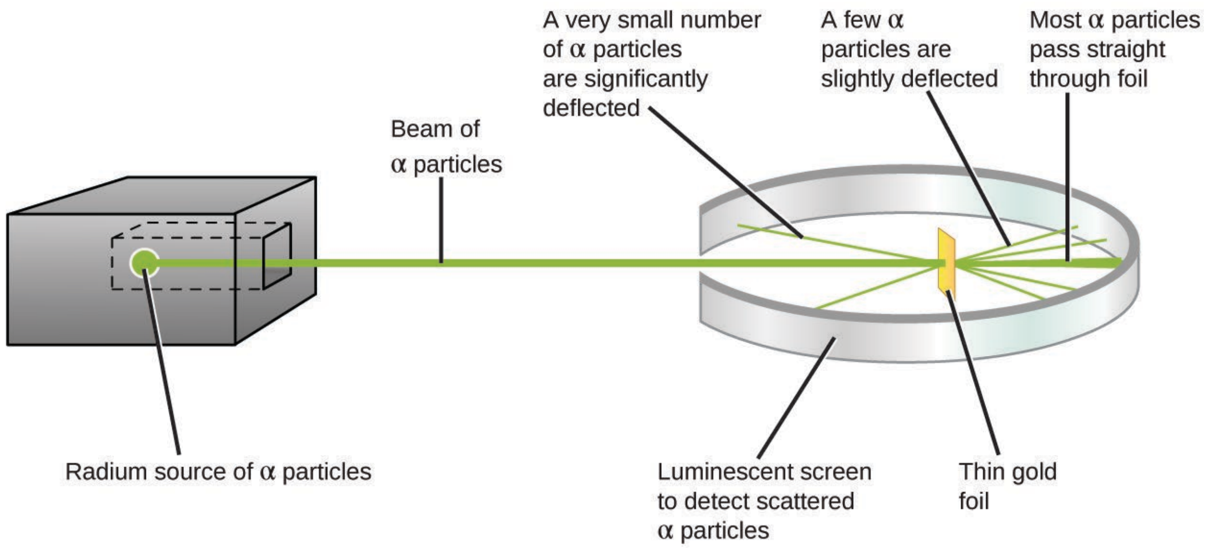


Figure 2.8 Rutherford's experiment set up

Geiger and Rutherford fired α particles at a piece of gold foil and detected where those particles went, as shown in this schematic diagram of their experiment. Most of the particles passed straight through the foil, but a few were deflected slightly and a very small number were significantly deflected.
Ref: www.openstax.org/

Here is what Rutherford deduced: Because most of the fast-moving α particles passed through the gold atoms undeflected, they must have traveled through essentially empty space inside the atom. Alpha particles are positively charged, so deflections arose when they encountered another positive charge (like charges repel each other). Since like charges repel one another, the few positively charged α particles that changed paths abruptly must have hit, or closely approached, another body that also had a highly concentrated, positive charge. Since the deflections occurred a small fraction of the time, this charge only occupied a small amount of the space in the gold foil. Analyzing a series of such experiments in detail, Rutherford drew two conclusions:

1. The volume occupied by an atom must consist of a large amount of empty space.
2. A small, relatively heavy, positively charged body, the nucleus, must be at the center of each atom.

This analysis led Rutherford to propose a model in which an atom consists of a very small, positively charged nucleus, in which most of the mass of the atom is concentrated, surrounded by the negatively charged electrons, so that the atom is electrically neutral. After many more experiments, Rutherford also discovered that the nuclei of other elements contain the hydrogen nucleus as a "building block," and he named this more fundamental particle the proton, the positively charged, subatomic particle found in the nucleus. With one addition, which you will learn next, this nuclear model of the atom, proposed over a century ago, is still used today.

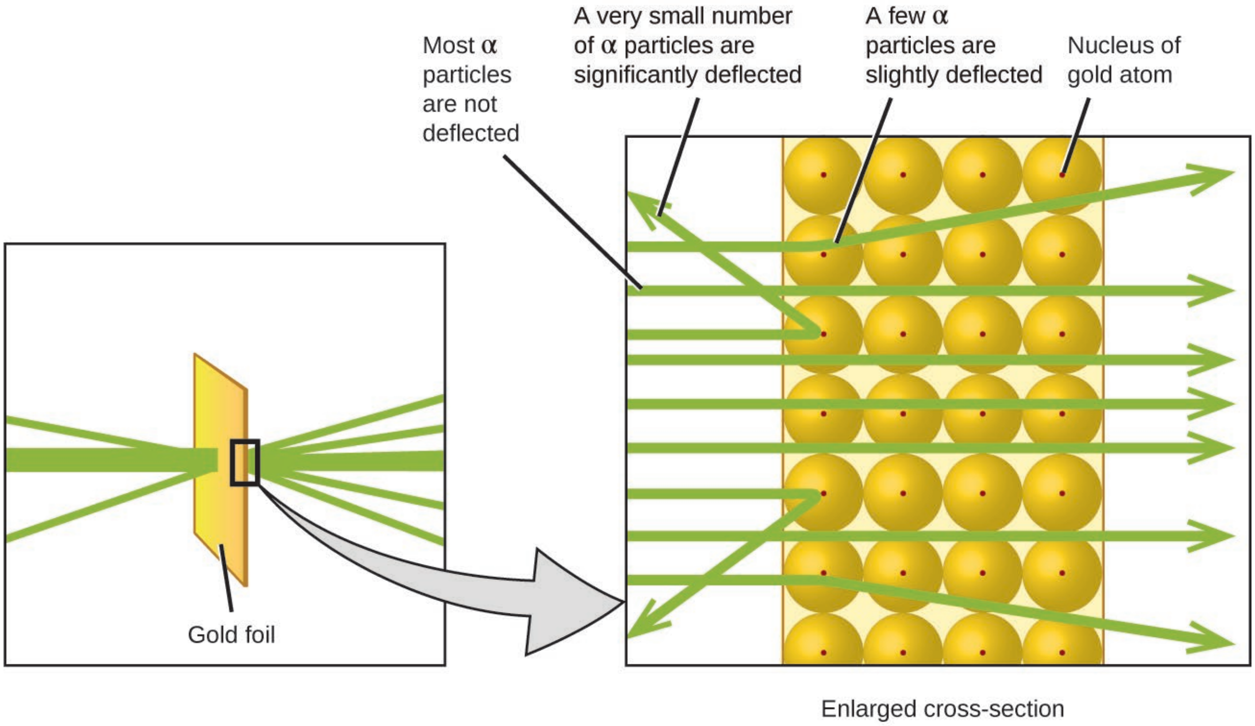
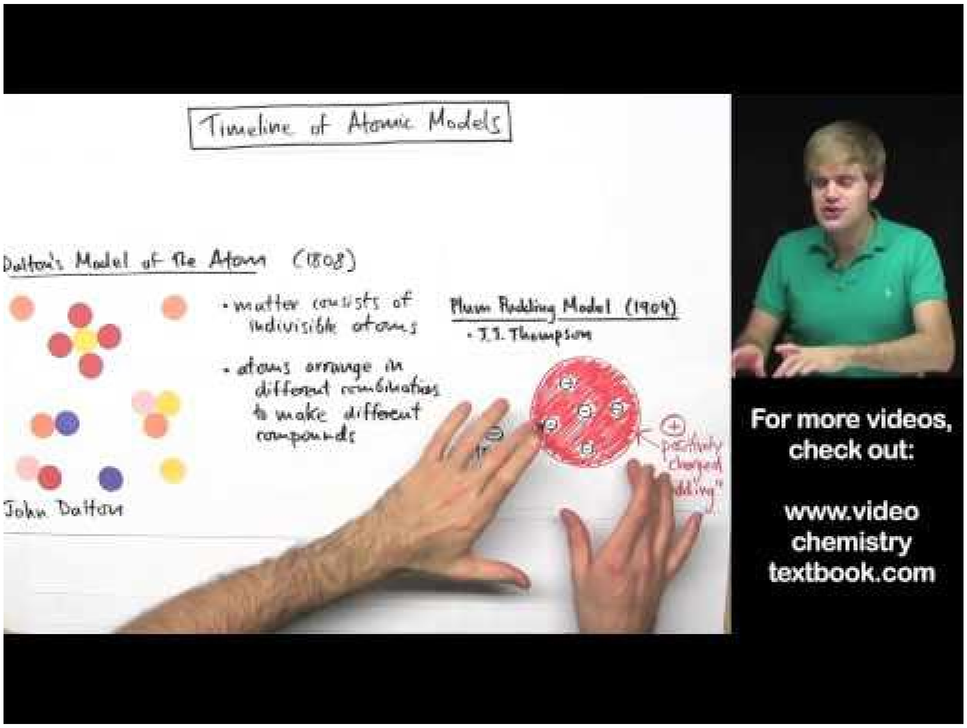


Figure 2.9. Rutherford's Experiment

The α particles are deflected only when they collide with or pass close to the much heavier, positively charged gold nucleus. Because the nucleus is very small compared to the size of an atom, very few α particles are deflected. Most pass through the relatively large region occupied by electrons, which are too light to deflect the rapidly moving particles.

Another important finding was the discovery of isotopes. During the early 1900s, scientists identified several substances that appeared to be new elements, isolating them from radioactive ores. For example, a "new element" produced by the radioactive decay of thorium was initially given the name mesothorium. However, a more detailed analysis showed that mesothorium was chemically identical to radium (another decay product), despite having a different atomic mass. This result, along with similar findings for other elements, led the English chemist Frederick Soddy to realize that an element could have types of atoms with different masses that were chemically indistinguishable. These different types are called isotopes—atoms of the same element that differ in mass. Soddy was awarded the Nobel Prize in Chemistry in 1921 for this discovery.

One puzzle remained: The nucleus was known to contain almost all of the mass of an atom, with the number of protons only providing half, or less, of that mass. Different proposals were made to explain what constituted the remaining mass, including the existence of neutral particles in the nucleus. As you might expect, detecting uncharged particles is very challenging, and it was not until 1932 that James Chadwick found evidence of neutrons, uncharged, subatomic particles with a mass approximately the same as that of protons. The existence of the neutron also explained isotopes: They differ in mass because they have different numbers of neutrons, but they are chemically identical because they have the same number of protons. This will be explained in more detail later in this chapter.



Section 2.3: Atomic Structure and Symbolism

The development of modern atomic theory revealed much about the inner structure of atoms. It was learned that an atom contains a very small nucleus composed of positively charged protons and uncharged neutrons, surrounded by a much larger volume of space containing negatively charged electrons. The nucleus contains the majority of an atom's mass because protons and neutrons are much heavier than electrons, whereas electrons occupy almost all of an atom's volume. The diameter of an atom is on the order of 10^{-10} m, whereas the diameter of the nucleus is roughly 10^{-15} m—about 100,000 times smaller. For a perspective about their relative sizes, consider this: If the nucleus were the size of a blueberry, the atom would be about the size of a football stadium.

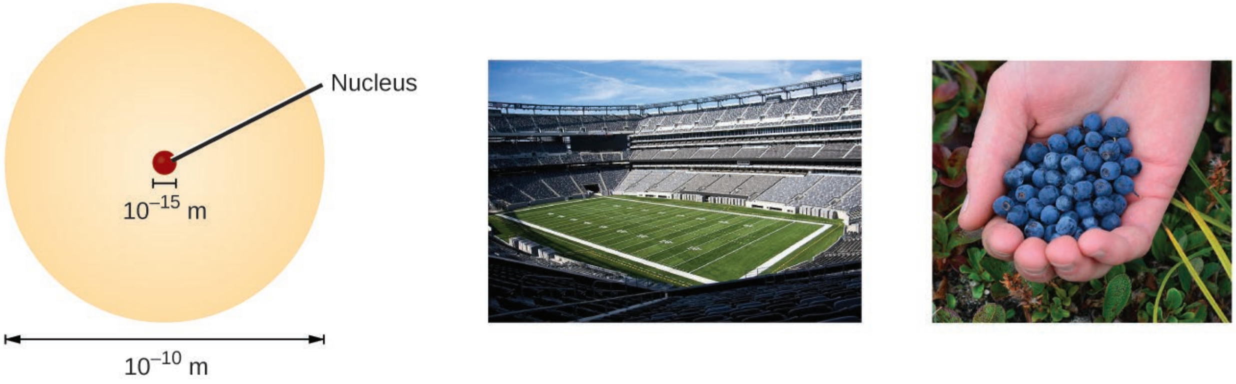


Figure 2.10. If an atom could be expanded to the size of a football stadium, the nucleus would be the size of a single blueberry.

Atoms—and the protons, neutrons, and electrons that compose them—are extremely small. For example, a carbon atom weighs less than 2×10^{-23} g, and an electron has a charge of less than 2×10^{-19} C (coulomb). When describing the properties of tiny objects such as atoms, we use appropriately small units of measure, such as the atomic mass unit (amu) and the fundamental unit of charge (e). The amu was originally defined based on hydrogen, the lightest element, then later in terms of oxygen. Since 1961, it has been defined with regard to the most abundant isotope of carbon, atoms of which are assigned masses of exactly 12 amu. (This isotope is known as "carbon-12" as will be discussed later in this module.) Thus, one amu is exactly 1 / 12 of the mass of one carbon-12 atom: 1 amu = 1.6605×10^{-24} g. The Dalton (Da) and the unified atomic mass unit (u) are alternative units that are equivalent to the amu. The fundamental unit of charge (also called the elementary charge) equals the magnitude of the charge of an electron (e) with $e = 1.602 \times 10^{-19}$ C.

A proton has a mass of 1.0073 amu and a charge of 1+. A neutron is a slightly heavier particle with a mass 1.0087 amu and a charge of zero; as its name suggests, it is neutral. The electron has a charge of 1− and is a much lighter particle with a mass of about 0.00055 amu (it would take about 1800 electrons to equal the mass of one proton.

Properties of Subatomic Particles					
Name	Location	Charge (C)	Unit Charge	Mass (amu)	Mass (g)
electron	outside nucleus	-1.602×10^{-19}	1−	0.00055	0.00091×10^{-24}
proton	nucleus	1.602×10^{-19}	1+	1.00727	1.67262×10^{-24}
neutron	nucleus	0	0	1.00866	1.67493×10^{-24}

Table 1. Properties of subatomic particles.

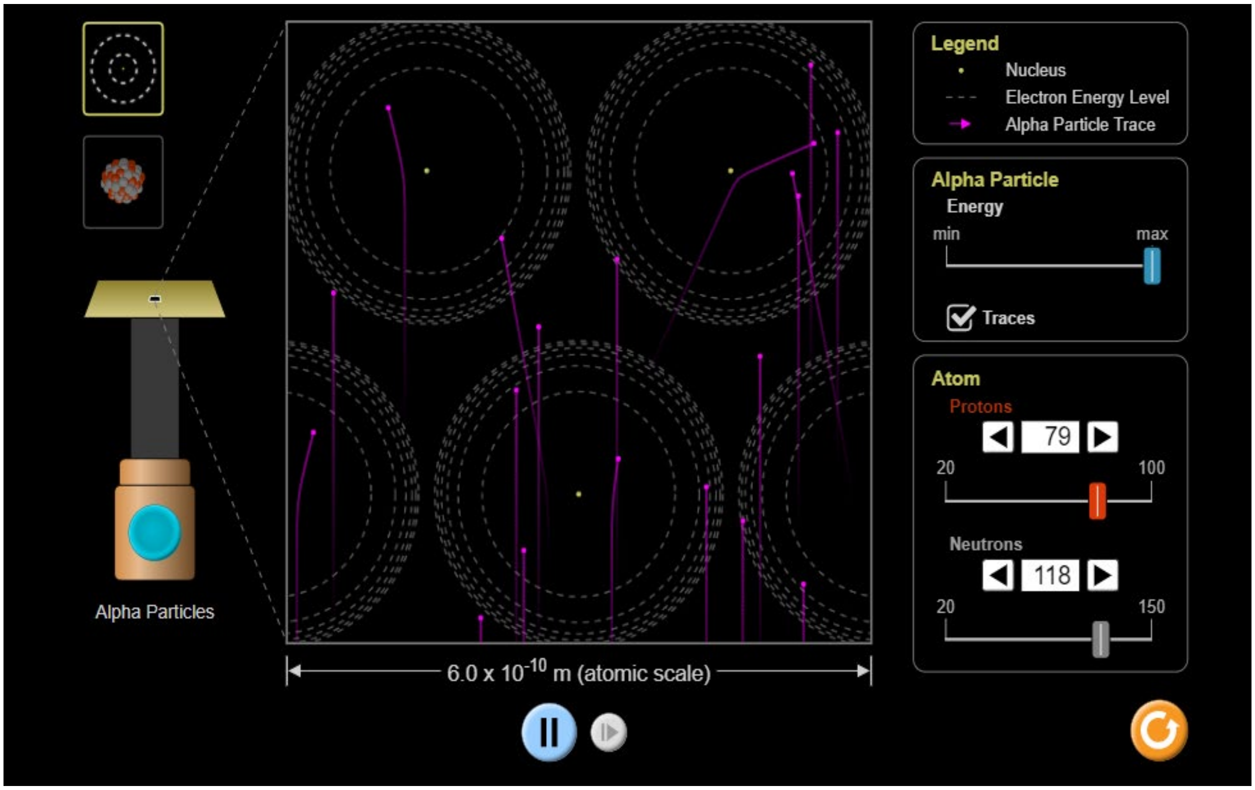
Activity:

Go to the following link and Perform Rutherford's experiment as well as Plum Pudding model experiment.

1. Click on the atom from left side menu
2. Click on Traces from the left top corner side menu
3. Adjust the alpha particle trace.
4. Click on the "play" button at the bottom of the page

What difference do you notice when you perform both experiments?

https://phet.colorado.edu/sims/html/rutherford-scattering/latest/rutherford-scattering_en.html



Questions

1. What postulate of atomic theory is partially correct and needs to be modified? Why?
2. What is the main discovery of Rutherford's experiment?

Ans: 1. Isotopes, atoms of same elements but not identical

2.Nucleus in an atom

The number of protons in the nucleus of an atom is its atomic number (Z). This is the defining trait of an element: Its value determines the identity of the atom. For example, any atom that contains six protons is the element carbon and has the atomic number 6, regardless of how many neutrons or electrons it may have. A neutral atom must contain the same number of positive and negative charges, so the number of protons equals the number of electrons. Therefore, the atomic number also indicates the number of electrons in an atom. The total number of protons and neutrons in an atom is called its mass number (A). The number of neutrons is therefore the difference between the mass number and the atomic number: A – Z = number of neutrons.

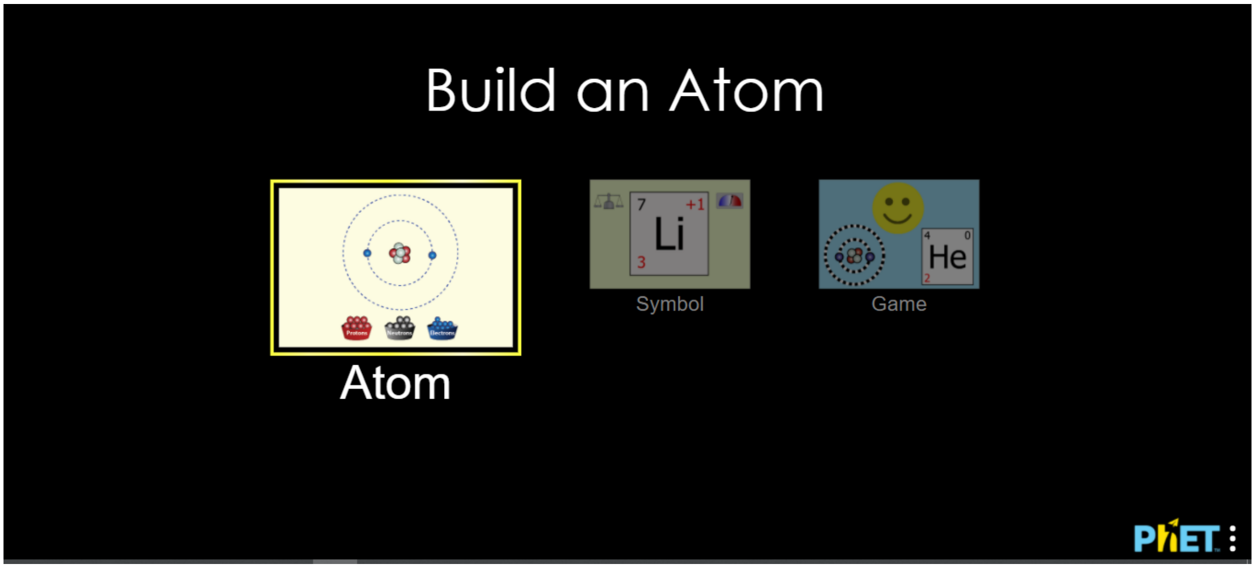
Atoms are electrically neutral if they contain the same number of positively charged protons and negatively charged electrons. When the numbers of these subatomic particles are *not* equal, the atom is electrically charged and is called an ion. The charge of an atom is defined as follows:

Atomic charge = number of protons − number of electrons

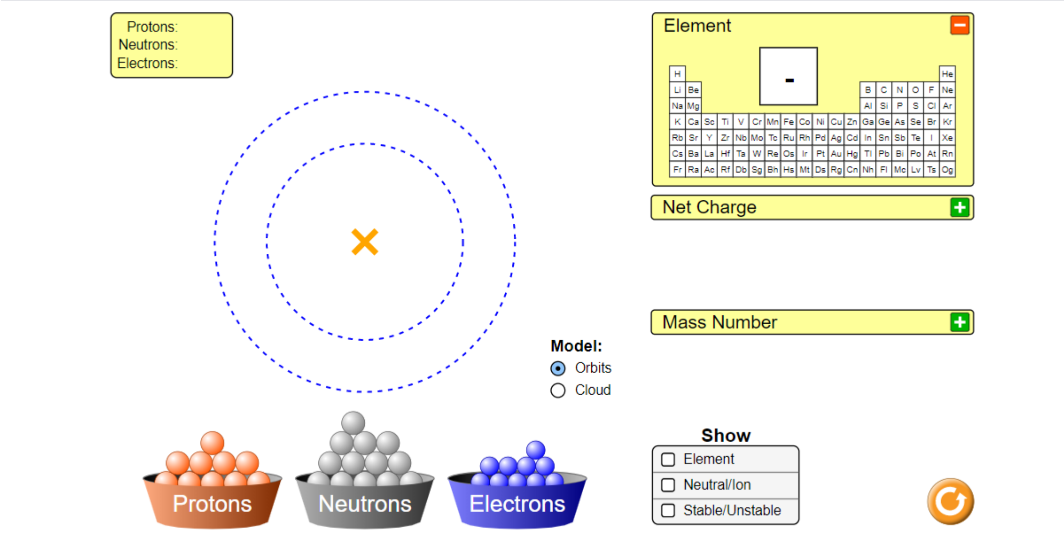
As will be discussed in more detail later in this chapter, atoms (and molecules) typically acquire charge by gaining or losing electrons. An atom that gains one or more electrons will exhibit a negative charge and is called an anion. Positively charged atoms called cations are formed when an atom loses one or more electrons. For example, a neutral sodium atom (Z = 11) has 11 electrons. If this atom loses one electron, it will become a cation with a 1+ charge (11 − 10 = 1+). A neutral oxygen atom (Z = 8) has eight electrons, and if it gains two electrons it will become an anion with a 2− charge (8 − 10 = 2−).

TRY THIS OUT!

https://phet.colorado.edu/en/simulation/build-an-atom



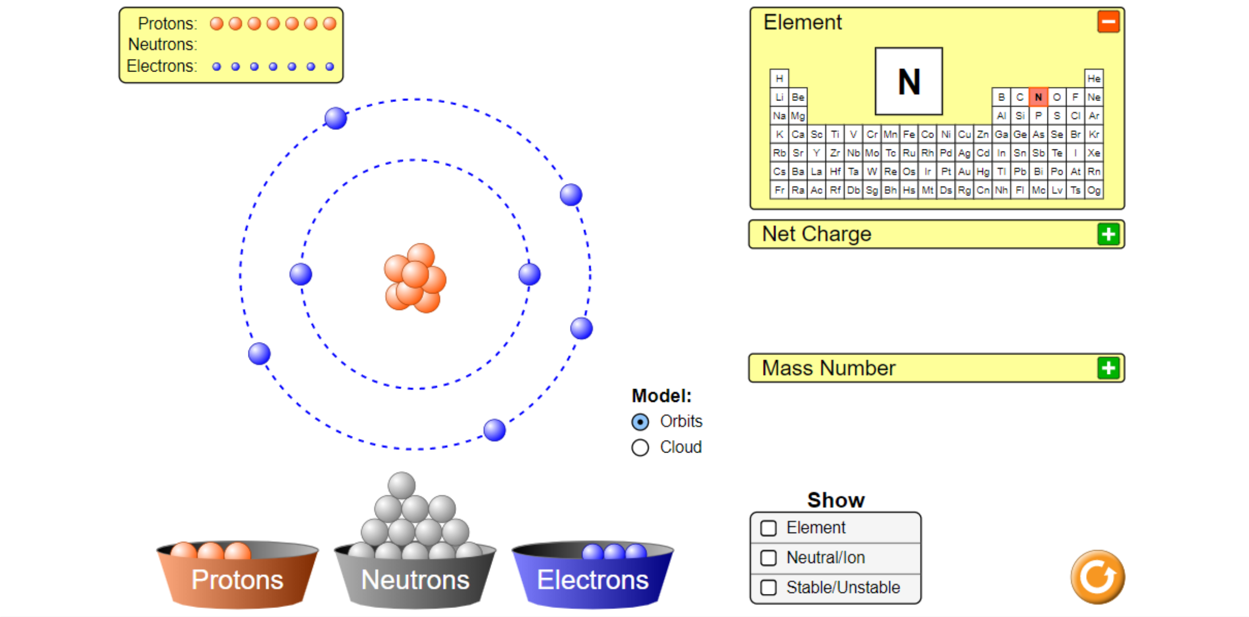
1. Go to the above activity and click on the first option "**Atom**". Then hide the mass number box and net charge box on the screen. Also choose the orbit model.



Model:
● Orbits
○ Cloud

Show
☐ Element
☐ Neutral/Ion
☐ Stable/Unstable

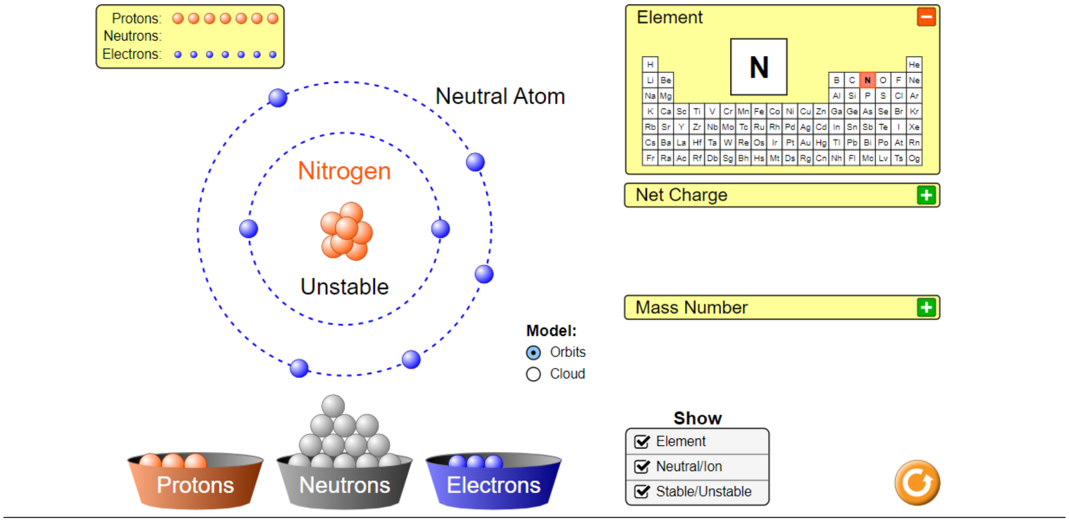
2. Drag and drop 7 protons and 7 electrons from the bucket and put in in the nucleus (“X “ marked) and dotted circles respectively. Can you predict which element is this?



Model:
● Orbits
○ Cloud

Show
☐ Element
☐ Neutral/Ion
☐ Stable/Unstable

3. Now check the boxes Element, Neutral/Ion and Stable/Unstable. You should see like the figure below.

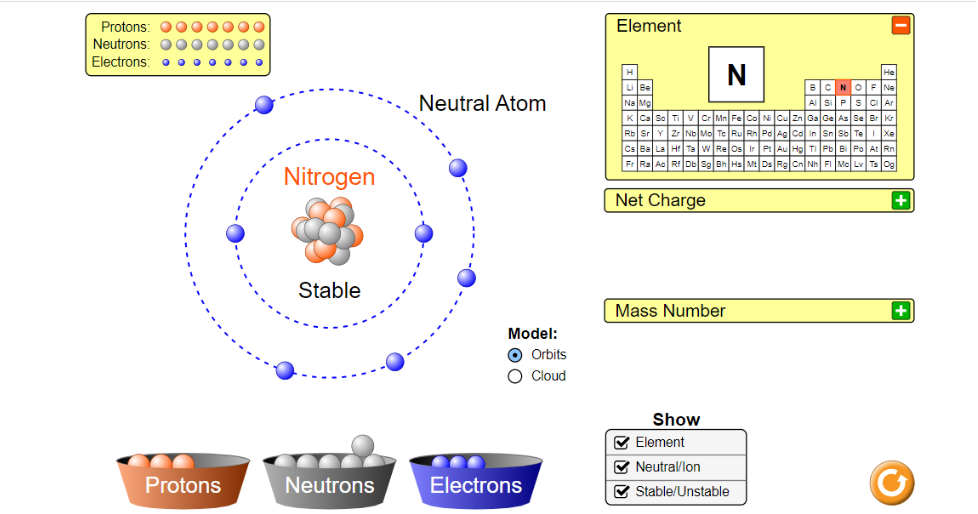


Model:
● Orbits
○ Cloud

Show
☑ Element
☑ Neutral/Ion
☑ Stable/Unstable

4. What are the atomic number of the element?
   Atomic #:

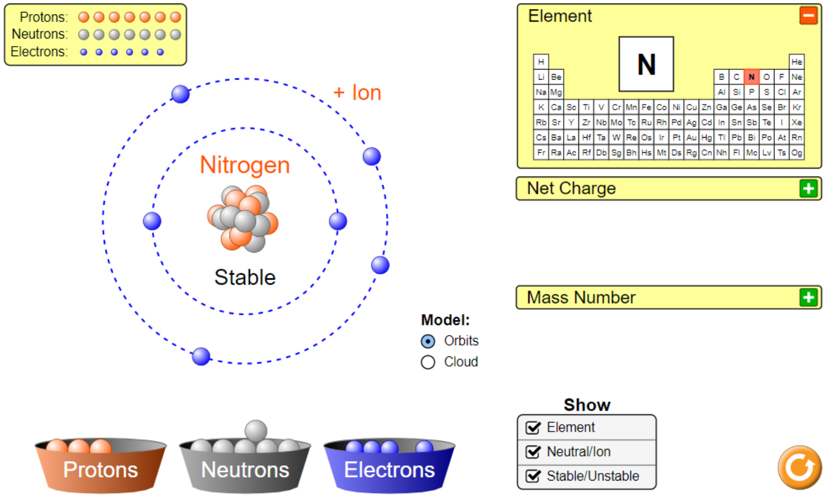
5. Why the atom is unstable? Add neutron one by one to the nucleus and until it becomes stable. Write the mass number of the element. Click on the box "Mass number" and compare to your values.
   Mass #:



Model:
● Orbits
○ Cloud

Show
☑ Element
☑ Neutral/Ion
☑ Stable/Unstable

6. Now take one electrons out from the atom. Why it is called “Ion”?. How many protons and electrons are now present in the atom? Is it positive or negative ion? Predict the charge of the ion. Then open the “Net Charge” box and compare to your results



Model:
● Orbits
○ Cloud

Show
☑ Element
☑ Neutral/Ion
☑ Stable/Unstable

Charge:

7. Add one more electron to the neutral atom. How many protons and electrons are now present in the atom? Is it positive or negative ion? Predict the charge of the ion.
Charge:

8. Add some more neutrons and observe the simulated picture. Can you predict when the atom will become unstable?

Example 3: Composition of an atom

Iodine is an essential trace element in our diet; it is needed to produce thyroid hormone. Insufficient iodine in the diet can lead to the development of a goiter, an enlargement of the thyroid gland.

(a) Insufficient iodine in the diet can cause an enlargement of the thyroid gland called a goiter.

(b) The addition of small amounts of iodine to salt, which prevents the formation of goiters, has helped eliminate this concern in the US where salt consumption is high.

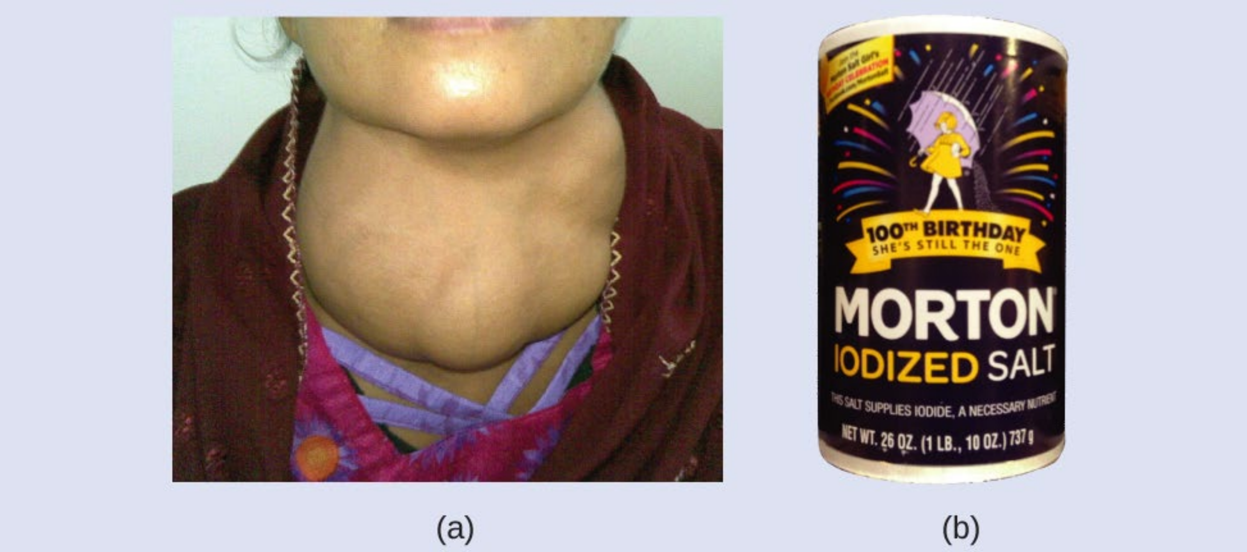


Figure 2.11 Iodine, An Element Present in Human Body

Ref: www.openstax.org/

The addition of small amounts of iodine to table salt (iodized salt) has essentially eliminated this health concern in the United States, but as much as 40% of the world's population is still at risk of iodine deficiency. The iodine atoms are added as anions, and each has a 1− charge and a mass number of 127. Determine the numbers of protons, neutrons, and electrons in one of these iodine anions.

Solution

The atomic number of iodine (53) tells us that a neutral iodine atom contains 53 protons in its nucleus and 53 electrons outside its nucleus. Because the sum of the numbers of protons and neutrons equals the mass number, 127, the number of neutrons is 74 (127 − 53 = 74). Since the iodine is added as a 1− anion, the number of electrons is 54 [53 – (1–) = 54].

Chemical Symbols

A chemical symbol is an abbreviation that we use to indicate an element or an atom of an element. For example, the symbol for mercury is Hg. We use the same symbol to indicate one atom of mercury (microscopic domain) or to label a container of many atoms of the element mercury (macroscopic domain).

The symbol Hg represents the element mercury regardless of the amount; it could represent one atom of mercury or a large amount of mercury.

Figure 2.11. The element of mercury, its chemical symbol is Hg.

Ref: www.openstax.org/

Some symbols are derived from the common name of the element; others are abbreviations of the name in another language. Most symbols have one or two letters, but three-letter symbols have been used to describe some elements that have atomic numbers greater than 112. To avoid confusion with other notations, only the first letter of a symbol is capitalized. For example, Co is the symbol for the element cobalt, but CO is the notation for the compound carbon monoxide, which contains atoms of the elements carbon (C) and oxygen (O). All known elements and their symbols are in the periodic table.

Some Common Elements and Their Symbols			
Element	Symbol	Element	Symbol
aluminum	Al	iron	Fe (from *ferrum*)
bromine	Br	lead	Pb (from *plumbum*)

Some Common Elements and Their Symbols			
Element	Symbol	Element	Symbol
calcium	Ca	magnesium	Mg
carbon	C	mercury	Hg (from *hydrargyrum*)
chlorine	Cl	nitrogen	N
chromium	Cr	oxygen	O
cobalt	Co	potassium	K (from *kalium*)
copper	Cu (from *cuprum*)	silicon	Si
fluorine	F	silver	Ag (from *argentum*)
gold	Au (from *aurum*)	sodium	Na (from *natrium*)

Some Common Elements and Their Symbols			
Element	Symbol	Element	Symbol
helium	He	sulfur	S
hydrogen	H	tin	Sn (from *stannum*)
iodine	I	zinc	Zn

Table 2. Common elements and their symbols.

Traditionally, the discoverer (or discoverers) of a new element names the element. However, until the name is recognized by the International Union of Pure and Applied Chemistry (IUPAC), the recommended name of the new element is based on the Latin word(s) for its atomic number. For example, element 106 was called unnilhexium (Unh), element 107 was called unnilseptium (Uns), and element 108 was called unniloctium (Uno) for several years. These elements are now named after scientists (or occasionally locations); for example, element 106 is now known as *seaborgium*(Sg) in honor of Glenn Seaborg, a Nobel Prize winner who was active in the discovery of several heavy elements.

The atomic number is the nuclear charge, and thus the number of electrons in the neutral atom

What single parameter uniquely characterizes the atom of a given element? It is not the atom's relative mass, as we will see in the section on isotopes below. It is, rather, the number of protons in the nucleus, which we call the ***atomic number*** and denote by the symbol *Z*. Each proton carries an electric charge of +1, so the atomic number also specifies the electric charge of the nucleus. In the neutral atom, the *Z protons* within the nucleus are balanced by *Z electrons* outside it.

Moseley searched for a measurable property of each element that increases linearly with atomic number. He found this in a class of X-rays emitted by an element when it is bombarded with electrons. The frequencies of these X-rays are unique to each element, and they increase uniformly in successive elements. Mosely found that the square roots of these frequencies give a straight line when plotted against Z; this enabled him to sort the elements in order of increasing atomic number.

See this example of his experimental plots.
Atomic numbers were first worked out in 1913 by Henry Moseley, a young member of Rutherford's research group in Manchester.

You can think of the atomic number as a kind of serial number of an element, commencing at 1 for hydrogen and increasing by one for each successive element. The chemical name of the element and its symbol are uniquely tied to the atomic number; thus the symbol "Sr" stands for strontium, whose atoms all have $Z = 38$.

Mass number

This is just the sum of the numbers of protons and neutrons in the nucleus. It is sometimes represented by the symbol A, so

$$A = Z + N$$

in which Z is the atomic number and N is the ***neutron number***.

Nuclides and their symbols

Because it is not always easy to display a subscript directly beneath a superscript, it is not uncommon to use constructions such as $_{12}\text{Mg}^{26}$, which will often be our practice in this document when it is necessary to show both Z and A explicitly.

The symbol for a specific isotope of any element is written by placing the mass number as a superscript to the left of the element symbol. The atomic number is sometimes written as a subscript preceding the symbol, but since this number defines the element's identity, as does its symbol, it is often omitted. For example, magnesium exists as a mixture of three isotopes, each with an atomic number of 12 and with mass numbers of 24, 25, and 26, respectively. These isotopes can be identified as ^{24}Mg, ^{25}Mg, and ^{26}Mg. These isotope symbols are read as "element, mass number" and can be symbolized consistent with this reading. For instance, ^{24}Mg is read as "magnesium 24," and can be written as "magnesium-24" or "Mg-24." ^{25}Mg is read as "magnesium 25," and can be written as "magnesium-25" or "Mg-25." All magnesium atoms have 12 protons in their nucleus. They differ only because a ^{24}Mg atom has 12 neutrons in its nucleus, a ^{25}Mg atom has 13 neutrons, and a ^{26}Mg has 14 neutrons.

The symbol for an atom indicates the element via its usual two-letter symbol, the mass number as a left superscript, the atomic number as a left subscript (sometimes omitted), and the charge as a right superscript.

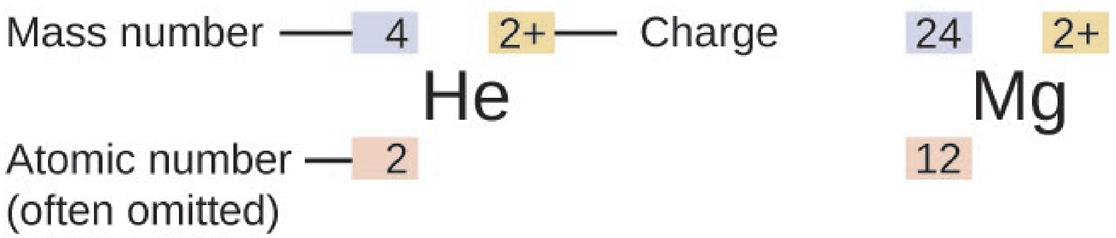
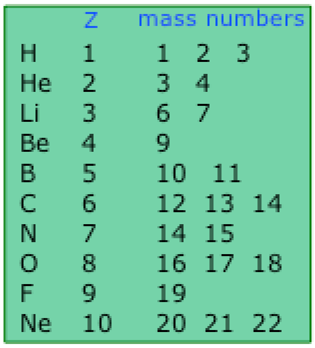


Figure 12. Chemical symbols for atoms.

Isotopes

Isotopes are nuclides having the same atomic number

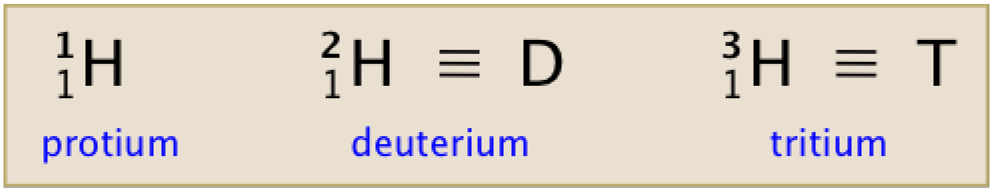
Two nuclides of the same element (and thus with identical atomic numbers) but different neutron numbers (and therefore different mass numbers) are known as ***isotopes***. Most elements occur in nature as mixtures of isotopes, but twenty-three of them (including beryllium and fluorine, shown in the table) are monoisotopic. For example, there are three *natural isotopes* of magnesium: ^{24}Mg (79% of all Mg atoms), ^{25}Mg (10%), and ^{26}Mg (11%); all three are present in all compounds of magnesium in about these same proportions. Approximately 290 isotopes occur in nature.



	Z	mass numbers
H	1	1 2 3
He	2	3 4
Li	3	6 7
Be	4	9
B	5	10 11
C	6	12 13 14
N	7	14 15
O	8	16 17 18
F	9	19
Ne	10	20 21 22

The best place to find out about the isotopes of individual elements is this page at the Lawrence Berkeley site, which covers both the natural isotopes and the artificially-produced ones.

The two heavy isotopes of hydrogen are especially important— so much so that they have names and symbols of their own:



Deuterium accounts for only about 15 out of every one million atoms of hydrogen. Tritium, which is radioactive, is even less abundant. All the tritium on the earth is a by-product of the decay of other radioactive elements.

Isotope effects: when different isotopes exhibit different chemical behavior

The chemical behavior of an element is governed by the number and arrangement of its electrons in relation to its nuclear charge (atomic number). Because these quantities are identical for all isotopes of a given element, they are generally considered to exhibit identical chemical properties.

However, it turns out that the mass differences between different isotopes can give rise to very slight differences in their physical behavior that can, in turn affect their chemical behavior as well. These *isotope effects* are most evident in the lighter elements, in which small differences in neutron number lead to greater differences in atomic mass.

Wikipedia article on **heavy water**

Thus no element is more subject to isotope effects than hydrogen: an atom of "heavy hydrogen" ${}_1H^2$ (also known as *deuterium* and often given the symbol D) has twice the mass of an atom of ${}_1H^2$. When this isotope is combined with oxygen, the resulting "heavy water" D_2O exhibits noticeably different physical and chemical properties: it melts at 3.8° C and boils at 101.4° C. D_2O apparently interferes with cell division in organisms; mammals given only heavy water typically die in about a week.

When two or more elements whose atoms contain multiple isotopes are present in a molecule, numerous isotopic modifications become possible.

For example, the two stable isotopes of hydrogen and of oxygen (O^{16} and O^{18}) give rise to combinations such as H_2O^{18}, HDO^{16}, etc., all of which are readily identifiable in the infrared spectra of water vapor.

Atomic Mass

Atoms are of course far too small to be weighed directly; weight measurements can only be made on the massive (but unknown) numbers of atoms that are observed in chemical reactions. The early combining-weight experiments of Dalton and others established that hydrogen is the lightest of the atoms, but the crude nature of the measurements and uncertainties about the formulas of many compounds made it difficult to develop a reliable scale of the relative weights of atoms. Even the most exacting weight measurements we can make today are subject to experimental uncertainties that limit the precision to four significant figures at best.

Atomic weights are *average relative* masses

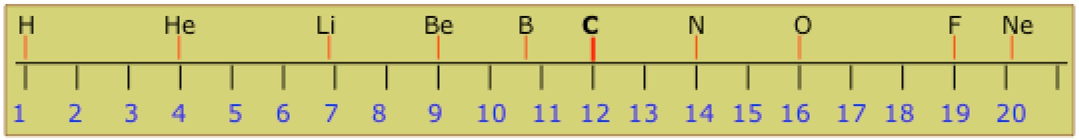
In the earlier discussion of relative weights of atoms, we explained how Dalton assigned a relative weight of unity to hydrogen, the lightest element, and used combining weights to estimate the relative weights of the others he studied. Later on, when it was recognized that more elements form simple compounds with oxygen, this element was used to define the atomic weight scale. Selecting O = 16 made it possible to retain values very close to those already assigned on the H=1 scale.

Finally, in 1961, carbon became the defining element of the atomic weight scale. But because, by this time, the existence of isotopes was known, it was decided to base the scale on one particular isotope of carbon, C-12, whose relative mass is defined as exactly 12.000. Because almost 99% of all carbon atoms on the earth consist of $_6C^{12}$, atomic weights of elements on the current scale are almost identical to those on the older O=16 scale.

Most elements possess more than one stable isotope in proportions that are unique to each particular element. For this reason, atomic weights are really weighted *averages* of the relative masses of each that are found on earth.

> Atomic weights are the ratios of the average mass of the atoms of an element to the mass of an identical number of $_6C^{12}$ atoms.

You can visualize the atomic weight scale as a long line of numbers that runs from 1 to around 280. The beginning of the scale looks like this:



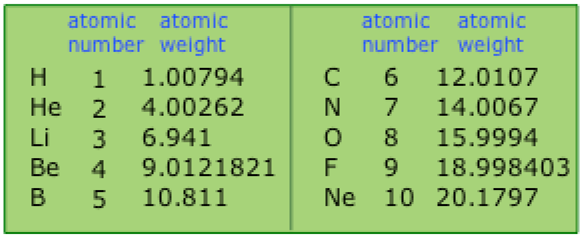
Atomic weights (relative atomic masses) of the first ten elements

The red vertical lines beneath each element symbol indicate where that element is located on the atomic weight scale.

Of these ten elements, only two, beryllium and fluorine, have a single isotope. The other eight atomic weights are weighted averages of the relative masses of the multiple isotopes that these (and most) elements possess. This is especially noticeable in the case of boron, whose average relative mass falls between 10 and 11. (Historically, observations of cases such as these led to the very concept of isotopes.)

For many elements, one particular isotope so dominates the natural mixture that the others have little effect on the average mass. For example, 99.99 percent of hydrogen atoms consist of $_1H^1$, whereas $_1H^2$, the other stable isotope, amounts to only 0.01 percent. Similarly, oxygen is dominated by $_8O^{16}$ (over 99.7 percent) to the near exclusion of its two other isotopes.

Atomic weights are listed in tables found in every chemistry textbook; you can't do much quantitative chemistry without them!
The "standard" values are updated every few years as better data becomes available.
You will notice that the precisions of these atomic weights, as indicated by the number of significant figures, vary considerably.



	atomic number	atomic weight		atomic number	atomic weight
H	1	1.00794	C	6	12.0107
He	2	4.00262	N	7	14.0067
Li	3	6.941	O	8	15.9994
Be	4	9.0121821	F	9	18.998403
B	5	10.811	Ne	10	20.1797

- Atomic weights of the 26 elements having a single stable isotope (*monoisotopic* elements) are the most precisely known. Two of these, boron and fluorine, appear in the above table.
- Owing to geochemical *isotopic fractionation* (discussed farther on), there is always some uncertainty in averaging the atomic weights of elements with two or more stable isotopes.
- Industrial processes associated mainly with nuclear energy and weapons production require the isolation or concentration of particular isotopes. When the by-product elements or compounds from which these isotopes have been depleted eventually get distributed in the environment or sold into the commercial marketplace, their atomic weights can vary from "official" values. This has occurred, for example, with lithium, whose isotope Li-6 has been used to produce hydrogen bombs.
- Naturally-occurring radioactive elements (all elements heavier than $_{82}$Pb) all gradually decay into lighter elements, most of which are themselves subject to radioactive decay. These *radioactive decay chains* eventually terminate in a stable element, the most common of which is one of the three stable isotopes of lead. Subsequent geochemical processes can cause lead ore bodies from such sources to mix with "primeval" Pb (derived from the cosmic dust that formed the solar system), leading to a range of possible average atomic weights. For these reasons, lead, with a listed average atomic weight of 207.2, has the least-certain mass of any stable element.

Weighing atoms: mass spectrometry

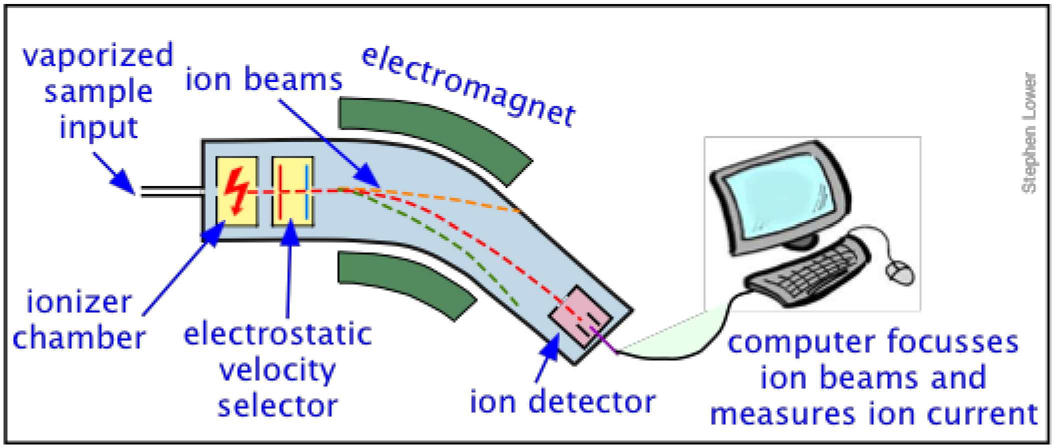
A major breakthrough in Chemistry occurred in 1913 when J.J. Thompson directed a beam of ionized neon atoms through both a magnetic field and an electrostatic field. Using a photographic plate as a detector, he found that the beam split into two parts, and suggested that these showed the existence of two isotopes of neon, now known to be Ne-20 and Ne-22.

This, combined with the finding made a year earlier by Wilhelm Wien that the degree of deflection of a particle in these fields is proportional to the ratio of its electric charge to its mass, opened the way to characterizing these otherwise invisible particles.

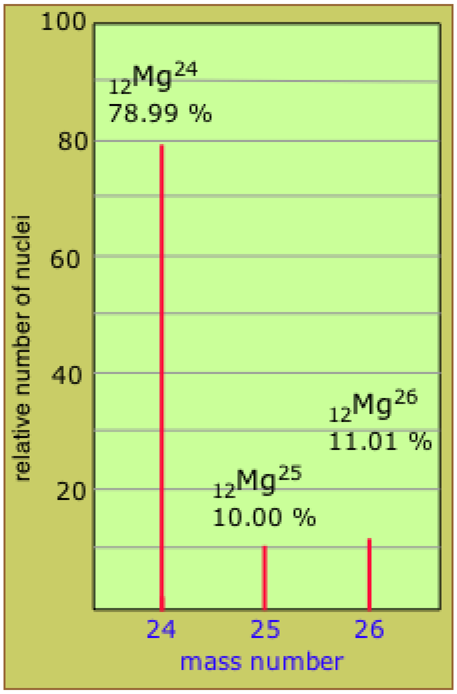
Thompson’s student F.W. Aston improved the apparatus, developing the first functional ***mass spectrometer***, and he went on to identify 220 of the 287 isotopes found in nature; this won him a Nobel prize in 1921. His work revealed that the mass numbers of all isotopes are nearly integers (that is, integer multiples of the mass number 1 of the protons and neutrons that make up the nucleus.

Neutral atoms, having no charge, cannot be accelerated along a path so as to form a beam, nor can they be deflected. They can, however, be made to *acquire* electric charges by directing an electron beam at them, and this was one of the major innovations by Aston that made mass spectrometry practical.

Mass spectrometry begins with the injection of a vaporized sample into an ionization chamber where an electrical discharge causes it to become ionized. An accelerating voltage propels the ions through an electrostatic field that allows only those ions having a fixed velocity (that is, a given charge) to pass between the poles of a magnet. The magnetic field deflects the ions by an amount proportional to the charge-to-mass ratios. The separated ion beams are detected and their



The mass spectrometer has become one of the most widely used laboratory instruments. Mass spectrometry is now mostly used to identify molecules. Ionization usually breaks a molecule up into fragments having different charge-to-mass ratios, each molecule resulting in a unique "fingerprint" of particles whose origin can be deduced by a jigsaw puzzle-like reconstruction. For many years, "mass-spec" had been limited to small molecules, but with the development of novel ways of creating ions from molecules, it has now become a major tool for analyzing materials and large biomolecules, including proteins.



The mass spectrum of magnesium shows that it consists of three isotopes of masses 24 through 26. The height of each peak shows the abundance of each isotope.

More on mass spectrometry

Mass Spectrometry: Atomic Structure & Properties

- How a mass spectrometer works

- Mass spectrometry and its applications
- Mass sectrometry history and timeline

Isotopic mixtures and abundances

Only 26 of the elements that occur on the Earth exist as a single isotope; these are said to be ***monoisotopic***. The remaining elements consist of mixtures of between two and ten isotopes. The total number of natural isotopes is 339; of these, 254 are stable, while the remainder are radioactive, meaning that they decay into stable isotopes.

Recalling that a given isotope (also known as a ***nuclide***) is composed of protons and neutrons, each having a mass number of unity, it should be apparent that the mass number of a given nuclide will be an integer, as seen in the mass spectrum of magnesium above.

It also follows that the relative atomic masses ("atomic weights") of monoisotopic elements will be very close to integers, while those of other elements, being weighted averages, can have any value.

Problem Example 4
Estimate the average atomic weight of magnesium from the isotopic abundance data shown in the above mass spectrometry plot.

Solution: We just take the weighted average of the mass numbers:

$(0.7899 \times 24) + (0.1000 \times 25) + (0.1101 \times 26) = \mathbf{24.32}$

Note: The measured atomic weight of Mg (24.305) is slightly smaller than this because atomic masses of nuclear components are not strictly additive, as will be explained further below.

When there are only two significantly abundant isotopes, you can estimate the relative abundances from the mass numbers and the average atomic weight.

Problem Example 5

The average atomic weight of chlorine is 35.45 and the element has two stable isotopes ${}_{17}Cl^{35}$ and ${}_{17}Cl^{37}$. Estimate the relative abundances of these two isotopes.

Solution: Here you finally get to put your high-school algebra to work! If we let x represent the fraction of Cl^{35}, then $(1-x)$ gives the fraction of Cl^{37}. The weighted average atomic weight is then

$35x + 37(1-x) = 35.45$

Solving for x gives $2x = 1.55$, $x = 0.775$, so the abundances are 77.5% Cl^{35} and 22.5% Cl^{37}.

[Problems of this kind almost always turn up in exams]

Problem Example 6

Elemental chlorine, Cl_2, is made up of the two isotopes mentioned in the previous example. How many peaks would you expect to observe in the mass spectrum
of Cl_2?

Solution: The mass spectrometer will detect a peak for each possible combination of the two isotopes in dichlorine: ^{35}Cl-^{35}Cl, ^{35}Cl-^{37}Cl, and ^{37}Cl-^{37}Cl.

Because each proton and each neutron contribute approximately one amu to the mass of an atom, and each electron contributes far less, the atomic mass of a single atom is approximately equal to its mass number (a whole number). However, the average masses of atoms of most elements are not whole numbers because most elements exist naturally as mixtures of two or more isotopes.

The mass of an element shown in a periodic table or listed in a table of atomic masses is a weighted, average mass of all the isotopes present in a naturally occurring sample of that element. This is equal to the sum of each individual isotope's mass multiplied by its fractional abundance.

average mass = fractional abundance} × isotopic mass

For example, the element boron is composed of two isotopes: About 19.9% of all boron atoms are ^{10}B with a mass of 10.0129 amu, and the remaining 80.1% are ^{11}B with a mass of 11.0093 amu. The average atomic mass for boron is calculated to be:

boron average mass = 0.199 × 10.0129 amu + 0.801 × 11.0093 amu = 1.99 amu + 8.82 amu =10.81 amu

It is important to understand that no single boron atom weighs exactly 10.8 amu; 10.8 amu is the average mass of all boron atoms, and individual boron atoms weigh either approximately 10 amu or 11 amu.

Example 4: Calculation of Average Atomic Mass

A meteorite found in central Indiana contains traces of the noble gas neon picked up from the solar wind during the meteorite's trip through the solar system. Analysis of a sample of the gas showed that it consisted of 91.84% 20Ne (mass 19.9924 amu), 0.47% 21Ne (mass 20.9940 amu), and 7.69% 22Ne (mass 21.9914 amu). What is the average mass of the neon in the solar wind?

Solution

average mass = 0.9184 × 19.9924 amu + 0.0047 × 20.9940 amu + 0.0769 × 21.9914 amu = 18.36 + 0.099 + 1.69 amu = 20.15 amu

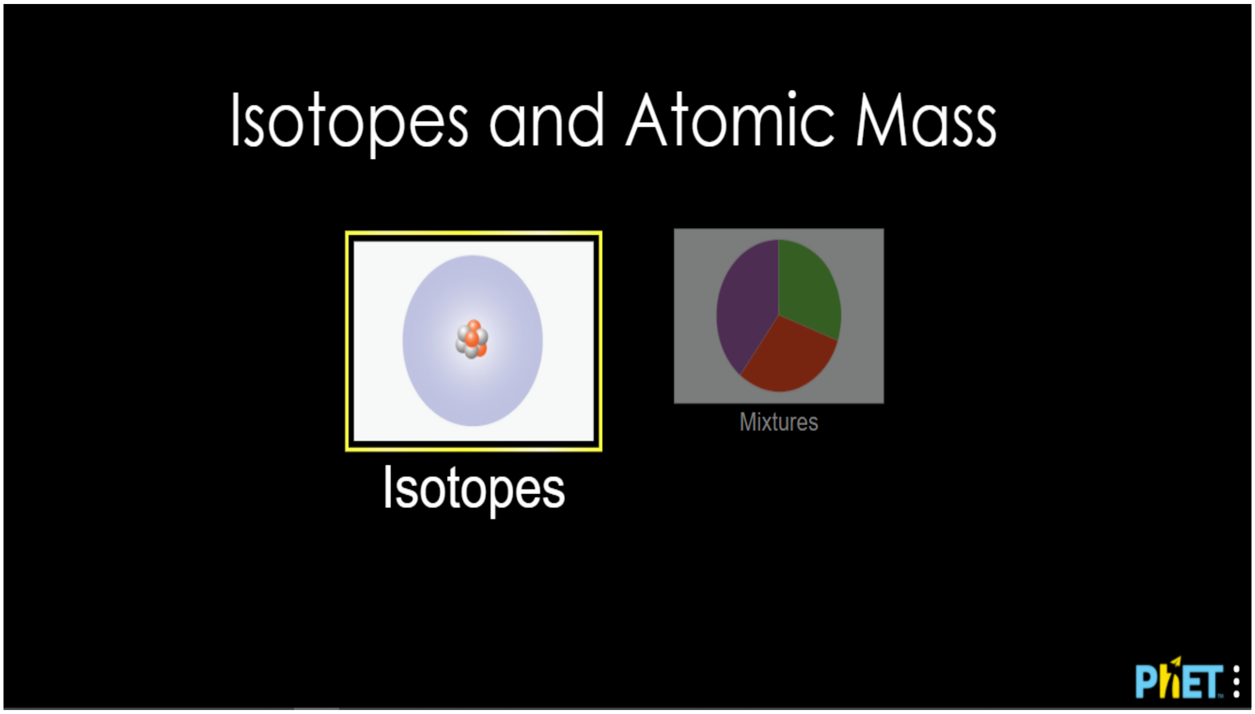
The average mass of a neon atom in the solar wind is 20.15 amu. (The average mass of a terrestrial neon atom is 20.1796 amu. This result demonstrates that we may find slight differences in the natural abundance of isotopes, depending on their origin.)

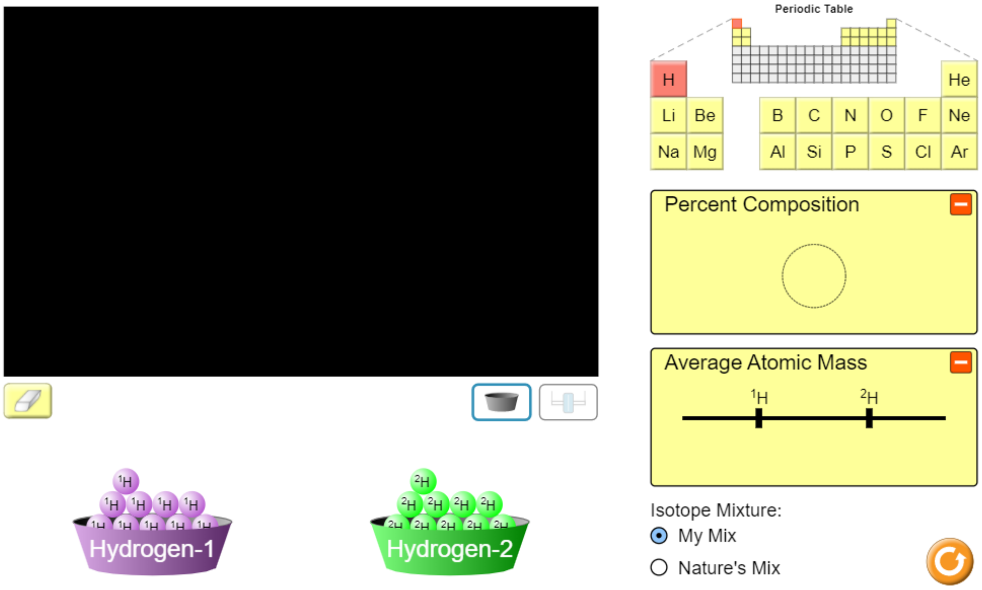
The occurrence and natural abundances of isotopes can be experimentally determined using an instrument called a mass spectrometer. Mass spectrometry (MS) is widely used in chemistry, forensics, medicine, environmental science, and many other fields to analyze and help identify the substances in a sample of material.

Let us use neon as an example. Since there are three isotopes, there is no way to be sure to accurately predict the abundances to make the total of 20.18 amu average atomic mass. Let us guess that the abundances are 9% Ne-22, 91% Ne-20, and only a trace of Ne-21. The average mass would be 20.18 amu. Checking the nature's mix of isotopes shows that the abundances are 90.48% Ne-20, 9.25% Ne-22, and 0.27% Ne-21, so our guessed amounts have to be slightly adjusted.

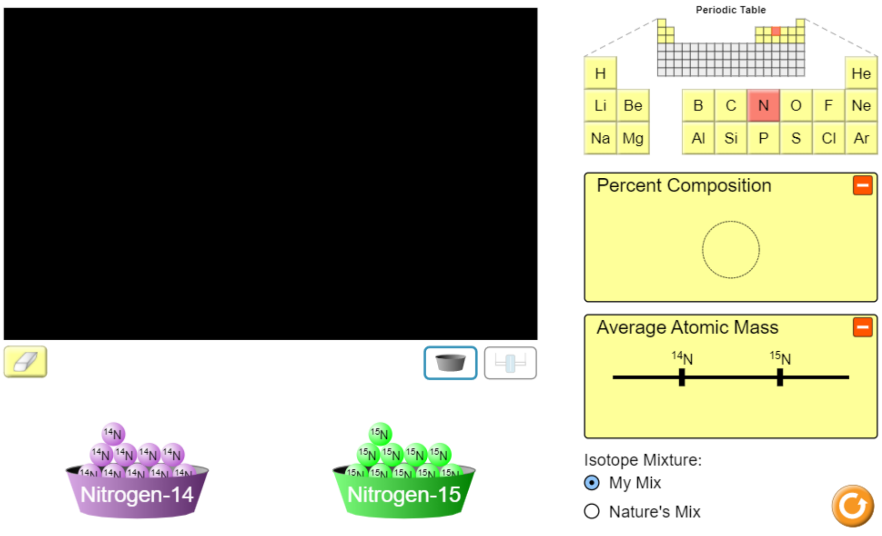
TRY THIS OUT!

https://phet.colorado.edu/en/simulation/isotopes-and-atomic-mass





Isotope Mixture:
● My Mix
○ Nature's Mix



Isotope Mixture:
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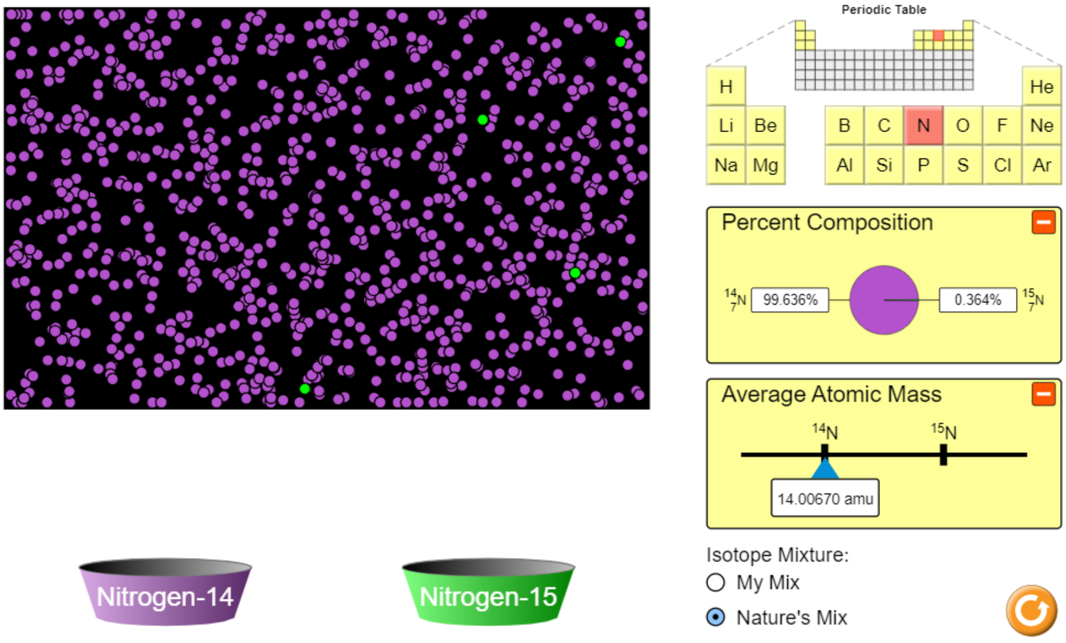
○ Nature's Mix

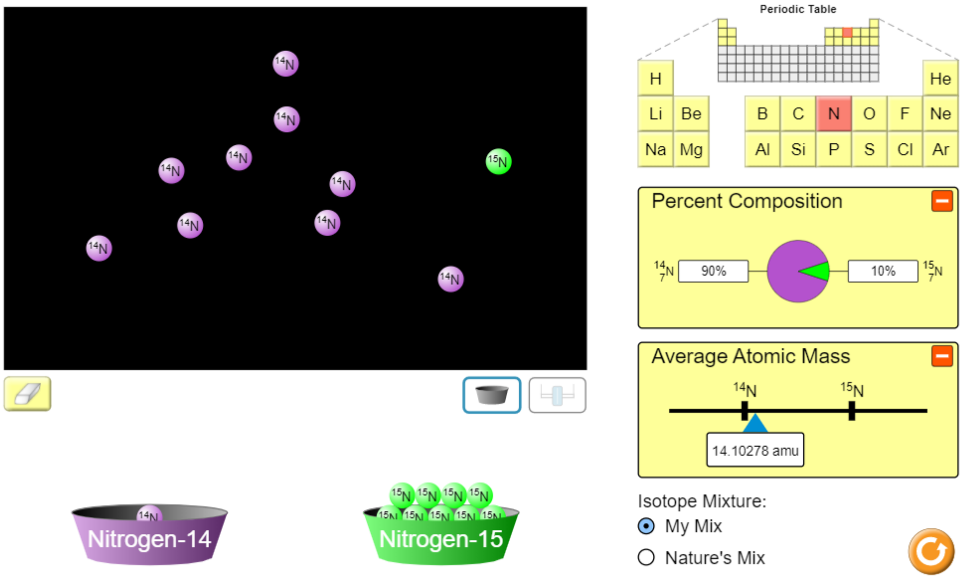


$^{14}_{7}N$ 99.636%
0.364% $^{15}_{7}N$

14.00670 amu

Isotope Mixture:
○ My Mix
● Nature's Mix

4. Now hide the percent composition and average atomic mass boxes. Click on my mix. Take 9 purple balls Nitrogen -14 atoms and 1 GREEN Nitrogen-15 atom.



Isotope Mixture:
● My Mix
○ Nature's Mix

5. Now estimate percent abundance from the visual represented and calculate average atomic mass. Open the Percent composition and average atomic mass boxes.

   Hint =[(14* # of purple balls) + (15*# of green balls)]/10

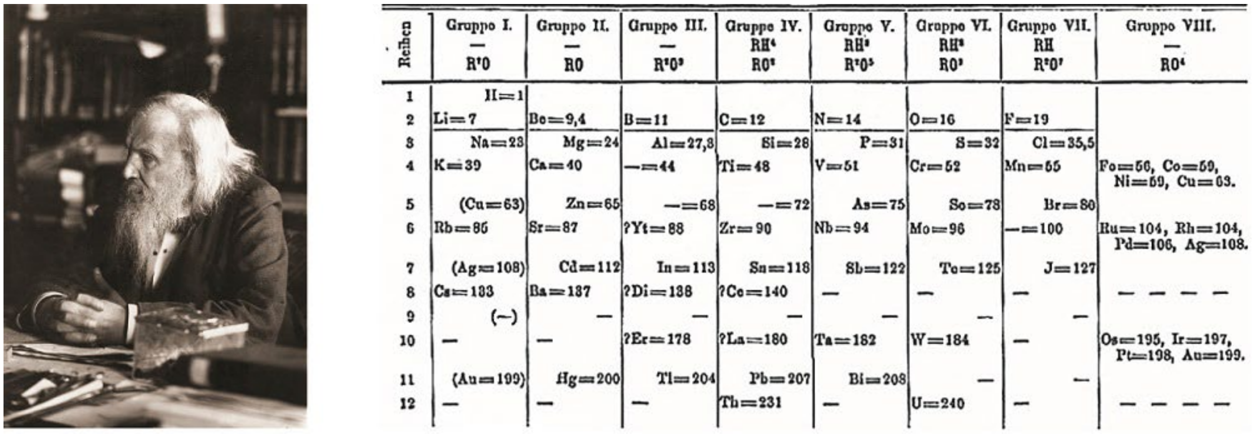
6. Compare your value with the values provided in the boxes. Explain the differences between your value and nature's mix values.

Section 2.4: The Periodic Table

As early chemists worked to purify ores and discovered more elements, they realized that various elements could be grouped together by their similar chemical behaviors. One such grouping includes lithium (Li), sodium (Na), and potassium (K): These elements all are shiny, conduct heat and electricity well, and have similar chemical properties. A second grouping includes calcium (Ca), strontium (Sr), and barium (Ba), which also are shiny, good conductors of heat and electricity, and have chemical properties in common. However, the specific properties of these two groupings are notably different from each other. For example: Li, Na, and K are much more reactive than are Ca, Sr, and Ba; Li, Na, and K form compounds with oxygen in a ratio of two of their atoms to one oxygen atom, whereas Ca, Sr, and Ba form compounds with one of their atoms to one oxygen atom. Fluorine (F), chlorine (Cl), bromine (Br), and iodine (I) also exhibit similar properties to each other, but these properties are drastically different from those of any of the elements above.

Watch this funny video:

Dimitri Mendeleev in Russia (1869) and Lothar Meyer in Germany (1870) independently recognized that there was a periodic relationship among the properties of the elements known at that time. Both published tables with the elements arranged according to increasing atomic mass. But Mendeleev went one step further than Meyer: He used his table to predict the existence of elements that would have the properties similar to aluminum and silicon, but were yet unknown. The discoveries of gallium (1875) and germanium (1886) provided great support for Mendeleev's work. Although Mendeleev and Meyer had a long dispute over priority, Mendeleev's contributions to the development of the periodic table are now more widely recognized (Figure 2.21).



(a)

(b)

Reihen	Gruppo I. — R^2O	Gruppo II. — RO	Gruppo III. — R^2O^3	Gruppo IV. RH^4 RO^2	Gruppo V. RH^3 R^2O^5	Gruppo VI. RH^2 RO^3	Gruppo VII. RH R^2O^7	Gruppo VIII. — RO^4
1	H=1							
2	Li=7	Be=9,4	B=11	C=12	N=14	O=16	F=19	
3	Na=23	Mg=24	Al=27,3	Si=28	P=31	S=32	Cl=35,5	
4	K=39	Ca=40	—=44	Ti=48	V=51	Cr=52	Mn=55	Fe=56, Co=59, Ni=59, Cu=63.
5	(Cu=63)	Zn=65	—=68	—=72	As=75	Se=78	Br=80	
6	Rb=85	Sr=87	?Yt=88	Zr=90	Nb=94	Mo=96	—=100	Ru=104, Rh=104, Pd=106, Ag=108.
7	(Ag=108)	Cd=112	In=113	Sn=118	Sb=122	Te=125	J=127	
8	Cs=133	Ba=137	?Di=138	?Ce=140	—	—	—	— — — —
9	(—)	—	—	—	—	—	—	
10	—	—	?Er=178	?La=180	Ta=182	W=184	—	Os=195, Ir=197, Pt=198, Au=199.
11	(Au=199)	Hg=200	Tl=204	Pb=207	Bi=208	—	—	
12	—	—	—	Th=231	—	U=240	—	— — — —

Figure 21. (a) Dimitri Mendeleev is widely credited with creating (b) the first periodic table of the elements. Lachinov; credit b: modification of work by "Den fjättrade ankan"/Wikimedia Commons)

By the twentieth century, it became apparent that the **periodic relationship** involved atomic numbers rather than atomic masses. **The modern statement of this relationship, the periodic law, is as follows:** ***the properties of the elements are periodic functions of their atomic numbers***. A modern periodic table arranges the elements in increasing order of their atomic numbers and groups atoms with similar properties in the same vertical column (Figure 22). Each box represents an element and contains its atomic number, symbol, average atomic mass, and (sometimes) name. The elements are arranged in seven horizontal rows, called periods or series, and 18 vertical columns, called groups. Groups are labeled at the top of each column. In the United States, the labels traditionally were numerals with capital letters. However, IUPAC recommends that the numbers 1 through 18 be used, and these labels are more common. For the table to fit on a single page, parts of two of the rows, a total of 14 columns, are usually written below the main body of the table.

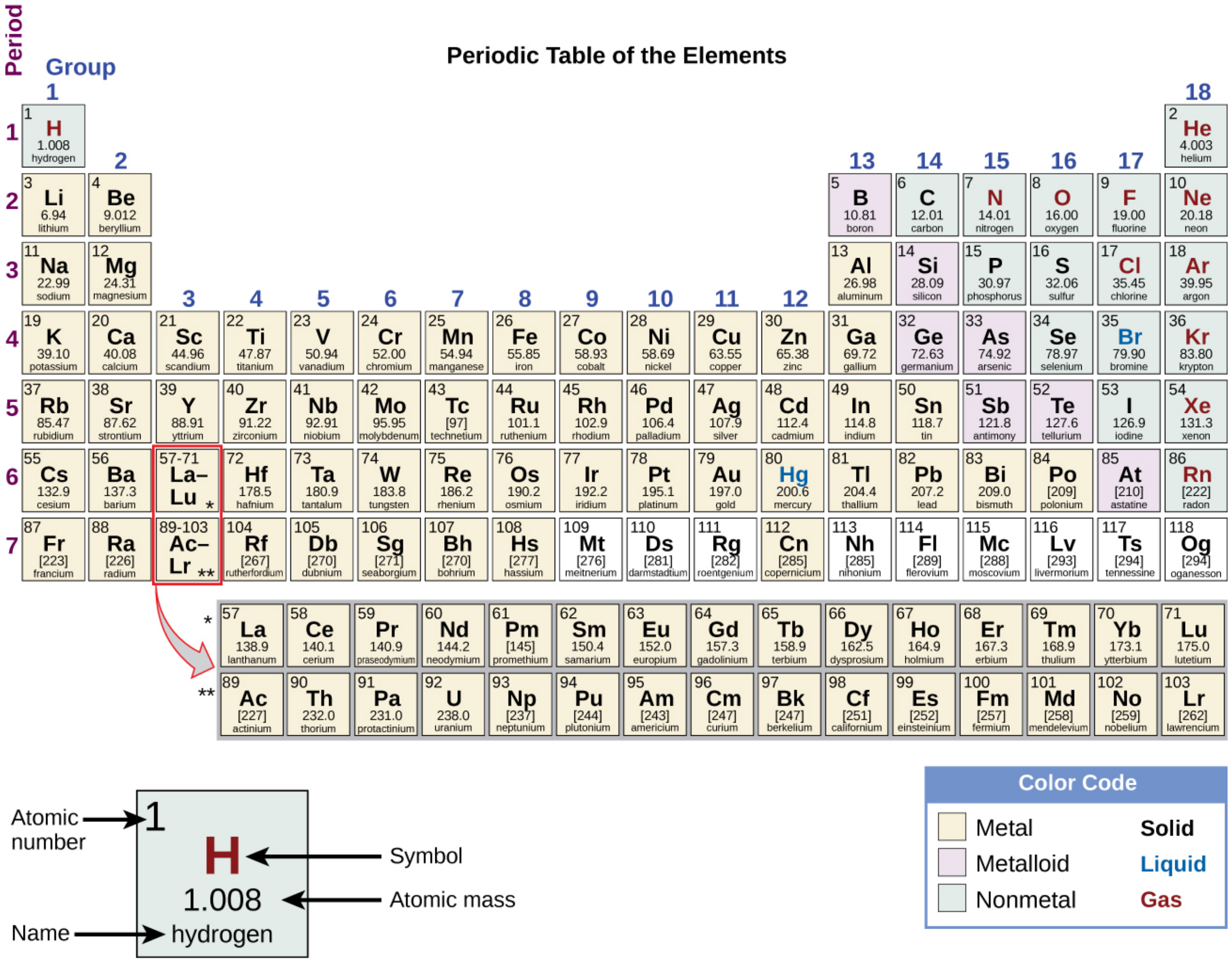


Figure 2. 22. Elements in the periodic table are organized according to their properties.

Ref: www.openstax.org/

Many elements differ dramatically in their chemical and physical properties, but some elements are similar in their behaviors. For example, many elements appear shiny, are malleable (able to be deformed without breaking) and ductile (can be drawn into wires), and conduct heat and electricity well. Other elements are not shiny, malleable, or ductile, and are poor conductors of heat and electricity. We can sort the elements into large classes with common properties: metals (elements that are shiny, malleable, good conductors of heat and electricity—shaded yellow); nonmetals (elements that appear dull, poor conductors of heat and electricity—shaded green); and metalloids (elements that conduct heat and electricity moderately well, and possess some properties of metals and some properties of nonmetals—shaded purple).

The elements can also be classified into the main-group elements (or representative elements) in the columns labeled 1, 2, and 13–18; the transition metals in the columns labeled 3–12; and inner transition metals in the two rows at the bottom of the table (the top-row elements are called lanthanides and the bottom-row elements are actinides; Figure 23). The elements can be subdivided further by more specific properties, such as the composition of the compounds they form. For example, the elements in group 1 (the first column) form compounds that consist of one atom of the element and one atom of hydrogen. These elements (except hydrogen) are known as alkali metals, and they all have similar chemical properties. The elements in group 2 (the second column) form compounds consisting of one atom of the element and two atoms of hydrogen: These are called alkaline earth metals, with similar properties among members of that group. Other groups with specific names are the pnictogens (group 15), chalcogens (group 16), halogens (group 17), and the noble gases (group 18, also known as inert gases). The groups can also be referred to by the first element of the group: For example, the chalcogens can be called the oxygen group or oxygen family. Hydrogen is a unique, nonmetallic element with properties similar to both group 1 and group 17 elements. For that reason, hydrogen may be shown at the top of both groups, or by itself.

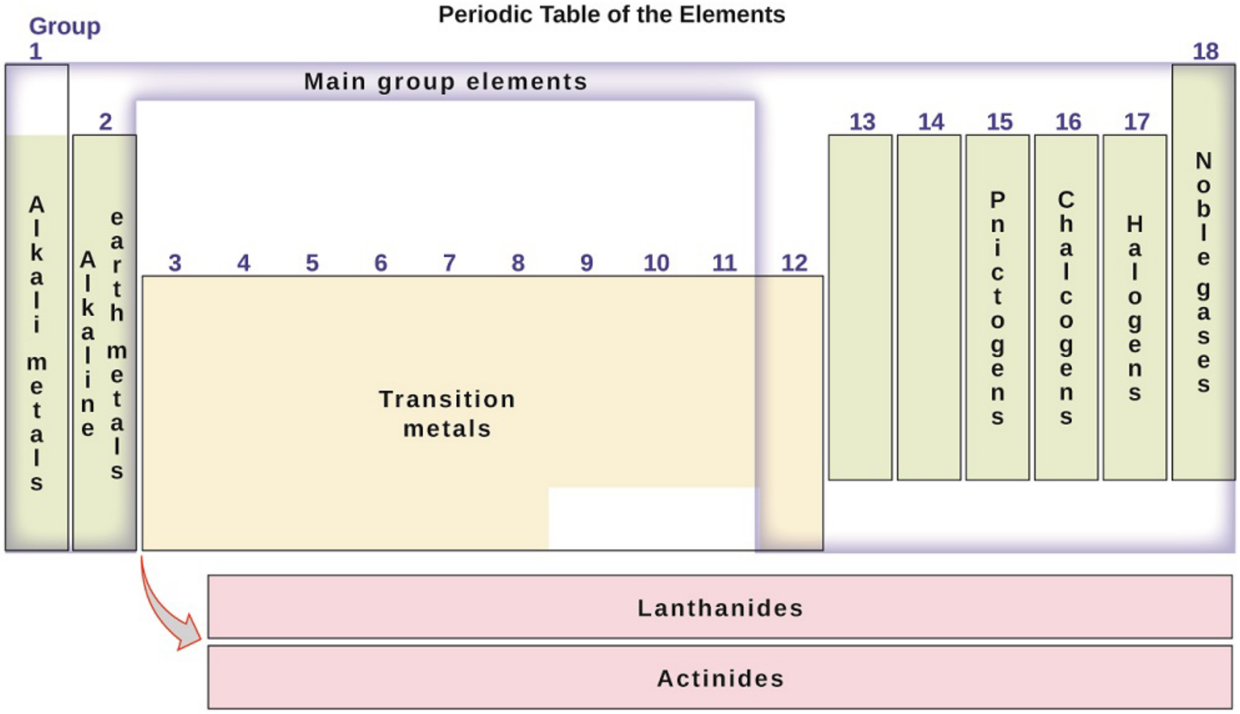


Figure 2.23: The periodic table organizes elements with similar properties into groups.

Ref: www.openstax.org/

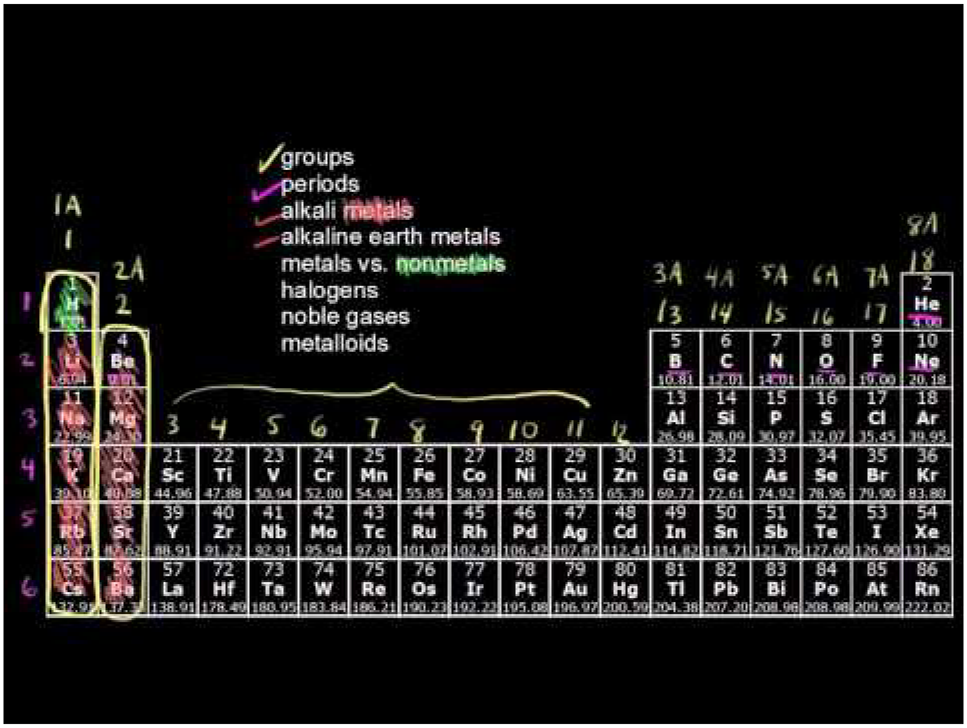
Example 6: Naming Groups of Elements

Atoms of each of the following elements are essential for life. Give the group name for the following elements:

chlorine
calcium
sodium
sulfur

Solution

The family names are as follows:
halogen
alkaline earth metal
alkali metal



In studying the periodic table, you might have noticed something about the atomic masses of some of the elements. Element 43 (technetium), element 61 (promethium), and most of the elements with atomic number 84 (polonium) and higher have their atomic mass given in square brackets. This is done for elements that consist entirely of unstable, radioactive isotopes (you will learn more about radioactivity in the nuclear chemistry chapter). An average atomic weight cannot be determined for these elements because their radioisotopes may vary significantly in relative abundance, depending on the source, or may not even exist in nature. The number in square brackets is the atomic mass number (and approximate atomic mass) of the most stable isotope of that element.

Section 2.5: Chemical Formulas

The structural formula for a compound gives the same information as its molecular formula (the types and numbers of atoms in the molecule) but also shows how the atoms are connected in the molecule. The structural formula for methane contains symbols for one C atom and four H atoms, indicating the number of atoms in the molecule (Figure 13). The lines represent bonds that hold the atoms together. (A chemical bond is an attraction between atoms or ions that holds them together in a molecule or a crystal.) We will discuss chemical bonds and see how to predict the arrangement of atoms in a molecule later. For now, simply know that the lines are an indication of how the atoms are connected in a molecule. A ball-and-stick model shows the geometric arrangement of the atoms with atomic sizes not to scale, and a space-filling model shows the relative sizes of the atoms.

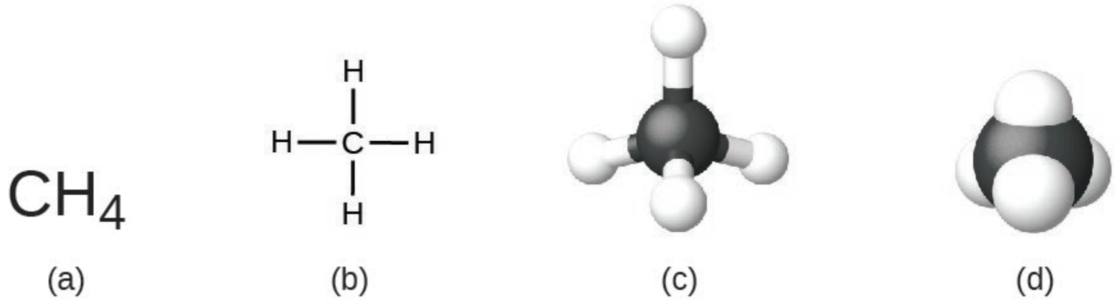


Figure 2. 13. A methane molecule can be represented as (a) a molecular formula, (b) a structural formula, (c) a ball-and-stick model, and (d) a space-filling model. Carbon and hydrogen atoms are represented by black and white spheres, respectively.

Ref: www.openstax.org/

Although many elements consist of discrete, individual atoms, some exist as molecules made up of two or more atoms of the element chemically bonded together. For example, most samples of the elements, hydrogen, oxygen, and nitrogen are composed of molecules that contain two atoms each (called diatomic molecules) and thus have the molecular formulas H_2, O_2, and N_2, respectively. Other elements commonly found as diatomic molecules are fluorine (F_2), chlorine (Cl_2), bromine (Br_2), and iodine (I_2). The most common form of the element sulfur is composed of molecules that consist of eight atoms of sulfur; its molecular formula is S_8 (Figure 14).

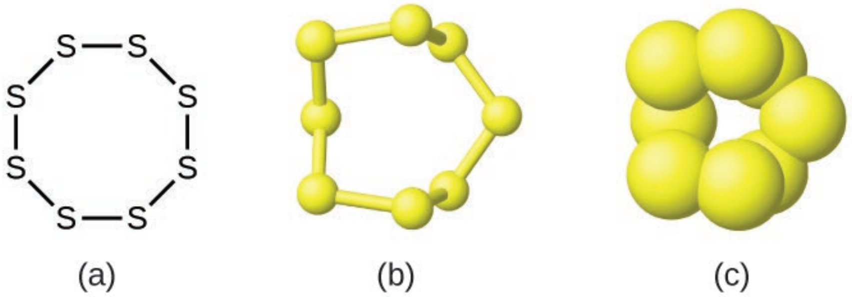


Figure 2.14. A molecule of sulfur is composed of eight sulfur atoms and is therefore written as S_8. It can be represented as (a) a structural formula, (b) a ball-and-stick model, and (c) a space-filling model. Sulfur atoms are represented by yellow spheres.

Ref: www.openstax.org/

It is important to note that a subscript following a symbol and a number in front of a symbol do not represent the same thing; for example, H_2 and 2H represent distinctly different species. H_2 is a molecular formula; it represents a diatomic molecule of hydrogen, consisting of two atoms of the element that are chemically bonded together. The expression 2H, on the other hand, indicates two separate hydrogen atoms that are not combined as a unit. The expression $2H_2$ represents two molecules of diatomic hydrogen (Figure 15).

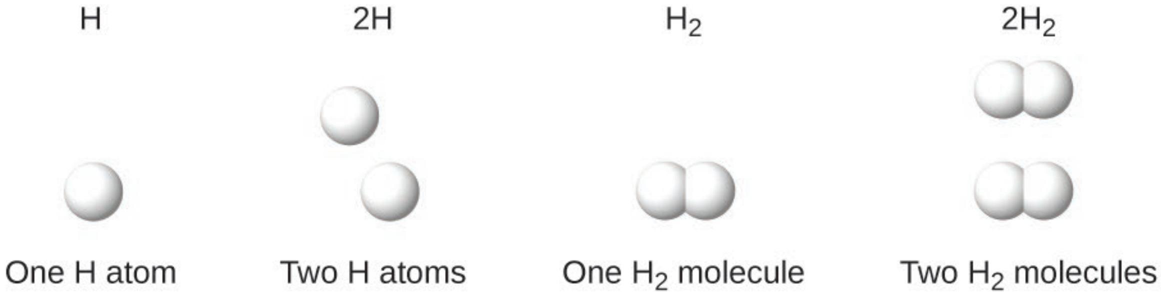


Figure 2.15. The symbols H, 2H, H_2, and $2H_2$ represent very different entities.

Ref: www.openstax.org/

Compounds are formed when two or more elements chemically combine, resulting in the formation of bonds. For example, hydrogen and oxygen can react to form water, and sodium and chlorine can react to form table salt. We sometimes describe the composition of these compounds with an empirical formula, which indicates the types of atoms present and the simplest whole-number ratio of the number of atoms (or ions) in the compound. For example, titanium dioxide (used as pigment in white paint and in the thick, white, blocking type of sunscreen) has an empirical formula of TiO_2. This identifies the elements titanium (Ti) and oxygen (O) as the constituents of titanium dioxide, and indicates the presence of twice as many atoms of the element oxygen as atoms of the element titanium (Figure 16).

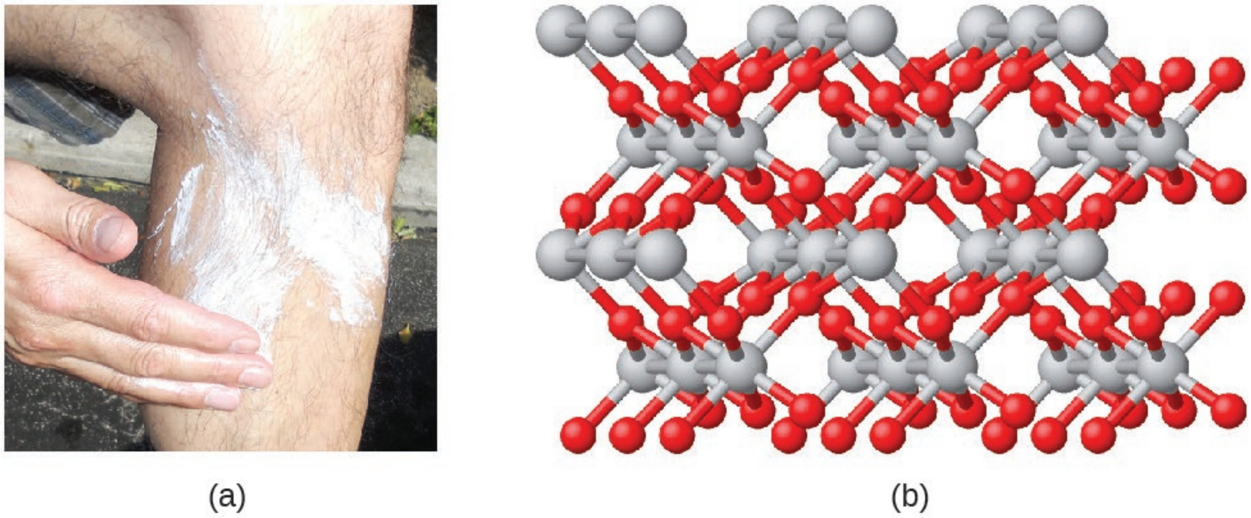


Figure 2.16. (a) The white compound titanium dioxide provides effective protection from the sun. (b) A crystal of titanium dioxide, TiO_2, contains titanium and oxygen in a ratio of 1 to 2. The titanium atoms are gray and the oxygen atoms are red. (credit a: modification of work by "osseous"/Flickr).

www.flickr.com/

As discussed previously, we can describe a compound with a molecular formula, in which the subscripts indicate the actual numbers of atoms of each element in a molecule of the compound. In many cases, the molecular formula of a substance is derived from experimental determination of both its empirical formula and its molecular mass (the sum of atomic masses for all atoms composing the molecule). For example, it can be determined experimentally that benzene contains two elements, carbon (C) and hydrogen (H), and that for every carbon atom in benzene, there is one hydrogen atom. Thus, the empirical formula is CH. An experimental determination of the molecular mass reveals that a molecule of benzene contains six carbon atoms and six hydrogen atoms, so the molecular formula for benzene is C_6H_6 (Figure 17).

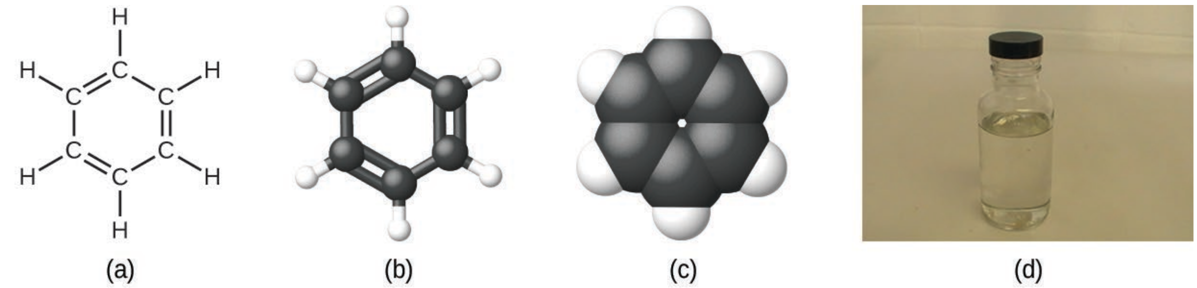


Figure 2.17. Benzene, C_6H_6, is produced during oil refining and has many industrial uses. A benzene molecule can be represented as (a) a structural formula, (b) a ball-and-stick model, and (c) a space-filling model. (d) Benzene is a clear liquid.

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If we know a compound's formula, we can easily determine the empirical formula. (This is somewhat of an academic exercise; the reverse chronology is generally followed in actual practice.) For example, the molecular formula for acetic acid, the component that gives vinegar its sharp taste, is $C_2H_4O_2$. This formula indicates that a molecule of acetic acid (Figure 18) contains two carbon atoms, four hydrogen atoms, and two oxygen atoms. The ratio of atoms is 2:4:2. Dividing by the lowest common denominator (2) gives the simplest, whole-number ratio of atoms, 1:2:1, so the empirical formula is CH_2O. Note that a molecular formula is always a whole-number multiple of an empirical formula.

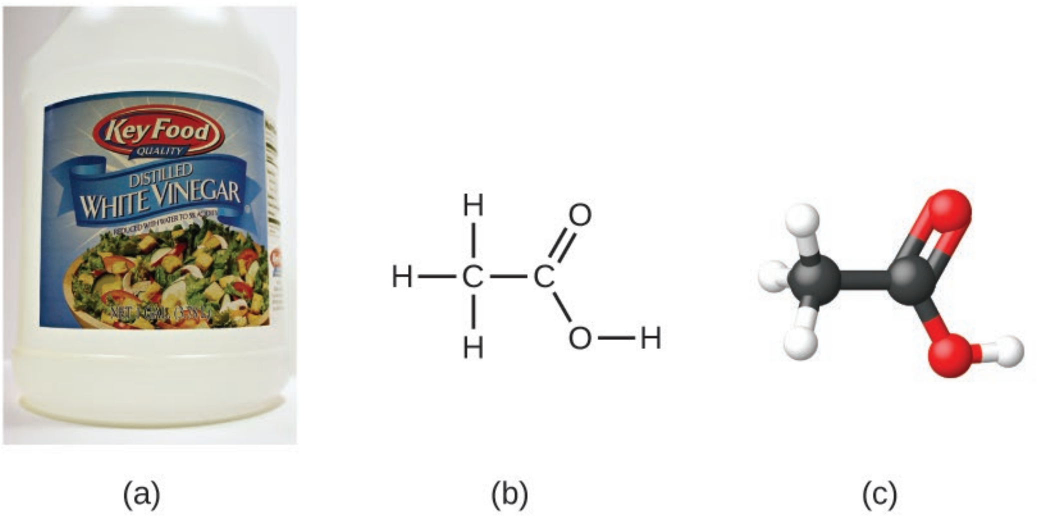

Figure 2.18. (a) Vinegar contains acetic acid, $C_2H_4O_2$, which has an empirical formula of CH_2O. It can be represented as (b) a structural formula and (c) as a ball-and-stick model.

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Example 5: Empirical and Molecular Formulas

Molecules of glucose (blood sugar) contain 6 carbon atoms, 12 hydrogen atoms, and 6 oxygen atoms. What are the molecular and empirical formulas of glucose?

Solution

The molecular formula is C6H12O6 because one molecule actually contains 6 C, 12 H, and 6 O atoms. The simplest whole-number ratio of C to H to O atoms in glucose is 1:2:1, so the empirical formula is CH_2O.

It is important to be aware that it may be possible for the same atoms to be arranged in different ways: Compounds with the same molecular formula may have different atom-to-atom bonding and therefore different structures. For example, could there be another compound with the same formula as acetic acid, $C_2H_4O_2$? And if so, what would be the structure of its molecules?

If you predict that another compound with the formula $C_2H_4O_2$ could exist, then you demonstrated good chemical insight and are correct. Two C atoms, four H atoms, and two O atoms can also be arranged to form methyl formate, which is used in manufacturing, as an insecticide, and for quick-drying finishes. Methyl formate molecules have one of the oxygen atoms between the two carbon atoms, differing from the arrangement in acetic acid molecules. Acetic acid and methyl formate are examples of isomers—compounds with the same chemical formula but different molecular structures (Figure 19). Note that this small difference in the arrangement of the atoms has a major effect on their respective chemical properties. You would certainly not want to use a solution of methyl formate as a substitute for a solution of acetic acid (vinegar) when you make salad dressing.

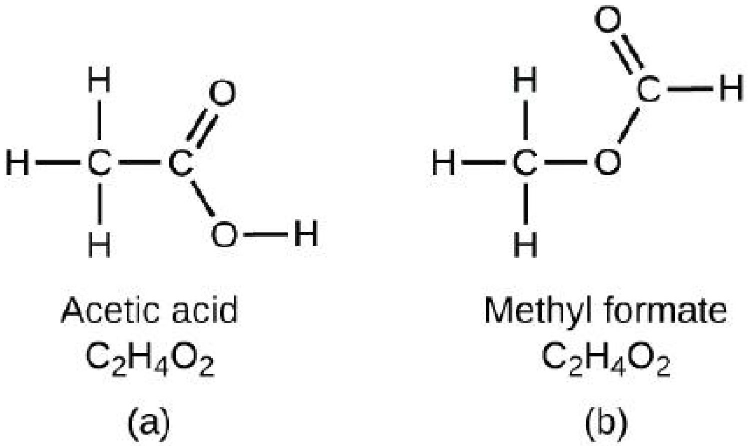

Figure 2.19. Molecules of (a) acetic acid and methyl formate (b) are structural isomers; they have the same formula ($C_2H_4O_2$) but different structures (and therefore different chemical properties).

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Many types of isomers exist (Figure 20). Acetic acid and methyl formate are structural isomers, compounds in which the molecules differ in how the atoms are connected to each other. There are also various types of spatial isomers, in which the relative orientations of the atoms in space can be different. For example, the compound carvone (found in caraway seeds, spearmint, and mandarin orange peels) consists of two isomers that are mirror images of each other. *S*-(+)-carvone smells like caraway, and *R*-(−)-carvone smells like spearmint.

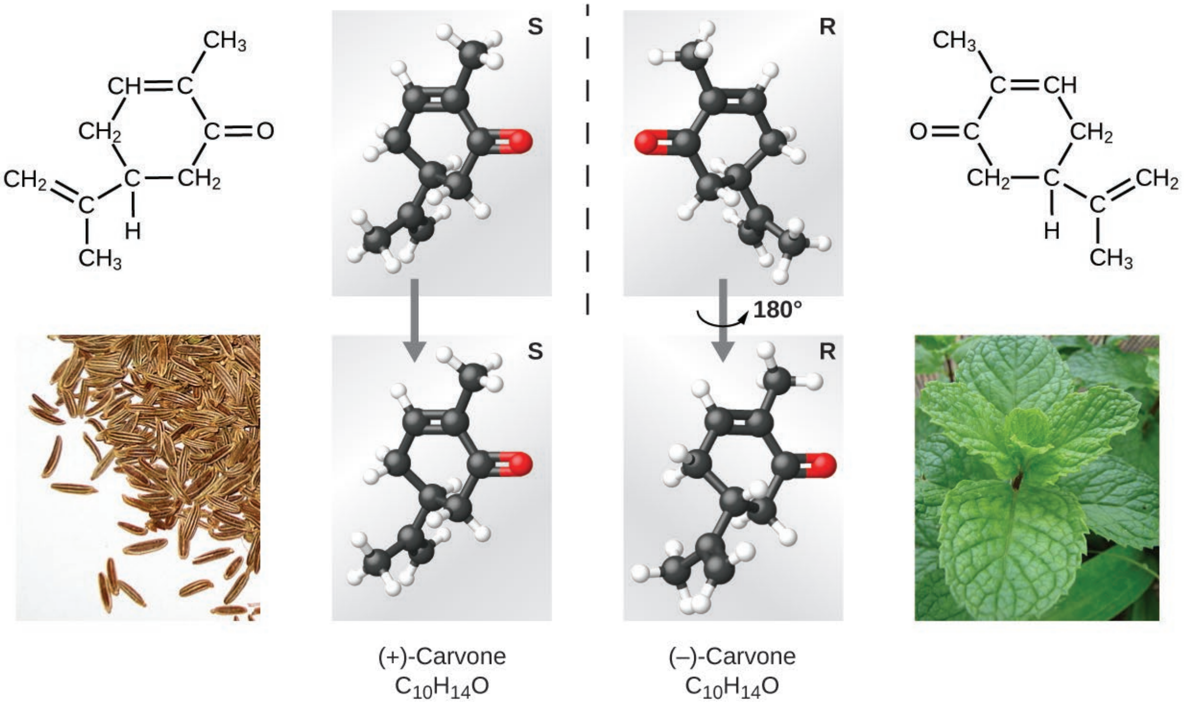

Figure 2.20: Molecules of carvone are spatial isomers; they only differ in the relative orientations of the atoms in space.

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Section 2.6: Molecular and Ionic Compounds

The atoms in all substances that contain more than one atom are held together by electrostatic interactions—interactions between electrically charged particles such as protons and electrons. Electrostatic attraction between oppositely charged species (positive and negative) results in a force that causes them to move toward each other, like the attraction between opposite poles of two magnets. In contrast, electrostatic repulsion between two species with the same charge (either both positive or both negative) results in a force that causes them to repel each other, as do the same poles of two magnets. Atoms form chemical compounds when the attractive electrostatic interactions between them are stronger than the repulsive interactions. Collectively, we refer to the attractive interactions between atoms as chemical bonds.

Chemical bonds are generally divided into two fundamentally different kinds: ionic and covalent. In reality, however, the bonds in most substances are neither purely ionic nor purely covalent, but they are closer to one of these extremes. Although purely ionic and purely covalent bonds represent extreme cases that are seldom encountered in anything but very simple substances, a brief discussion of these two extremes helps us understand why substances that have different kinds of chemical bonds have very different properties. Ionic compounds consist of positively and negatively charged ions held together by strong electrostatic forces, whereas covalent compounds generally consist of molecules, which are groups of atoms in which one or more pairs of electrons are shared between bonded atoms. In a covalent bond, the atoms are held together by the electrostatic attraction between the positively charged nuclei of the bonded atoms and the negatively charged electrons they share. We begin our discussion of structures and formulas by describing covalent compounds.

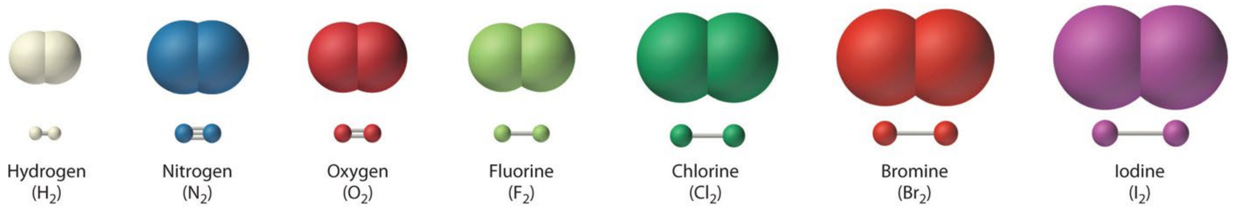
Note the Pattern

Ionic compounds consist of ions of opposite charges held together by strong electrostatic forces, whereas pairs of electrons are shared between bonded atoms in covalent compounds.

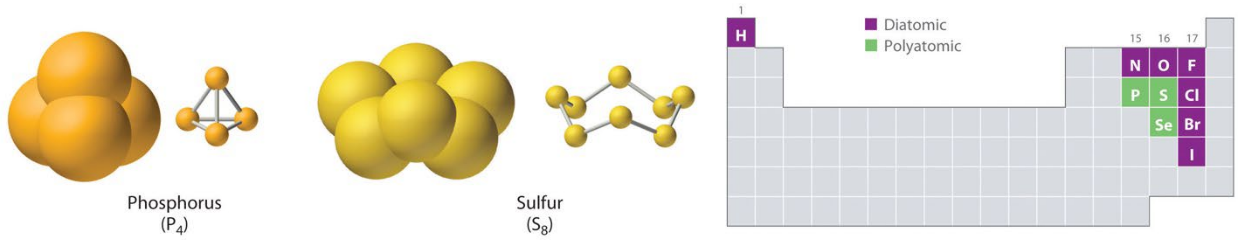
Covalent Molecules and Compounds

Just as an atom is the simplest unit that has the fundamental chemical properties of an element, a molecule is the simplest unit that has the fundamental chemical properties of a covalent compound. Some pure elements exist as covalent molecules. Hydrogen, nitrogen, oxygen, and the halogens occur naturally as the *diatomic* ("two atoms") molecules H_2, N_2, O_2, F_2, Cl_2, Br_2, and I_2 (Figure 24). Similarly, a few pure elements are polyatomic ("many atoms") molecules, such as elemental phosphorus and sulfur, which occur as P_4 and S_8 (Figure 24).

Each covalent compound is represented by a molecular formula, which gives the atomic symbol for each component element, in a prescribed order, accompanied by a subscript indicating the number of atoms of that element in the molecule. The subscript is written only if the number of atoms is greater than 1. For example, water, with two hydrogen atoms and one oxygen atom per molecule, is written as H_2O. Similarly, carbon dioxide, which contains one carbon atom and two oxygen atoms in each molecule, is written as CO_2.



(a) Elements that exist as diatomic molecules



(b) Elements that exist as polyatomic molecules

Figure 2.24. (a) Several elements naturally exist as diatomic molecules, in which two atoms (E) are joined by one or more covalent bonds to form a molecule with the general formula E_2. (b) A few elements naturally exist as polyatomic molecules, which contain more than two atoms. For example, phosphorus exists as P_4 tetrahedra—regular polyhedra with four triangular sides—with a phosphorus atom at each vertex. Elemental sulfur consists of a puckered ring of eight sulfur atoms connected by single bonds. Selenium is not shown due to the complexity of its structure.

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Covalent compounds that contain predominantly carbon and hydrogen are called organic compounds. The convention for representing the formulas of organic compounds is to write carbon first, followed by hydrogen and then any other elements in alphabetical order (e.g., CH_4O is methyl alcohol, a fuel). Compounds that consist primarily of elements other than carbon and hydrogen are called inorganic compounds; they include both covalent and ionic compounds. In inorganic compounds, the component elements are listed beginning with the one farthest to the left in the periodic table, such as we see in CO_2 or SF_6. Those in the same group are listed beginning with the lower element and working up, as in ClF. By convention, however, when an inorganic compound contains both hydrogen and an element from groups 13–15, the hydrogen is usually listed last in the formula. Examples are ammonia (NH_3) and silane (SiH_4). Compounds such as water, whose compositions were established long before this convention was adopted, are always written with hydrogen first: Water is always written as H_2O, not OH_2. The conventions for inorganic acids, such as hydrochloric acid (HCl) and sulfuric acid (H_2SO_4), are described later in the chapter.

Note the Pattern

For organic compounds: write C first, then H, and then the other elements in alphabetical order. For molecular inorganic compounds: start with the element at far left in the periodic table; list elements in same group beginning with the lower element and working up.

Example 7: Nomenclature

Write the molecular formula of each compound.

The phosphorus-sulfur compound that is responsible for the ignition of so-called strike anywhere matches has 4 phosphorus atoms and 3 sulfur atoms per molecule.

Ethyl alcohol, the alcohol of alcoholic beverages, has 1 oxygen atom, 2 carbon atoms, and 6 hydrogen atoms per molecule.

Freon-11, once widely used in automobile air conditioners and implicated in damage to the ozone layer, has 1 carbon atom, 3 chlorine atoms, and 1 fluorine atom per molecule.

Solution

Given: identity of elements present and number of atoms of each
Asked for: molecular formula

Strategy:

A. Identify the symbol for each element in the molecule. Then identify the substance as either an organic compound or an inorganic compound.
B. If the substance is an organic compound, arrange the elements in order beginning with carbon and hydrogen and then list the other elements alphabetically. If it is an inorganic compound, list the elements beginning with the one farthest left in the periodic table. List elements in the same group starting with the lower element and working up.
C. From the information given, add a subscript for each kind of atom to write the molecular formula.

Solution:

A. The molecule has 4 phosphorus atoms and 3 sulfur atoms. Because the compound does not contain mostly carbon and hydrogen, it is inorganic. B Phosphorus is in group 15, and sulfur is in group 16. Because phosphorus is to the left of sulfur, it is written first. C Writing the number of each kind of atom as a right-hand subscript gives P_4S_3 as the molecular formula.
B. Ethyl alcohol contains predominantly carbon and hydrogen, so it is an organic compound. B The formula for an organic compound is written with the number of carbon atoms first, the number of hydrogen atoms next, and the other atoms in alphabetical order: CHO. C Adding subscripts gives the molecular formula C_2H_6O.
C. Freon-11 contains carbon, chlorine, and fluorine. It can be viewed as either an inorganic compound or an organic compound (in which fluorine has replaced hydrogen). The formula for Freon-11 can therefore be written using either of the two conventions. According to the convention for inorganic compounds, carbon is written first because it is farther left in the periodic table. Fluorine and chlorine are in the same group, so they are listed beginning with the lower element and working up: CClF. Adding subscripts gives the molecular formula CCl_3F.
   We obtain the same formula for Freon-11 using the convention for organic compounds. The number of carbon atoms is written first, followed by the number of hydrogen atoms (zero) and then the other elements in alphabetical order, also giving CCl_3F.

Representations of Molecular Structures

Molecular formulas give only the elemental composition of molecules. In contrast, structural formulas show which atoms are bonded to one another and, in some cases, the approximate arrangement of the atoms in space. Knowing the structural formula of a compound enables chemists to create a three-dimensional model, which provides information about how that compound will behave physically and chemically.

The structural formula for H_2 can be drawn as H–H and that for I_2 as I–I, where the line indicates a single pair of shared electrons, a single bond. Two pairs of electrons are shared in a double bond, which is indicated by two lines— for example, O_2 is O=O. Three electron pairs are shared in a triple bond, which is indicated by three lines—for example, N_2 is N≡N (Figure 25). Carbon is unique in the extent to which it forms single, double, and triple bonds to itself and other elements. The number of bonds formed by an atom in its covalent compounds is *not* arbitrary.

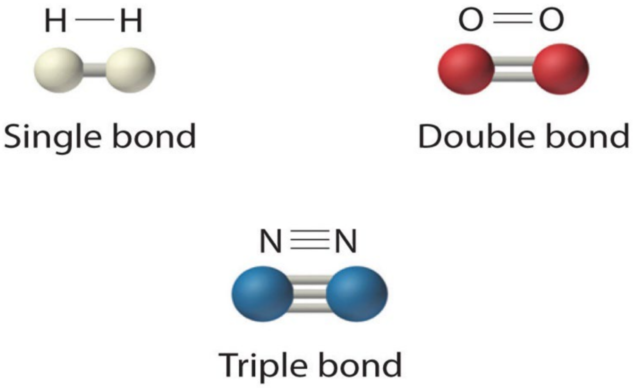
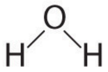
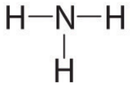


Figure 2.25. Hydrogen (H_2) has a single bond between atoms. Oxygen (O_2) has a double bond between atoms, indicated by two lines (=). Nitrogen (N_2) has a triple bond between atoms, indicated by three lines (≡). Each bond represents an electron pair.

The structural formula for water can be drawn as follows:



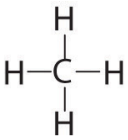
Because the latter approximates the experimentally determined shape of the water molecule, it is more informative. Similarly, ammonia (NH_3) and methane (CH_4) are often written as planar molecules:



$$\begin{array}{c}\text{H}-\text{N}-\text{H}\\ | \\ \text{H}\end{array}$$

Ammonia

and



$$\begin{array}{c}\text{H}\\ | \\ \text{H}-\text{C}-\text{H}\\ | \\ \text{H}\end{array}$$

Methane

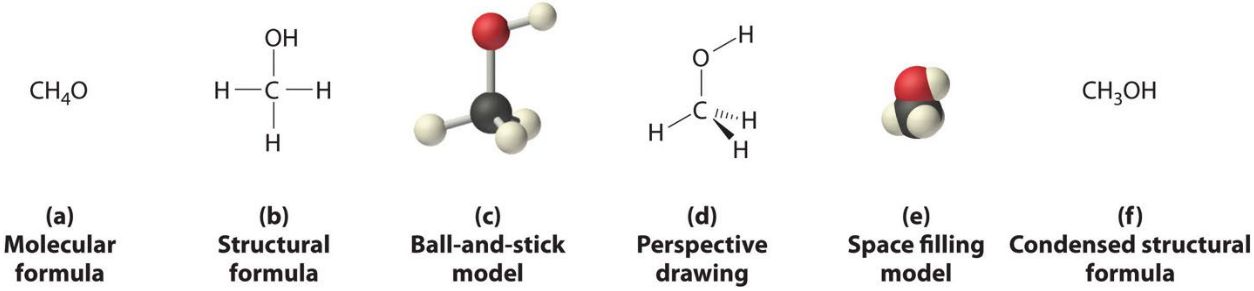


Figure 2.26. Different ways of representing the structure of a molecule (a) The molecular formula for methanol gives only the number of each kind of atom present. (b) The structural formula shows which atoms are connected. (c) The ball-and-stick model shows the atoms as spheres and the bonds as sticks. (d) A perspective drawing (also called a wedge-and-dash representation) attempts to show the three-dimensional structure of the molecule. (e) The space-filling model shows the atoms in the molecule but not the bonds. (f) The condensed structural formula is by far the easiest and most common way to represent a molecule.

Ref: www.openstax.org/

Although a structural formula, a ball-and-stick model, a perspective drawing, and a space-filling model provide a significant amount of information about the structure of a molecule, each requires time and effort. Consequently, chemists often use a *condensed structural formula* (part (f) in figure 26, which omits the lines representing bonds between atoms and simply lists the atoms bonded to a given atom next to it. Multiple groups attached to the same atom are shown in parentheses, followed by a subscript that indicates the number of such groups. For example, the condensed structural formula for methanol is CH_3OH, which tells us that the molecule contains a CH_3 unit that looks like a fragment of methane (CH_4). Methanol can therefore be viewed either as a methane molecule in which one hydrogen atom has been replaced by an –OH group or as a water molecule in which one hydrogen atom has been replaced by a $–CH_3$ fragment. Because of their ease of use and information content, we use condensed structural formulas for molecules throughout this text. Ball-and-stick models are used when needed to illustrate the three-dimensional structure of molecules, and space-filling models are used only when it is necessary to visualize the relative sizes of atoms or molecules to understand an important point.

Example 8

Write the molecular formula for each compound. The condensed structural formula is given.

Sulfur monochloride (also called disulfur dichloride) is a vile-smelling, corrosive yellow liquid used in the production of synthetic rubber. Its condensed structural formula is ClSSCl.

Ethylene glycol is the major ingredient in antifreeze. Its condensed structural formula is $HOCH_2CH_2OH$.

Trimethylamine is one of the substances responsible for the smell of spoiled fish. Its condensed structural formula is $(CH_3)_3N$.

Solution

Given: condensed structural formula
Asked for: molecular formula

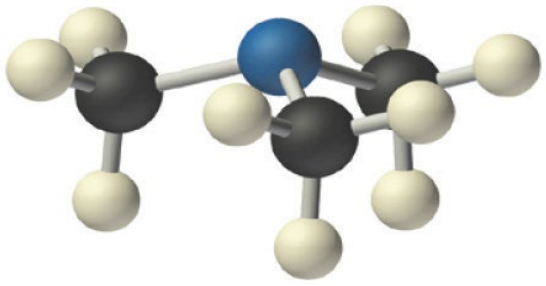
Strategy:

A. Identify every element in the condensed structural formula and then determine whether the compound is organic or inorganic.
B. As appropriate, use either organic or inorganic convention to list the elements. Then add appropriate subscripts to indicate the number of atoms of each element present in the molecular formula.

Solution:

The molecular formula lists the elements in the molecule and the number of atoms of each.

B. Sulfur lies to the left of chlorine in the periodic table, so it is written first in the formula. Adding subscripts gives the molecular formula S_2Cl_2.
C. Counting the atoms in ethylene glycol, we get six hydrogen atoms, two carbon atoms, and two oxygen atoms per molecule. The compound consists mostly of carbon and hydrogen atoms, so it is organic. As with all organic compounds, C and H are written first in the molecular formula. Adding appropriate subscripts gives the molecular formula $C_2H_6O_2$.
D. The condensed structural formula shows that trimethylamine contains three CH_3 units, so we have one nitrogen atom, three carbon atoms, and nine hydrogen atoms per molecule. Because trimethylamine contains mostly carbon and hydrogen, it is an organic compound. According to the convention for organic compounds, C and H are written first, giving the molecular formula C_3H_9N.



Trimethylamine

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Ionic Compounds

The substances described in the preceding discussion are composed of molecules that are electrically neutral; that is, the number of positively charged protons in the nucleus is equal to the number of negatively charged electrons. In contrast, **ions** are atoms or assemblies of atoms that have a net electrical charge. Ions that contain fewer electrons than protons have a net positive charge and are called **cations**. Conversely, ions that contain more electrons than protons have a net negative charge and are called **anions**. Ionic compounds contain both cations and anions in a ratio that results in no net electrical charge.

Note the Pattern

Ionic compounds contain both cations and anions in a ratio that results in zero electrical charge.

In covalent compounds, electrons are shared between bonded atoms and are simultaneously attracted to more than one nucleus. In contrast, ionic compounds contain cations and anions rather than discrete neutral molecules. Ionic compounds are held together by the attractive electrostatic interactions between cations and anions. In an ionic compound, the cations and anions are arranged in space to form an extended three-dimensional array that maximizes the number of attractive electrostatic interactions and minimizes the number of repulsive electrostatic interactions. As equation 1 shows, the electrostatic energy of the interaction between two charged particles is proportional to the product of the charges on the particles and inversely proportional to the distance between them:

Equation 1

$$\text{electrostatic energy} \propto Q1Q2r$$

where Q_1 and Q_2 are the electrical charges on particles 1 and 2, and r is the distance between them. When Q_1 and Q_2 are both positive, corresponding to the charges on cations, the cations repel each other and the electrostatic energy is positive. When Q_1 and Q_2 are both negative, corresponding to the charges on anions, the anions repel each other and the electrostatic energy is again positive. The electrostatic energy is negative only when the charges have opposite signs; that is, positively charged species are attracted to negatively charged species and vice versa. As shown in figure 28. The strength of the interaction is proportional to the *magnitude* of the charges and decreases as the *distance* between the particles increases.

Note the Pattern

If the electrostatic energy is positive, the particles repel each other; if the electrostatic energy is negative, the particles are attracted to each other.

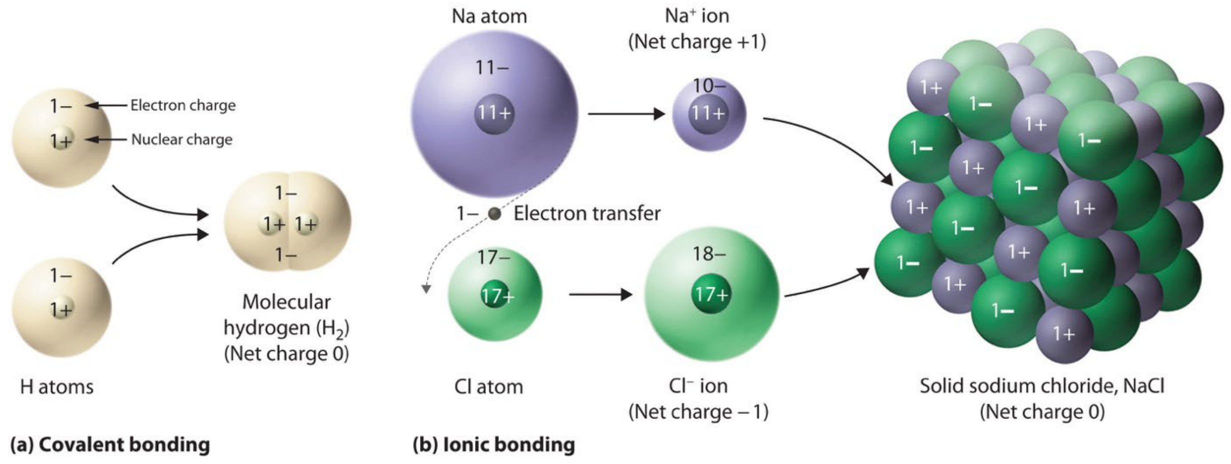

Figure 2.27. Comparison of covalent and ionic bonding. (a) In molecular hydrogen (H_2), two hydrogen atoms share two electrons to form a covalent bond. (b) The ionic compound NaCl forms when electrons from sodium atoms are transferred to chlorine atoms. The resulting Na^+ and Cl^- ions form a three-dimensional solid that is held together by attractive electrostatic interactions. \

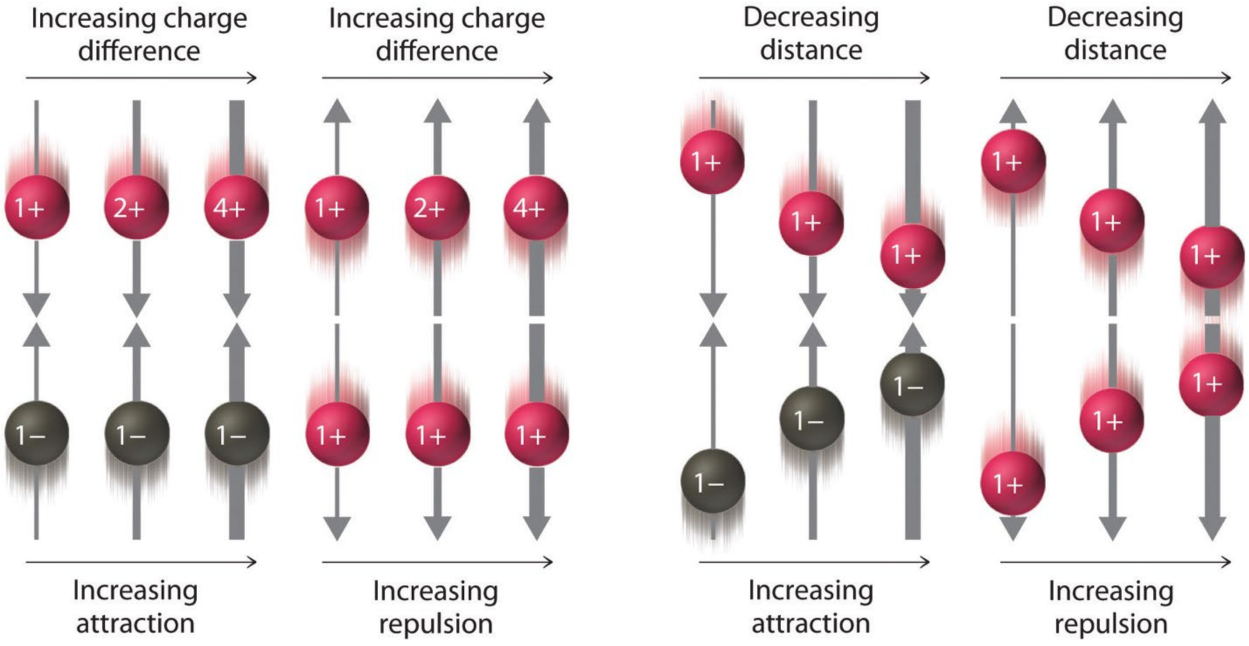

Figure 2.28. As the charge on ions increases or the distance between ions decreases, so does the strength of the attractive (−…+) or repulsive (−…− or +…+) interactions. The strength of these interactions is represented by the thickness of the arrows.

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One example of an ionic compound is sodium chloride (NaCl; Figure 27), formed from sodium and chlorine. In forming chemical compounds, many elements have a tendency to gain or lose enough electrons to attain the same number of electrons as the noble gas closest to them in the periodic table. When sodium and chlorine come into contact, each sodium atom gives up an electron to become a Na^+ ion, with 11 protons in its nucleus but only 10 electrons (like neon), and each chlorine atom gains an electron to become a Cl^- ion, with 17 protons in its nucleus and 18 electrons (like argon), as shown in part (b) in Figure 27. Solid sodium chloride contains equal numbers of cations (Na^+) and anions (Cl^-), thus maintaining electrical neutrality. Each Na^+ ion is surrounded by 6 Cl^- ions, and each Cl^- ion is surrounded by 6 Na^+ ions. Because of the large number of attractive Na^+Cl^- interactions, the total attractive electrostatic energy in NaCl is great.

Consistent with a tendency to have the same number of electrons as the nearest noble gas, when forming ions, elements in groups 1, 2, and 3 tend to *lose* one, two, and three electrons, respectively, to form cations, such as Na^+ and Mg^{2+}. They then have the same number of electrons as the nearest noble gas: neon. Similarly, K^+, Ca^{2+}, and Sc^{3+} have 18 electrons each, like the nearest noble gas: argon. In addition, the elements in group 13 *lose* three electrons to form cations, such as Al^{3+}, again attaining the same number of electrons as the noble gas closest to them in the periodic table. Because the lanthanides and actinides formally belong to group 3, the most common ion formed by these elements is M^{3+}, where M represents the metal. Conversely, elements in groups 17, 16, and 15 often react to *gain* one, two, and three electrons, respectively, to form ions such as Cl^-, S^{2-}, and P^{3-}. Ions such as these, which contain only a single atom, are called monatomic ions. You can predict the charges of most monatomic ions derived from the main group elements by simply looking at the periodic table and counting how many columns an element lies from the extreme left or right. For example, you can predict that barium (in group 2) will form Ba^{2+} to have the same number of electrons as its nearest noble gas, xenon, that oxygen (in group 16) will form O^{2-} to have the same number of electrons as neon, and cesium (in group 1) will form Cs^+ to also have the same number of electrons as xenon. Note that this method does not usually work for most of the transition metals.

Note the Pattern

Elements in groups 1, 2, and 3 tend to form 1+, 2+, and 3+ ions, respectively; elements in groups 15, 16, and 17 tend to form 3−, 2−, and 1− ions, respectively.

Group 1	Group 2	Group 3	Group 13	Group 15	Group 16	Group 17
Li^+ lithium	Be^{2+} beryllium			N^{3-} nitride (azide)	O^{2-} oxide	F^- fluoride
Na^+ sodium	Mg^{2+} magnesium		Al^{3+} aluminum	P^{3-} phosphide	S^{2-} sulfide	Cl^- chloride

Group 1	Group 2	Group 3	Group 13	Group 15	Group 16	Group 17
K^+ potassium	Ca^{2+} calcium	Sc^{3+} scandium	Ga^{3+} gallium	As^{3-} arsenide	Se^{2-} selenide	Br^- bromide
Rb^+ rubidium	Sr^{2+} strontium	Y^{3+} yttrium	In^{3+} indium		Te^{2-} telluride	I^- iodide
Cs^+ cesium	Ba^{2+} barium	La^{3+} lanthanum				

Table 3. Some Common Monatomic Ions and Their Names

Example 9

Predict the charge on the most common monatomic ion formed by each element.

aluminum, used in the quantum logic clock, the world's most precise clock
selenium, used to make ruby-colored glass
yttrium, used to make high-performance spark plugs

Solution
Given: element
Asked for: ionic charge

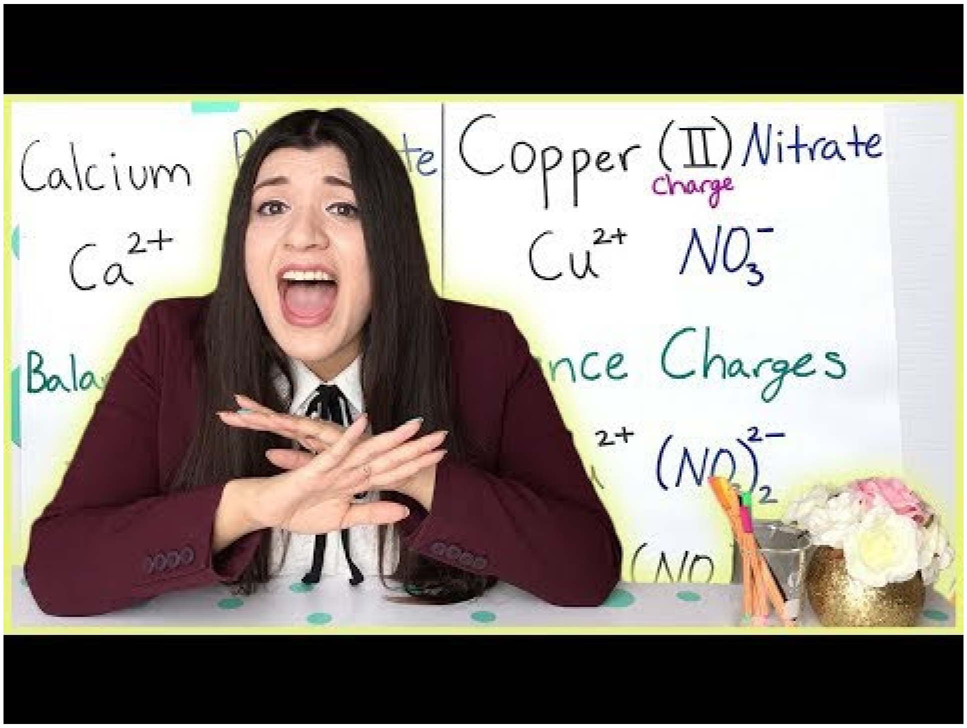
Strategy:

A. Identify the group in the periodic table to which the element belongs. Based on its location in the periodic table, decide whether the element is a metal, which tends to lose electrons; a nonmetal, which tends to gain electrons; or a semimetal, which can do either.
B. After locating the noble gas that is closest to the element, determine the number of electrons the element must gain or lose to have the same number of electrons as the nearest noble gas.

Solution:

A. Aluminum is a metal in group 13; consequently, it will tend to lose electrons. B The nearest noble gas to aluminum is neon. Aluminum will lose three electrons to form the Al3+ ion, which has the same number of electrons as neon.
B. Selenium is a nonmetal in group 16, so it will tend to gain electrons. B The nearest noble gas is krypton, so we predict that selenium will gain two electrons to form the Se2− ion, which has the same number of electrons as krypton.

C. Yttrium is in group 3, and elements in this group are metals that tend to lose electrons. B The nearest noble gas to yttrium is krypton, so yttrium is predicted to lose three electrons to form Y3+, which has the same number of electrons as krypton.



Polyatomic Ions

Polyatomic ions are charged species, consisting of group of atoms. They are composed on more than one element. In polyatomic ion, one central nonmetal attached to either oxygen or hydrogen. Central nonmetals are mainly from period 2 and 3 like N, S, P, Cl. Some metalloids also form polyatomic ions. The names of polyatomic cations end in the suffix -onium. Many polyatomic anions have names that end in the suffix-ate or ite.

Only one positively charged or polyatomic cation is NH_4^+.

Only two polyatomic anions that have end name -ide (OH^-)are hydroxide and cyanide (CN^-)

Most polyatomic ions contain oxygen. That is why sometimes they are called oxo anion. Oxo anions have end name either r -ate or -ite. Lower number of oxygen containing polyatomic ion is named as -ite and higher number of oxygen containing polyatmic ions are named as -ate. Example: NO_2^-: nitrite, NO_3^- : nitrate

When a H^+ is added to a polyatomic ion, the negative charge of the ion is decreased by one unit.

Example: PO_4^{3-} : phosphate ion, HPO_4^{2-}: hydrogen phosphate ion

Cations

+1
Ammonium, NH_4^+

Anions

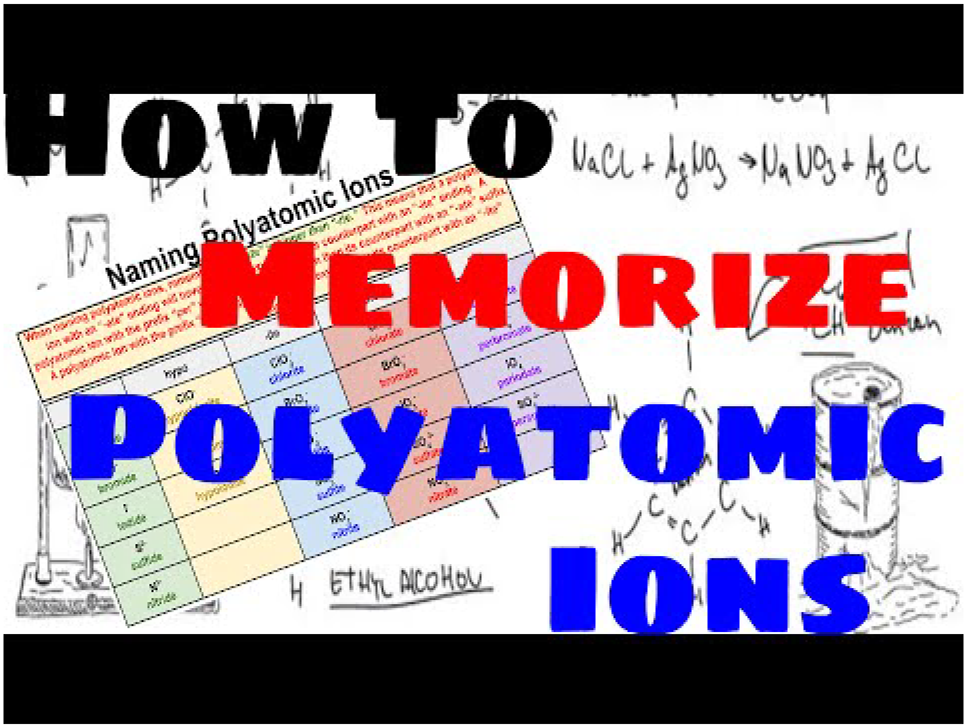
-1	-2	-3
Hypochlorite, ClO^- Chlorite, ClO_2^- Chlorate, ClO_3^- Perchlorate, ClO_4^-	Sulfite, SO_3^{2-} Sulfate, SO_4^{2-}	Phosphate, PO_4^{3-}
Nitrite, NO_2^- Nitrate, NO_3^- Bicarbonate, HCO_3^-	Carbonate, CO_3^{2-}	
Hydroxide, OH^-	Peroxide, O_2^{2-}	
Acetate, $C_2H_3O_2^-$	Oxalate, $C_2O_4^{2-}$ Silicate, SiO_3^{2-} Thiosulfate, $S_2O_3^{2-}$	
Permanganate, MnO_4^-	Chromate, CrO_4^{2-} Dichromate, $Cr_2O_7^{2-}$	
Cyanide, CN^- Thiocyanate, SCN^-		

More important polyatomic ions are marked with asterisk below.

<u>Common Polyatomic Ions</u>

Formula	**Name**
*NH_4^+	Ammonium
*NO_2^-	Nitrite
*NO_3–	Nitrate
*SO_3^{2-}	Sulfite
*SO_4^{2-}	Sulfate
*HSO_4^-	Hydrogen sulfate (bisulfate)
*OH^-	Hydroxide
*CN^-	Cyanide
*PO_4^{3-}	Phosphate
*CO_3^{2-}	Carbonate
*HCO_3^-	Hydrogen carbonate (bicarbonate)
*ClO_3^-	Chlorate
*$C2H_3O_2^-$	Acetate
(or CH3COO–)	

The following video might help to memorize the polyatomic molecules.



The following video explains in detail how to write ionic compounds with polyatomic ions.

When cations combine with polyatomic ions ionic compounds are formed. When the charges are switched to form neutral compound, parenthesis is used to use for polyatomic ions.

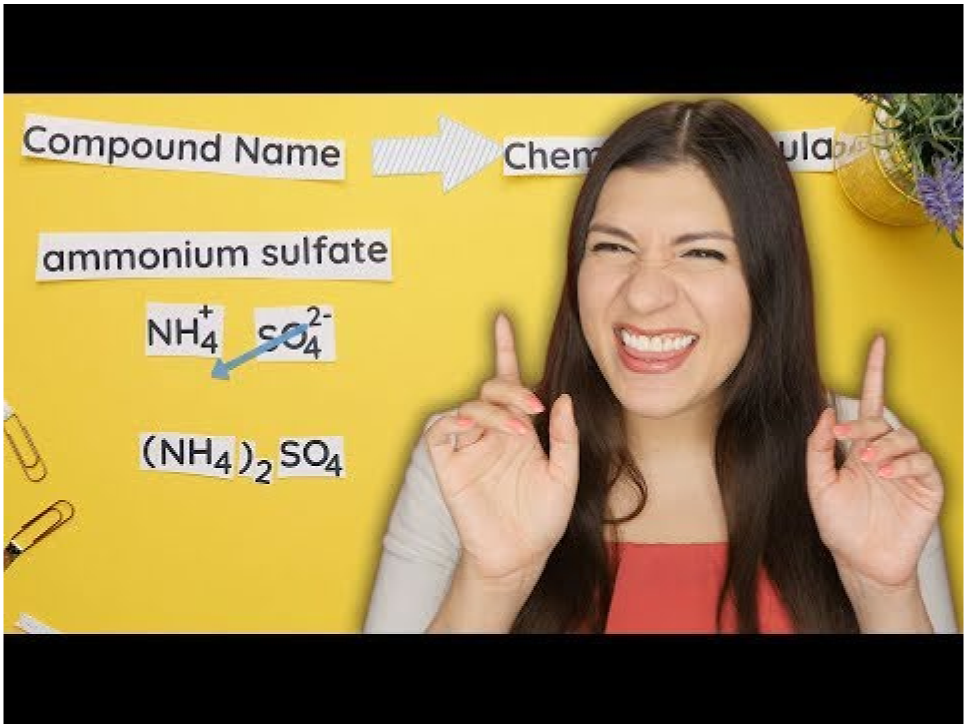
For example: $Na^{+} + SO_4^{2-} \rightarrow Na_2SO4$

But when Ca^{2+} is combined with PO_4^{3-}, the formula of the compound is::

$Ca^{2+} + PO_4^{3-} \rightarrow Ca_3(PO_4)_2$

Here is another video to practice writing ionic compounds with polyatomic ions.

https://www.youtube.com/watch?v=PPfLDdIfOVA



Questions

Name the formula of the ionic compound formed from $Fe^{3+}$and each anion. Then name each compound.

1. OH^-
2. CO_3^{2-}
3. HPO_4^{2-}
4. NO_2^-
5. PO_4^{3-}
6. $C_2H_3O_2^-$

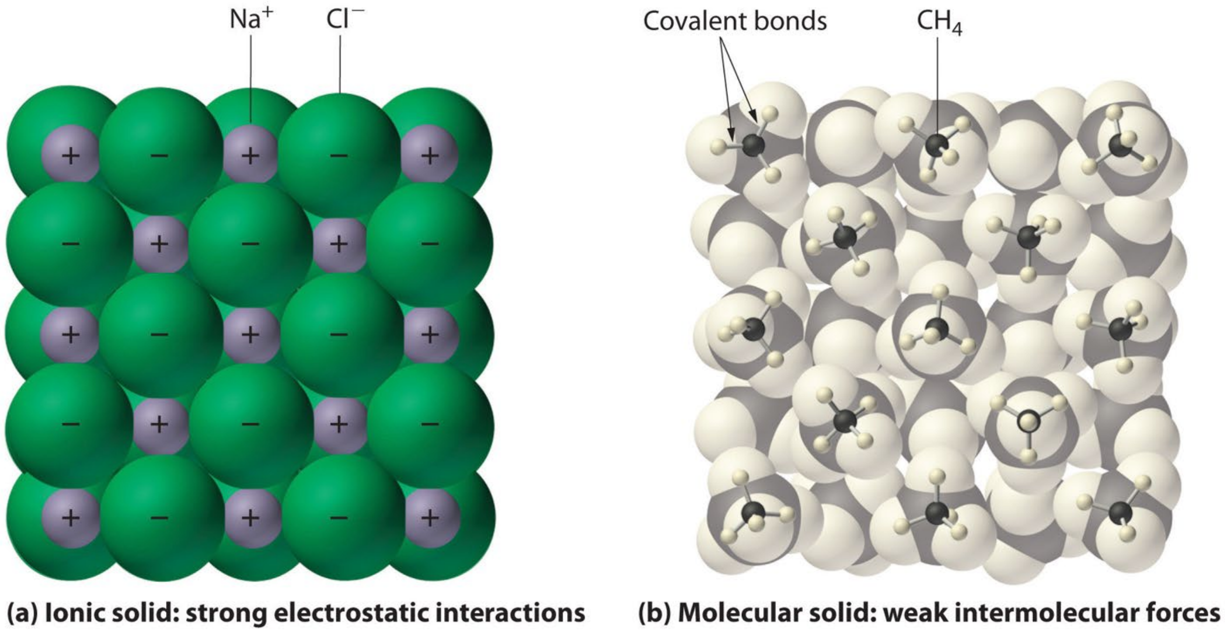
Ans: a) $Fe(OH)_3$, Iron(III) Hydroxide
b) $Fe_2(CO_3)_3$: Iron(III) Carbonate
c) $Fe(NO_2)_3$: Iron(III) Nitrite
d) FePO4, Iron(III) Phosphate
e) $Fe(C_2H_3O_2)_3$, iron(III) Acetate

Physical Properties of Ionic and Covalent Compounds

In general, ionic and covalent compounds have different physical properties. Ionic compounds usually form hard crystalline solids that melt at rather high temperatures and are *very* resistant to evaporation. These properties stem from the characteristic internal structure of an ionic solid, illustrated schematically in part (a) in Figure 29, which shows the three-dimensional array of alternating positive and negative ions held together by **strong electrostatic attractions**. In contrast, as shown in part (b) in Figure 29, most covalent compounds consist of discrete molecules held together by comparatively **weak intermolecular** forces (the forces between molecules), even though the atoms within each molecule are held together by **strong intramolecular** covalent bonds (the forces within the molecule). Covalent substances can be gases, liquids, or solids at room temperature and pressure, depending on the strength of the intermolecular interactions. Covalent molecular solids tend to form soft crystals that melt at rather low temperatures and evaporate relatively easily. Some covalent substances, however, are not molecular but consist of infinite three-dimensional arrays of covalently bonded atoms and include some of the hardest materials known, such as diamond. The covalent bonds that hold the atoms together in the molecules are unaffected when covalent substances melt or evaporate, so a liquid or vapor of discrete, independent molecules is formed. For example, at room temperature, methane, the major constituent of natural gas, is a gas that is composed of discrete CH_4 molecules. A comparison of the different physical properties of ionic compounds and covalent molecular substances is given in Table 4.

Ionic Compounds	Covalent Molecular Substances
hard solids	gases, liquids, or soft solids
high melting points	low melting points
nonvolatile	volatile

Table 4. The physical properties of typical ionic compounds and covalent molecular substances.



(a) Ionic solid: strong electrostatic interactions (b) Molecular solid: weak intermolecular forces

Figure 2.29. Interactions in ionic and covalent solids. (a) The positively and negatively charged ions in an ionic solid such as sodium chloride (NaCl) are held together by strong electrostatic interactions. (b) In this representation of the packing of methane (CH_4) molecules in solid methane, a prototypical molecular solid, the methane molecules are held together in the solid only by relatively weak intermolecular forces, even though the atoms within each methane molecule are held together by strong covalent bonds.

Ref: www.openstax.org/

Section 2.7: Chemical Nomenclature

As with ionic compounds, the system that chemists have devised for naming covalent compounds enables us to write the molecular formula from the name and vice versa. In this and the following section, we describe the rules for naming simple covalent compounds. We begin with inorganic compounds and then turn to simple organic compounds that contain only carbon and hydrogen.

Binary Inorganic Compounds

Binary covalent compounds—that is, covalent compounds that contain only two elements—are named using a procedure similar to that used to name simple ionic compounds, but prefixes are added as needed to indicate the number of atoms of each kind. The procedure, diagrammed in Figure 30, uses the following steps:

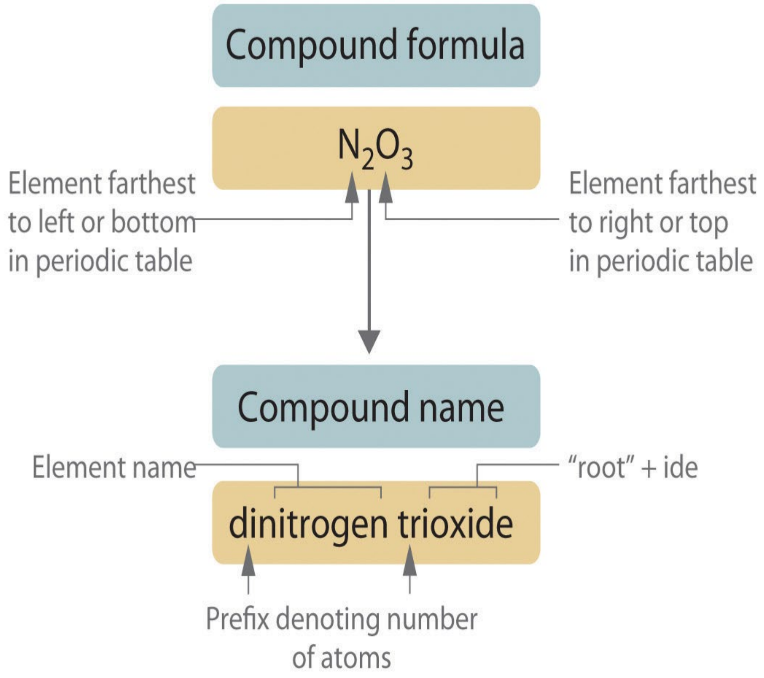


Figure 2.30. Naming a Covalent Inorganic Compound

1. Place the elements in their proper order.
    1. The element farthest to the left in the periodic table is usually named first. If both elements are in the same group, the element closer to the bottom of the column is named first.
    2. The second element is named as if it were a monatomic anion in an ionic compound (even though it is not), with the suffix *-ide* attached to the root of the element name.
2. Identify the number of each type of atom present. Prefixes derived from Greek stems are used to indicate the number of each type of atom in the formula unit (Table 5). The prefix *mono-* ("one") is used only when absolutely necessary to avoid confusion, just as we omit the subscript 1 when writing molecular formulas. To demonstrate steps 1 and 2a, we name HCl as hydrogen chloride (because hydrogen is to the left of chlorine in the periodic table) and PCl_5 as phosphorus pentachloride.
   The order of the elements in the name of BrF_3, bromine trifluoride, is determined by the fact that bromine lies below fluorine in group 17.

Prefix	Number
mono-	1
di-	2

Prefix	Number
tri-	3
tetra-	4
penta-	5
hexa-	6
hepta-	7
octa-	8
nona-	9
deca-	10
undeca-	11
dodeca-	12

Table 5. Prefixes for Indicating the Number of Atoms in Chemical Names

1. If a molecule contains more than one atom of both elements, then prefixes are used for both. Thus N_2O_3 is *di*nitrogen *tri*oxide, as shown in.
2. In some names, the final *a* or *o* of the prefix is dropped to avoid awkward pronunciation. Thus, OsO_4 is osmium tetroxide rather than osmium tetraoxide.

3. Write the name of the compound.

Binary compounds of the elements with oxygen are generally named as "element oxide," with prefixes that indicate the number of atoms of each element per formula unit. For example, CO is carbon monoxide. The only exception is binary compounds of oxygen with fluorine, which are named as oxygen fluorides.

1. Certain compounds are *always* called by the common names that were assigned long ago when names rather than formulas were used. For example, H_2O is water (not dihydrogen oxide); NH_3 is ammonia; PH_3 is phosphine; SiH_4 is silane; and B_2H_6, a *dimer* of BH_3, is diborane. For many compounds, the systematic name and the common name are both used frequently, so you must be familiar with them. For example, the systematic name for NO is nitrogen monoxide, but it is much more commonly called nitric oxide. Similarly, N_2O is usually called nitrous oxide rather than dinitrogen monoxide. Notice that the suffixes -*ic* and -*ous* are the same ones used for ionic compounds.

Note the Pattern

Start with the element at the far left in the periodic table and work to the right. If two or more elements are in the same group, start with the bottom element and work up.

Example 10

Write the name of each binary covalent compound.

SF_6
N_2O_4
ClO_2

Solution

Given: molecular formula
Asked for: name of compound

Strategy:

A. List the elements in order according to their positions in the periodic table. Identify the number of each type of atom in the chemical formula and then use Table 2.6 "Prefixes for Indicating the Number of Atoms in Chemical Names" to determine the prefixes needed.
B. If the compound contains oxygen, follow step 3a. If not, decide whether to use the common name or the systematic name.

Solution:

A. Because sulfur is to the left of fluorine in the periodic table, sulfur is named first. Because there is only one sulfur atom in the formula, no prefix is needed. B There are, however, six fluorine atoms, so we use the prefix for six: hexa- (Table 2.6 "Prefixes for Indicating the Number of Atoms in Chemical Names"). The compound is sulfur hexafluoride.
B. Because nitrogen is to the left of oxygen in the periodic table, nitrogen is named first. Because more than one atom of each element is present, prefixes are needed to indicate the number of atoms of each. According to Table 2.6 "Prefixes for Indicating the Number of Atoms in Chemical Names", the prefix for two is di-, and the prefix for four is tetra-. B The compound is dinitrogen tetroxide (omitting the a in tetra- according to step 2c) and is used as a component of some rocket fuels.
C. Although oxygen lies to the left of chlorine in the periodic table, it is not named first because ClO2is an oxide of an element other than fluorine (step 3a). Consequently, chlorine is named first, but a prefix is not necessary because each molecule has only one atom of chlorine. B Because there are two oxygen atoms, the compound is a dioxide. Thus the compound is chlorine dioxide. It is widely used as a substitute for chlorine in municipal water treatment plants because, unlike chlorine, it does not react with organic compounds in water to produce potentially toxic chlorinated compounds.

Example 11

Write the formula for each binary covalent compound.

sulfur trioxide
diiodine pentoxide

Given: name of compound
Asked for: formula

Solution

Strategy:

List the elements in the same order as in the formula to identify the number of each type of atom present, and then indicate this quantity as a subscript to the right of that element when writing the formula.

Solution:

Sulfur has no prefix, which means that each molecule has only one sulfur atom. The prefix tri- indicates that there are three oxygen atoms. The formula is therefore SO3. Sulfur trioxide is produced industrially in huge amounts as an intermediate in the synthesis of sulfuric acid.
The prefix di- tells you that each molecule has two iodine atoms, and the prefix penta- indicates that there are five oxygen atoms. The formula is thus I2O5, a compound used to remove carbon monoxide from air in respirators.

The empirical and molecular formulas discussed in the preceding section are precise and highly informative, but they have some disadvantages. First, they are inconvenient for routine verbal communication. For example, saying “C-A-three-P-O-four-two” for $Ca_3(PO_4)_2$ is much more difficult than saying “calcium phosphate.” In addition, you will see that many compounds have the same empirical and molecular formulas, but different arrangements of atoms, which result in very different chemical and physical properties. In such cases, it is necessary for the compounds to have different names that distinguish among the possible arrangements.

Many compounds, particularly those that have been known for a relatively long time, have more than one name: **a common name** (sometimes more than one) and a **systematic name**, which is the name assigned by adhering to specific rules. Like the names of most elements, the common names of chemical compounds generally have historical origins, although they often appear to be unrelated to the compounds of interest. For example, the systematic name for KNO_3 is potassium nitrate, but its common name is saltpeter.

In this text, we use a systematic nomenclature to assign meaningful names to the millions of known substances. Unfortunately, some chemicals that are widely used in commerce and industry are still known almost exclusively by their common names; in such cases, you must be familiar with the common name as well as the systematic one. The objective of this and the next two sections is to teach you to write the formula for a simple inorganic compound from its name—and vice versa—and introduce you to some of the more frequently encountered common names.

We begin with *binary ionic compounds*, which contain only two elements. The procedure for naming such compounds is outlined in Figure 2.10 "Naming an Ionic Compound" and uses the following steps:

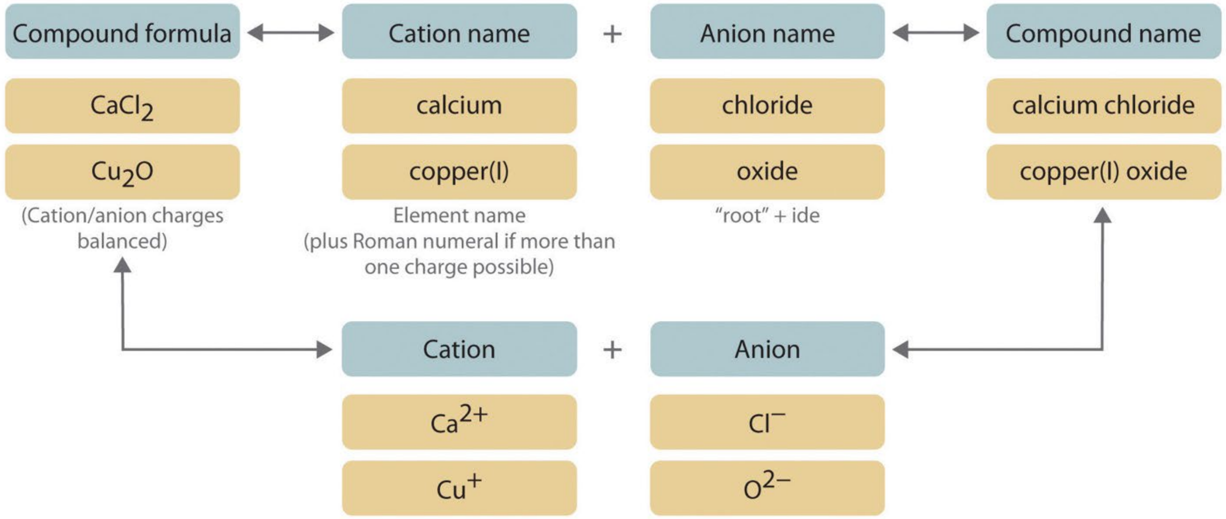


Figure 2.31. Naming an Ionic Compound

Ref: commons.wikimedia.org/

1. Place the ions in their proper order: cation and then anion.
2. Name the cation.
    1. Metals that form only one cation. As noted before, these metals are usually in groups 1–3, 12, and 13. The name of the cation of a metal that forms only one cation is the same as the name of the metal (with the word ion added if the cation is by itself). For example, Na^+ is the sodium ion, Ca^{2+} is the calcium ion, and Al^{3+} is the aluminum ion.
    2. Metals that form more than one cation. As shown before, many metals can form more than one cation. This behavior is observed for most transition metals, many actinides, and the heaviest elements of groups 13–15. In such cases, the positive charge on the metal is indicated by a roman numeral in parentheses immediately following the name of the metal. Thus Cu^+ is copper (I) (read as "copper one"), Fe^{2+} is iron (II), Fe^{3+} is iron (III), Sn^{2+} is tin (II), and Sn^{4+} is tin (IV).

An older system of nomenclature for such cations is still widely used, however. The name of the cation with the *higher* charge is formed from the root of the element's Latin name with the suffix -ic attached, and the name of the cation with the lower charge has the same root with the suffix -ous. The names of Fe^{3+}, Fe^{2+}, Sn^{4+}, and Sn^{2+} are therefore ferric, ferrous, stannic, and stannous, respectively. Even though this text uses the systematic names with roman numerals, you should be able to recognize these common names because they are still often used. For example, on the label of your dentist's fluoride rinse, the compound chemists call tin (II) fluoride is usually listed as stannous fluoride.

Some examples of metals that form more than one cation are in table 6, along with the names of the ions. Note that the simple Hg^+ cation does not occur in chemical compounds. Instead, all compounds of mercury(I) contain a dimeric cation, Hg_2^{2+}, in which the two Hg atoms are bonded together.

Cation	Systematic Name	Common Name	Cation	Systematic Name	Common Name
Cr^{2+}	chromium(II)	chromous	Cu^{2+}	copper(II)	cupric
Cr^{3+}	chromium(III)	chromic	Cu^{+}	copper(I)	cuprous
Mn^{2+}	manganese(II)	manganous*	Hg^{2+}	mercury(II)	mercuric
Mn^{3+}	manganese(III)	manganic*	Hg_2^{2+}	mercury(I)	mercurous†
Fe^{2+}	iron(II)	ferrous	Sn^{4+}	tin(IV)	stannic
Fe^{3+}	iron(III)	ferric	Sn^{2+}	tin(II)	stannous
Co^{2+}	cobalt(II)	cobaltous*	Pb^{4+}	lead(IV)	plumbic*
Co^{3+}	cobalt(III)	cobaltic*	Pb^{2+}	lead(II)	plumbous*
* Not widely used.					
†The isolated mercury(I) ion exists only as the gaseous ion.					

Table 6. Common Cations of Metals That Form More Than One Ion

    3. Polyatomic cations. The names of the common polyatomic cations that are relatively important in ionic compounds, such as the ammonium ion.
3. Name the anion.
    1. Monatomic anions. Monatomic anions are named by adding the suffix -*ide* to the root of the name of the parent element; thus, Cl^- is chloride, O^{2-} is oxide, P^{3-} is phosphide, N^{3-} is nitride (also called azide), and C^{4-} is carbide. Because the charges on these ions can be predicted from their position in the periodic table, it is *not* necessary to specify the charge in the name.
    2. Polyatomic anions. Polyatomic anions typically have common names that you must learn. Polyatomic anions that contain a single metal or nonmetal atom plus one or more oxygen atoms are called oxoanions (or oxyanions). In cases where only two oxoanions are known for an element, the name of the oxoanion with more oxygen atoms ends in -ate, and the name of the oxoanion with fewer oxygen atoms ends in -ite. For example, NO_3^- is nitrate and NO_2^- is nitrite. The halogens and some of the transition metals form more extensive series of oxoanions with as

many as four members. In the names of these oxoanions, the prefix per- is used to identify the oxoanion with the most oxygen (so that ClO_4^- is perchlorate and ClO_3^- is chlorate), and the prefix *hypo-* is used to identify the anion with the fewest oxygen (ClO_2^- is chlorite and ClO^- is hypochlorite). Differentiating the oxoanions in such a series is no trivial matter. For example, the hypochlorite ion is the active ingredient in laundry bleach and swimming pool disinfectant, but compounds that contain the perchlorate ion can explode if they come into contact with organic substances.

4. Write the name of the compound as the name of the cation followed by the name of the anion.

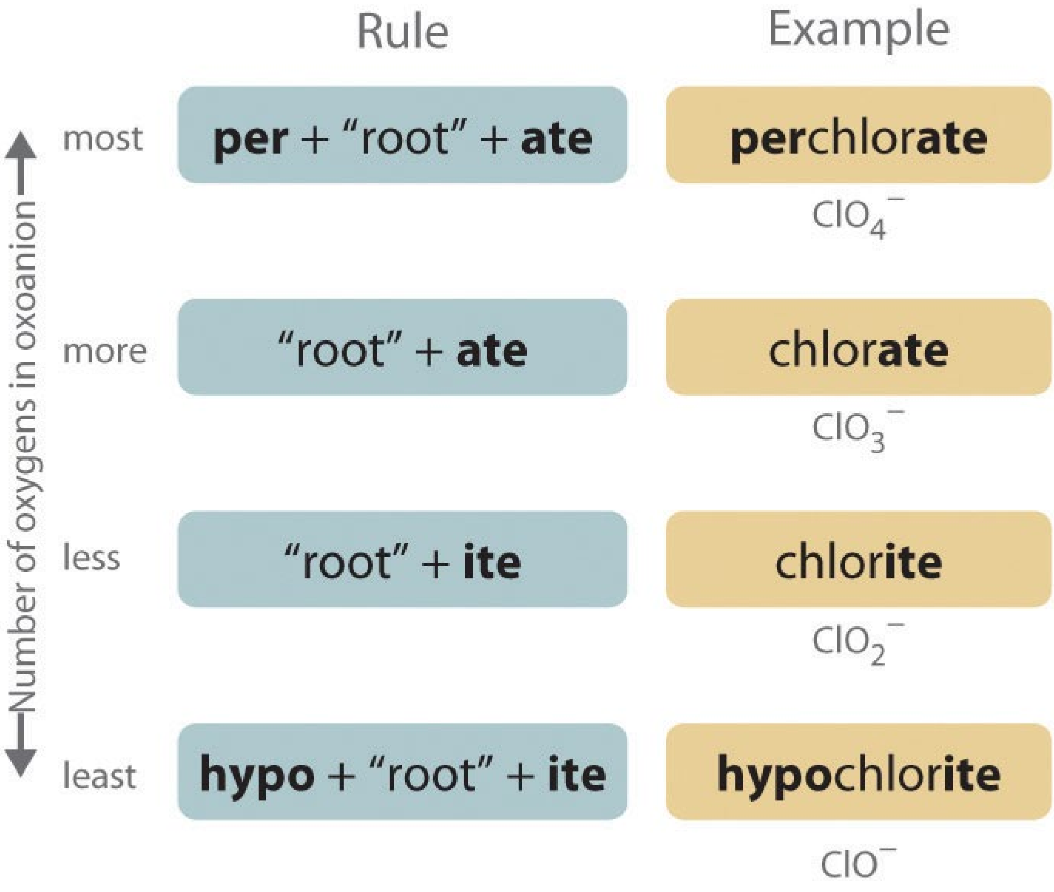
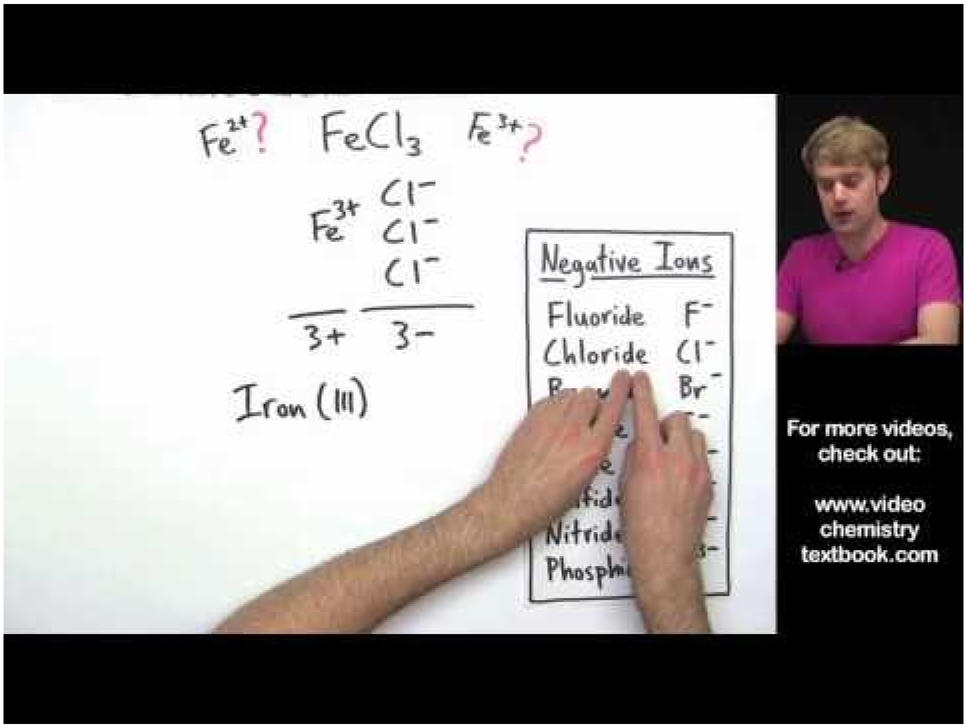


Figure 2.32. The relationship between the Names of oxoanions and the number of oxygen atoms present

Ref: commons.wikimedia.org/

Note the Pattern

Cations are always named before anions.
Most transition metals, many actinides, and the heaviest elements of groups 13–15 can form more than one cation.



Example 12

Write the systematic name (and the common name if applicable) for each ionic compound.

LiCl
$MgSO_4$
$(NH_4)_3$PO4
Cu_2O

Solution

Given: empirical formula
Asked for: name

Strategy:

A. If only one charge is possible for the cation, give its name. If the cation can have more than one charge, specify the charge using roman numerals.
B. If the anion does not contain oxygen, name it according to step 3a. For polyatomic anions that contain oxygen, use the appropriate prefix and suffix listed in step 3b.
C. Beginning with the cation, write the name of the compound.

Solution:

A. Lithium is in group 1, so we know that it forms only the Li^+ cation, which is the lithium ion. Similarly, chlorine is in group 7, so it forms the Cl^- anion, which is the chloride ion. Because we begin with the name of the cation, the name of this compound is lithium chloride, which is used medically as an antidepressant drug.
B. The cation is the magnesium ion, and the anion, which contains oxygen, is sulfate. Because we list the cation first, the name of this compound is magnesium sulfate. A hydrated form of magnesium sulfate ($MgSO_4 \cdot 7H_2O$) is sold in drugstores as Epsom salts, a harsh but effective laxative.
C. The cation is the ammonium ion and the anion is phosphate. The compound is therefore ammonium phosphate, which is widely used as a fertilizer. It is not necessary to specify that the formula unit contains three ammonium ions because three are required to balance the negative charge on phosphate.
D. The cation is a transition metal that often forms more than one cation. We must therefore specify the positive charge on the cation in the name: copper (I) or, according to the older system, cuprous. The anion is oxide. The name of this compound is copper (I) oxide or, in the older system, cuprous oxide. Copper (I) oxide is used as a red glaze on ceramics and in antifouling paints to prevent organisms from growing on the bottoms of boats. Cu_2O. The bottom of a boat is protected with a red antifouling paint containing copper (I) oxide, Cu_2O.

Naming Acids

Acids

An **acid** can be defined in several ways. The most straightforward definition is that an acid is a molecular compound that contains one or more hydrogen atoms and produces hydrogen ions $(H^+)(H^+)$ when dissolved in water.

Figure 2.33: (A) Vinegar comes in a variety of types, but all contain acetic acid. (B) Citrus fruits like grapefruit contain citric and ascorbic acids.
Ref: commons.wikimedia.org/

This is a different type of compound than the others we have seen so far. Acids are molecular, which means that in their pure state they are individual molecules and do not adopt the extended three-dimensional structures of ionic compounds like NaCl-NaCl. However, when these molecules are dissolved in water, the chemical bond between the hydrogen atom and the rest of the molecule breaks, leaving a positively-charged hydrogen ion and an anion. This can be symbolized in a chemical equation:

$$HCl \rightarrow H++Cl-$$

Since acids produce H+H+ cations upon dissolving in water, the HH of an acid is written first in the formula of an inorganic acid. The remainder of the acid (other than the HH) is the anion after the acid dissolves. Organic acids are also an important class of compounds, but will not be discussed here.

Naming Acids

Since all acids contain hydrogen, the name of an acid is based on the anion that goes with it. These anions can either be monatomic or polyatomic.

Naming Binary acids (in aqueous form)

A **binary acid** is an acid that consists of hydrogen and one other element. The most common binary acids contain a halogen. The acid name begins with the prefix *hydro-*. followed by the base name of the anion, followed by the suffix *-ic*.

Hydro- and Base name of Non metal and *-ic + acid*

Example: $HCl_{(aq)}$

Cl^-, chloride ion

hydrochloric acid

Naming Oxyacids

An **oxyacid** is an acid that consists of hydrogen, oxygen, and a third element. The third element is usually a nonmetal.

a. Oxyanions with ***-ite*** ending.

Base name of oxyanion and *-ous+ acid*

Example: $H_2SO_{3(aq)}$

SO_3^{2-}, sulfite ion

sulfurous acid

b. Oxyanions with ***-ate*** ending.

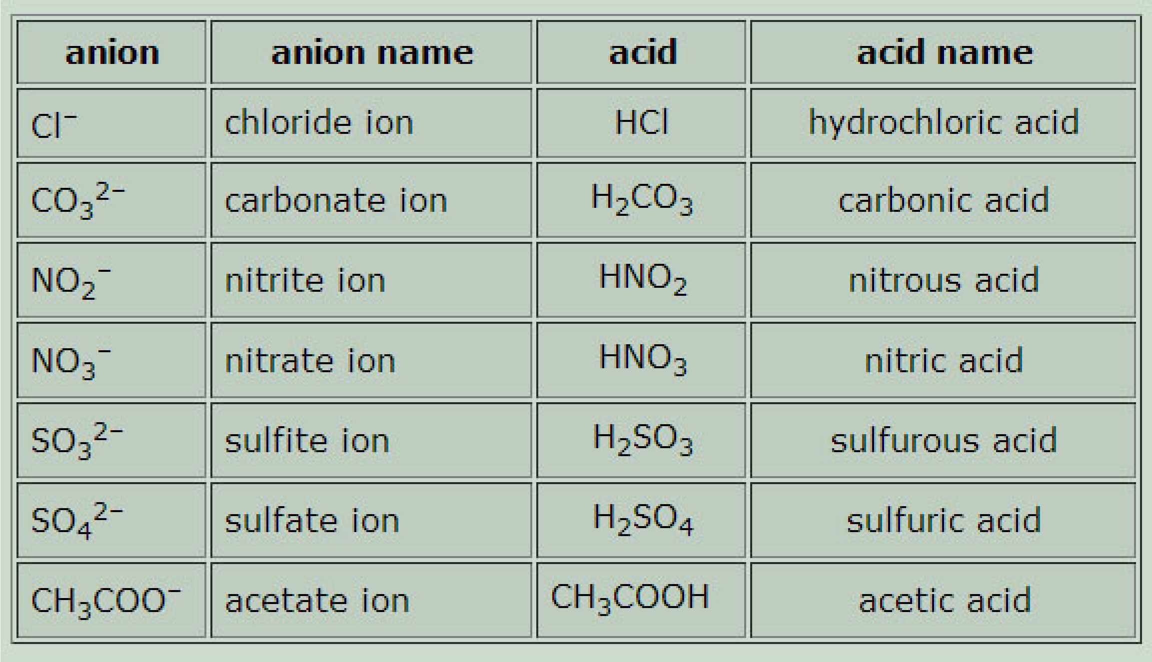
The name of the acid is the root of the anion followed by the suffix ***-ic***. There is no prefix.

Base name of oxyanion and -ic+ acid

Example: $H_3PO_{4(aq)}$

PO_4^{3-} phosphate ion

phosphoric acid



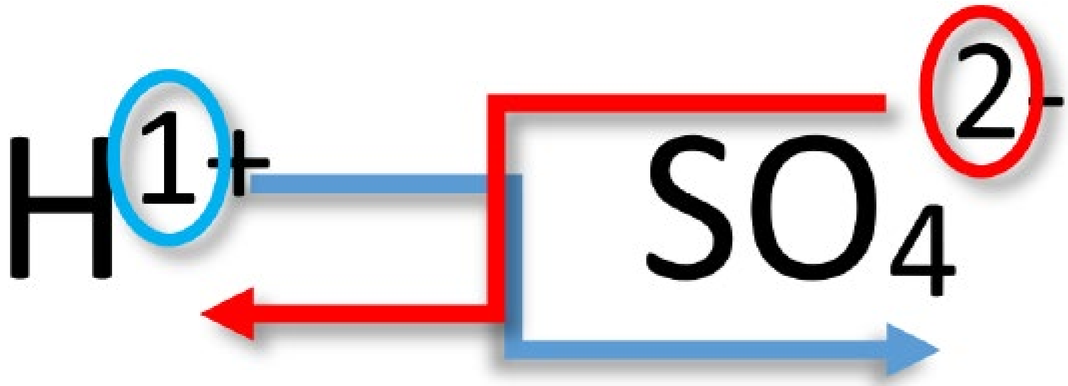
anion	anion name	acid	acid name
Cl^-	chloride ion	HCl	hydrochloric acid
CO_3^{2-}	carbonate ion	H_2CO_3	carbonic acid
NO_2^-	nitrite ion	HNO_2	nitrous acid
NO_3^-	nitrate ion	HNO_3	nitric acid
SO_3^{2-}	sulfite ion	H_2SO_3	sulfurous acid
SO_4^{2-}	sulfate ion	H_2SO_4	sulfuric acid
CH_3COO^-	acetate ion	CH_3COOH	acetic acid

Nomenclature of common acids This chart provides the nomenclature of some common anions and acids

Note:

The base name for sulfur containing oxyacid is *sulfur-* instead of just **sulf-**. The same is true for a phosphorus containing oxyacid. The base name is *phosphor-* instead of simply *phosph-*.

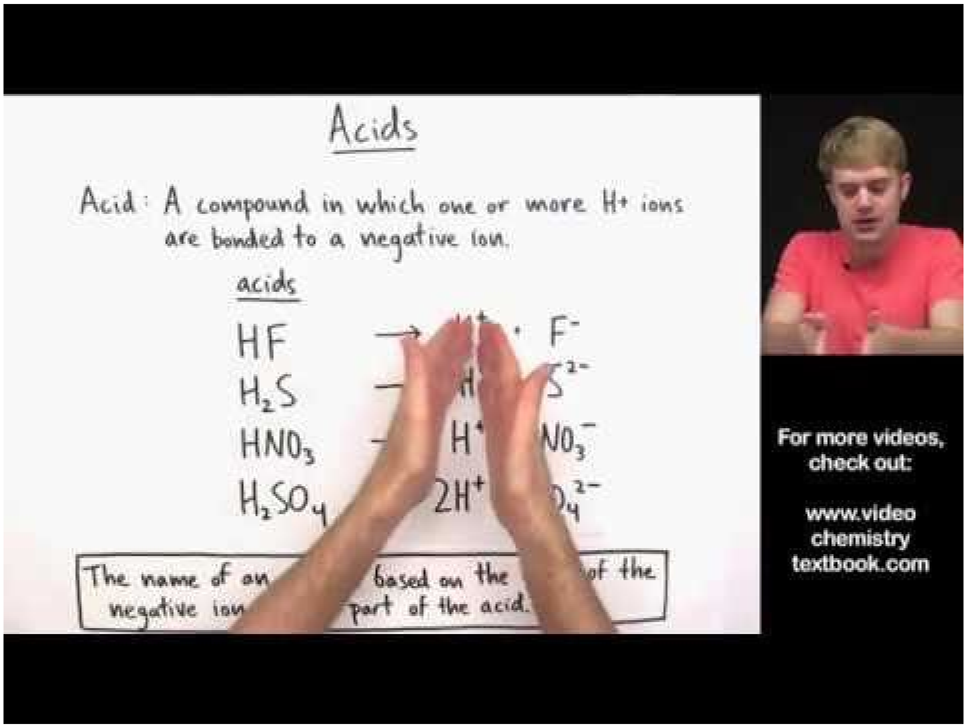
Writing Formulas for Acids



Formula: H_2SO_4

Figure 2.34 **:** *Crisscross approach to writing formula for sulfuric acid.*

Ref: *www.libretext.org/*



Acids

Acid: A compound in which one or more H^+ ions are bonded to a negative ion.

acids

$HF \rightarrow$ F^-

H_2S S^{2-}

HNO_3 H^+ NO_3^-

H_2SO_4 $2H^+$ O_4^{2-}

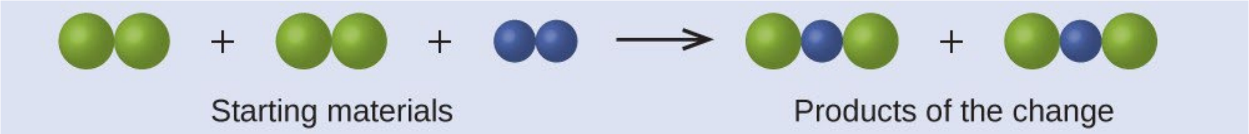
The name of an based on the of the negative ion part of the acid.

For more videos, check out:

www.video chemistry textbook.com

End of the chapter questions/problems

1. In the following drawing, the green spheres represent atoms of a certain element. The purple spheres represent atoms of another element. If the spheres touch, they are part of a single unit of a compound. Does the following chemical change represented by these symbols violate any of the ideas of Dalton's atomic theory? If so, which one?



1. A sample of compound X (a clear, colorless, combustible liquid with a noticeable odor) is analyzed and found to contain 14.13 g carbon and 2.96 g hydrogen. A sample of compound Y (a clear, colorless, combustible liquid with a noticeable odor that is slightly different from X's odor) is analyzed and found to contain 19.91 g carbon and 3.34 g hydrogen. Are these data an example of the law of definite proportions, the law of multiple proportions, or neither? What do these data tell you about substances X and Y?
2. The existence of isotopes violates one of the original ideas of Dalton's atomic theory. Which one?
3. Dalton originally thought that all atoms of a particular element had identical properties, including mass. Thus, the concept of isotopes, in which an element has different masses, was a violation of the original idea. To account for the existence of isotopes, the second postulate of his atomic theory was modified to state that atoms of the same element must have identical chemical properties.
4. How are electrons and protons similar? How are they different?
5. How are protons and neutrons similar? How are they different?
6. Both are subatomic particles that reside in an atom's nucleus. Both have approximately the same mass. Protons are positively charged, whereas neutrons are uncharged.
7. Predict and test the behavior of α particles fired at a "plum pudding" model atom.
8. (a) Predict the paths taken by α particles that are fired at atoms with a Thomson's plum pudding model structure. Explain why you expect the α particles to take these paths.
9. (b) If α particles of higher energy than those in (a) are fired at plum pudding atoms, predict how their paths will differ from the lower-energy α particle paths. Explain your reasoning.

10. (c) Now test your predictions from (a) and (b). Open the Rutherford Scattering simulation and select the "Plum Pudding Atom" tab. Set "Alpha Particles Energy" to "min," and select "show traces." Click on the gun to start firing α particles. Does this match your prediction from (a)? If not, explain why the actual path would be that shown in the simulation. Hit the pause button, or "Reset All." Set "Alpha Particles Energy" to "max," and start firing α particles. Does this match your prediction from (b)? If not, explain the effect of increased energy on the actual paths as shown in the simulation.

11. Predict and test the behavior of α particles fired at a Rutherford atom model.

12. (a) Predict the paths taken by α particles that are fired at atoms with a Rutherford atom model structure. Explain why you expect the α particles to take these paths.

13. (b) If α particles of higher energy than those in (a) are fired at Rutherford atoms, predict how their paths will differ from the lower-energy α particle paths. Explain your reasoning.

14. (c) Predict how the paths taken by the α particles will differ if they are fired at Rutherford atoms of elements other than gold. What factor do you expect to cause this difference in paths, and why?

15. (d) Now test your predictions from (a), (b), and (c). Open the Rutherford Scattering simulation and select the "Rutherford Atom" tab. Due to the scale of the simulation, it is best to start with a small nucleus, so select "20" for both protons and neutrons, "min" for energy, show traces, and then start firing α particles. Does this match your prediction from (a)? If not, explain why the actual path would be that shown in the simulation. Pause or reset, set energy to "max," and start firing α particles. Does this match your prediction from (b)? If not, explain the effect of increased energy on the actual path as shown in the simulation. Pause or reset, select "40" for both protons and neutrons, "min" for energy, show traces, and fire away. Does this match your prediction from (c)? If not, explain why the actual path would be that shown in the simulation. Repeat this with larger numbers of protons and neutrons. What generalization can you make regarding the type of atom and effect on the path of α particles? Be clear and specific.

16. (a) The Rutherford atom has a small, positively charged nucleus, so most α particles will pass through empty space far from the nucleus and be undeflected. Those α particles that pass near the nucleus will be deflected from their paths due to positive-positive repulsion. The more directly toward the nucleus the α particles are headed, the larger the deflection angle will be. (b) Higher-energy α particles that pass near the nucleus will still undergo deflection, but the faster they travel, the less the expected angle of deflection. (c) If the nucleus is smaller, the positive charge is smaller and the expected deflections are smaller—both in terms of how closely the α particles pass by the nucleus undeflected and the angle of deflection. If the nucleus is larger, the positive charge is larger and the expected deflections are larger—more α particles will be deflected, and the deflection angles will be larger. (d) The paths followed by the α particles match the predictions from (a), (b), and (c).

17. A sample of magnesium is found to contain 78.70% of 24Mg atoms (mass 23.98 amu), 10.13% of 25Mg atoms (mass 24.99 amu), and 11.17% of 26Mg atoms (mass 25.98 amu). Calculate the average mass of a Mg atom.
18. Naturally occurring copper consists of 63Cu (mass 62.9296 amu) and 65Cu (mass 64.9278 amu), with an average mass of 63.546 amu. What is the percent composition of Cu in terms of these two isotopes?
19. In what way are isotopes of a given element always different? In what way(s) are they always the same?

20. Write the symbol for each of the following ions:

    (a) the ion with a 1+ charge, atomic number 55, and mass number 133

    (b) the ion with 54 electrons, 53 protons, and 74 neutrons

    (c) the ion with atomic number 15, mass number 31, and a 3− charge

    (d) the ion with 24 electrons, 30 neutrons, and a 3+ charge

    (a) $^{133}Cs^{+}$; (b) $^{127}I^{-}$; (c) $^{31}P^{3-}$; (d) $^{57}Co^{3+}$

21. Write the symbol for each of the following ions:

    (a) the ion with a 3+ charge, 28 electrons, and a mass number of 71

    (b) the ion with 36 electrons, 35 protons, and 45 neutrons

    (c) the ion with 86 electrons, 142 neutrons, and a 4+ charge

    (d) the ion with a 2+ charge, atomic number 38, and mass number 87

22. Determine the number of protons, neutrons, and electrons in the following isotopes that are used in medical diagnoses:

    (a) atomic number 9, mass number 18, charge of 1−

    (b) atomic number 43, mass number 99, charge of 7+

    (c) atomic number 53, atomic mass number 131, charge of 1−

    (d) atomic number 81, atomic mass number 201, charge of 1+

    (e) Name the elements in parts (a), (b), (c), and (d).

23. The following are properties of isotopes of two elements that are essential in our diet. Determine the number of protons, neutrons and electrons in each and name them.

    (a) atomic number 26, mass number 58, charge of 2+

(b) atomic number 53, mass number 127, charge of 1−

24. An element has the following natural abundances and isotopic masses: 90.92% abundance with 19.99 amu, 0.26% abundance with 20.99 amu, and 8.82% abundance with 21.99 amu. Calculate the average atomic mass of this element.

25. Average atomic masses listed by IUPAC are based on a study of experimental results. Bromine has two isotopes ^{79}Br and ^{81}Br, whose masses (78.9183 and 80.9163 amu) and abundances (50.69% and 49.31%) were determined in earlier experiments. Calculate the average atomic mass of bromine based on these experiments.

26. Variations in average atomic mass may be observed for elements obtained from different sources. Lithium provides an example of this. The isotopic composition of lithium from naturally occurring minerals is 7.5% ^{6}Li and 92.5% ^{7}Li, which have masses of 6.01512 amu and 7.01600 amu, respectively. A commercial source of lithium, recycled from a military source, was 3.75% ^{6}Li (and the rest ^{7}Li). Calculate the average atomic mass values for each of these two sources.

27. The average atomic masses of some elements may vary, depending upon the sources of their ores. Naturally occurring boron consists of two isotopes with accurately known masses (^{10}B, 10.0129 amu and ^{11}B, 11.0931 amu). The actual atomic mass of boron can vary from 10.807 to 10.819, depending on whether the mineral source is from Turkey or the United States. Calculate the percent abundances leading to the two values of the average atomic masses of boron from these two countries. Turkey source: 26.49% (of 10.0129 amu isotope); US source: 25.37% (of 10.0129 amu isotope)

28. The ^{18}O:^{16}O abundance ratio in some meteorites is greater than that used to calculate the average atomic mass of oxygen on earth. Is the average mass of an oxygen atom in these meteorites greater than, less than, or equal to that of a terrestrial oxygen atom?

29. A molecule of metaldehyde (a pesticide used for snails and slugs) contains 8 carbon atoms, 16 hydrogen atoms, and 4 oxygen atoms. What are the molecular and empirical formulas of metaldehyde?
30. Give the group name for each of the following elements:
    1. krypton
    2. selenium
    3. barium
    4. lithium
31. Write the molecular formula for each compound.
    1. Nitrous oxide, also called “laughing gas,” has 2 nitrogen atoms and 1 oxygen atom per molecule. Nitrous oxide is used as a mild anesthetic for minor surgery and as the propellant in cans of whipped cream.
    2. Sucrose, also known as cane sugar, has 12 carbon atoms, 11 oxygen atoms, and 22 hydrogen atoms.
    3. Sulfur hexafluoride, a gas used to pressurize “unpressurized” tennis balls and as a coolant in nuclear reactors, has 6 fluorine atoms and 1 sulfur atom per molecule.
32. Predict the charge on the most common monatomic ion formed by each element.

   1. calcium, used to prevent osteoporosis
   2. iodine, required for the synthesis of thyroid hormones
   3. zirconium, widely used in nuclear reactors

33. Ionic and covalent compounds are held together by electrostatic attractions between oppositely charged particles. Describe the differences in the nature of the attractions in ionic and covalent compounds. Which class of compounds contains pairs of electrons shared between bonded atoms?
34. Which contains fewer electrons than the neutral atom—the corresponding cation or the anion?
35. What is the difference between an organic compound and an inorganic compound?
36. What is the advantage of writing a structural formula as a condensed formula?
37. The majority of elements that exist as diatomic molecules are found in one group of the periodic table. Identify the group.
38. Discuss the differences between covalent and ionic compounds with regard to
39. the forces that hold the atoms together.
40. melting points.
41. physical states at room temperature and pressure.
42. Why do covalent compounds generally tend to have lower melting points than ionic compounds?
43. What is the total number of electrons present in each ion?
    1. F−
    2. Rb+
    3. Ce3+
    4. Zr4+
    5. Zn2+
    6. Kr2+
    7. B3+
44. What is the total number of electrons present in each ion?
    1. Ca2+
    2. Se2−
    3. In3+
    4. Sr2+
    5. As3+
    6. N3−
    7. Tl+
45. Predict how many electrons are in each ion.
    1. an oxygen ion with a −2 charge
    2. a beryllium ion with a +2 charge
    3. a silver ion with a +1 charge
    4. a selenium ion with a +4 charge
    5. an iron ion with a +2 charge
    6. a chlorine ion with a −1 charge
    7. Predict how many electrons are in each ion.
    8. a copper ion with a +2 charge

    9. a molybdenum ion with a +4 charge
    10. an iodine ion with a −1 charge
    11. a gallium ion with a +3 charge
    12. an ytterbium ion with a +3 charge
    13. a scandium ion with a +3 charge
    14. Predict the charge on the most common monatomic ion formed by each element.
    15. chlorine
    16. phosphorus
    17. scandium
    18. magnesium
    19. arsenic
    20. oxygen
46. Predict the charge on the most common monatomic ion formed by each element.
    1. sodium
    2. selenium
    3. barium
    4. rubidium
    5. nitrogen
    6. aluminum
47. Write the name of each binary covalent compound.
    1. IF7
    2. N2O5
    3. OF2
48. Write the name of each binary covalent compound.
    a. IF_7
    b. N_2O_5
    c. OF_2
49. Name each cation: K^+, $Al3^+$, NH_4^+, Mg_2^+, Li^+
50. Name each anion: Br^-, CO_3^{2-}, S^{2-}, NO_3^-, HCO^{2-}, F^-, ClO^-, $C_2O_4^{2-}$
51. Name each anion: PO_4^{3-}, Cl^-, SO_3^{2-}, CH_3CO^{2-}, HSO_4^-, ClO_4^-,NO_2^-, O_2^-
52. Name each anion: SO_4^{2-}, CN^-, $Cr_2O_7^{2-}$, N_3^-, OH^-, I^-, O_2^{2-}
53. Name each compound: $MgBr_2$, NH_4CN, CaO, $KClO_3$, K_3PO_4, $NH4NO_2$, NaN_3
54. Name each compound: $NaNO_3$, $Cu_3(PO_4)_2$, NaOH
55. For each ionic compound, name the cation and the anion and give the charge on each ion: BeO, Pb(OH)2, BaS, $Na_2Cr_2O_7$
56. Write the formula for each compound: magnesium carbonate, aluminum sulfate, potassium phosphate, lead(IV) oxide, silicon nitride, sodium hypochlorite, titanium(IV) chloride, disodium ammonium phosphate
57. Using the periodic table, classify each of the following elements as a metal or a nonmetal, and then further classify each as a main-group element, transition metal, or inner transition metal:

    a. uranium

    b. bromine

c. strontium
d. neon
e. gold
f. americium
g. rhodium
h. sulfur
i. carbon
j. potassium

58. Using the periodic table, identify the lightest member of each of the following groups:
   a. noble gases
   b. alkaline earth metals
   c. alkali metals
   d. chalcogens

59. Use the periodic table to give the name and symbol for each of the following elements:
(a) the noble gas in the same period as germanium
(b) the alkaline earth metal in the same period as selenium
(c) the halogen in the same period as lithium
(d) the chalcogen in the same period as cadmium

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Chapter 3: Stoichiometry

Key Concepts

3.1 The Concept of Moles and the Formula Mass
3.2 The Concept of Empirical Formula and Molecular Formula
3.3 Solution's Different Concentrations
3.4 Concentrations Calculations in Chemical Reactions
3.5 Mole Definition and Mass Percent Calculations and Reviews

I. The Concept of Moles and the Formula Mass

What is the Mole?

Owing to their tiny size, atoms and molecules cannot be counted by direct observation. But much as we do when "counting" beans in a jar, we can estimate the number of particles in a sample of an element or compound if we have some idea of the volume occupied by each particle and the volume of the container.

Figure 3.1 Counting Jelly Beans

Once this has been done, we know the number of formula units (to use the most general term for any combination of atoms we wish to define) in any arbitrary weight of the substance. The number will of course depend both on the formula of the substance and on the weight of the sample. But if we consider a weight of substance *that is the same as its formula (molecular) weight expressed in grams*, *we have only one number to know*: ***Avogadro's number***, 6.022141527 × 10^{23}, usually designated by N_A.

The mole is defined as the mass of compound or element that contains the same number of fundamental units as there are atoms in 12.000 grams of ^{12}C (Carbon – 12 isotope).

This means that the atomic mass or atomic weight (12 grams) of carbon is equal to exactly 1 mole of carbon.

The mole as word was introduced by the German Chemist Wilhelm Ostwald in 1894 as a German unit in chemistry called Mol which was rooted from the German Molekül (molecule).

Furthermore, one mole equals 6.022 X 10^{23} particles. These particles can be atoms, molecules or formula units.

You should know it to three significant figures:

$N_A = 6.02 \times 10^{23}$

6.02×10^{23} of *what*? Well, of anything you like: apples, stars in the sky, burritos. But the only *practical* use for N_A is to have a more convenient way of expressing the huge numbers of the tiny particles such as atoms or molecules that we deal with in chemistry. Avogadro's number is a *collective number*, just like a dozen.

Think of 6.02×10^{23} as the "chemist's dozen".

Example:

Each carbon atom weighs about 1.99625×10^{-23} g, hence”

$[1.99625 \times 10^{-23}$ g / atoms$] \times [6.02214179 \times 10^{23}$ atoms$] = 12.0217$ g of Carbon – 12 isotope.

The value of 6.022×10^{23} is called Avogadro’s number.

Now we can define 1 mole of a matter is given in the table below:

1 mole of a matter equals	**6.022×10^{23} atoms**
	6.022×10^{23} molecules
	6.022×10^{23} formula units (ions)

Things to understand about Avogadro's number N_A

- It is a *number*, just as is "dozen", and thus is *dimensionless*.
- It is a *huge* number, far greater in magnitude than we can visualize; see here for some interesting comparisons with other huge numbers.
- Its practical use is limited to counting tiny things like atoms, molecules, "formula units", electrons, or photons.
- The value of N_A can be known only to the precision that the number of atoms in a measurable weight of a substance can be estimated. Because large numbers of atoms cannot be counted directly, a variety of ingenious indirect measurements have been made involving such things as Brownian motion and X-ray scattering.
- The current value was determined by measuring the distances between the atoms of silicon in an ultrapure crystal of this element that was shaped into a perfect sphere. (The measurement was made by X-ray scattering.) When combined with the measured mass of this sphere, it yields Avogadro's number. But there are two problems with this: 1) The silicon sphere is an artifact, rather than being something that occurs in nature, and thus may not be perfectly reproducible. 2) The standard of mass, the kilogram, is not precisely known, and its value appears to be changing. For these reasons, there are proposals to revise the definitions of both N_A and the kilogram. See here for more, and stay tuned!

History of the determination of Avogadro's number

Wikipedia has a good discussion of Avogadro's number

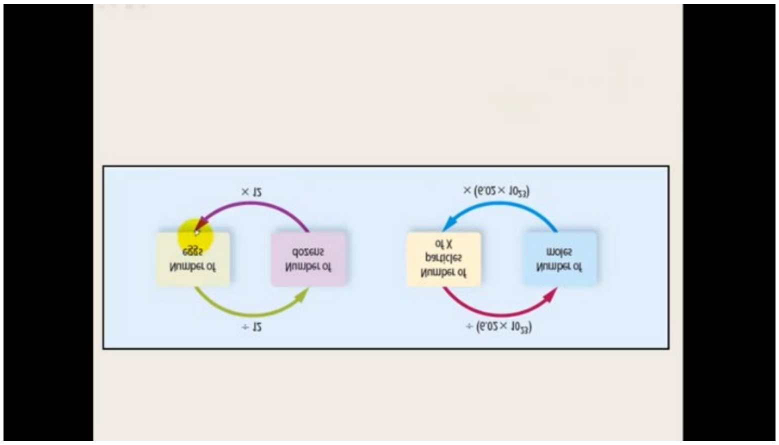
What is the Formula Mass?

The formula mass of a substance is the sum of the average weighed atomic masses of each atom present in the chemical formula and is expressed in atomic mass units (amu). The formula mass of a covalent compound is also called the molecular mass. The mass in grams of 1 mole of substance is its molar mass and it has the unit of (g/mol)

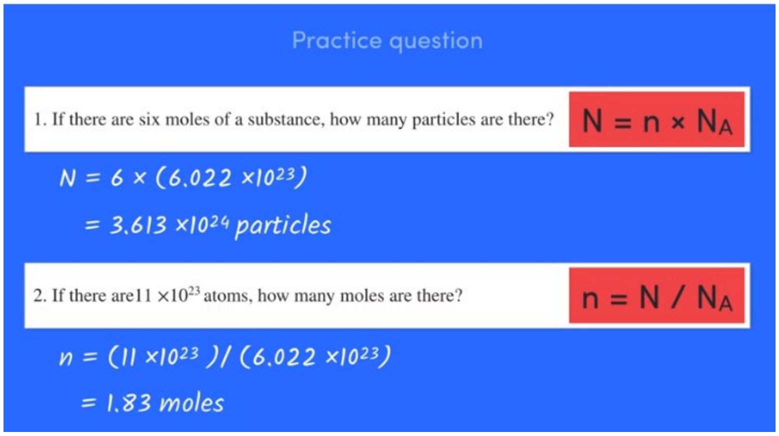
Examples are posted in table below:

Element Name	**Element Symbol**	**Average Weighed Atomic Mass in amu (atomic mass units)**	**Atomic Mass in g/mol**	**Atoms / 1 mole**
Phosphorous	**P**	**30.973762**	**30.973762**	**6.022×10^{23}**
Carbon	**C**	**12.0107**	**12.0107**	**6.022×10^{23}**
Uranium	**U**	**238.02891**	**238.02891**	**6.022×10^{23}**
Barium	**Ba**	**137.327**	**137.327**	**6.022×10^{23}**
Silicon	**Si**	**28.0855**	**28.0855**	**6.022×10^{23}**
Xenon	**Xe**	**131.293**	**131.293**	**6.022×10^{23}**

The two videos explain the concept of the mole:



https://www.youtube.com/watch?v=wORiAOnvw8g&feature=youtu.be



Practice question

1. If there are six moles of a substance, how many particles are there? $N = n \times N_A$

$N = 6 \times (6.022 \times 10^{23})$

$= 3.613 \times 10^{24}$ particles

2. If there are11 $\times 10^{23}$ atoms, how many moles are there? $n = N / N_A$

$n = (11 \times 10^{23}) / (6.022 \times 10^{23})$

$= 1.83$ moles

https://www.youtube.com/watch?v=jCynTWTwjpw

Now let us look into the conversion of moles into grams for elements and compounds or molecules and vice versa.

Molar Mass

The molar mass is the mass of one mole of a substance, reported in grams. The molar mass is numerically equal to the formula weight but the units are different (g/mol or amu).

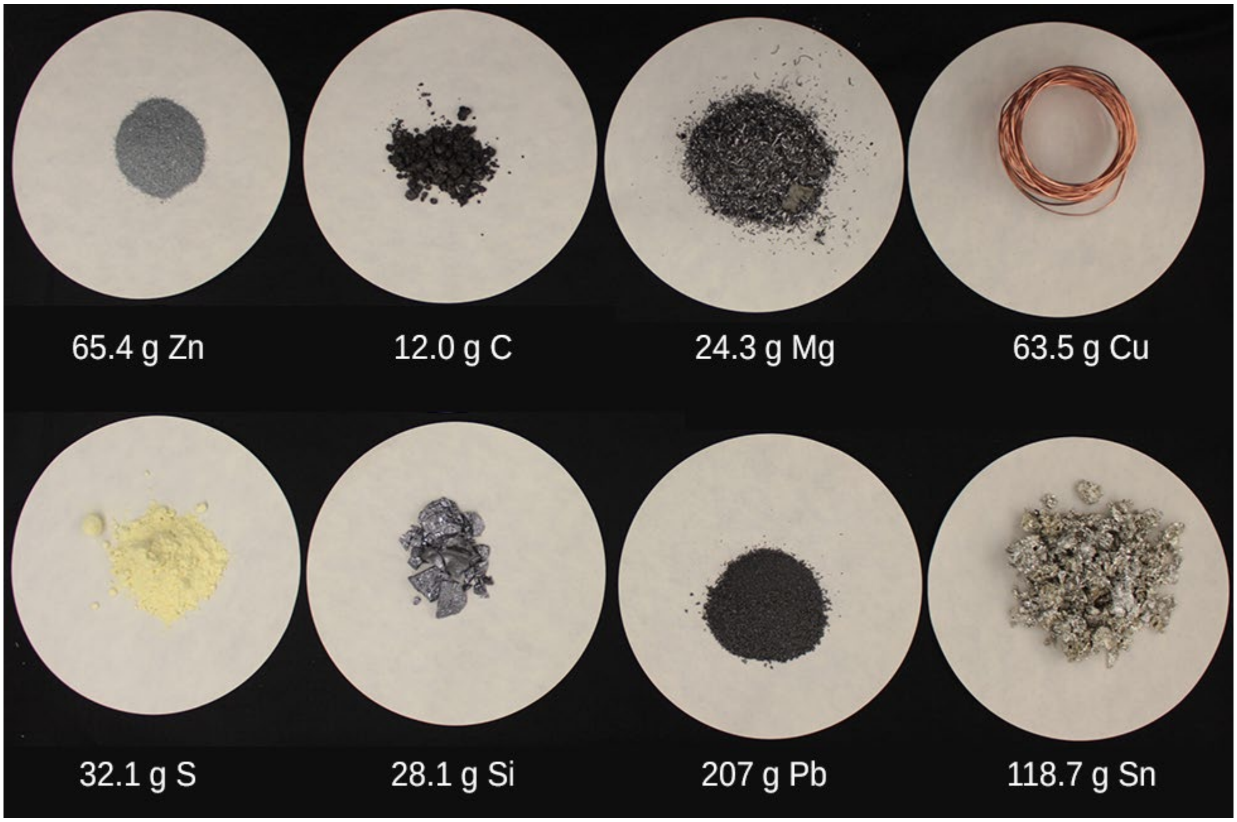
Calculation of molar mass: use the average atomic mass from periodic table. For example: molar mass of carbon 12.01 g/mol, Hydrogen 1.008 g/mol.
Below is a picture of 1 mol of different element in grams.

Molar mass of a compound is determined using the formula. Individual molar mass of the elements in a compound is taken and multiplied by its coefficients and added all together.

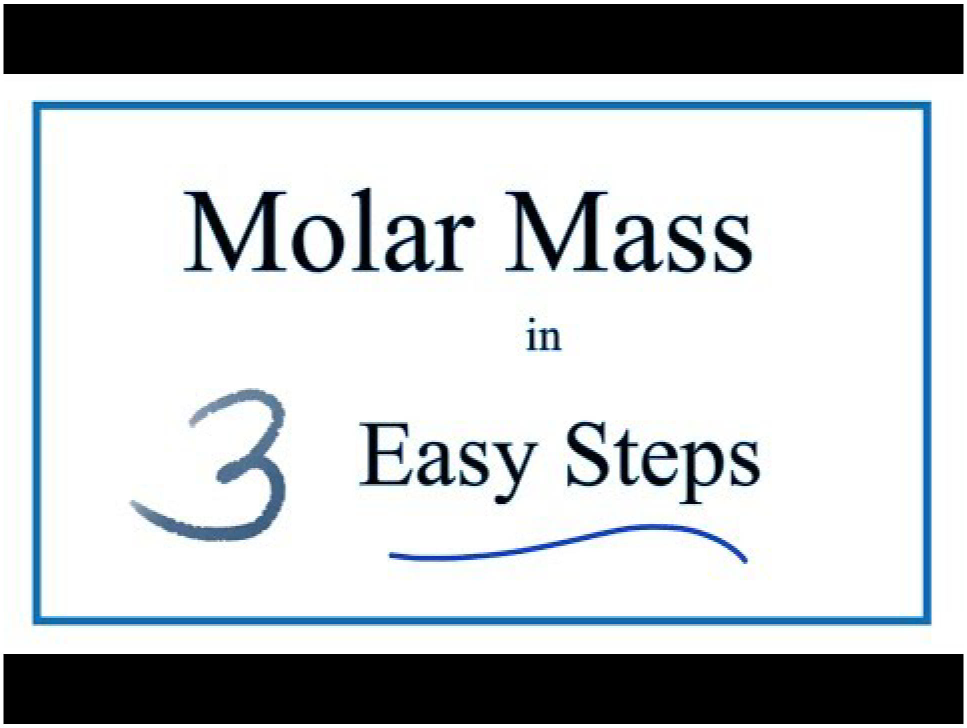
Example: Determine the molar mass of Glucose: $C_6H_{12}O_6$

Molar mass C → 6*12.01 = (72.06 g/mol)+
H →(12*1.008= (12.096 g/mol) +
O→(6* 16.00)= (96 .00g/mol)

180.16 g/mol



Watch the following video:
https://www.youtube.com/watch?v=o3MMBO8WxjY



Questions:

1. Determine the molar mass of Eu.

2. What is the molar mass of water, H_2O?

3. What is the formula weight ammonium carbonate, $(NH_4)_2CO_3$?

Ans: 1. 151.965 g/mol

2.18.02 g/mol

3. 96.07 amu

Conversion of moles into grams for elements:

Example:

How many grams can be calculated in 10.5 moles of Helium?

First of all, we should look at the average weighed atomic mass of Helium from the periodic table which turns to be 4.003 amu (atomic mass units). This value has the same unit of gram / mole.

Grams of Helium = 10.5 moles X 4.003 grams / moles = 42.0315 grams of Helium = 42.0 grams of Helium

Conversion of moles into grams for compounds or molecules:

Example:

How many grams can be calculated for 20.25 moles of sodium chloride NaCl?

When dealing with compounds or molecules, one should start calculating the molar mass of the compound or molecule first:

Molar mass of NaCl = the sum of average weighed atomic masses of each atom involved in the compound or molecule:

Molar mass of NaCl = Na + Cl = 23.0 g/mole + 35.5 g/mole = 58.5 g/mole

Grams of NaCl = 20.25 moles NaCl X 58.5 g/mole NaCl = 1184.625 g = 1.18×10^3 g NaCl

Conversion of grams into moles for elements:

Example:

How many moles can be calculated for 42.0 grams of Helium?

Moles of Helium = 42.0 g He X [mole / 4.003 g He] = 10.5 moles He

Conversion of grams into moles for compounds or molecules:

Example:

How may moles can be calculated for 1.18 X 10^3 grams NaCl?

Molar mass of NaCl = Na + Cl = 23.0 g/mole + 35.5 g/mole = 58.5 g/mole

Moles of NaCl = [1.18 X 10^3 grams NaCl] X [moles / 58.5g NaCl] = 20.2 moles NaCl

Conversion of number of atoms, molecules or ions (formula units) of a matter into number of grams of the matter and vice versa:

The general scheme is shown below:

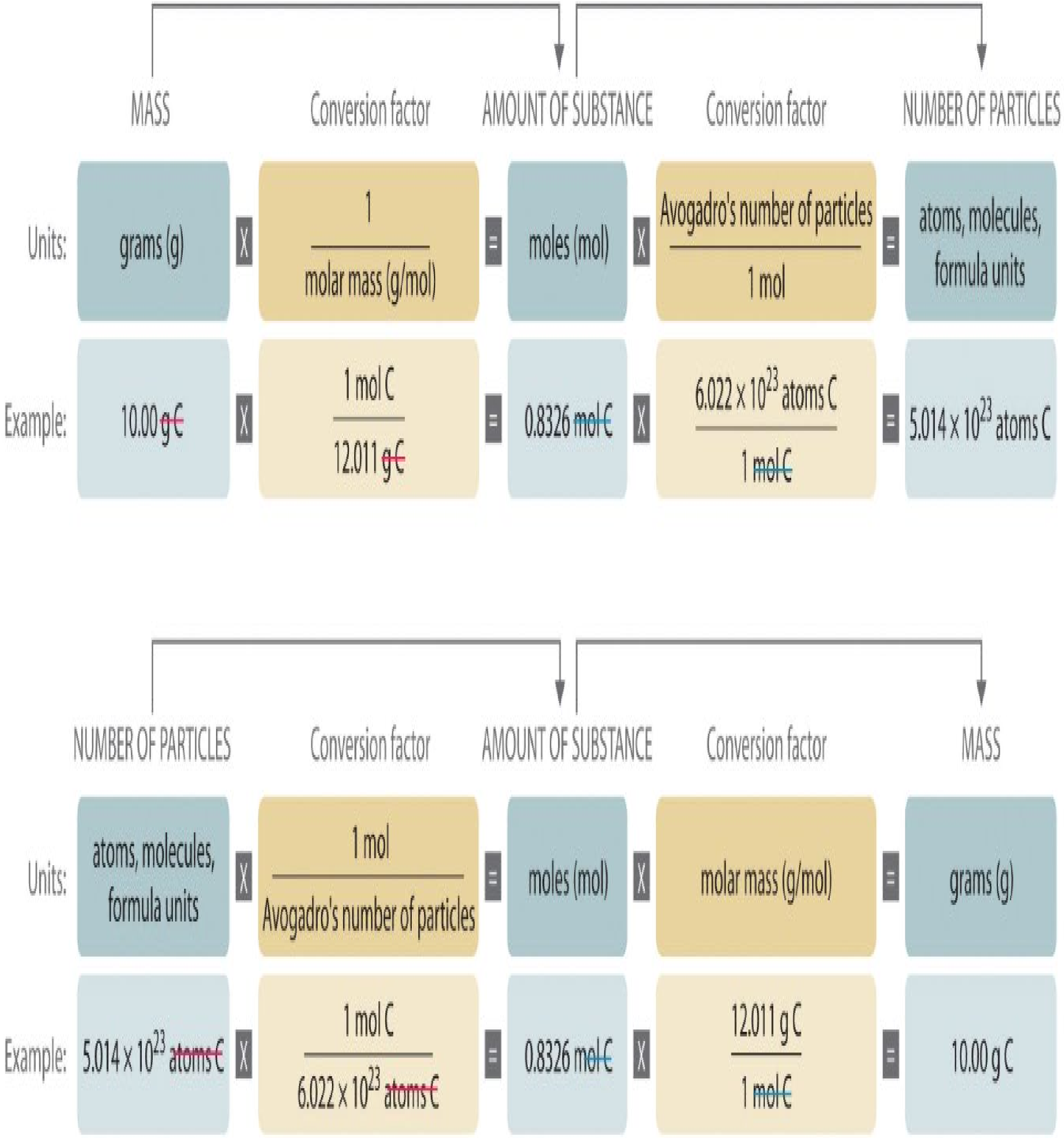
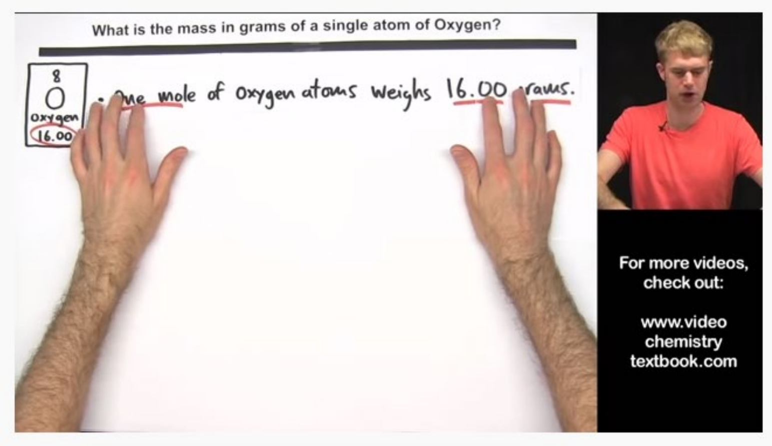


Figure 3.2 Concept Map of mass to mols

Ref: Commons.wikimedia.org/

Reference:
https://chem.libretexts.org/Courses/Howard_University/General_Chemistry%3A_An_Atoms_First_Approach/Unit_1%3A__Atomic_Structure/Chapter_1%3A_Introduction/Chapter_1.7%3A__The_Mole_and_Molar_Mass

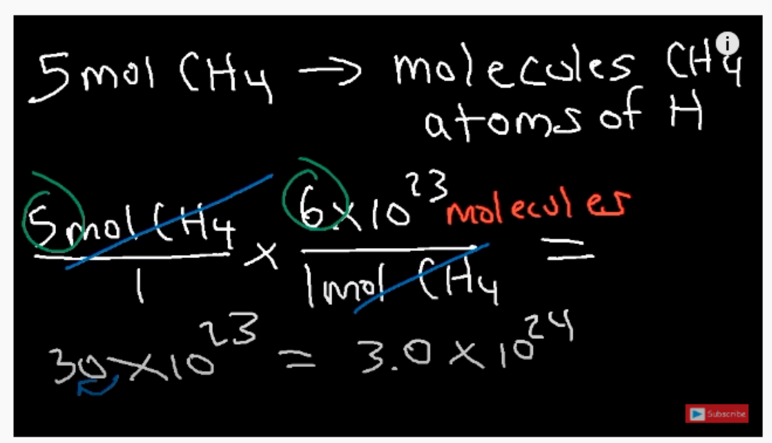
Videos covering the conversion of atoms, molecules, ions (formula units into grams of matter and vice versa are given below:



What is the mass in grams of a single atom of Oxygen?

One mole of Oxygen atoms weighs 16.00 grams.

https://www.youtube.com/watch?v=BO9M1hbs88s

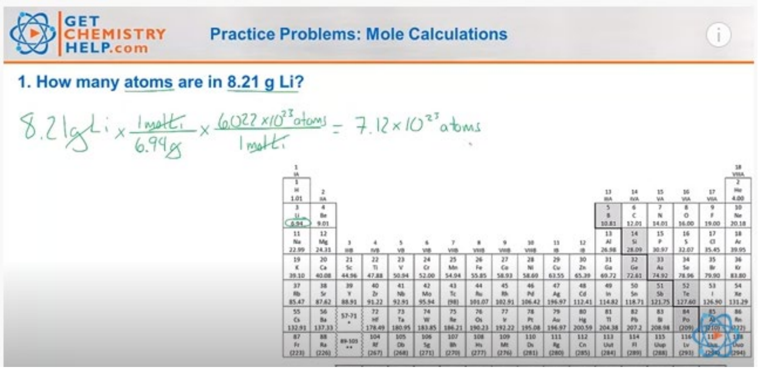


$5\ \text{mol CH}_4 \rightarrow$ molecules CH_4, atoms of H

$$\frac{5\ \cancel{\text{mol CH}_4}}{1} \times \frac{6\times10^{23}\ \text{molecules}}{1\ \cancel{\text{mol CH}_4}} =$$

$$30\times10^{23} = 3.0\times10^{24}$$

https://www.youtube.com/watch?v=74-X94OP2XI



Practice Problems: Mole Calculations

1. How many atoms are in 8.21 g Li?

$$8.21\ \cancel{\text{g Li}} \times \frac{1\ \text{mol Li}}{6.94\ \text{g}} \times \frac{6.022\times10^{23}\ \text{atoms}}{1\ \text{mol Li}} = 7.12\times10^{23}\ \text{atoms}$$

https://www.youtube.com/watch?v=w2-Pcfj60fA

Examples:

The following activity has been taken from American Association of Chemical teachers (AACT)

Calculating Moles in Daily Life

Background

Now that we have discussed Avogadro's number and molar mass, we are going to use these quantities to do some analysis of common items in your life. We're going to look at a nickel, water, chalk and sugar and determine the number of particles within a given sample.

Prelab Questions

1. Define Avogadro's number:

2. Define molar mass:

Objective

In this activity you will make a series of mass measurements. You will then convert these measurements to moles and molecules.

Safety

- Always wear safety goggles when handling chemicals in the lab.
- Wash your hands thoroughly before leaving the lab.
- Follow the teacher's instructions for cleanup of materials and disposal of chemicals.
- Do not consume lab solutions, even if they're otherwise edible products.

Procedure & Data Collection

1. Make the following measurements and calculations:

Mass of Nickel	
Mass of a nickel	g

Mass of 30 mL of Water: this is about how much water is in one gulp	
Mass of cup and water (before pouring 30mL)	g
Mass of cup and water (after pouring 30mL)	g
Mass of 30 mL water	g

Mass of Sugar: Don’t open the sugar packet, see teacher for empty mass	
Mass of Sugar in packet	g
Mass of empty packet (from teacher)	g
Mass of sugar	g

Mass of Signature	
Mass of chalk (before writing your name 3 times)	g
Mass of chalk (after writing your name 3 times)	g
Mass of chalk used in 3 signatures	g
Mass of chalk used in 1 signature	g

Calculations
Use information that you have collected above to help complete the following calculations. Please show your work with proper dimensional analysis and significant figures.

1. A **nickel** is composed of 25.0% nickel and 75.0% copper.
    a. Calculate the mass of nickel in the coin.
    b. Calculate the number of moles of nickel in the coin.
    c. Calculate the number of atoms of nickel in the coin.
    d. Calculate the mass of copper in the coin.
    e. Calculate the number of moles of copper in the coin.
    f. Calculate the number of atoms of copper in the coin.
2. **Water**
    a. Calculate the molar mass of water
    b. Calculate the number of moles of water swallowed
    c. Calculate the number of molecules of water swallowed
3. **Table sugar** (sucrose, $C_{12}H_{22}O_{11}$)

    a. Calculate the molar mass of sucrose

    b. Calculate the number of moles of sugar in the packet

    c. Calculate the number of molecules of sugar in the packet

    d. Calculate the number of atoms on carbon in the packet

4. Assume the **chalk** was 100% calcium carbonate.

    a. Using what we learned about naming chemicals, write the formula for calcium carbonate

    b. Calculate the molar mass of calcium carbonate

    c. Calculate the number of moles of calcium carbonate used in a single signature

    d. Calculate the number of oxygen atoms in your signature

Analysis

1. What is the difference between calculations made for the nickel and the other materials? (hint: consider the composition of each material)

2. What other household items do you think we could perform similar calculations with? Make several suggestions and explain if necessary.

3. What household item wouldn't work for such simple calculations and why not?

4. Why might a person be interested in this type of calculation?

5. Write a brief summary of what you learned in this lab that includes how the objective was met.

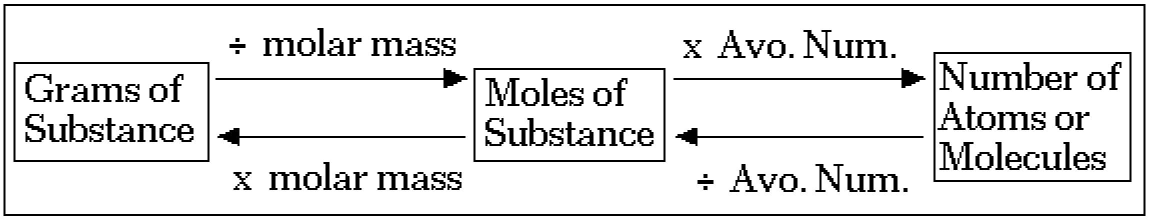


Figure 3.3 Conversion of Mass to mols to atoms or molecules

Ref: Commons.wikimedia.org/

Example#1: How many mols are present in 24.02 g of Carbon?

Since it is grams to mol conversion, molar mass is the conversion factor.

According to Periodic table molar mass of C= 12.01 g/mol

24.02 g C * 1 mol C = 2.00mols of C

12.01 g C

Example#2: How many mols are present in 54.1 g of Carbon?

Since it is grams to mols, molar mass is the conversion factor.

Molar mass of H_2O= 1.008 + 2* 16.00= 18.02 g/mol

54.1 g H_2O * 1mol H_2O =3.00 mols of H_2O
18.02 g H2O

Example #3: How many grams are in 3.57 mols of CO_2?

Since it is mols to grams, molar mass is the conversion factor.

Molar mass of CO_2= 12.01 + (4*16.00)= 44.01 g/mol

3.57 mols of CO_2 * 44.01 1g CO_2 = 157 g of CO_2

1 mol CO_2

Example#4 : How many atoms are present in 35.0 g of Cu?

We will use both conversion factor, molar mass and avogadro’s number to solve this problem.

Pathway:

$$35.0\text{ g Cu} * \frac{1\text{mol Cu}}{63.5\text{ g Cu}} * \frac{6.022 * 10^{23}\text{ atoms Cu}}{1\text{ mol Cu}} = 3.32 * 10^{23}\text{ atoms of Cu}$$

Practice Questions

1. **How many mols of H_2O are in 75.0 g of H_2O?**

2. **How many grams are in 3.46 mols of NaCl?**

3. **How many molecules are present in one mole of glucose, $C_6H_{12}O_6$?**

4. **You have a sample of 3.01×10^{23} atoms of silver. How much does this sample weigh?**

5. **A typical deposit of cholesterol, $C_{27}H_{46}O$, in an artery has a mass of 3.90 mg. How many molecules of cholesterol are present in this deposit?**

Ans: 1. 4.16 mols H_2O

2. 202.2g NaCl

3. $6.02 * 10^{23}$

4. 53.9 g Ag

5. $6.10 * 10^{18}$ molecules

More Practice: Calculate the mass of each of the following item in grams.

CHECK WITH YOUR INSTRUCTOR FOR CORRECT ANSWER:

Items	Material	Calculation
1	One mole of aluminum	
2	0.250 moles of NaCl	

3	5.6 x 10^{23} atoms of copper		
4	3.45 moles of water		
5	9.0 x 10^{22} molecules of chalk, $CaCO_3$		
6	8.9 x 10^{23} atoms of hydrogen in water		

II. The Concept of Empirical Formula and Molecular Formula

Empirical of "simplest" formulas

Empirical formulas give the *relative* numbers of the different elements in a sample of a compound, expressed in the smallest possible integers. The term *empirical* refers to the fact that formulas of this kind are determined experimentally; such formulas are also commonly referred to as ***simplest formulas***.

Problem Example 2: *Simplest formula from molecular formula*

Glucose (the "fuel" your body runs on) is composed of molecular units having the formula $C_6H_{12}O_6$. What is the empirical formula of glucose?

Solution: The glucose molecule contains twice as many atoms of hydrogen as carbons or oxygens, so we divide through by 6 to get $\mathbf{CH_2O}$.

Note: this simplest formula, which applies to all 6-carbon sugars, indicates that these compounds are "composed" of carbon and water, which explains why sugars are known as *carbohydrates*.

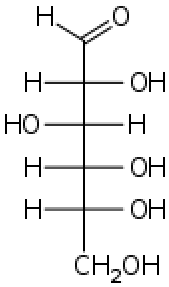


Figure 3.4 Carbohydrate Structure

Some solid compounds do not exist as discrete molecular units, but are built up as extended two- or three-dimensional lattices of atoms or ions. The compositions of such compounds are commonly described by their simplest formulas. In the very common case of *ionic solids*, such a formula also expresses the minimum numbers of positive and negative ions required to produce an electrically neutral unit, as in NaCl or $CuCl_2$.

Problem Example 3: *Molecular formula from ionic charges*

a) Write the formula of ferric bromide, given that the ferric (iron-III) ion is Fe^{3+} and the bromide ion carries a single negative charge.

b) Write the formula of bismuth sulfide, formed when the ions Bi^{3+} and S^{2-} combine.

Solution:

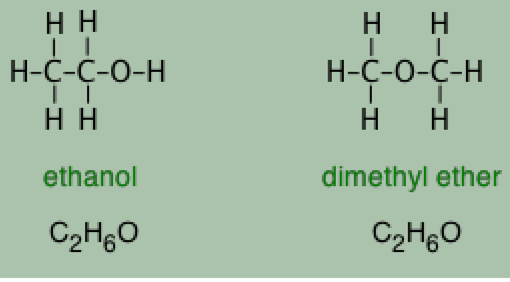
a) Three Br^- ions are required to balance the three positive charges of Fe^{3+}, hence the formula $\mathbf{FeBr_3}$.

b) The only way to get equal numbers of opposite charges is to have six of each, so the formula will be $\mathbf{Bi_2S_3}$.

What formulas *don't* tell us

The formulas we ordinarily write convey no information about the compound's ***structure***— that is, the order in which the atoms are connected by chemical bonds or are arranged in three-dimensional space. This limitation is especially significant in organic compounds, in which hundreds if not thousands of different molecules may share the same empirical formula.

The compounds ethanol and dimethyl ether both have the *simplest formula* C_2H_6O. *The structural formulas* reveal the very different nature of these two molecules:



Formulas can be made to convey structural information

It is often useful to write formulas in such as way as to convey at least some information about the structure of a compound. For example, the formula of the solid $(NH_4)_2CO_3$ is immediately identifiable as ammonium carbonate, and essentially a compound of ammonium and carbonate ions in a 2:1 ratio, whereas the *simplest* or *empirical* formula $N_2H_8CO_3$ obscures this information.

Similarly, the distinction between ethanol and dimethyl ether can be made by writing the formulas as C_2H_5OH and $CH_3–O–CH_3$, respectively. Although neither of these formulas specifies the structures precisely, anyone who has studied organic chemistry can work them out, and will immediately recognize the –OH (hydroxyl) group which is the defining characteristic of the large class of organic compounds known as *alcohols*. The –O– atom linking two carbons is similarly the defining feature of *ethers*.

Formulas imply molar masses

Several related terms are used to express the mass of one mole of a substance.

- **Molecular weight** This is analogous to atomic weight: it is the relative weight of one formula unit of the compound, based on the carbon-12 scale. The molecular weight is found by adding atomic weights of all the atoms present in the formula unit. Molecular weights, like atomic weights, are dimensionless; i.e., they have no units.
- **Formula weight** The same thing as molecular weight. This term is sometimes used in connection with ionic solids and other substances in which discrete molecules do not exist.
- **Molar mass** The mass (in grams, kilograms, or anyother mass unit) of one mole of particles or formula units. When expressed in grams, the molar mass is numerically the same as the molecular weight, but it must be accompanied by the mass unit.

Problem Example 4: ***Formula weight and molar mass***
a) Calculate the formula weight of copper(II) chloride, $CuCl_2$.

b) How would you express this same quantity as a *molar mass*?

Solution:

a) The atomic weights of Cu and Cl are, respectively 63.55 and 35.45; the sum of each atomic weight, multiplied by the numbers of each kind of atom in the formula unit, yields 63.55 + 2(25.35) = **134.45**.

b) The masses of one mole of Cu and Cl atoms are, respectively, 63.55 g and 35.45 g; the mass of one mole of $CuCl_2$ units is (63.55 g) + 2(25.35 g) = **134.45 g**.

Mole ratios and mole fractions from formulas

The information contained in formulas can be used to compare the compositions of related compounds as in the following example:

Problem Example 5: ***mole ratio calculation***

The ratio of hydrogen to carbon is often of interest in comparing different fuels. Calculate these ratios for methanol (CH_3OH) and ethanol (C_2H_5OH).

Solution: the H:C ratios for the two alcohols are 4:1 = 4.0 for methanol and 6:2 (3.0) for ethanol.

Alternatively, one sometimes uses mole fractions to express the same thing. The mole fraction of an element M in a compound is just the number of atoms of M divided by the total number of atoms in the formula unit.

Problem Example 6: ***mole fraction and mole percent***

Calculate the mole fraction and mole-percent of carbon in ethanol (C_2H_5OH).

Solution: The formula unit contains nine atoms, two of which are carbon. The mole fraction of carbon in the compound is 2/9 = .22. Thus 22 percent of the atoms in ethanol are carbon.

Percent composition and elemental masses from formulas

Since the formula of a compound expresses the ratio of the numbers of its constituent atoms, a formula also conveys information about the relative masses of the elements it contains. But in order to make this connection, we need to know the relative masses of the different elements.

Problem Example 7: ***mass of each element in a given mass of compound***

Find the masses of carbon, hydrogen and oxygen in one mole of ethanol (C_2H_5OH).

Solution: Using the atomic weights (molar masses) of these three elements, we have

carbon: (2 mol)(12.0 g mol^{-1}) = 24 g of C
hydrogen: (6 mol)(1.01 g mol^{-1}) = 6 g of H
oxygen: (1 mol)(16.0 g mol^{-1}) = 16 g of O

The ***mass fraction*** of an element in a compound is just the ratio of the mass of that element to the mass of the entire formula unit. Mass fractions are always between 0 and 1, but are frequently expressed as percent.

Problem Example 8: ***mass fraction and mass percent of an element in a compound***

Find the mass fraction and mass percentage of oxygen in ethanol (C_2H_5OH)

Solution: Using the information developed in the preceding example, the molar mass of ethanol is (24 + 6 + 16)g mol^{-1} = 46 g mol^{-1}. Of this, 16 g is due to oxygen, so its mass fraction in the compound is (16 g)/(46 g) = 0.35 which corresponds to 35%.

Finding the **percentage composition** of a compound from its formula is a fundamental calculation that you must master; the technique is exactly as shown above. Finding a mass fraction is often the first step in solving related kinds of problems:

Problem Example 9: ***mass of an element in a given mass of compound***

How many tons of potassium are contained in 10 tons of KCl?

Solution: The mass fraction of K in KCl is 39.1/74.6=.524; 10 tons of KCl contains(39.1/74.6) × 10 tons of K, or **5.24 tons** of K. (Atomic weights: K = 39.1, Cl = 35.5.)

Note that there is no need to deal explicitly with moles, which would require converting tons to kg.

Problem Example 10: *mass of compound containing given mass of an element*

How many grams of KCl will contain 10 g of potassium?

Solution: The mass ratio of KCl/K is 74.6 ÷ 39.1; 10 g of potassium will be present in (74.6/39.1) × 10 grams of KCl, or **19 grams**.

Mass ratios of two elements in a compound can be found directly from the mole ratios that are expressed in formulas.

Problem Example 11: ***Mass ratio of elements from formula***

Molten magnesium chloride ($MgCl_2$) can be decomposed into its elements by passing an electric current through it. How many kg of chlorine will be released when 2.5 kg of magnesium is formed? (Mg = 24.3, Cl = 35.5)

Solution: *Solution*: The mass ratio of Cl/Mg is (35.5 ×2)/24.3, or 2.9; thus 2.9 kg of chlorine will be produced for every kg of Mg, or (2.9 × 2.5) = 7.2 kg of chlorine for 2.5 kg of Mg
(Note that is is not necessary to know the formula of elemental chlorine (Cl_2) in order to solve this problem.)

Simplest formulas from experimental data

As was explained above, the ***simplest formula*** (***empirical formula***) is one in which the relative numbers of the various elements are expressed in the smallest possible whole numbers. Aluminum chloride, for example, exists in the form of structural units having the composition Al_2Cl_6; the simplest formula of this substance is $AlCl_3$.

Simplest formulas from atom ratios

Some methods of analysis provide information about the relative numbers of the different kinds of atoms in a compound.

The process of finding the formula of a compound from an analysis of its composition depends on your ability to recognize the decimal equivalents of common integer ratios such as 2:3, 3:2, 4:5, etc.

Problem Example 12: ***Simplest formula from mole ratio***

Analysis of an aluminum compound showed that 1.7 mol of Al is combined with 5.1 mol of chlorine. Write the simplest formula of this compound.

Solution: The formula $Al_{1.7}Cl_{5.1}$ expresses the relative numbers of moles of the two elements in the compound. It can be converted into the simplest formula by dividing both subscripts by the smaller one, yielding $\mathbf{AlCl_3}$.

Simplest formulas from mass composition

More commonly, an arbitrary mass of a compound is found to contain certain masses of its elements. These must be converted to moles in order to find the formula.

Problem Example 13: ***Simplest formula from combustion masses***

When 10.0 g of a certain organic compound containing only C, H, and O undergoes combustion in the presence of excess O_2, 9.56 g of CO_2 and 3.92 g of H_2O are formed. Find the simplest formula of this substance.

Solution: Begin by calculating the moles of the two combustion products:
CO_2: (9.56 g) / (44 g mol^{-1}) = .217 mol
H_2O: (3.92 g) / (18 g mol^{-1}) = .218 mol (containing 2 × .218 mol = .436 mol of hydrogen.)

We can now write a preliminary formula of the compound as $C_{.217}H_{.436}O_x$, leaving the value of x to be determined. The easiest way to do this is by calculating the difference between the 10.0-g mass of the unknown compound and the total mass of carbon plus hydrogen in the combustion products. The latter quantities work out as follows: C: (.217 mol × 12 g mol^{-1}) = 2.60 g; H: (.436 mol × 1.01 g mol^{-1}) = .440 g. The mass of oxygen in the compound is (10.0 g) â€“ (.440 + 2.60) g = 6.96 g, corresponding to (6.96 g / 16 g mol^{-1}) = .435 mol. Inserting this quantity into the preliminary formula gives $C_{.217}H_{.436}O_{.435}$. Allowing for experimental- and roundoff error, this reduces to $\mathbf{CH_2O_2}$.

Comment: This problem may at first seem very complicated, but it's really just a combination of a number of almost trivially-simple calculations, carried out in a logical sequence. Your ability to construct this sequence is an essential part of solving practical problems of these kinds. it's worth taking the time to work through this exerciset on your own, perhaps starting with 5.0 g of the compound, which will produce proportionally smaller quantites of products.

Problem Example 14: ***Simplest formula from element masses***

A 4.67-g sample of an aluminum compound was found to contain 0.945 g of Al and 3.72 g of Cl. Find the simplest formula of this compound. Atomic weights: Al = 27.0, Cl=35.45.

Solution: The sample contains (.945 g)/(27.0 g mol^{-1}) = .035 mol of aluminum and (3.72 g)(35.45) = 0.105 mol of chlorine. The formula $Al_{.035}Cl_{.105}$ expresses the relative numbers of moles of the two elements in the compound. It can be converted into the simplest formula by dividing both subscripts by the smaller one, yielding **$AlCl_3$**.

Simplest formulas from mass ratios

The composition of a binary (two-element) compound is sometimes expressed as a mass ratio. The easiest approach here is to treat the numbers that express the ratio as masses, thus turning the problem into the kind described immediately above.

Problem Example 15: *Simplest formula from element mass ratio*

A compound composed of only carbon and oxygen contains these two elements in a mass ratio C:H of 0.375. Find the simplest formula.

Solution: Express this ratio as 0.375 g of C to 1.00 g of O.

moles of carbon: (.375 g)/(12 g/mol) = .03125 mol C;
moles of oxygen: (1.00 g)/(16 g/mol) = .0625 mol O
mole ratio of C/O = .03125/.0625 = 0.5;
this corresponds to the formula $C_{0.5}O$, which we express in integers as **CO_2**.

Simplest formulas from percent composition

The composition-by-mass of a compound is most commonly expressed as weight percent (grams per 100 grams of compound). The first step is again to convert these to relative numbers of moles of each element in a fixed mass of the compound. Although this fixed mass is completely arbitrary (there is nothing special about 100 grams!), the *ratios* of the mole amounts of the various elements are not arbitrary: these ratios must be expressible as integers, since they represent ratios of integral numbers of atoms.

Problem Example 16: *Simplest formula from mass-percent composition*

Find the simplest formula of a compound having the following mass-percent composition. Atomic weights are given in parentheses.

36.4 % Mn (54.9), 21.2 % S (32.06), 42.4 % O (16.0)

Solution: 100 g of this compound contains:

Mn: (36.4 g) / (54.9 g mol^{-1}) = 0.663 mol
S: (21.2 g) / (32.06 g mol^{-1}) = 0.660 mol
O: (42.4 g) / (16.0 g mol^{-1}) = 2.65 mol

The formula $Mn_{.663}S_{.660}O_{2.65}$ expresses the relative numbers of moles of the three elements in the compound. It can be converted into the simplest formula by dividing all subscripts by the smallest one, yielding $Mn_{1.00}S_{1.00}O_{4.01}$ which we write as **$MnSO_4$**.

Note: because experimentally-determined masses are subject to small errors, it is usually necessary to neglect small deviations from integer values.

Problem Example 17: *Simplest formula from mass-percent composition*

Find the simplest formula of a compound having the following mass-percent composition. Atomic weights are given in parentheses.

27.6 % Mn (54.9), 24.2 % S (32.06), 48.2 % O (16.0)

Solution: A preliminary formula based on 100 g of this compound can be written as

$Mn_{(27.6 / 54.9)} S_{(24.2 / 32.06)} O_{(42.4 / 16.0)}$ or $Mn_{.503} S_{.754} O_{3.01}$

Dividing through by the smallest subscript yields $Mn_1 S_{1.5} O_6$. Inspection of this formula suggests that multiplying each subscript by 2 yields the all-integer formula $\mathbf{Mn_2S_3O_{12}}$.

More on elemental analysis

Elemental analysis in the laboratory

One of the most fundamental operations in chemistry consists of breaking down a compound into its elements (a process known as *analysis*) and then determining the simplest formula from the relative amounts of each kind of atom present in the compound. In only a very few cases is it practical to carry out such a process directly: thus heating mercury(II) sulfide results in its direct decomposition: $2\,HgS \rightarrow 2Hg + O_2$. Similarly, electrolysis of water produces the gases H_2 and O_2 in a 2:1 volume ratio.

Most elemental analyses must be carried out indirectly, however. The most widely used of these methods has traditionally been the *combustion analysis* of organic compounds. An unknown hydrocarbon $C_aH_bO_c$ can be characterized by heating it in an oxygen stream so that it is completely decomposed into gaseous CO_2 and H_2O. These gases are passed through tubes containing substances which absorb each gas selectively. By careful weighing of each tube before and after the combustion process, the values of *a* and *b* for carbon and hydrogen, respectively, can be calculated. The subscript *c* for oxygen is found by subtracting the calculated masses of carbon and hydrogen from that of the original sample.

Right: Illustration from Mark Bishop's *An Introduction to Chemistry: an online textbook*.
This page also contains detailed examples of empirical formula calculations.

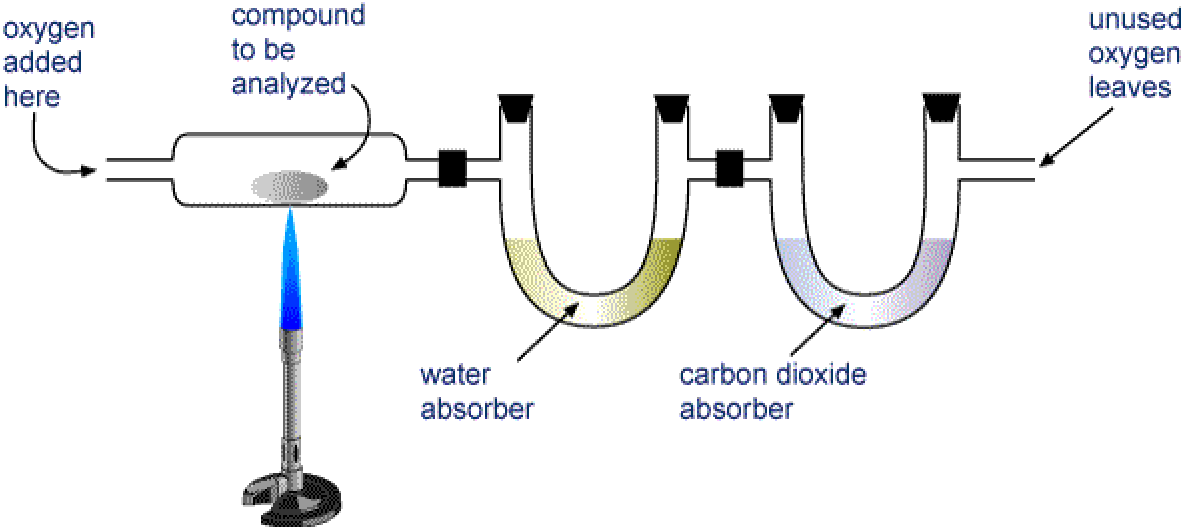


Figure 3.5 Combustion Analysis Experiment

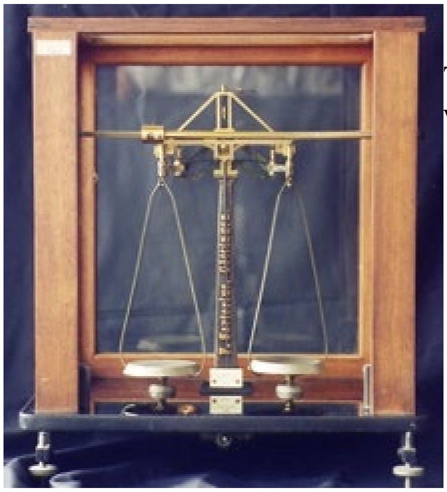
Figure 3.6 Combustion Analysis Instrument

← Since the 1970s, it has been possible to carry out combustion analyses with automated equipment. This one can also determine nitrogen and sulfur.

For analyses of compounds containing elements other than C, H, and O, spectroscopic methods based on atomic absorption and inductively-coupled plasma atomic absorption are now widely used.

The analytical balance

Measurements of mass or weight have long been the principal tool for understanding chemical change in a quantitative way. Balances and weighing scales have been in use for commercial and pharmaceutical purposes since the beginning of recorded history, but these devices lacked the 0.001-g precision required for quantitative chemistry and elemental analysis carried out on the laboratory scale.



The classic equal-arm analytical balance and set of calibrated weights

Figure 3.7 Equal arm Balance

Figure 3.8 Weights for Balance

> It was not until the mid-18th century that the Scottish chemist Joseph Black invented the *equal arm **analytical balance***. The key feature of this invention was a lightweight, rigid beam supported on a knife-edged fulcrum; additional knife-edges supported the weighing pans. The knife-edges greatly reduced the friction that limited the sensitivity of previous designs; it is no coincidence that accurate measurements of combining weights and atomic weights began at about this time.

Analytical balances are enclosed in a glass case to avoid interference from air currents, and the calibrated weights are handled with forceps to prevent adsorption of moisture or oils from bare fingers.

Anyone who was enrolled in college-level general chemistry up through the 1960's will recall the training (and tedium) associated with these devices. These could read directly to 1 milligram and allow estimates to ±0.1 mg. Later technical refinements added magnetic damping of beam swinging, pan brakes, and built-in weight sets operated by knobs. The very best research-grade balances achieved precisions of 0.001 mg.

Beginning in the 1970's, **electronic balances** have come into wide use, with single-pan types being especially popular. A single-pan balance eliminates the need for comparing the weight of the sample with that of calibrated weights. Addition of a sample to the pan causes a displacement of a *load cell* which generates a compensating electromagnetic field of sufficient magnitude to raise the pan to its original position. The current required to accomplish this is sensed and converted into a weight measurement. The best research-grade electronic balances can read to 1 microgram, but 0.1-mg sensitivities are more common for student laboratory use.

Figure 3.9 Digital Analytical balance

An empirical formula expresses the relative ratios of the atoms in a compound or a molecule. The ratio of the atoms within the compound and molecule is held for the atomic level as well the molar level.

$MgCl_2$ is made of 1 atom of Mg (magnesium atom) and 2 atoms of Cl (chlorine atom) → (atomic level)

$MgCl_2$ is made of 1.0 mole of Mg and 2.0 moles of Cl → (molar level)

Knowing the molar ratio of each element within a molecule or a compound, one can determine the empirical formula of such molecule or compound.

Steps how to calculate the empirical formula from known mass percent (%):can be seen below:

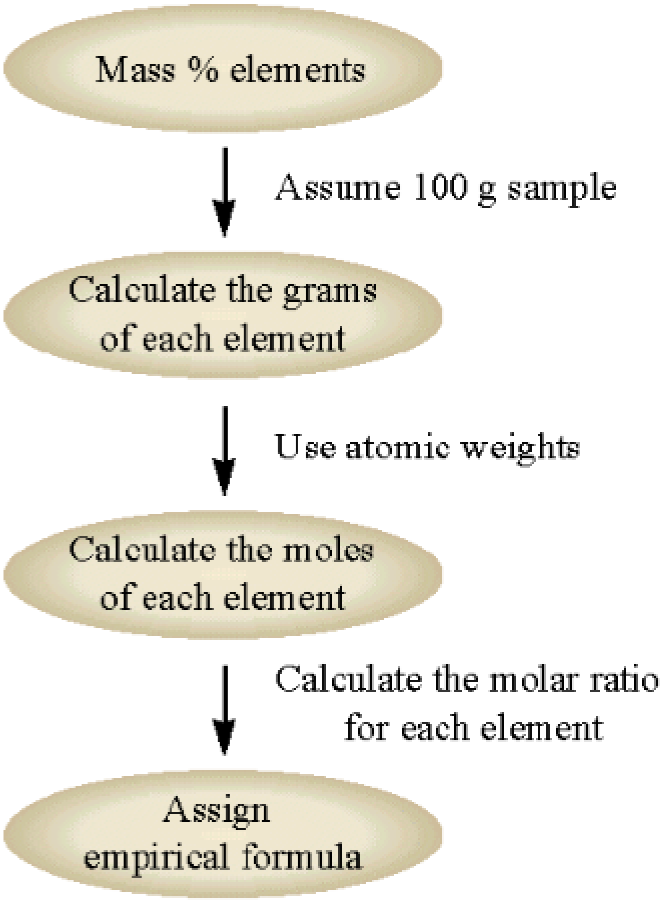
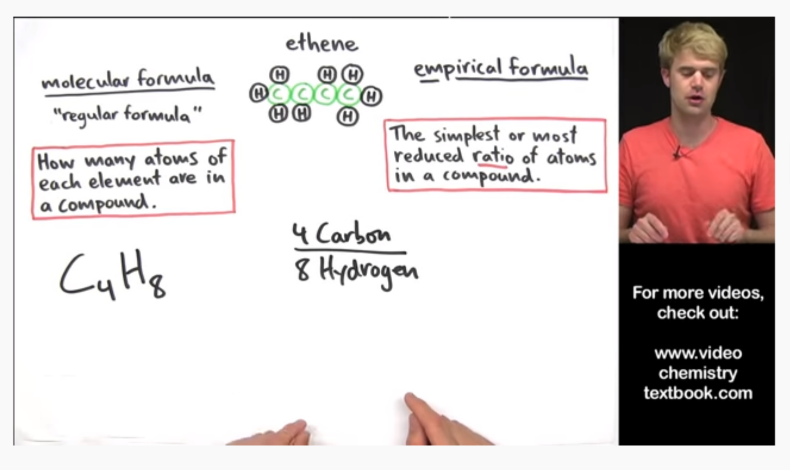


Figure 3.10 Concept Map for Empirical Formula Determination

Reference:
https://chem.libretexts.org/Courses/Heartland_Community_College/HCC%3A_Chem_161/3%3A_Chemical_Reactions_and_Quantities/3.4%3A_Determing_an_Empirical_and_Molecular_Formula#:~:text=Chemical%20formulas%20tell%20you%20how,same%20as%20the%20chemical%20formula.

The videos below illustrates with examples the concept of the empirical formula:



ethene

molecular formula

"regular formula"

How many atoms of each element are in a compound.

C_4H_8

empirical formula

The simplest or most reduced ratio of atoms in a compound.

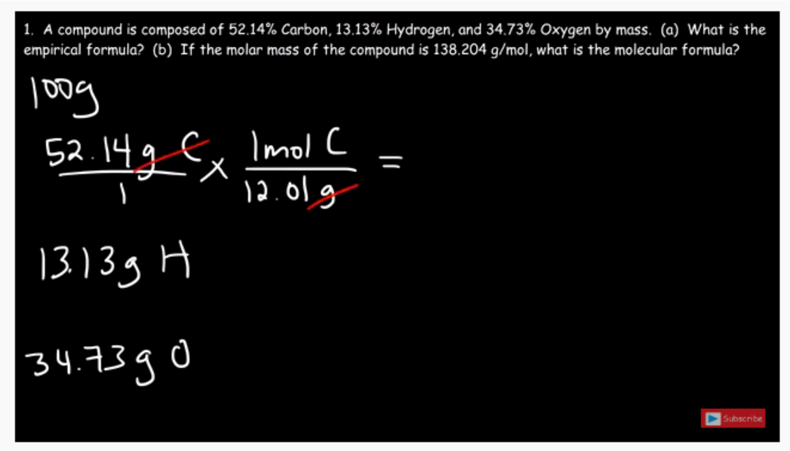
4 Carbon

8 Hydrogen

For more videos, check out:

www.video chemistry textbook.com

https://www.youtube.com/watch?v=wnRaBWvhYKY



1. A compound is composed of 52.14% Carbon, 13.13% Hydrogen, and 34.73% Oxygen by mass. (a) What is the empirical formula? (b) If the molar mass of the compound is 138.204 g/mol, what is the molecular formula?

100g

$$\frac{52.14\,\cancel{g}\,\cancel{C}}{1} \times \frac{1\,mol\,C}{12.01\,\cancel{g}} =$$

13.13g H

34.73g O

https://www.youtube.com/watch?v=JeSSucG-CVw

Calculation of the percent composition from the molecular formula:

Examples:

Calculate the % composition in 3 significant figures:

1. the percent composition of ammonia, NH_3
2. the percent composition of $Na_2S_2O_3$
3. Determine the percent water in $CuSO_4 \cdot 5H_2O$ to three significant figures.

1.The percent composition of ammonia, NH_3

First one has to determine the molar mass of the NH_3 which is:
1N + 3H = [1x 14.0] g/mole + [3 x 1.00] g/mole = 17.0 g/mole

N% = { [1 x 14.0 g/mole] / [17.0 g/mole] } x 100% = 82.4 %
H% = { [3 x 1.00 g/mole] / [17.0 g/mole] } x 100% = 17.6 %

2.The percent composition of $Na_2S_2O_3$

First one has to determine the molar mass of the $Na_2S_2O_3$ which is:

[2 Na + 2 S + 3 O] = [2 x 23.0] g/mole + [2 x 32.0] g/mole + [3 x 16.0] g/mole = 158.0 g/mol

Na% = { [2 x 23.0 g/mole] / [158.0 g/mole] } x 100% = 29.1%
S% = { [2 x 32.0 g/mole] / [158.0 g/mole] } x 100% = 40.5%
O% = { [3 x 16.0 g/mole] / [158.0 g/mole] } x 100% = 30.4 %

3.Determine the percent water in $CuSO_4{\cdot}5H_2O$ to three significant figures.

First one has to determine the molar mass of the $CuSO_4{\cdot}5H_2O$ which is:
$CuSO_4$ molar mass:

[1 Cu + 1 S + 4 O] = [1 x 63.5 g/mole] + [1 x 32.0 g/mole] + [4 x 16.0 g/mole] = 159.6 g/mole

5 H_2O molar mass:

5 x [2 H + 1 O] = 5{ [2 x 1.00 g/mole] + [1 x 16.0 g/mole] } = 5 x 18.0 g/mole = 90.0 g/mole

Total molar mass of $CuSO_4{\cdot}5H_2O$ = [159.6 g/mole + 90.0 g/mole] = 249.6 g/mole

H_2O% = { [90.0 g/mole] / [249.6 g/mole] } x 100% = 36.1 %

Calculation of the percent composition from the masses of the elements:

Example:

A 24.81-g sample of a gaseous compound containing only carbon, oxygen, and chlorine is determined to contain 3.01 g C, 4.00 g O, and 17.81 g Cl. What is this compound's percent composition?

C% = { [3.01 g C] / [24.81 g compound] } x 100% = 12.1 %

O% = { [4.00 g O] / [24.81 g compound] } x 100% = 16.1%

Cl% = { [17.81 g Cl] / [24.81 g compound] } x 100% = 71.8%

How to Calculate the Empirical Formula from the mass percent of each element or actual mass of each element:

Example:

Chloroform has percent composition of chloroform is 10.06% carbon, 0.85% hydrogen, and 89.09% chlorine. Determine its empirical formula

1. **Assume that the sample 100 g (corresponds to 100%):**

Then:

1. C = 10.06 g
2. H = 0.85 g
3. Cl = 89.09 g

2. **Convert numbers of grams of each into moles by dividing the grams by the atomic mass of each element in the molecule or the compound:[use 3 significant figures]**

C = 10.06 g / [1 mole / 12.0 g] = 0.838 moles

H = 0.85 g / [1 mole / 1.00 g] = 0.850 moles

Cl = 89.09 g / [1 mole / 35.5 g] = 2.51 moles

3. **Divide number of moles of each element by the smallest number of moles [in this problem 0.838 moles is the smallest number of moles]:**

C = 0.838 moles / 0.838 moles = 1.00

H = 0.850 moles / 0.838 moles = 1.01 rounded as 1.00

Cl = 2.51 moles / 0.838 moles = 2.995 = rounded as 3.00

4. **The empirical formula is $C_1H_1Cl_3$ or $CHCl_3$ [Chloroform]**

Example:

3.23 g of a compound has 0.728 grams of phosphorous and 2.50 grams chlorine. What is the empirical formula of this compound?

Convert the grams of each element into moles by dividing each element by its atomic mass:

P = 0.728 g / [mole / 31.0 g] = 0.0235 moles [3 sig. figs]

Cl = 2.50 g / [mole / 35.5 g] = 0.0704 moles [3 sig. figs]

The ratio of the elements within this compound is:

$\mathbf{P_{0.0235}Cl_{0.0704}}$

Divide by smallest number of moles:

P = 0.0235 moles / 0.0235 moles = 1.00

Cl = 0.0704 moles / 0.0235 moles = 2.995 = 3.00

The empirical formula of this compound is:

P_1Cl_3 or PCl_3

Calculating Molecular Formulas for a Compound by Using its Empirical Formula

What is the difference between Empirical Formula and Molecular Formula?

Empirical Formula: The smallest whole number ratio of elements within a compound or a molecule or a formula unit (ion).

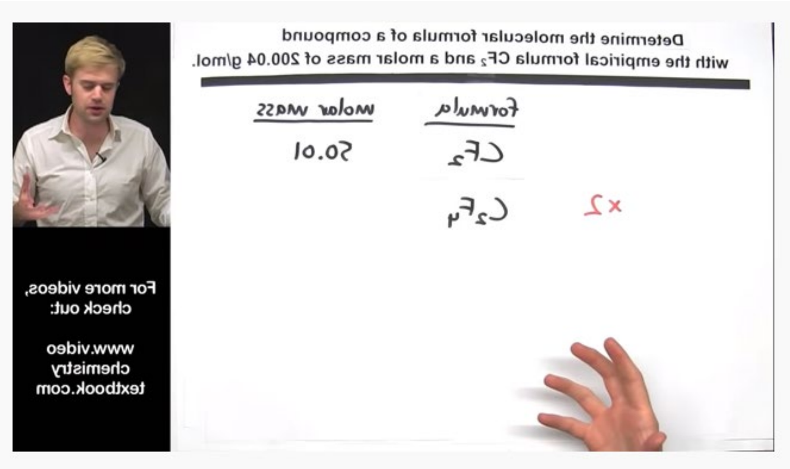
Molecular Formula: The actual number of the atoms of each element within a compound or a molecule or a formula unit (ion).

The relationship between Molecular Formula (molar mass) and Empirical Formula (empirical formula mass) is given below:

$$\frac{\text{molecular or molar mass}\left(\text{amu or }\dfrac{\text{g}}{\text{mol}}\right)}{\text{empirical formula mass}\left(\text{amu or }\dfrac{\text{g}}{\text{mol}}\right)} = n\ \text{formula units/molecule}$$

Molecular or molar mass (amu or g/mole) =[n formula units/molecule] x [empirical formula mass (amu or g/mole]

The video below illustrates this relationship:



Determine the molecular formula of a compound with the empirical formula CF_2 and a molar mass of 200.04 g/mol.

https://www.youtube.com/watch?v=J_MtVs0aBdU

Example:

The empirical formula of hexane C_3H_7. The molecular weight is 86.2 amu.

What is the molecular formula of hexane?

Empirical formula weight of hexane C_3H_7 = 3 C + 7 H = [3 x 12.0] + [7 x 1.00] = 43.0 amu.

Following the formula given above:

86.2 amu / 43.0 amu = n = 2.00

Molecular formula = 2 x [C_3H_7] = C_6H_{14}

Example:

Reference: http://www.chem.uiuc.edu/rogers/Text6/Tx65/tx65fr.html

The compound dioxane contains only carbon, hydrogen, and oxygen. When 0.956 g dioxane is burned, 1.91 g carbon dioxide and 0.782 g water are formed. In another experiment, it was determined that 6.04x10-3 mol dioxane weighs 0.532 g. What is the molecular formula of dioxane?

1. Calculate the mass of carbon, hydrogen, and oxygen in 0.956 g dioxane.

$$?\text{ g C} = 1.91\text{ g }CO_2 \times \frac{1\text{ mol }CO_2}{44.0\text{ g }CO_2} \times \frac{1\text{ mol C}}{1\text{ mol }CO_2} \times \frac{12.0\text{ g C}}{1\text{ mol C}} = 0.521\text{ g C}$$

$$?\text{ g H} = 0.782\text{ g }H_2O \times \frac{1\text{ mol }H_2O}{18.0\text{ g }H_2O} \times \frac{2\text{ mol H}}{1\text{ mol }H_2O} \times \frac{1.0\text{ g H}}{1\text{ mol H}} = 0.087\text{ g H}$$

$$?\text{ g O} = 0.956\text{ g dioxane} - 0.521\text{ g C} - 0.087\text{ g H} = 0.348\text{ g O}$$

2. Using the data from step 1 above, calculate the empirical formula of dioxane.

$$?\text{ g mol C} = 0.521\text{ g C} \times \frac{1\text{ mol C}}{12.01\text{ g C}} = 0.043\text{ mol C}$$

$$?\text{ g mol H} = 0.087\text{g H} \times \frac{1\text{ mol H}}{1.008\text{ g H}} = 0.087\text{mol H}$$

$$?\text{ g mol O} = 0.348\text{ g O} \times \frac{1\text{ mol O}}{12.01\text{ g O}} = 0.022\text{ mol O}$$

The empirical formula is:

$C_{0.043}H_{0.087}O_{0.022}$

3. Calculate the molecular weight of dioxane.

$$\text{Molecular weight} = \frac{\text{grams}}{\text{mole}} = \frac{0.532 \text{ g dioxane}}{6.04 \times 10^{-3} \text{ mol dioxane}} = 88.1 \text{ g/mol}$$

4. Calculate the molecular formula of dioxane.

The empirical formula weight is 2(12.0) + 4(1.01) + 16.0 = 44.0. The molecular weight is 88.08. The ratio of molecular weight to empirical weight is:

$$\frac{\text{Molecular weight}}{\text{Empirical weight}} = \frac{88.0}{44.0} = 2$$

Thus the molecular of dioxane formula is: $C_4H_8O_2$.

Example:

The compound ethylene glycol is often used as an antifreeze. It contains 38.7% carbon, 9.75% hydrogen, and the rest oxygen. The molecular weight of ethylene glycol is 62.07 g. What is the molecular formula of ethylene glycol?

1. Calculate the empirical formula. Assume 100 g of the compound, which will contain 38.70 g carbon, 9.75 g hydrogen and the rest oxygen

? g O = 100 g - 38.70 g C - 9.75 g H = 51.55 g O.

2. Calculate the moles of each element present:

$$? \text{ g mol C} = 38.70 \text{ g C} \times \frac{1 \text{ mol C}}{12.01 \text{ g C}} = 3.22 \text{ mol C}$$

$$? \text{ g mol H} = 9.75 \text{ g H} \times \frac{1 \text{ mol H}}{1.008 \text{ g H}} = 9.67 \text{ mol H}$$

$$? \text{ g mol O} = 51.55 \text{ g O} \times \frac{1 \text{ mol O}}{12.01 \text{ g O}} = 3.22 \text{ mol O}$$

3. Next calculate the ratio of molecular weight to empirical formula weight. The molecular weight is given. The empirical formula is CH3O, so the empirical formula weight is 12.01 + 3(1.008) + 16.00 = 31.03.

$$\frac{\text{molecular weight}}{\text{empirical formula weight}} = \frac{62.07}{31.03} = 2$$

Therefore the molecular formula is twice the empirical formula: $C_2H_6O_2$

III. Solution's Different Concentrations

Introducing solutions

Solutions are ***homogeneous*** (single-phase) mixtures of two or more ***components***. For convenience, we often refer to the majority component as the ***solvent***; minority components are ***solutes***. But there is really no fundamental distinction between them.

Solutions play a very important role in Chemistry because they allow intimate and varied encounters between molecules of different kinds, a condition that is essential for rapid chemical reactions to occur. Several more explicit reasons can be cited for devoting a significant amount of effort to the subject of solutions:

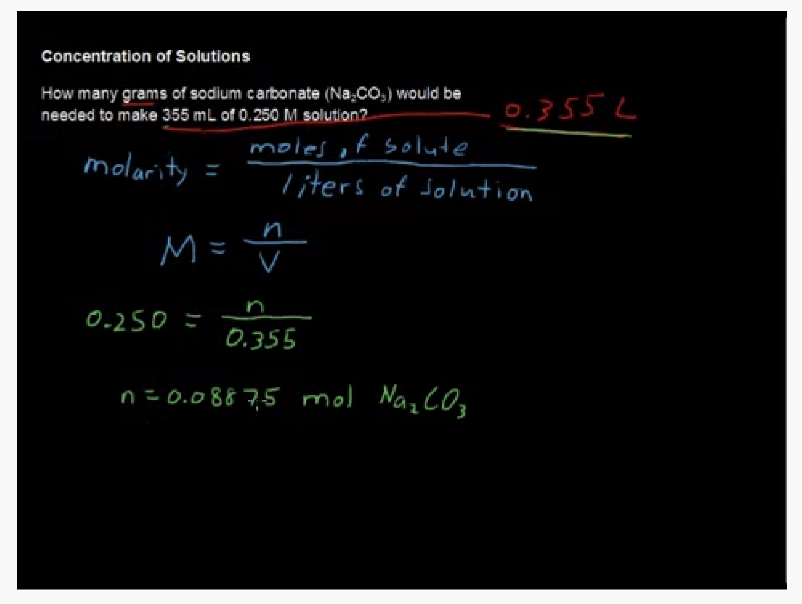
- For the reason stated above, most chemical reactions that are carried out in the laboratory and in industry, and that occur in living organisms, take place in solution.
- Solutions are so common; very few pure substances are found in nature.
- Solutions provide a convenient and accurate means of introducing known small amounts of a substance to a reaction system. Advantage is taken of this in the process of titration, for example.
- The physical properties of solutions are sensitively influenced by the balance between the intermolecular forces of like and unlike (solvent and solute) molecules. The physical properties of solutions thus serve as useful experimental probes of these intermolecular forces.

We usually think of a solution as a liquid made by adding a gas, a solid or another liquid *solute* in a liquid *solvent*. Actually, solutions can exist as gases and solids as well. Gaseous mixtures don't require any special consideration. Solid solutions are very common; most natural minerals and many metallic alloys are solid solutions.

Still, it is liquid solutions that we most frequently encounter and must deal with. Experience has taught us that sugar and salt dissolve readily in water, but that oil and water don't mix. Actually, this is not strictly correct, since all substances have at least a slight tendency to dissolve in each other. This raises two important and related questions: why do solutions tend to form in the first place, and what factors limit their mutual solubilities? These questions will be answered in Chem II course but here we will discuss the concentration and reactions of aqueous solutions.

2 How solution concentrations are expressed

Concentration is a general term that expresses the quantity of solute contained in a given amount of solution. Various ways of expressing concentration are in use; the choice is usually a matter of convenience in a particular application. You should become familiar with all of them.



Concentration of Solutions

How many grams of sodium carbonate (Na_2CO_3) would be needed to make 355 mL of 0.250 M solution?

$0.355\ L$

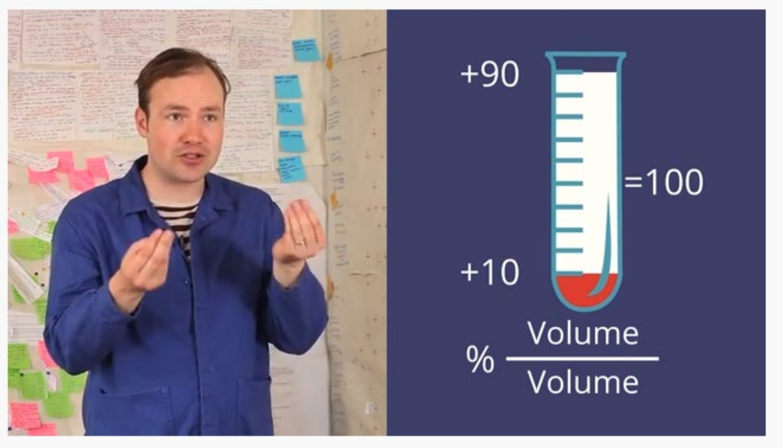
$$\text{molarity} = \frac{\text{moles of solute}}{\text{liters of solution}}$$

$$M = \frac{n}{V}$$

$$0.250 = \frac{n}{0.355}$$

$$n = 0.08875\ \text{mol}\ Na_2CO_3$$

https://www.youtube.com/watch?v=UMPyExRPsuw



https://www.youtube.com/watch?v=yuGNzipRXE4

The concentration of a solution is referred to as the ratio of the solute amount to the amount of the solution (or a solvent in some specific cases).

The below is the table summarizing all types of concentrations formulas used in this chapter

Name of the Concentration	Formula	Unit of solute	Unit of solution (solvent)	Overall unit of the formula

(Mass/volume)%	={[mass of the solute]/[volume of the solution]} x100%	Grams (g)	Milliliters (mL)	[g/mL]%
(Mass/mass)% or mass%	=[mass of the solute]/[mass of the solution]x100% Note that: Mass of solution = mass of solute + mass of solvent	Grams (g)	Grams (g)	[g/g]%
(Volume/volume)% or volume%	=[volume of the solute]/[volume of the solution]x100% Note that: Volume of the solution = volume in solute + volume of the solvent	Milliliters (mL)	Milliliters (mL)	[mL/mL]%
(Molarity)	= [moles of the solute]/[liter of solution]	Moles (mol)	Liter (L)	[mol/L] Also can be expressed as M or molar
(Molality)	= [moles of the solute]/[Kilogram of solvent	Moles (mol)	Kilogram (kg)	[mol/kg] Also can be expressed as m or molal
Equivalent molarity of the electrolytes	= [milliequivalents/Liter of solution]	Milliequivalents (mEq)	Liter (L)	[mEq/L]
Dilution	$C_1xV_1 = C_2xV_2$ or sometimes is given in: $M_1xV_1=M_2xV_2$ Where C_1 and M_1 are the concentration and the molarity of the stock solution respectively. C_2 and $M_2$are the concentration and molarity of the diluted solution respectively V_1 is the volume of the stock solution and V_2 is the volume of diluted solution	Moles (mol)	Liter (L)	[mol/L] Also can be expressed as M or molar
Part per million (ppm) Part per billion (ppb)	ppm = {[mass of solute] / [mass of solution]} x 1 x 10^6	ppm ppb		

	ppb = {[mass of solute] / [mass of solution]} x 1 x 10^9			

Let us now go over some workout problems in some details covering all the formulas.

1. (Mass/volume)%

a. What is the mass/volume percent by of a solution formed by mixing 25.0 grams of sodium chloride NaCl with 455 mL of water?

Solution:

(Mass/volume)% = {[mass of the solute]/[volume of the solution]} x100%

= {[25.0 g NaCl] / [455 mL solution]} x100% = 5.494505494505495%
(answer from calculator and it should be rounded off to the correct significant figures which is 3.

Final answer after the significant figures rule consideration is 5.50% (g/mL %)

b. Calculate amount of grams of solute potassium nitrate aqueous solution which is 38.5% (mass/mL%) if the solution made with 1.00 Liter of water.

Solution:

Let us set up the formula and replacing it with the given data:

(Mass/volume)% = {[mass of the solute]/[volume of the solution]} x100%

First the volume should be converted from Liter into milli Liter (mL)

[38.5 g/mL]% = { [X] / [1000 mL] } x 100%

Cross x Multiply

[38.5 g/mL] / [100] = [X] / [1000 mL]

X = 385 g potassium nitrate KNO_3

Verifying the answer:

(Mass/volume)% = {[mass of the solute]/[volume of the solution]} x100%

= [385 g / 1000 mL] x100% = (38.5 g/mL)%

Conclusion the answer is correct.

2. (Mass/mass)% or mass%

   a. A solution is formed by adding 48 g of Lithium sulfate to 250 g of water. What is the percent by mass of Lithium sulfate?

(Mass/mass)% or mass% = [mass of the solute]/[mass of the solution]x100%

Note that:

Mass of solution = mass of solute + mass of solvent

(Mass/mass)% = {[48 g of Lithium sulfate] /[48 g of Lithium sulfate + 250 g water]} x 100%

= 16.10738255033557% from calculator and it should be rounded off to the correct significant figures

Final answer = 16% [g/g]%

b. What is the mass of solvent (water) in grams for a solution made of 10.5% mass percent of each component in the mixture formed by adding 2.00 g of Aluminum nitrate in water?

(Mass/mass)% or mass% =[mass of the solute]/[mass of the solution]x100%

Note that:

Mass of solution = mass of solute + mass of solvent

Mass of the whole solution is not known and it will be referred to as X

[10.5 / 100] = [2.00 g Aluminum nitrate] / [X]

Cross / Multiply:

[0.105] * [X] = 2.00

X = [2.00 /0.105] = 19.04761904761905 = 19.0

X = amount of water in grams = 19.0 – 2.00 = 17.0 grams water

Verifying the answer:

[Mass/mass]% = [2.00 /(2.00 + 17.0)] x 100% = 10.52631578947368% = 10.5%

The answer is correct.

3. (Volume/volume)% or volume%

a. What is the percent by volume of a solution formed by added 25 L of ethanol to 155 L of water?

(Volume/volume)% or volume% = [volume of the solute]/[volume of the solution]x100%

Note that:

Volume of the solution = volume in solute + volume of the solvent

(Volume/volume)% = [25 L] /[25L + 155 L] x 100 % = [25 L] / [180 L] = 13.88888888888 %. The answer is from calculator and it should be rounded off to the correct significant figures

Final answer is 14 % (two significant figures).

b. A 5.50% volume percent solution is made by adding certain amount of volume of a solute acetone to 255 mL water as solvent. Calculate the amount of the acetone in mL added.

(Volume/volume)% or volume% = [volume of the solute]/[volume of the solution]x100%

Note that:

Volume of the solution = volume in solute + volume of the solvent

Amount of the solute is unknown and it will be referred to as X

5.50% = [X] / [X + 255 mL]

0.0550 = [X] / [X + 255 mL]

0.0550 [X + 255 mL] = [X]

0.0550 X + (0.0550*255) = [X]

Solving for X

0.0550*255 = X – 0.0550 X = 0.945 X

X = 14.8 mL (3 significant figures)

Verifying the answer:

Volume/volume)% = { [14.8 mL] / [14.8 mL + 255 mL] } x 100% = 5.485544848035582 % rounded to 3 significant figures = 5.50 %. The answer is correct.

4. Molarity

Molarity = [moles of the solute]/[liter of solution]

a. Calculate the molarity of solution made by dissolving 35.0 grams of sodium chloride solid in 97890. mL distilled water.

Molarity = [moles of the solute]/[liter of solution]

First one has to calculate the number of moles of sodium chloride with given mass of 35.0 grams. Therefore, one has to use the molar mass of sodium chloride in calculating number of moles with given number of grams.

Molar mass of sodium chloride = NaCl using the atomic masses of Na and Cl, the molar mass is:

23.0 g/mole + 35.5 g/mol = 58.5 g/mol

Number of moles of sodium chloride = (35.0 g) / (58.5 g/mol) = 0.598 moles NaCl

Second one has to convert the mL into Liters by dividing by 1000 =(97890. mL) / (1L / 1000 mL) = 97.890 L

Molarity = [0.598 moles NaCl] / [97.890 L} = 0.006108897742363877 mol/L. This the calculator's answer and it will be rounded off to the correct significant figures (3 significant figures).

Molarity = 0.00611 mol/L or 0.00611 M or 0.00611 molar.

b. A solution of a molarity of 2.675 M is prepared by dissolving 8.50 gram of magnesium nitrate in certain amount of distilled water as a solvent. Calculate the amount of the distilled water.

First one has to calculate the number of moles of magnesium nitrate with given mass of 8.50 grams.

Therefore, one has to use the molar mass of magnesium nitrate in calculating number of moles with given number of grams.

Molar mass of magnesium nitrate = $Mg(NO_3)_2$ using the atomic masses of Mg and 2 (NO_3), the molar mass is: 24.3 g/mol + 2x (14.0 g/mol) + 2 (3 x 16.0 g/mol) =148.3 g/mol

Number of moles of magnesium nitrate = [8.50 g $Mg(NO_3)_2$] / [148.3 g $Mg(NO_3)_2$ / mol $Mg(NO_3)_2$]

Number of moles of magnesium nitrate = 0.0573 moles

2.675 M = 2.675 mol /L = [0.0573 mol] / [X]

X = amount of the solution or solvent in Liters

Solving for X, one can obtain:

2.675 X = 0.0573

X = 0.0573 / 2.675 = 0.02142056074766355 Liters. The correct rounded off answer has to have three significant figures. The final correct answer is 0.0214 Liters

Verifying the answer: = [0.0573 mol] / [0.0214 Liters] = 2.6775700934579439 = 2.678 mol/L

The answer is correct. Note that the verified answer is not exactly the given molarity of 2.675 mol/L. This is because of the in between rounding off and rounding off the atomic masses.

c. 10.00 x 10^{26} molecules of acetone dissolved to make 3500. mL of water of solvent. Calculate the molarity of acetone solution.

First one has to calculate the number of moles of acetone with given number of molecules.

Number of moles of acetone = [10.00 x 10^{26} molecules of acetone] x [1 mole acetone/6.022 x 10^{23} molecules of acetone]

One has to use the Avogadro's number of 6.022 x 10^{23} to calculate number of moles:

1 mole of acetone = 6.022 x 10^{23} molecules of acetone

Moles of acetone = 1660.577881102624 moles

The volume of solution is 3500. mL = 3.500 L (volume is converted into Liters)

Molarity = [1660.577881102624 moles] / [3.500 L] = 474.4508231721783 mol/L = 474.5 M or 474.5 mol/L or 474.5 molar.

The answer is rounded to the correct 4 significant figures.

5. Molality = [moles of the solute]/[Kilogram of solvent

a. What is the molality of a solution made of 9.384 grams of aluminum nitrate has been dissolved in 5500.0 g water

   First the number of moles of aluminum nitrate is calculated using the molar mass of aluminum nitrate.
   Molar mass of aluminum nitrate= $Al(NO_3)_3$ = Al + 3N + 9O = 27.0 g/mol + (3 x 14.0) g/mol + (9 x 16.0 g/mol) = 213.0 g/mol
   Number of moles = [9.384 grams of aluminum nitrate] / [mol aluminum nitrate /(= 213.0 g/mol)] = 0.04405633802816902 moles aluminum nitrate.

   Second to convert 5500.0 g water into kilo grams water by diving by 1000 = 5.500 kg water

   Molality = [0.04405633802816902 moles aluminum nitrate] / [5.500 kg water] = 0.008010243277848913 mol/kg. The answer should be rounded off to the correct significant figures of 4.
   The final correct answer is 0.008010 mol/kg or m or molal.

b. What mass of water is required to dissolve 45.0 grams calcium chloride to prepare a 2.50 m solution?

   First the number of moles of calcium chloride is calculated using the molar mass of calcium chloride.
   Molar mass of calcium chloride $CaCl_2$ = Ca + 2 Cl = 40.0 g/mol + 2x 35.5 g/mol = 111.0 g/mol
   Number of moles $CaCl_2$ = [45.0 g calcium chloride] / [111.0 g/mol] = 0.4054054054054054 moles = 0.405 moles $CaCl_2$

   Second the molality formula is used:

   2.50 m = [2.50 CaCl2 mol / kg water] = [0.405 moles $CaCl_2$] / X
   Where X is the amount of water

   Solving for X yields:
   X = 0.405 / 2.50 = 0.162 kg water

Verifying:

Molality = [0.405 moles $CaCl_2$] / [0.162 kg water] = 2.50 m

6. Equivalent molarity of the electrolytes

Milliequivalents (mEq) calculations are covered in greater details in the link below:

https://www.researchgate.net/file.PostFileLoader.html?id=546acea8d4c1182b638b473a&assetKey=AS:273639646138393@1442252184176

Milliequivalents calculations cover the three topics:

a. Converting milliequivalents to weight
b. Converting weight to milliequivalents
c. Converting milligrams% into milliequivalents

Each electrolyte such as Na^+ is measured in equivalent (Eq).For example 1 mole of an ionic compound of NaCl dissolved in water will produce 1 mole of Na^+ 1 mole of and Cl^-. Each Na^+ and Cl^- which equal to 1 equivalent each.

The table below illustrates the relationship between the electrolytes charge and number of the equivalents.

ion	Ion charge	Ion Oxidation number	Number of Equivalents per 1 mole
Li^+, Na^+, $K^+NH_4^+$	1+	+1	1 Eq
Mg^{2+}, Ca^{2+}, Ba^{2+}	2+	+2	2 Eq
Al^{3+}, Cr^{3+}, Fe^{3+}	3+	+3	3 Eq
Br^-, I^-, F^-	1-	-1	1 Eq
CO_3^{2-}, SO_4^{2-}	2-	-2	2 Eq
PO_4^{3-}	3-	+3	3 Eq

a. Converting milliequivalents to weight

What is the concentration of a solution contains 8.50 mEq/L of NaCl?

First the molar mass of NaCl should be calculated. NaCl molar mass is calculated in the above examples and it equals 58.5 g/mol

Second use the general formula for the calculation of the milligram/L from mEq/L:

Mg/L = [(mEq/L) x (atomic mass or molar mass)] / [number of the equivalent)

Mg/L = [(8.50 mEq/L) x (58.5 g /mol)] / [1 Eq/ 1 mol] = 497.25 mg / L

Final answer is 497 mg / L (3 significant figures).

b. Converting weight to milliequivalents

How many mEq of NaCl are in 10.5 g of NaCl?

First the molar mass of NaCl should be calculated. NaCl molar mass is calculated in the above examples and it equals 58.5 g/mol

Second use the setup that relates mEq to mass of electrolytes using molar mass:

mEq = {[10.5 g of NaCl] / [58.5 g NaCl/mol]} * [Eq /1 mol] * [1000 mEq/ 1Eq] = 179 mEq

c. Converting milligrams% into milliequivalents

Convert the expression 15.0 mg% of Ba^{2+} to mEq/L

Ba^{2+} atomic mass = 137.3 g/mol

Ba has 2+ ion and hence 2 Eq

Equivalent mass of Ba^{2+} = [137.3 g/mol] / [2 Eq/mol] = 68.65 g/Eq = 68.7 g per Eq

1mEq Ba^{2+} = [68.7 g] / [1 g/1000 mg] = 0.0687 mg

15.0 mg% = [15.0 mg Ba^{2+}] / [100 mL solvent] = [15.0 mg/ 100 mL]*[1000 mL/1L] = 150. mg/L

0.0687 mg/ 1 mEq = 150. mg/ X mEq

Solving for X = 150. / 0.0687 = 2183.406113537118 mEq/L rounded off to 2180 mEq/L (3 significant figures) or expressed in scientific notation 2.18 X 10^3 mEq/L

7. Dilution
   $C_1xV_1 = C_2xV_2$ or sometimes is given in:
   $M_1xV_1=M_2xV_2$
   Where C_1 and M_1 are the concentration and the molarity of the stock solution respectively.
   C_2 and $M_2$are the concentration and molarity of the diluted solution respectively
   V_1 is the volume of the stock solution and V_2 is the volume of diluted solution
   The stock solution is considered as the most concentrated solution.

Examples:

a. If 75.5 mL of water are added to 875.0 mL of a 0.125 M HNO_3 solution, what will be the new molarity of the diluted solution?
   $C_1xV_1 = C_2xV_2$
   Total volume = V_2 = 75.5 + 875.0 = 950.5 mL
   0.125 M x 875.0 mL = C_2 x 950.5 mL
   C_2 = [0.125 M x 875.0 mL] / [950.5 mL] = 0.115 M

b. If 500.0 mL are added to 0.150 M HCl solution until the final volume is 650.0 mL, what will be the molarity of the diluted solution?

$C_1xV_1 = C_2xV_2$
Total volume $= V_2 = 650.0$ mL
0.150 M x 500.0 mL $= C_2$ x 650.0 mL
$C_2 =$ [0. 0.150 M x 500.0 mL] / [650.0 mL] = 0.115 M

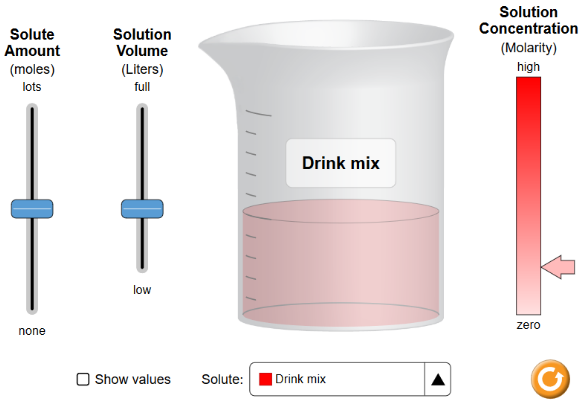
c. How much water should be added to 985 mL of a 6.55 M NaOH solution to make a 1.00 M solution?
$C_1xV_1 = C_2xV_2$
Total volume $= V_2 = X + 985$ mL
X = volume of water
6.55 M x 985 mL = 1.00 M x V_2
$V_2 =$ [6.55 M x 985 mL] / [1.00 M] = 6451.75 mL
X + 985 mL = 6451.75 mL
X = 5466.75 mL = 5470 mL rounded off to 3 significant figures

d. 450.5 mL of a 2.660 M KNO_3 solution. If one boils the water until the volume of the solution is half of its amount, what will be the molarity of the solution after the boiling?
$C_1xV_1 = C_2xV_2$
Total volume $= V_2 = 450.5/2$ mL = 225.3 mL
450.5 mL x 2.660 M $KNO_3 = C_2$ x 225.3 mL
$C_2 =$ [450.5 x 2.660] / [225.3] = 5.319 M [Boiling the stock solution had led to higher concentration of the new boiled solution]

After going over couple examples of the concentrations, let us look at some available simulation activities for the concentrations of the solution.

A Phet molarity simulation activity is given below:

https://phet.colorado.edu/sims/html/molarity/latest/molarity_en.html



In this simulation, the students will use the information below:

Solution volume is the combined volume of solute and water.

By design, not all solutions will reach saturation. The number of moles that can be added is limited to the range of 0.2-1.0 moles so that students can explore some solutions for the full concentration range (0-5 M).

Drink mix is assume to have the same solubility as sucrose.

Solubility of each solution listed was calculated at 25^0 C, except for $AuCl_3$ and Drink mix, which were based on data taken at 20^0 C.

Activity:

Determine the qualitative relationships between molarity, moles, and liters before completing quantitative problems or data collection.

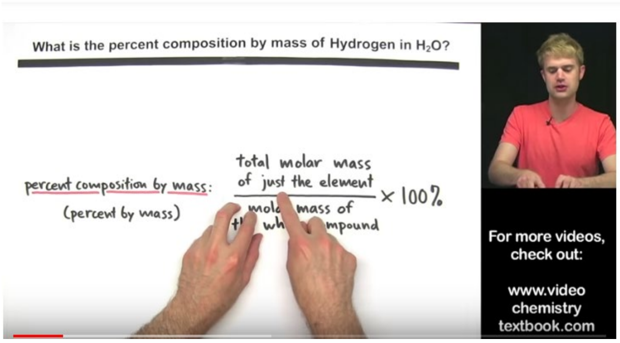
The simulation demonstrates saturation but does not explain why different solutes have different solubilities. The Drink Mix example provides a real-world link to the concept of concentration to help the students make connections to the chemical examples. Determine the saturation molarity in mol/L for all salts (solutes) in the simulation.

Questions:

1. Which one of the salts (solutes) used has the largest saturation concentration
2. Which one of the salts (solutes) used has the smallest saturation concentration
3. Arrange the salts (solutes) in increasing order of saturation concentration. Explain the difference in the saturation concentrations among the salts (solutes).

Several You Tube videos discussing the concentration of solution:

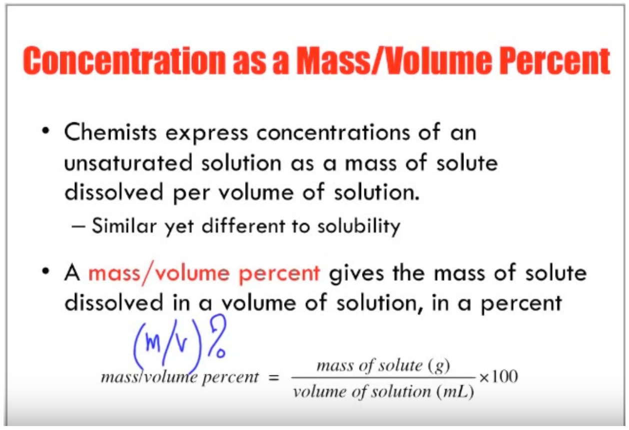
(Mass) %



What is the percent composition by mass of Hydrogen in H_2O?

https://www.youtube.com/watch?v=lywmGCfIUIA

(Mass/volume) %:



Concentration as a Mass/Volume Percent

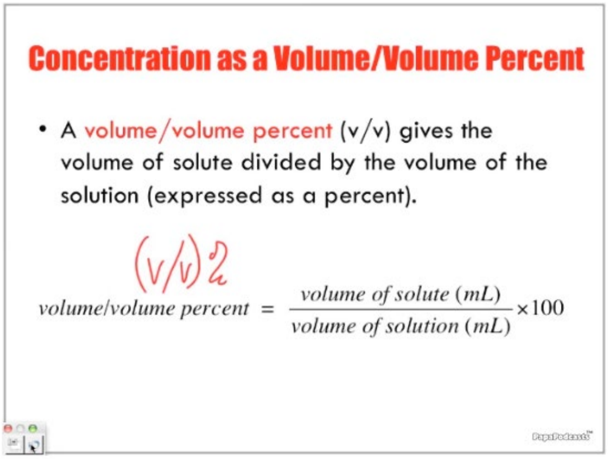
- Chemists express concentrations of an unsaturated solution as a mass of solute dissolved per volume of solution.
  - Similar yet different to solubility
- A mass/volume percent gives the mass of solute dissolved in a volume of solution, in a percent

(M/V)%

$$\text{mass/volume percent} = \frac{\text{mass of solute (g)}}{\text{volume of solution (mL)}} \times 100$$

https://www.youtube.com/watch?v=dl6G_p6gsJc

(Volume/volume) %



Concentration as a Volume/Volume Percent

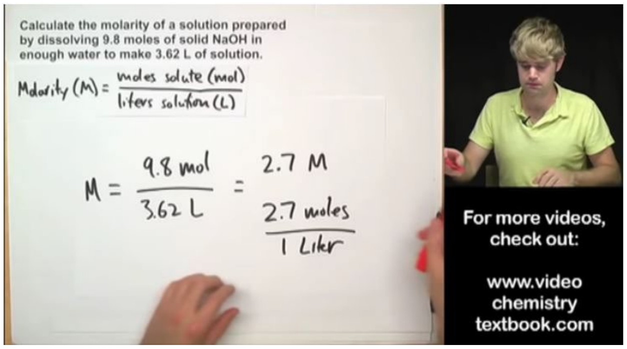
- A volume/volume percent (v/v) gives the volume of solute divided by the volume of the solution (expressed as a percent).

(V/V)%

$$\text{volume/volume percent} = \frac{\text{volume of solute (mL)}}{\text{volume of solution (mL)}} \times 100$$

https://www.youtube.com/watch?v=RCbhk3yyM88

Molarity:



Calculate the molarity of a solution prepared by dissolving 9.8 moles of solid NaOH in enough water to make 3.62 L of solution.

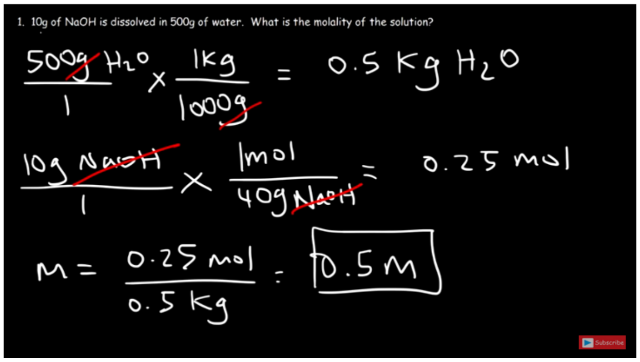
$$\text{Molarity (M)} = \frac{\text{moles solute (mol)}}{\text{liters solution (L)}}$$

$$M = \frac{9.8\ \text{mol}}{3.62\ \text{L}} = \frac{2.7\ \text{M}}{\frac{2.7\ \text{moles}}{1\ \text{Liter}}}$$

https://www.youtube.com/watch?v=SXf9rDnVFao

Molality:

https://www.youtube.com/watch?v=uj1u7Nx9JUc



1. 10g of NaOH is dissolved in 500g of water. What is the molality of the solution?

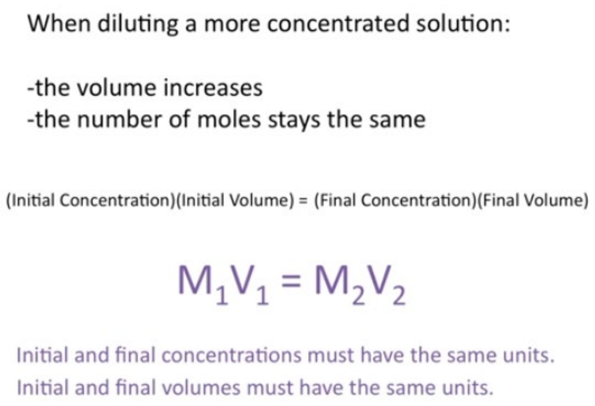
$$\frac{500\cancel{g}\ H_2O}{1} \times \frac{1kg}{1000\cancel{g}} = 0.5\ Kg\ H_2O$$

$$\frac{10g\ \cancel{NaOH}}{1} \times \frac{1mol}{40g\ \cancel{NaOH}} = 0.25\ mol$$

$$M = \frac{0.25\ mol}{0.5\ Kg} = \boxed{0.5\ M}$$

https://www.youtube.com/watch?v=uj1u7Nx9JUc

Dilution:



When diluting a more concentrated solution:

-the volume increases
-the number of moles stays the same

(Initial Concentration)(Initial Volume) = (Final Concentration)(Final Volume)

$$M_1V_1 = M_2V_2$$

Initial and final concentrations must have the same units.
Initial and final volumes must have the same units.

https://www.youtube.com/watch?v=v6dnEp58mVk

Part Per Million (ppm) and Part Per Billion (ppb):

Parts per million (ppm) and parts per billion (ppb) may be converted from one to the other using this relationship: 1 part per million = 1,000 parts per billion.

ppm = {[mass of solute] / [mass of solution]} x 1 x 10^6

ppb = {[mass of solute] / [mass of solution]} x 1 x 10^9

Examples:

The solubility of NaCl is 284 grams/100 grams of water. What is this concentration in ppm?

$\underline{284}$ X 1,000,000 = **2840000 ppm**

100

The solubility of AgCl is 0.008 grams/100 grams of water. What is this concentration in ppm?

$\underline{.008}$ X 1000000 = **80 ppm**

100

A certain pesticide has a toxic solubility of 5.0 grams/Kg of body weight. What is this solubility in ppm?

$\underline{1\ \cancel{Kg}}$ X $\underline{1000\ g}$ = 1000 g $\underline{\quad 5 \quad}$ X 1,000,000 = **5000 ppm**

1   1~~Kg~~   1000

Change 50 ppm to ppb.

50 ppm = 50 X 1,000,000 = 50,000,000   50,000,000 X 1,000=50,000,000,000

X(ppm) = X(ppb) / 1000

ppb = 1000 ppm

50 ppm = 50 x 1000 ppb = **50,000 ppb**

How many parts per million (ppm) is 1mg/L?

1 ppm

IV. Concentrations Calculations in Chemical Reactions

Concentrations and moles calculations in chemical reactions are known as stoichiometry. In most cases, one reactant is used in excess and the other reactant is used in limiting amount. The concentration of the product or the yield of the product is calculated based on the limited reactant amount because it is consumed completely during the chemical reaction.

In the example below, the molarity and the volume of the reactant are used to determine the molarity of the other reactant molarity and/or volume:

Example:

$2\ Na_3PO_4(aq) + 3\ Ca(NO_3)_2(aq) \rightarrow Ca_3(PO_4)_2(s) + 6\ NaNO_3(aq)$

If 355.0 mL of 0.380 M Na_3PO_4 are required to react with 0.135 M $Ca(NO_3)_2$ to produce $Ca_3(PO_4)_2$.

Calculate the amount of the volume $Ca(NO_3)_2$ needed for this reaction.

Solution:

Step 1: number of moles of a given reactant using its molarity and volume:

Number of moles of Na_3PO_4:

355.0 mL are converted into Liters and multiplied with molarity 0.380 mol/L = 0.3550 L X 0.380 mol/L = 0.1349 moles Na_3PO_4

Step 2: using the mole ratio of both reactants from the chemical equation above, one can calculate number of moles of the other reactant:

Mole ratio = 2 moles Na_3PO_4 / 3 moles $Ca(NO_3)_2$ or 3 moles $Ca(NO_3)_2$ / 2 moles Na_3PO_4

Moles of $Ca(NO_3)_2$ = [3 moles $Ca(NO_3)_2$ / 2 moles Na_3PO_4] x [0.1349 moles Na_3PO_4] = 0.20235 moles

Step 3: amount of the volume of $Ca(NO_3)_2$ can be calculated using its molarity and number of moles:

Amount of $Ca(NO_3)_2$ needed = [0.20235 moles $Ca(NO_3)_2$] / [0.135 mol / L $Ca(NO_3)_2$ = 1.50 L (3 significant figures)

Example:

How many liters of 0.188 M hydrochloric acid HCl would be required to react completely with 2.85 grams of sodium hydroxide NaOH according to the reaction below?

$HCl(aq) + NaOH(aq) \rightarrow NaCl(aq) + H_2O(l)$

Step 1: number of moles of NaOH is calculated with the help of the molar mass of NaOH:

Molar mass of NaOH = Na + O + H = 23.0 + 16.0 + 1.0 = 40.0 g/mol

NaOH number of moles = [(2.85 g) / (40.0 g/mol)] = 0.07125 mol

Step 2: using the mol ratio from the chemical equation:

Mole ratio = 1 mol HCl / 1 mol NaOH = 1:1

HCl moles = NaOH moles = 0.07125 mol

Step 3: with the help of molarity of HCl and its number of moles, its volume can be calculated

Volume of HCl = [0.07125 mol HCl / (0.188 mol/L)] = 0.379 L

SUPPLEMENTAL

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V. Mole Definition and Mass Percent Calculations and Reviews

A) Mole Definition and Reviews

The Mole is the ratio between the mass of the matter (element, chemical compound or molecule) to its atomic mass or molar mass.

Mole = [mass of the matter] / [atomic mass or molar mass]

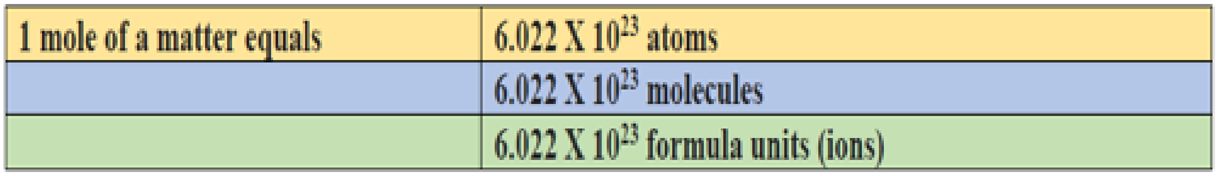
Molar mass = sum of all atomic masses of the elements making the matter of the molecule of compound

Also the Mole is defined in connection to the particles of the matter (atoms, molecules and formula units (ions)):

The Mole is defined as the mass of the compound or the element that contains the same number of fundamental units as there are found in 12.000 grams of ^{12}C (Carbon – 12 isotope).

This means that the atomic mass of Carbon atom of (12 grams) is equal exactly equal 1 mole of Carbon.

Using Avogadro's number, one can define the mole to be:



1 mole of a matter equals	6.022 X 10^{23} atoms
	6.022 X 10^{23} molecules
	6.022 X 10^{23} formula units (ions)

Examples:

1) How many moles are in 40.0 grams of water?

$$\mathbf{40.0\ g\ H_2O\ \ x\ \frac{1\ mole\ H_2O}{18.01\ \ g\ H_2O} = 2.22\ mole\ H_2O}$$

2) How many grams are in 3.7 moles of Na_2O?

$$\mathbf{3.7\ \ moles\ Na_2O\ \ x\ \frac{62\ g\ Na_2O}{1\ mole\ Na_2O}\ = 230\ g\ Na_2O}$$

3) How many atoms are in 14 moles of cadmium?

$$\mathbf{14\ mole\ Cd\ x\ \frac{6.022\ x\ 10^{23}\ atoms\ \ Cd}{1\ mole\ Cd} = 8.4\ x\ 10^{23}\ atoms\ \ Cd}$$

4) How many moles are in 4.3 x 10^{22} molecules of $H_3P0\ 4$?

$$\mathbf{4.3\ \ x\ 10^{22}\ molecules\ H_3PO_4\ x\ \frac{1\ mole\ \ H_3PO_4}{6.022\ \ x\ \ 10^{23}\ molecules\ \ H_3PO_4} = 7.1\ x\ 10\text{-}^{2}\ moles\ H_3PO_4}$$

5) How many molecules are in 48.0 grams of NaOH?

$$\mathbf{48.0\ molecules\ NaOH\ \ x\ \frac{1\ mole\ NaOH}{40\ \ g\ NaOH}\ x\ \frac{6.022\ x\ 10^{23}\ molecules\ NaOH}{1\ mole\ NaOH}}$$

$$\mathbf{= 7.23\ x\ 10^{23}\ molecules\ NaOH}$$

6) How many grams are in 4.63 x 10^{24} molecules of CCl4?

$$\mathbf{4.63 \times 10^{24} \text{ molecules } CCl_4 \times \frac{1 \text{ mole } CCl_4}{6.022 \times 10^{23} \text{ molecules } CCl_4} \times \frac{153.8 \text{ g } CCl_4}{1 \text{ mole } CCl_4} = 1180 \text{ g } CCl_4}$$

7) **How many moles** are in 15 grams of lithium? **(molar mass of lithium is 6.94 g/mole)**

$$\cancel{15} \text{ grams} \times \frac{1 \text{ mole}}{\cancel{6.94}\text{grams lithium}} = 2.1614 \qquad \boxed{= 2.2 \text{ moles Li}}$$

8) **How many grams** are in 2.4 moles of sulfur? **(molar mass of sulfur is 32.07 g/mole)**

$$\cancel{2.4} \text{ moles} \times \frac{32.07 \text{ grams}}{1 \text{ } \cancel{\text{mole}}} = 76.97 \text{ grams sulfur} \qquad \boxed{77 \text{ g Sulfur}}$$

9) How many grams are in 4.5 moles of sodium fluoride, NaF?

(molar mass of NaF is 22.99 + 19.00 = 41.99 g/ mole)

$$\cancel{4.5} \text{ moles} \times \frac{41.99 \text{ grams}}{1 \text{ Mole}} = 188.955 \text{ g NaF} \qquad \boxed{= 190 \text{ g NaF}}$$

10) How many moles are in 98.3 grams of aluminum hydroxide, $Al(OH)_3$?

(molar mass of $Al(OH)_3$ is 26.98 + (3 x 16.00) + (3 x 1.01) = 78.01 g/ mole)

$$\cancel{98.3} \text{ grams} \times \frac{1 \text{ mole}}{\cancel{78}.01 \text{ grams}} = 1.2601 \text{ moles } Al(OH)_3 \qquad \boxed{1.26 \text{ moles } Al(OH)_3}$$

11) How many moles are in 25.0 grams of water?

1.39 moles

1 mole H_2O = 18.0 g H_2O

25 g H_2O	**1 mol H_2O**

= 1.39 mol H_2O

12) How many grams are in 4.500 moles of Li_2O?

134.6 grams

1 mole Li_2O = 29.90 g Li_2O

4.500 mol Li_2O	**29.90 g Li_2O**

= 134.6 g Li_2O

13) How many molecules are in 23.0 moles of oxygen?

1.38 x 10^{25} molecules

1 mole oxygen molecules = 6.02 x 10^{23} oxygen molecules

23.0 mol O_2	**6.02 x 10^{23} O_2 molecules**
	1 mol O_2

= 1.38 x 10^{25} O_2 molecules

14) How many moles are in 3.4×10^{23} molecules of H_2SO_4?

0.56 moles

1 mole anything = 6.02×10^{23} anything

3.4×10^{23} molecules H_2SO_4	**1 mol H_2SO_4**
	6.02×10^{23} molecules H_2SO_4

= 0.56 mol H_2SO_4

15) How many molecules are in 25.0 grams of NH_3?

8.85×10^{23} molecules

1 mole NH_3 = 17.0 g NH_3

1 mole anything = 6.02×10^{23} anything

25.0 g NH_3	**1 mol NH_3**	**6.02×10^{23} molecules NH_3**
	17.0 g NH_3	**1 mol NH_3**

= 8.85×10^{23} molecules

16) How many grams are in 8.200×10^{22} molecules of N_2I_6?

107.5 grams

1 mole N_2I_6 = 789.4 g N_2I_6

1 mole anything = 6.02×10^{23} anything

8.200×10^{22} molecules N_2I_6	**1 mol N_2I_6**	**789.4 g N_2I_6**
		1 mol N_2I_6

= 107.5 g N_2I_6

17) How many moles are in 15 grams of lithium?

? moles Li = 15 g Li X [1 mol Li / 6.941 g Li] = 2.2 mol Li

18) How many grams are in 2.4 moles of sulfur?

? grams S = 2.4 mol S X [32.066 g S / 1 mol S] = 77 g S

19) How many moles are in 3.5 grams of $K_2Cr_2O_7$?

First determine the molar mass of $K_2Cr_2O_7$

= 2 K + 2 Cr + 7 O = [2x (39.0983)] + [2x(51.996)] + [7x(15.9994)] = 294.185 g /mol $K_2Cr_2O_7$

? moles $K_2Cr_2O_7$ = 3.5 g $K_2Cr_2O_7$ X [1 mol K2Cr2O7 / 294.185 g $K_2Cr_2O_7$] = 0.012 mol $K_2Cr_2O_7$

20) How many grams are found in 2.5 moles of $Al(OH)_3$?

First determine the molar mass of $Al(OH)_3$

= 1 Al + 3 O + 3 H
= [1x(26.98154)] + [3x(15.9994)] + [3x(1.00797)] = 78.0036 g $Al(OH)_3$ / mol $Al(OH)_3$

? grams $Al(OH)_3$ = 2.5 mol $Al(OH)_3$ X [78.0036 g $Al(OH)_3$ / mol $Al(OH)_3$] = 195.009 g $Al(OH)_3$ = **2.0 X 10^2 g $Al(OH)_3$**
Note that the answer is rounded to sig. figs.

Now, please watch these videos below:

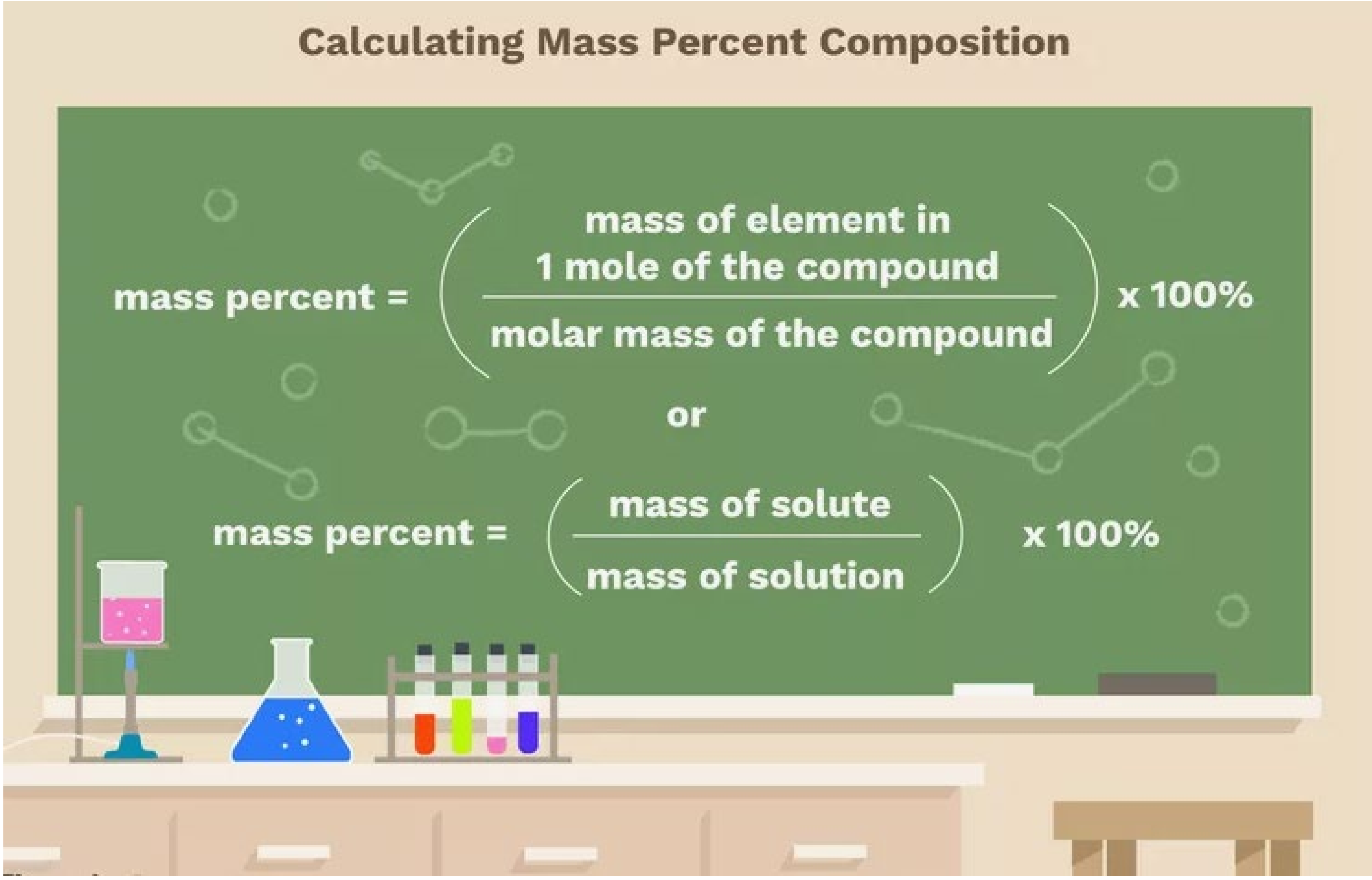
https://www.youtube.com/watch?v=e_KMPemSVPc https://www.youtube.com/watch?v=hQ6_BxJwvB0

B) Mass Percent Calculations Review

Mass Percent covers the mass of an elements to the some of the elements within a molecule or a compound.

It covers the mass of the solute to the total mass of the solution which includes the mass of the solute and the solvent.

The mass % is defined as illustrated in the figure below:



https://www.thoughtco.com/mass-percent-composition-example-609567

Examples:

1) 5.0 grams of sugar are dissolved in 150. g of water What is the mass percent of sugar in the solution?

{ (5.0 g) / [(5.0 g + 150. g)] } * 100 % =

{ (5.0 g) / [(155. g)] } * 100 % = 3.2 %

2) 200.0 gram solution of alcohol contains 180.0 mL of water. What is the mass percent of alcohol? (Remember water's density is 1.000 g /mL)

The mass of 180. mL of water = [180.0 mL * 1.000 g / mL] = 180.0 g

Mass of the solute = 200.0 g – 180.0 g = 20.0 g

[(20.0 g) / (200.0 g)] * 100 %] = 10.0%

3) How many grams of NaBr are needed to make 50. g of a 5.0% solution?

Set the formula up:

5.0 % = X / 50. g

5.0 g NaBr / 100 g solution = X / 50. g solution

Solving for X

Cross multiply yields:

{ [5.0 g NaBr / 100 g solution] * [50. g solution] } = X

Cancelling g solution:

{ [5.0 g NaBr / 100 ~~g solution~~] * [50. ~~g solution~~] } = X

{ [5.0 g NaBr / 100] * [50.] } = 2.5 g NaBr

4) How many grams of LiOH are needed to make 25 g of a 4.0 % solution?

Set the formula up:

4.0 % = X / 25 g solution

[4.0 g LiOH / 100 g solution] = X / 25 g solution

Solving for X

Cross multiply yields:

[4.0 g LiOH / 100 g solution] * [25 g solution] = X

[4.0 g LiOH / 100 ~~g solution~~] * [25 ~~g solution~~] = X

[4.0 g LiOH / 100 ~~g solution~~] * [25 ~~g solution~~] = 1.0 g LiOH

5) What mass of NaF must be mixed with 25 mL of water to create a 3.5% by mass solution? (Remember water's density is 1.000 g /mL)

Set the formula up:

X = mass of NaF in g

Mass of water = 25 mL = 25 g

Mass of the solution = (X + 25) g

3.5 % = X / X + 25 g solution

[3.5 g Na F / 100 g solution] = X / (X + 25 g) solution

Cancelling g solution from both sides:

[3.5 g Na F / 100 ~~g solution~~] = X / (X + 25 ~~g) solution~~

[3.5 g Na F / 100] = X / (X + 25)

$$\frac{3.5\text{ g NaF}}{100} = \frac{X}{(X+25)}$$

(X + 25) * (3.5 g Na F) = 100 X

3.5 X + 87.5 g = 100 X

Moving 3.5 X to the right side of the equation:

87.5 g = 100 X – 3.5 X

87.5 g = 96.5 X

X = (87.5 g / 96.5) = 0.906 g = 0.91 g

6) An 800.0 g solution of Kool-Aid contains 780.0 g of water. What is the mass percent of solute in this solution?

Mass of solute (Kool – Aid) = 800.0 – 780.0 = 20.0 g

Mass of the solution = 800.0 g

Mass % = [(20.0 g) / (800.0 g)] * 100% = 2.50 %

7) What is the mass percent of a solution created by adding 10.0 g of olive oil to 90.0 g of vegetable oil?

Mass of the solute = 10.0 g olive oil

Mass of the solvent = 90.0 g of vegetable oil.

Mass of the solution = 10.0 + 90.0 = 100.0 g solution

Mass % = 10.0 g olive oil / 100.0 g solution = 10.0 %

8) If 4000.0 g solution of salt water contains 40.0 g of salt, what is its mass percent?

Mass of the solute = 40.0 g salt water

Mass of the solution = 4000.0 g solution

Mass % = 40.0 g salt water / 4000.0 g solution = 1.00 %

Percentage Composition of Water in Salts (Hydrates Percentage Composition)

Example:

9) What is the composition of water in copper sulfate pentahydrate?

copper sulfate pentahydrate has the following formula:

$CuSO_4$ $5H_2O$

From the formula one can deduce that in 1 mol of $CuSO_4$ $5H_2O$ has 5 mol of water.

First we have to calculate the molar mass of the whole molecule/compound:

H_2O = 5 x [2H + 1 O] = 2 [2 x 1.00797 g/mol + 1 x 15.9994 g/mol] = 18.01534 g/mol

$CuSO_4$ = [1 Cu + 1 S + 4 O] = [1 x 63.546 g/mol + 1 x 32.06 g/mol + 4 x 15.9994 g/mol]
$CuSO_4$ = 159.609 g/mol

The molar mass of the $CuSO_4$ $5H_2O$ = [5 x18.01534 g/mol + 159.609 g/mol] = 249.686 g/mol

Mass % of H_2O = { [5 X 18.01534 g/mol] x [249.686 g/mol] } * 100% = 36.07599% = 36.076 %

Mass composition of an Element within its Compound

Example:

10) Find the mass percentages (mass %) of Na, H, C, and O in sodium hydrogen carbonate $NaHCO_3$.

First, look up the atomic masses for the elements from the Periodic Table. The atomic masses are found to be:

Na is 22.99 g/mol

H is 1.01 g/mol

C is 12.01 g/mol

O is 16.00 g/mol

Next, determine how many grams of each element are present in one mole of $NaHCO_3$:

22.99 g in 1 mol of Na

1.01 g in 1 mol of H

12.01 g in 1 mol C

48.00 g (3 mol x 16.00 g/mol) in 3 mol O

The mass of one mole of $NaHCO_3$ is:

22.99 g + 1.01 g + 12.01 g + 48.00 g = 84.01 g in 1 mol $NaHCO_3$

Mass percentages of each element are

mass % Na = 22.99 g / 84.01 g x 100 = 27.36 %

mass % H = 1.01 g / 84.01 g x 100 = 1.20 %

mass % C = 12.01 g / 84.01 g x 100 = 14.30 %

mass % O = 48.00 g / 84.01 g x 100 = 57.14 %

Verification: Adding all the mass % it should make 100%

27.36 + 14.30 + 1.20 + 57.14 = 100.00 %

Mass Percent of an Element within its Compound

Example:

11) What the mass % of S and O in SO_3?

Atomic mass of S = 32.06 g/mol

Atomic mass of O = 16.00 g/mol

The molar mass of SO_3 = 1 S + 3 O = [32.06 g/mol + 3 x 16.00 g/mol] = 80.06 g/mol

Mass % S = [32.06 g/mol / 80.06 g/mol] x 100% = 40.05 %

Mass %) = { [3 x 16.00 g/mol] / [80.06] } x 100% = 59.95%

Verification:

Adding both mass % should yield 100% = 40.05 % + 59.95 % = 100.00 %

End of Chapter Questions:

1. How many atoms are in the following compounds?

a) CaCl$_2$ __3
b) NH$_4$OH ______7
c) NaCl __2
d) N$_2$O$_7$ __9
e) P$_2$O$_5$ __7

a) KNO$_3$ ______5
b) Al$_2$(CO$_3$)$_3$ __14
c)Na$_3$PO$_4$ 8__
d) Mg(NO$_3$)$_2$ __9_____

2. **Calculate the molar mass of the following compounds:**

a) NaCl 58.5 g/mol
b) Fe$_2$O$_3$ 159.6 g/mol
c) LiOH 23.9 g/mol
d) NH$_3$ 17.0 g/mol
e) AlPO$_4$ 122.3 g/mol

3. **Mole-to-Gram/Gram-to-Mole Conversions**

How many grams of Ca are present in 3.28 moles?

132 g Ca

How many grams of S are present in 5.39 moles?

173 g S

How many moles of Ag are there in 4.98 gram?

0.0462 mol

How many moles of Mg are present in 303 grams?

12.5 mol Mg

3. **Conversions using Avogadro's number**

How many atoms are present in 34.69 moles of Mg?

2.09×10^{25} atoms

How many atoms are present in 0.529 moles of Li?

3.18×10^{23} atoms

How many moles of Mn are present in 4.09×10^{24} atoms of Mn?

6.79 mol

How many moles of Ni are present in 5.88×10^{19} atoms? 0.0000977 mol

4. Grams ↔ Moles ↔ Particles OR Atoms OR Molecules

Calculate the number of molecules in 8.33 grams of O_2

1.57 X 10^{23} molecules

Calculate the number of atoms in 43.33 grams of iron, Fe?

4.67 X 10^{23} atoms

Calculate the number of particles in 32.8 grams of Cu_2S.

4.12 X 10^{20} particles

Calculate the number of grams of lithium in 5.44 x 10^{21} atoms of lithium.

0.0624 g

Calculate the number of grams of SO_3 in 3.92 x 10^{25} molecules of sulfur trioxide.

5220

5. Using Avogadro's number to convert from molecules or atoms to moles.
A chemical species is either an atom (e.g. K, Ag, S) , an ion (e.g. K^+,SO_4^{2-}, S^{2-}) or a molecule (e.g. H_2O, K_2CrO_4, $Sr(NO_3)_2$, I_2).

e) 2.57 x 10^{11} atoms of silver equals how many moles of silver? [What is the chemical symbol of silver?]

4.27 x 10-13 mol Ag

f) 2.845 x 10^{12} potassium ions [What is the chemical symbol of the potassium ion?] equals how many moles of potassium ions?

4.73 x 10-12 mol K+

g) 0.0524 moles of H_2O equals how many molecules of water?

3.15 x 1022 molecules H2O

h) 347865 atoms of xenon are equal to how many moles of Xe?

5.78 x 10-19 mol Xe

i) 3.25 x 10^{25} atoms of neon gas equals how many moles of neon gas?

54.0 mol Ne

j) How many moles of H_2SO_4 do you have if you there are 1.64 x 10^{12} molecules of H_2SO_4?

2.72 10^{-12} mol H_2SO_4

6. If there are 8.24 x 10^{22} molecules of NaCl in a salt shaker, what is the mass of the salt? First find the number of moles, then convert to grams.

8.00 g NaCl

Empirical Formula:

1. **State the empirical formula for each of the following compounds: a) C_4H_8; b) $C_2H_6O_2$; c) N_2O_5; d) $Ba_3(PO_4)_2$; e) Te_4I_{16}**

a) CH_2; b) CH_3O; c) N_2O_5; d) $Ba_3(PO_4)_2$; e) TeI_4.

2. **What is the empirical formula for a compound that contains 0.063 mol chlorine and 0.22 mol oxygen?**

a)Step 1 is already done, so we will start with step 2:

$$Cl \square \frac{0.063mol}{0.063mol} \square 1 \qquad O \square \frac{0.22mol}{0.063mol} \square 3.5$$

Step 3 is necessary:

Cl = 1•2 = 2 O = 3.5•2 = 7

Step 4: Cl_2O_7 – **dichlorine heptaoxide**

3. **What is the empirical formula for a compound that contains 26.1% carbon, 4.3% hydrogen and 69.6 % oxygen?**

Step 1:

$C \square 26.1\left|\frac{1mol}{12.01g}\right| \square 2.17mol$ $\quad H \square 4.3g\left|\frac{1mol}{1.008g}\right| \square 4.27mol$

$O \square 69.6g\left|\frac{1mol}{16.00g}\right| \square 4.35mol$

Step 2:

$C \square \frac{2.17mol}{2.17mol} \square 1$ $\quad H \square \frac{4.27mol}{2.17mol} \square 1.9$ $\quad O \square \frac{4.35mol}{2.17mol} \square 2.0$

Step 3 isn't necessary. Step 4: CH_2O_2

4. An oxide of nitrogen contains 30.45% N and 69.55% O. What is its empirical formula?

Step 1: $N = 30.45g\left|\frac{1mol}{14.01g}\right| = 2.17mol$ $\quad O = 69.55g\left|\frac{1mol}{16.00g}\right| = 4.35mol$

Step 2: $N = \frac{2.17mol}{2.17mol} = 1$ $\quad O = \frac{4.35mol}{2.17mol} = 2.0$

Step 3: isn't necessary. Step 4: NO_2

Molecular Formulas:

5. The molar mass of the oxide of nitrogen is 92 g/mol. What is its molecular formula?

Step 1 was done as above, so we will start with Step 2:

$$\frac{92\frac{g}{mol}}{46.01\frac{g}{mol}} = 2$$

Step3: N = 1•2 = 2

O = 2•2 = 4

N_2O_4 = Dinitrogen tetroxide

6. 84.9% Hg and the remainder Cl, with a molecular weight of 472.2 g/mol.

6. Step 1: % Si = 100% - 79.1% = 20.9%

$$Cl = 79.1g\left|\frac{1mol}{35.45g}\right| = 2.23mol \qquad Si = 20.9g\left|\frac{1mol}{28.09g}\right| = 0.744mol$$

$$Cl = \frac{2.23mol}{0.744mol} = 2.99 \qquad Si = \frac{0.744mol}{0.744mol} = 1 \qquad \text{Empirical: } SiCl_3$$

Step 2: $\dfrac{269\frac{g}{mol}}{134.44\frac{g}{mol}} = 2$ Step 3: $Si = 1 \cdot 2 = 2$

$Cl = 3 \cdot 2 = 6$

Si_2Cl_6 – disilicon hexachloride

7. 12.26% N, 3.54% H, 28.1% S, and 56.1% O. The molecular weight is 228.2 g/mol. The formula is known to contain the NH_4^+ grouping. Write your formula accordingly.

7. Step 1:

$$C = 69.6g\left|\frac{1mol}{12.01g}\right| = 5.80mol \qquad H = 8.34g\left|\frac{1mol}{1.008g}\right| = 8.27mol$$

$$O = 22.1g\left|\frac{1mol}{16.00g}\right| = 1.38mol$$

$$C = \frac{5.80mol}{1.38mol} = 4.20 \qquad H = \frac{8.27mol}{1.38mol} = 5.99 \qquad O = \frac{1.38mol}{1.38mol} = 1$$

$C = 4.2 \cdot 5 = 21$ $H = 6 \cdot 5 = 30$ $O = 1 \cdot 5 = 5$ Empirical: $C_{21}H_{30}O_5$

Step 2: $\dfrac{362.47\frac{g}{mol}}{362.45\frac{g}{mol}} = 1$ Step 3: all subscripts will be the same

$C_{21}H_{30}O_5$ – Cortisol

8. 71.5% Hg, 5.0% N, 17.1% O, and 6.4% H_2O, with molecular weight of 561.2 g/mol

Step 1:

$C = 77.4g \left| \frac{1mol}{12.01g} \right| = 6.44mol$ $H = 12.9g \left| \frac{8.27mol}{1.008mol} \right| = 12.8mol$

$O = 10.2g \left| \frac{1mol}{16.00g} \right| = 0.638mol$

$C = \frac{6.44mol}{0.638mol} = 10.1$ $H = \frac{12.8mol}{0.638mol} = 20.0$ $O = \frac{0.638mol}{0.638mol} = 1$

Empirical: $C_{10}H_{20}O$

Step 2: $\frac{156.3\frac{g}{mol}}{156.26\frac{g}{mol}}$ Step 3: all subscripts will be the same

$C_{10}H_{20}O$ – Menthol

……

END OF CHAPTER QUIZ:

1. The molar mass of carbon is 12 g /mol. How many moles are there in 3g of carbon?
    a) 0.25 mol
    b) 0.4 mol
    c) 4 mol
    d) 36 mol

    Answer: A

2. The concentration of a solution is expressed as the number of moles in which of the following volumes?
    a) 1 L
    b) 1 mL
    c) 1 kL
    d) 1 dL

    Answer: A

3. 25 mL is equivalent to how many Liters (L)?
    a) 0.025
    b) 0.25
    c) 2.5
    d) 0.0025

    Answer: A

4. What is the concentration in percent mass/volume of 150. mL of solution containing 30.0 g of solute?
    a) 25.0%
    b) 20.0%
    c) 50.5%
    d) 60.5%

    Answer: B

5. What is the concentration by % m/v if 67 g are dissolved to make 1.2 L of solution?
    a) 5.6%
    b) 12%
    c) 45%
    d) 92%

    Answer: A

6. What volume of a 40.0 % m/v solution contains 70.0 g of solute?
    a) 169 mL

b) 124 mL
c) 155 mL
d) 175 mL

Answer: D

7. What amount of solute is dissolved to make 0.500 L of a 20.0 % m/v solution?
   a) 178 g
   b) 124 g
   c) 100. g
   d) 254 g

Answer: C

8. What amount of a 75 % m/v solution will be made if 50 g of solute are dissolved?
   a) 185 mL
   b) 66.7 mL
   c) 143 mL
   d) 127 mL

Answer: B

9. What is the concentration in % m/v if 0.55 kg of solute is dissolved to make 1.5 L of solution?
   a) 52.8%
   b) 33.3%
   c) 36.7%
   d) 78.9%

Answer: C

10. 5.0 grams of sugar are dissolved in 150 g of water. What is the mass percent of sugar in the solution?
    a) 59%
    b) 3.2%
    c) 4.5%
    d) 6.2%

Answer: B

11. A 200.- gram solution of alcohol contains 180. mL of water. What is the mass percent of alcohol? (Remember water's density.)
    a) 10.0%
    b) 6.19%
    c) 8.05%
    d) 6.22%

Answer: A

12. How many grams of NaBr are needed to make 50 g of a 5.0% solution?
    a) 5.2 g

b) 3.5 g
c) 4.2 g
d) 2.5 g

Answer: D

13. How many grams of LiOH are needed to make 25 g of a 4.0 % solution?
    a) 2.8 g
    b) 1.0 g
    c) 3.8 g
    d) 5.5 g

    Answer: B

14. What mass of NaF must be mixed with 25 mL of water to create a 3.5% by mass solution?
    a) 0.56 g
    b) 0.55 g
    c) 0.91 g
    d) 0.88 g

    Answer: D

15. An 800. g solution of Kool-Aid contains 780. g of water. What is the mass percent of solute in this solution?
    a) 3.66 g
    b) 2.50 g
    c) 4.75 g
    d) 2.98 g

    Answer: B

16. What is the mass percent of a solution created by adding 10.0 g of olive oil to 90.0 g of vegetable oil?
    a) 20.0%
    b) 30.0%
    c) 10.0%
    d) 40.0%

    Answer: C

17. If a 4000. g solution of salt water contains 40. g of salt, what is its mass percent?
    a) 1.0%
    b) 2.0%
    c) 3.0%
    d) 4.0%

    Answer: A

18. Determine the volume/volume percent solution made by combining 25.0 mL of ethanol with enough water to produce 200. mL of the solution.
    a) 10.5 %
    b) 12.5 %
    c) 9.56%
    d) 11.7%

    Answer: B

19. A solution is prepared by dissolving 90.0 mL of hydrogen peroxide in enough water to make 3000. mL of solution. Identify the concentration of the hydrogen peroxide solution.
    a) 5.00 %
    b) 3.00 %
    c) 4.00 %
    d) 2.00 %

    Answer: B

20. How would you prepare 250. mL of 70 % (v/v) of rubbing alcohol ?
    a) You would add enough water to 165 mL of rubbing alcohol to make a total of 250. mL of solution.
    b) You would add enough water to 185 mL of rubbing alcohol to make a total of 250. mL of solution.
    c) You would add enough water to 175 mL of rubbing alcohol to make a total of 250. mL of solution.
    d) You would add enough water to 195 mL of rubbing alcohol to make a total of 250. mL of solution.

    Answer: C

21. If 2.0 moles of salt is dissolved to form 1.0 liter of solution, calculate the molarity of the solution.
    a) 1.0 M solution
    b) 1.5 M solution
    c) 2.0 M solution
    d) 2.5 M solution

    Answer: C

22. Calculate the molarity of a sugar solution if 4 liters of the solution contains 8 moles of sugar?
    a) 0.5 M
    b) 8 M

c) 2 M
d) 80 M

Answer: C

23. What is the molarity of a solution containing 5.00 moles of solute in 250. milliliters of solution?
a) 20.0 M
b) 15.0 M
c) 0.104 M
d) 1.25 M

Answer: A

24. How many moles of NaOH are needed to dissolve in water to make 4.0 liters of a 2.0 M solution?
a) 0.50 M
b) 2.0 M
c) 8.0 mol
d) 0.50 mol

Answer: C

25. How many moles of Na are needed to make 4.5 liters of a 1.5 M Na solution?
a) 6.75 mol
b) 0.33 M
c) 0.33 mol
d) 3.0 M

Answer: A

26. Molarity of a solution can be defined as the:
a) atomic mass of an element
b) moles of solution per liter of solute
c) moles of solute per liter of solution
d) mass of solvent per liter of solution

Answer: C

27. To calculate the Molarity of a solution when the solute is given in grams and the volume of the solution is given in milliliters, you must first:
a) Convert grams to moles, but leave the volume of solution in milliliters
b) Convert volume of solution in milliliters to liters, but leave grams to moles
c) Convert grams to moles, and convert volume of solution in milliliters to liters
d) None of the above
Answer: C

28. The molarity of an aqueous solution of $CaCl_2$ is defined as the
a) moles of $CaCl_2$ per milliliter of solution
b) grams of $CaCl_2$ per liter of water
c) grams of $CaCl_2$ per milliliter of solution
d) moles of $CaCl_2$ per liter of solution

29. How many grams of NaCl are contained in 350. mL of a 0.250 M solution of sodium chloride?
   a) 41.7 g
   b) 14.6 g
   c) 5.11 g
   d) 87.5 g
   e) None of these

   Answer: C

30. The molarity of Cl^- available in 110. mL of a solution containing 5.55 g of $CaCl_2$ is:
   a) 0.00550 M
   b) 0.668 M
   c) 50.5 M
   d) 0.455 M
   e) 0.909 M

   Answer: Answer: E

31. A 51.24 g sample of $Ba(OH)_2$ is dissolved in enough water to make 1.20 liters of solution. How many mL is this solution must be diluted with water in order to make 1.00 liter of 0.100 M $Ba(OH)_2$?
   a) 401 mL
   b) 333 mL
   c) 278 mL
   d) 1.20×10^3 mL
   e) none of these

   Answer: A

32. How many grams of NaOH are contained in 5.0×10^2 mL of a 0.80 M sodium hydroxide solution?
   a) 16 g
   b) 80. g
   c) 20. g
   d) 64 g
   e) None of the above

   Answer: A

33. 25.0 mL of 0.20 M K_2SO_4 is added to 50.0 mL of 0.40 M KOH. Calculate the concentration of K^+ ions in solution.
   a) 0.20 M
   b) 0.33 M

c) 0.40 M
d) 0.60 M
e) 0.66 M

Answer: B

34. What is the molarity of a solution that contains 122 g of MgSO4 in 3.50 L of solution?

a) 0.271 M
b) 0.550 M
c) 0.630 M
d) 0.290 M

Answer: D

35. How many moles of KI are present in 0.8500 L of a 0.5500 M KI solution?
a) 0.9350 mol
b) 0.4675 mol
c) 3.100 mol
d) 1.550 mol

Answer: B

36. You are given 100.0 ml of a 2.00 M solution of KOH. What would be the molarity of the solution if it is diluted to a volume of 1000. ml?
a) 2.00 M
b) 0.002 M
c) 0.200 M
d) 0.0200 M

Answer: C

37. How many milliliters of 2.00 M NaCl solution are required to make 1 liter of 0.400 M NaCl solution?
a) 5,000 mL
b) 800. mL
c) 200. mL
d) 0.200

Answer: D

38. Determine the number of grams of $NaHCO_3$ that are in one liter of a 2.100 M solution
a) 2.5.50 g
b) 176.4 g
c) 205.0 g
d) 155.0 g

Answer: B

39. Determine the number of grams of $NaNO_3$ that are present in 500.0 mL of a 1.0 M solution.
    a) 122.0 g
    b) 33.55 g
    c) 345.0 g
    d) 42.50 g

    Answer: D

40. Determine the number of grams of CCl_4 in 450.0 mL of a 3.200 M solution.
    a) 45.50 g
    b) 874.0 g
    c) 221.8 g
    d) 345.0 g

    Answer: C

41. You need to make 300. mL of a 0.400 M solution of sodium chloride. The only available solution is 1.0 M. Determine how to make the needed dilution.
    a) 125 mL 1.0 M solution + 180 mL water
    b) 120 mL 1.0 M solution + 180 mL water
    c) 130 mL 1.0 M solution + 180 mL water
    d) 140 mL 1.0 M solution + 180 mL water

    Answer: B

42. You have to make 500. mL of a 0.500 M $BaCl_2$. You have 2.00 M barium chloride solution available. Determine how to make the needed dilution
    a) 135 mL 2.0M solution + 375 mL of water
    b) 145 mL 2.0M solution + 375 mL of water
    c) 155 mL 2.0M solution + 375 mL of water
    d) 125 mL 2.0M solution + 375 mL of water

    Answer: D

43. You need to make 10.0 L of 1.20 M KNO_3 . What molarity would the potassium nitrate solution need to be if you were to use only 2.50 L of it?
    a) 4.80 M
    b) 5.50 M
    c) 3.55 M
    d) 2.86 M

Answer: A

44.If 45 mL of water are added to 250 mL of a 0.75 M K_2SO_4 solution, what will be the molarity of the diluted solution be?

a) 0.89 M
b) 0.64 M
c) 0.15 M
d) 0.35 M

Answer: B

45.If water is added to 175 mL of a 0.45 M KOH solution until the volume is 250 mL, what will be the molarity of the diluted solution be?

a) 0.25 M
b) 0.45 M
c) 0.32 M
d) 0.15 M

Answer: C

46.How much 0.075 M NaCl solution can be made by diluting 450 mL of 9.0 M NaCl?

a) 45 L
b) 54 L
c) 43 L
d) 34 L

Answer: B

47.If 550. mL of a 3.50 M KCl solution are set aside and allowed to evaporate until the volume of the solution is 275 mL, what will the molarity of the solution be?

a) 7.00 L
b) 6.00 L
c) 5.00 L
d) 4.00 L

Answer: A

48.How much water would need to be added to 750 mL of a 2.8 M HCl solution to make a1.0 M solution?

a) 2.5 L
b) 1.1 L
c) 2.1 L
d) 3.5 L

Answer: C

Chapter 4: Chemical Reactions Stoichiometry

Key Concepts

- 4.1 Introduction to History of Chemical Reactions
- 4.2 Balancing Chemical Reactions
- 4.3 Chemical Reactions Types
- 4.4 Chemical Reactions Stoichiometry
- 4.5 Yields of Reactions
- 4.6 Quantitative Chemical Analysis

I. Introduction to History of Chemical Reactions

The first known chemical equation was written in 1615 in the first chemistry textbook called Tyrocinium Chymicum (meaning "Begin Chemistry") by the French scientist Jean Beguin. The chemical equation was presented as a diagram rather than symbols:

Jean Beguin used antimony sulfide to react with chloride of mercury. The mercury became vapor, leaving behind a residue of antimony oxychloride.

In 1747, William Cullen an English chemist and a professor at University of Glasgow had written lecture notes for chemical equations which were closer to what we have today. In addition, he had classified 4 types of chemical reactions:

In 1774, a French chemist Antoine Lavoisier had developed that the mass of the reactants equal the mass of the products which then was known as mass conservation. This was the first crucial step to understand how to balance the chemical equation.

Figure 4.1 Antoine Lavoisier

At same period of time, Lavosier, Joseph Proust a French scientist had developed Law of definite proportions which stated that in any given compound, the elements occur in fixed ratios, regardless of their source.

In 1803, English chemist John Dalton combined all these laws and concepts together and proposed that matter is made of atoms of unique substances that could not be created or destroyed.

Figure 4.2 John Dalton

Identifying Chemical Reactions

Chemical reactions can be broadly classified in five categories.

$$2H_2O \longrightarrow 2H_2 + O_2$$

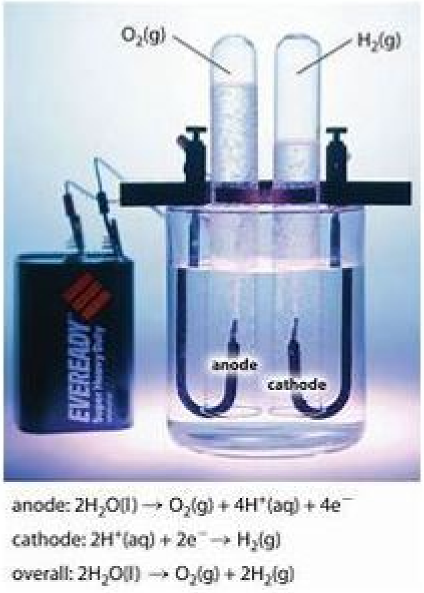


Figure 4.**3** Electrolysis of water

Ref: commons.wikimedia.org/

- **Combination reaction:** When two or more reactants join together to form one single product, the reaction is called combination or synthesis reaction. Here are some example of combination reaction.

$$8Fe + S_8 \longrightarrow 8FeS$$

3) Single replacement reaction:

- An active element replaces another element in a compound.

$$Mg + 2H_2O \longrightarrow Mg(OH)_2 +$$

Figure 4.4 Reaction of Mg with water

Ref: commons.wikimedia.org/

In the above example, Magnesium replaces Hydrogen from water to form Hydrogen gas(H_2) and Magnesium Hydroxide is formed.($Mg(OH)_2$)

4) **Double replacement Reactions:**

Ref: commons.wikimedia.org/

Figure 4.5 Formation of yellow PbI_2 precipitate

$$Pb(NO_3)_2 + 2KI \longrightarrow PbI_2 + 2KNO_3$$

In the above example

When the cations of two ionic compounds switch places to form products, the reaction is classified as double displacement reaction. When Potassium Iodide(KI) is added to colorless Lead Nitrate solution ($Pb(NO_3)_2$) , yellow precipitate of Lead Iodide (PbI_2) is formed.

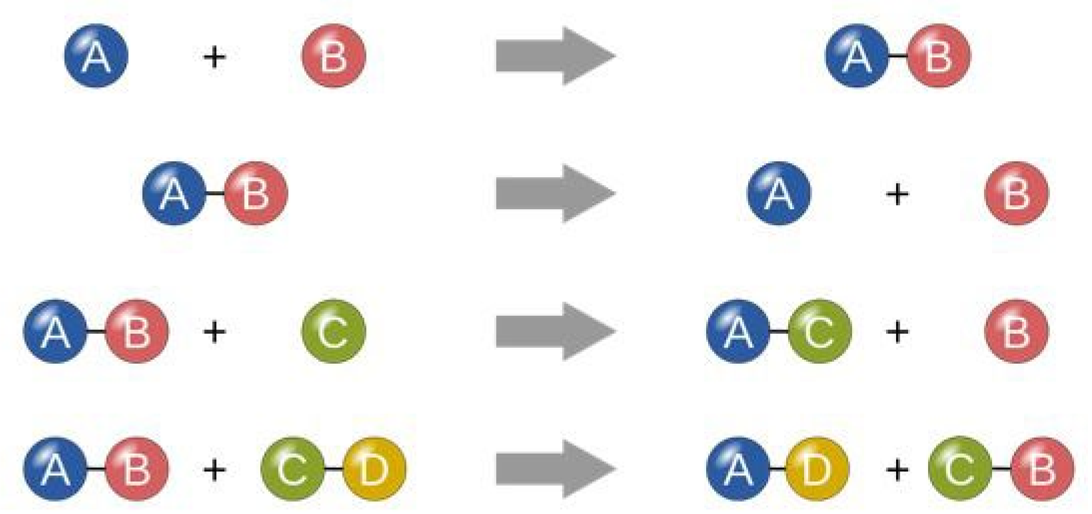


Figure 4.6 Classification of Different types of reactions

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Figure 4.7 Combustion Reaction

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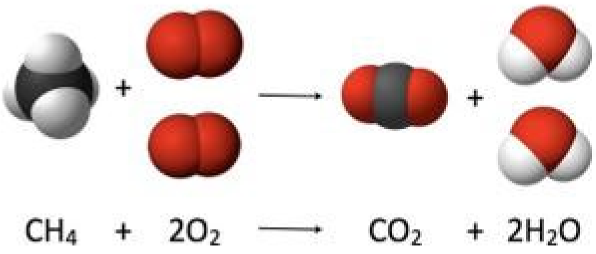

Figure 4.8 Combustion Reaction

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There are many other categories of reactions like acid-base reactions, precipitation reactions, etc. These reactions will be described under respective chapters. Only redox reaction is described in this chapter.

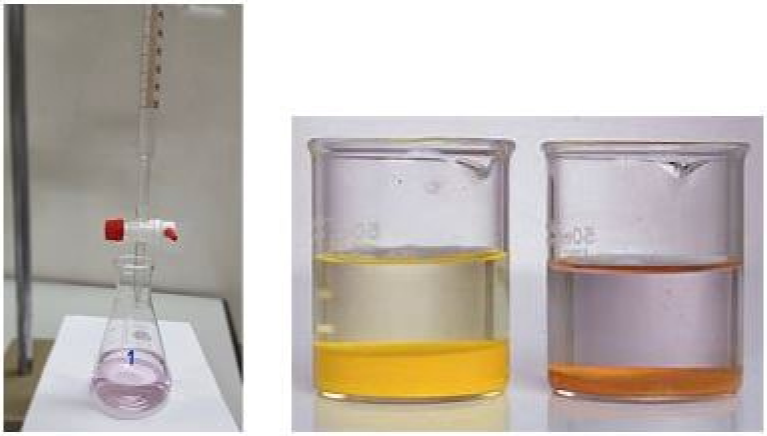

Figure 4.9 Combustion Reaction

Ref: commons.wikimedia.org/

Questions:

1. Classify the following reactions:

1. a) $N_2 + 3H_2 \longrightarrow 2NH_3$
2. b) $Na_2SO_3 + H_3PO_4 \longrightarrow H_2SO_3 + Na_3PO_4$

Ans: a) combination, b) double displacement

/

II. Balancing Chemical Reactions

In a *chemical reaction*, one or more reactants are transformed into products:

reactants → products

The purpose of a *chemical equation* is to express this relation in terms of the formulas of the actual reactants and products that define a particular chemical change. For example, the reaction of mercury with oxygen to produce mercuric oxide would be expressed by the equation

$Hg + O2 \rightarrow HgO$

Sometimes, for convenience, it is desirable to indicate the physical state (gas, liquid or solid) of one or more of the species by appropriate abbreviations:

$Hg(l) + O2(g) \rightarrow HgO(s)$

$C(graphite) + O2(g) \rightarrow CO2(g)$

$C(diamond) + O2(g) \rightarrow CO2(g)$

However, this is always optional.

Chemical equations must be balanced!

Basically, this means that chemical equations must be consistent with the law of conservation of mass:

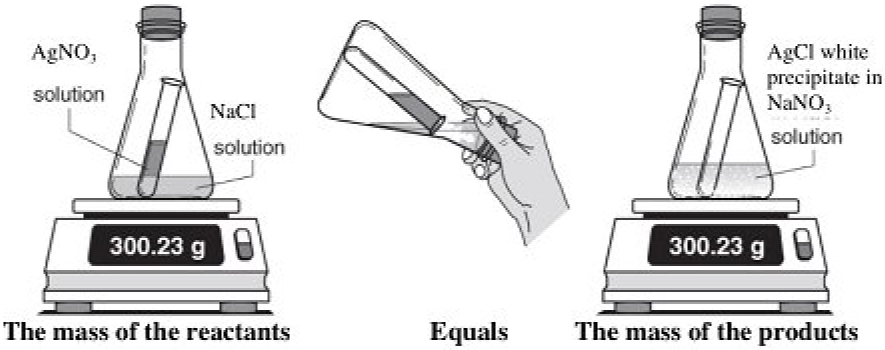

Figure 4.10 Combustion Reaction

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In the context of an ordinary chemical reaction, conservation of mass means that atoms are neither created nor destroyed. This requirement is easily met by making sure that there are equal numbers of all atoms on both sides of the equation.

When we balance an equation, we simply make it consistent with the observed fact that individual atoms are conserved in chemical changes.

A chemical Equation is made of reactants at the left side of the chemical equation. These reactants are compounds being reacting to produce new compounds called the products at right side of the chemical equation Both reactants and products are separated with an arrow.

If the reaction goes mostly to completion, then one arrow is used but if the reaction does not go to completion, then double arrows are used which means that both the reactants and the products are found in reaction in appreciative amount at the end of the reaction and the reaction does not give only products.

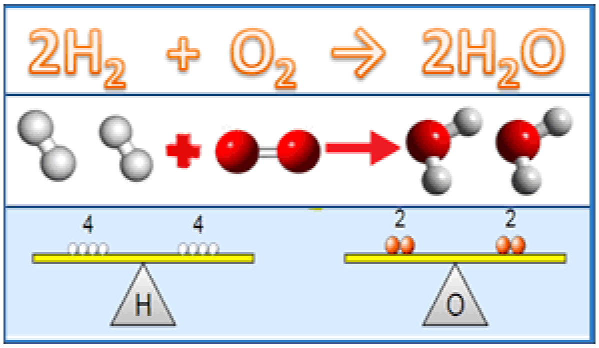

Figure 4.11 Balancing Chemical Requation

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Reaction goes to completion: (Using One Arrow to Separate the Reactants from the Products)

Here are few more examples:

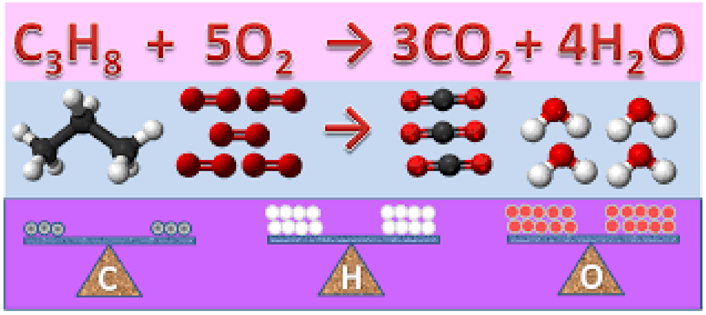

Figure 4.12 Balancing Chemical Equation

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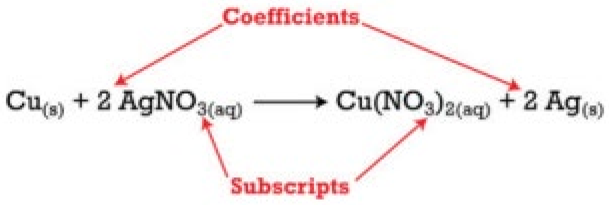
Some Reactions do not go to completion also known as chemical equilibrium: (Using Double Arrows to Separate the Reactants from the Products)

Figure 4.13 Chemical Equation

Ref: commons.wikimedia.org/

Furthermore, one to differentiate between numbers of moles (also called coefficients) appearing at the front of the products or the reactants which are changed till the chemical equations are balanced, and the numbers appearing within the molecular formula as subscripts which are fixed and should not be touched when balancing chemical equations.

Example:



Reference:
https://chem.libretexts.org/Bookshelves/Introductory_Chemistry/Map%3A_Introductory_Chemistry_(Tro)/07%3A_Chemical_Reactions/7.03%3A_How_to_Write_Balanced_Chemical_Equations

General Procedure to balance chemical equation:

a) Balance the polyatomic anions on both sides of the chemical equation as one unit
b) Look at a standalone element or a molecule, balance them at the end
c) Balance the remaining atoms, and if necessary use fractional coefficients. If a fractional coefficients have been used, multiply both sides of the equation by the denominator to obtain whole numbers for the coefficients. Remember there are no fractional atoms
d) Count the numbers of atoms of identical type at both sides of the equation to make sure their amounts at both side are identical and hence the equation is balanced

Example:

$C_4H_{10} + O_2 \rightarrow CO_2 + H_2O + \text{Heat}$

Let us make a table:

Number of Atoms or Number of Polyatomic Anions	Number of Atoms or Number of Polyatomic Anions Left Side (Reactants' Side)	Number of Atoms or Number of Polyatomic Anions Right Side (Products Side)	Status of the Balancing
C atom	4	1	Not Balanced
H atom	10	2	Not Balanced
O atom	2	3	Not Balanced

Now let us multiply the Carbon atom at the right side by 4 and Hydrogen atom by 5 to balance them at both sides.

$C_4H_{10} + O_2 \rightarrow 4\ CO_2 + 5\ H_2O + \text{Heat}$

Number of Atoms or Number of Polyatomic Anions	Number of Atoms or Number of Polyatomic Anions Left Side (Reactants' Side)	Number of Atoms or Number of Polyatomic Anions Right Side (Products Side)	Status of the Balancing
C atom	4	4	Balanced
H atom	10	10	Balanced
O atom	2	13	Not Balanced

Now look at the chemical reaction. Everything is balanced except oxygen. General rule of thumb; if one atom at one side has an even number (i.e. like oxygen atom at the left side 2) and odd number at the other side (i.e. like oxygen atom at the right side 130, one has to go through fraction to balance the chemical equation:

$C_4H_{10} + 13/2\ O_2 \rightarrow 4\ CO_2 + 5\ H_2O$

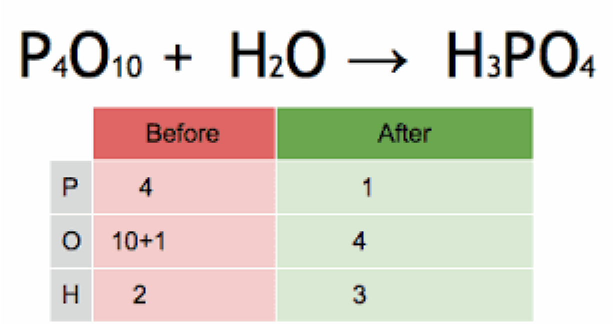
Since nature does not support fractional atoms, both side of the chemical equations have to be multiplied with the denominator which is 2:

$2 \times [C_4H_{10} + 13/2\ O_2 \rightarrow 4\ CO_2 + 5\ H_2O$

The final balance chemical equation is then:

$$2\ C_4H_{10} + 13\ O_2 \rightarrow 8\ CO_2 + 10\ H_2O$$

Practice: try this one!



$$P_4O_{10} + H_2O \longrightarrow H_3PO_4$$

	Before	After
P	4	1
O	10+1	4
H	2	3

Figure 4.14 Balancing Chemical Equation

Ref: commons.wikimedia.org/

What are the coefficients of the balanced equation of the above equation?

Try this Balancing app(free): "Reactions" with more than 400 equations for practicing balancing. Look for the app in app store on any mobile device.

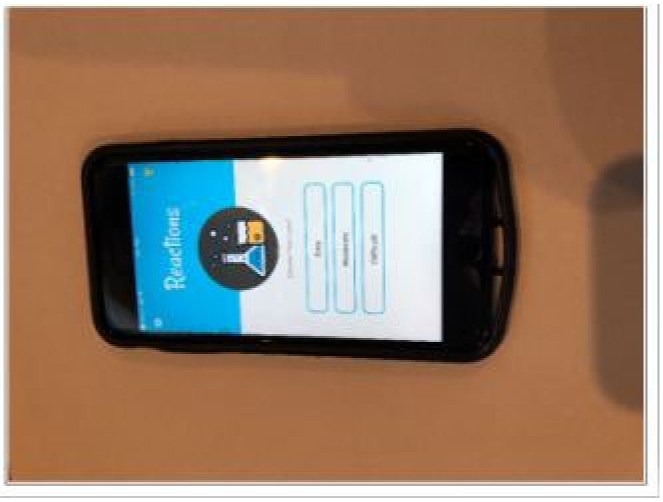


Figure 4.15 Balancing App

Ref: commons.wikimedia.org/

In case of polyatomic ion containing equations, it is always recommended to consider them as unit rather than broken down to individual atoms if they appear on both sides of the equation.

$LiOH + H_3PO4 \rightarrow Li_2HPO4 + H_2O$ *(unbalanced)*

To balance Li, we have to put coefficient 2 in front of LiOH. That will give total number H on the left hand side= 5 and O=2, keeping PO_4 unit separate from other elements. We can put coefficient 2 in front of H_2O to form 4 H and 2 O, remaining one H is present in Li_2HPO4. PO_4 unit is same on left and right hand side. So the final number of atoms look like :

Left side: Li -2	Right side: Li-2
O-2	O-2
H-5	H-5
PO4-1	PO4-1

Balanced equation is

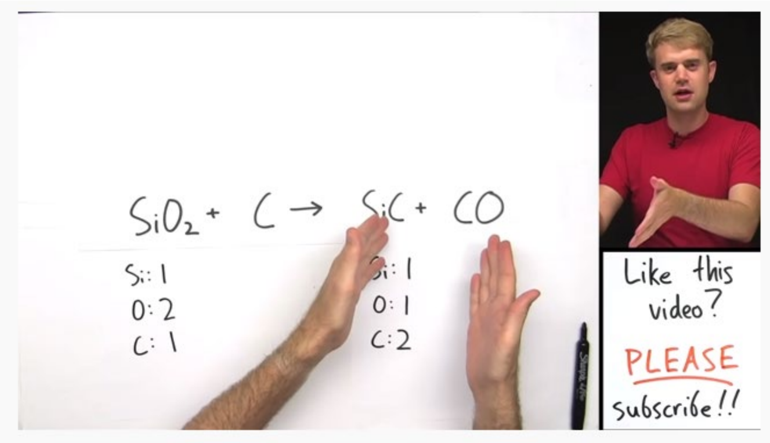
$2LiOH + H_3PO4 \rightarrow Li_2HPO4 + 2H_2O$ *(balanced)*

Always lowest number of coefficients are used to balance a chemical equation. For example, $2H_2O \rightarrow 2H_2 + O_2$, this equation can also be balanced by $4H_2O \rightarrow 4H_2 + O_2$

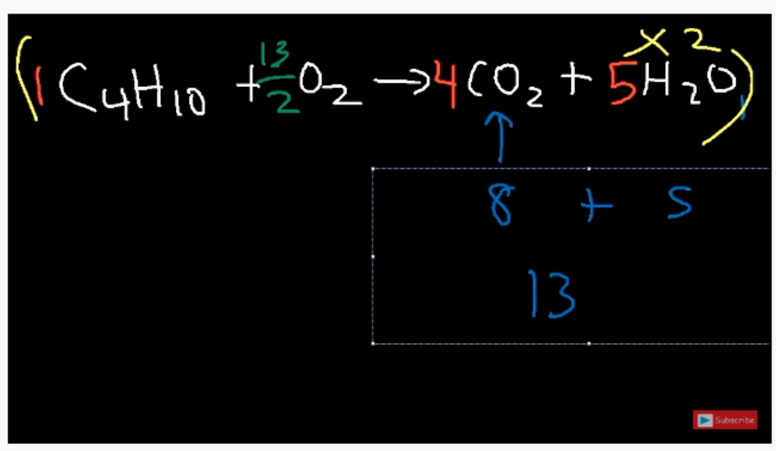
But we always use lowest set of whole numbers to balance an equation.

The following video might help you to understand more this topic.

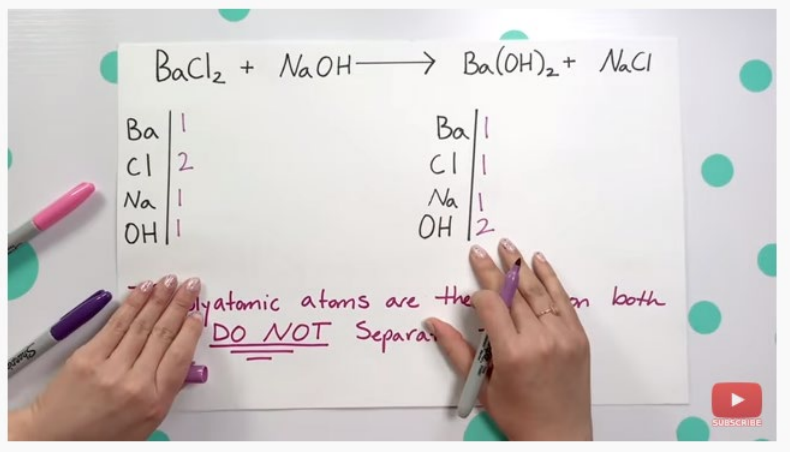
Now let us review the videos below:



https://www.youtube.com/watch?v=eNsVaUCzvLA&t=500s



https://www.youtube.com/watch?v=e_C-V5vJv80&t=169s



https://www.youtube.com/watch?v=jy6F0Lbvjm8&t=71s

Chemical equations should exhibit the status of the chemical compounds involved in the chemical reactions such liquids (l), solids (s), gases (g) and aqueous (aq).

Furthermore, the status of the heat being absorbed (taken in) or given away:

$2\ C_4H_{10}(g) + 13\ O_2(g) \rightarrow 8\ CO_2(g) + 10\ H_2O(g)$ + Heat [Exothermic]

$HgCO_3(s) \xrightarrow{\Delta} HgO(s) + CO_2(g)$ [Exothermic]

Heat + $NH_4Cl(g) \leftrightarrow NH_3(g) + HCl(g)$ [Endothermic]

The chemical equations of ionic compounds in aqueous solution (dissolved in water) represent very unique sets of balancing:

a) Complete molecular ionic chemical equation
b) Complete ionic chemical equation
c) Net ionic chemical equation

Complete molecular ionic chemical equation:

This is an ionic chemical equation that keeps the ionic compounds and they are not taken apart in ions.

Example:

$NaI(aq) \quad + \quad Pb(NO_3)_2(aq) \rightarrow PbI_2(s) \quad + \quad NaNO_3(aq)$

Balancing this molecular ionic chemical equation:

$\mathbf{2\ NaI(aq) \quad + \quad Pb(NO_3)_2(aq) \rightarrow PbI_2(s) \quad + \quad 2\ NaNO_3(aq)}$

Complete ionic chemical equation:

Each aqueous ionic compound in the ionic chemical equation will be taken apart to its original ions, keeping all solids, liquids and gaseous compounds **untouched**:

$2\ NaI(aq) \quad + \quad Pb(NO_3)_2(aq) \rightarrow PbI_2(s) \quad + \quad 2\ NaNO_3(aq)$

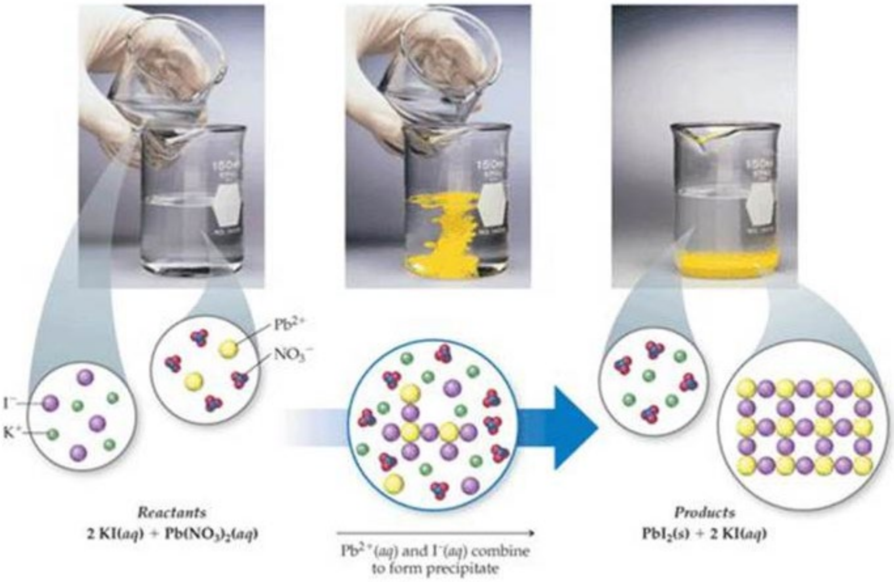
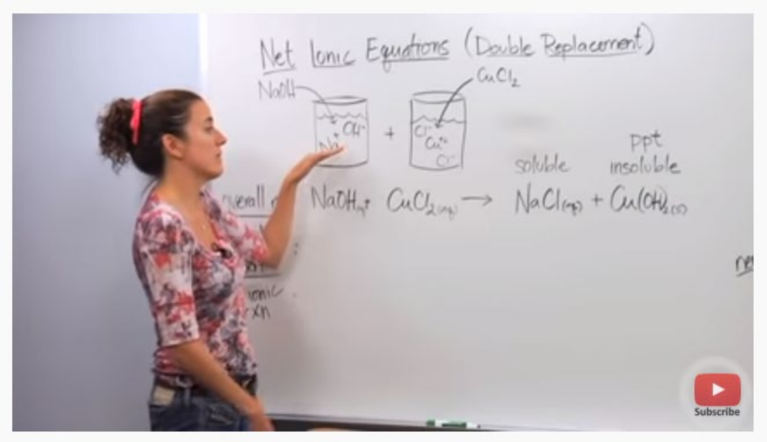


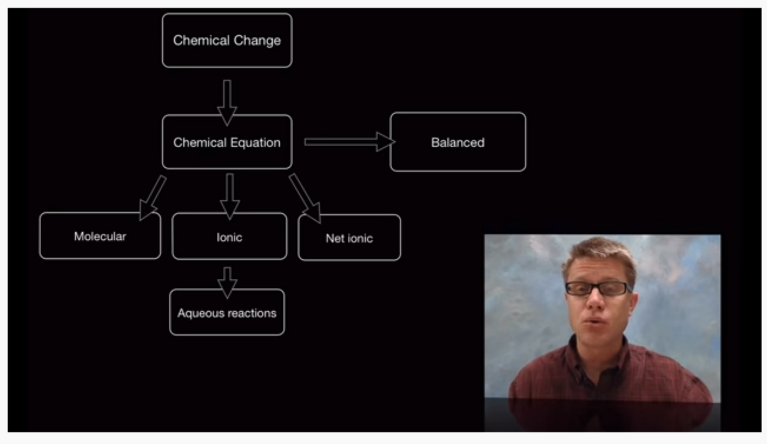
Figure 4.16 Precipitation Reaction

Reference: https://microbenotes.com/introduction-to-precipitation-reaction/

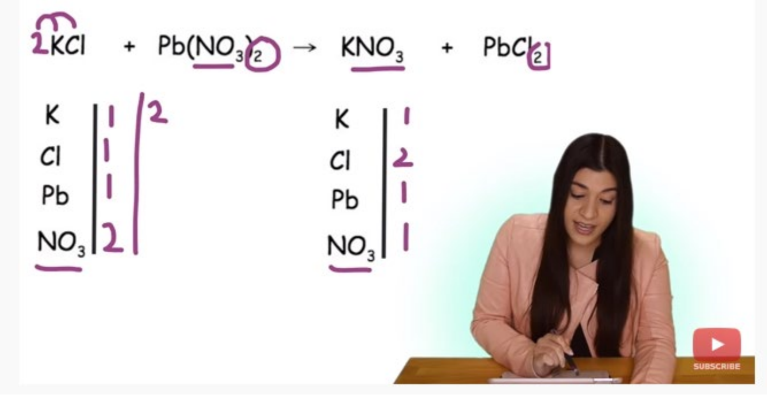
The videos below illustrate the net ionic chemical equations set up and balancing:



https://www.youtube.com/watch?v=dXqelH1MxGw



https://www.youtube.com/watch?v=wxvERNlUdBQ



https://www.youtube.com/watch?v=MJy5CNzd6sY

The simulation below helps understand the concept of balancing chemical equation:

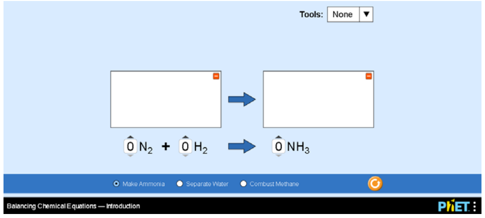
Simulation Activity Instructions:

https://phet.colorado.edu/sims/html/balancing-chemical-equations/latest/balancing-chemical-equations_en.html

Learning Goals: Students will be able to:

a) Describe what “reactants” and “products” in a chemical equation mean.
b) Explain the importance of knowing the difference between “coefficients” and “subscripts”.
c) Use pictures and calculations to show how the number of atoms for each product or reactant is found.
d) Identify the relationship between “reactants” and “products” atoms.
e) Balance a chemical equation using the relationships identified.
f) Given a chemical equation, draw molecular representations of the reaction and explain how the representations were derived.
g) Given a molecular drawing of a chemical reaction, write the equation and explain how the symbols were derived.

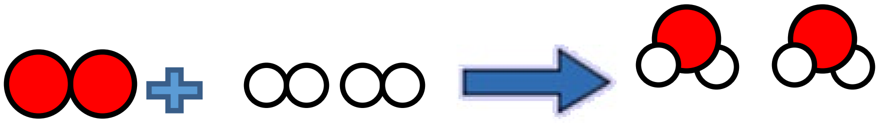
Develop your understanding: Open the **Introduction** screen, then explore to develop your own ideas about what it means to “balance a chemical equation”.


Tools: None

● Make Ammonia ○ Separate Water ○ Combust Methane

Explain your understanding:

1. How does the sim provide information to help you learn the goals?
2. What things did you have to research outside the sim (cite references)?
3. How can you use the simulation to check your learning?
4. Use this balanced reaction to show that you can write the equation that makes chemical sense. Explain how your symbols were derived in paragraph form.

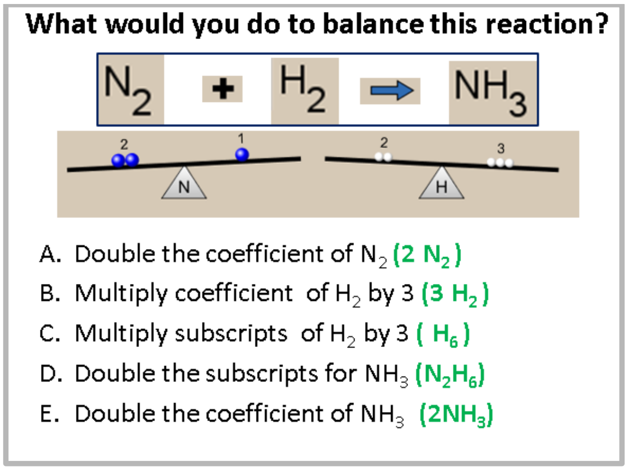


5. Use this reaction to show that you can draw molecular representations of a balanced reaction. Explain how your representations were derived in paragraph form.

$$CO_2 + H_2O \rightarrow C_2H_6 + O_2$$

Test your understanding: For each question, write your answer and give your reasoning with evidence from the simulation.

Question 1

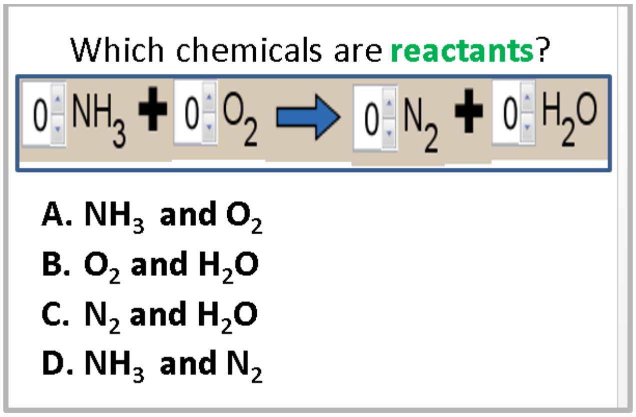

What would you do to balance this reaction?

$N_2 + H_2 \rightarrow NH_3$

A. Double the coefficient of N_2 ($2\ N_2$)
B. Multiply coefficient of H_2 by 3 ($3\ H_2$)
C. Multiply subscripts of H_2 by 3 (H_6)
D. Double the subscripts for NH_3 (N_2H_6)
E. Double the coefficient of NH_3 ($2NH_3$)

Your answer and explanation:

Question 2

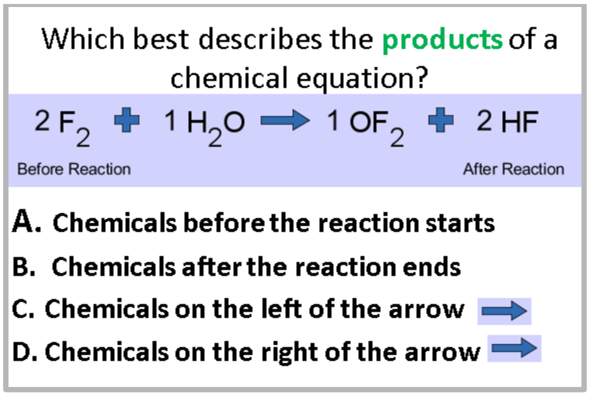

Which chemicals are **reactants**?

$0\ NH_3 + 0\ O_2 \rightarrow 0\ N_2 + 0\ H_2O$

A. NH_3 and O_2
B. O_2 and H_2O
C. N_2 and H_2O
D. NH_3 and N_2

Your answer and explanation:

Question 3



Which best describes the products of a chemical equation?

$2 F_2 + 1 H_2O \rightarrow 1 OF_2 + 2 HF$

Before Reaction

After Reaction

A. Chemicals before the reaction starts

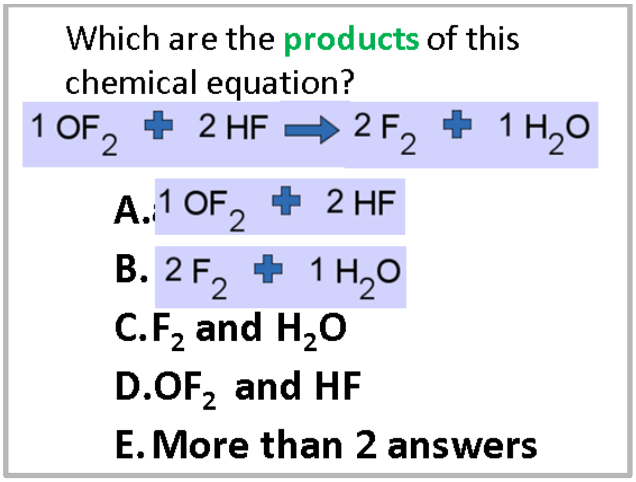
B. Chemicals after the reaction ends

C. Chemicals on the left of the arrow →

D. Chemicals on the right of the arrow →

Your answer and explanation:

Question 4



Which are the products of this chemical equation?

$1 OF_2 + 2 HF \rightarrow 2 F_2 + 1 H_2O$

A. $1 OF_2 + 2 HF$

B. $2 F_2 + 1 H_2O$

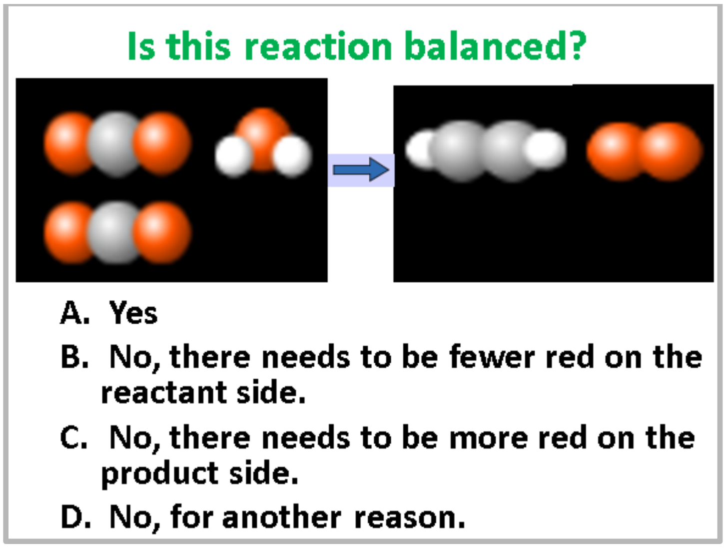
C. F_2 **and** H_2O

D. OF_2 **and HF**

E. More than 2 answers

Your answer and explanation:

Question 5



Is this reaction balanced?

A. Yes

B. No, there needs to be fewer red on the reactant side.

C. No, there needs to be more red on the product side.

D. No, for another reason.

Your answer and explanation:

Test your understanding and skill application:

Open the full simulation Balancing Chemical Equations, then open the **Game** screen. Use ideas you have from the learning goals. You may need to use the Intro and Balance Lab screens to learn.

1. Play Level 1of the Balancing Chemical Equations game
    a. Did you have to change your thinking or do you have other ideas to make you get a better score? Include screen captures from the simulation to help explain.

    b. When you get a wrong answer, how did the "Show Why" help you?

Great!

★★★★☆

Score: 8 out of 10

2. Play Level 2 of the game
    a. Explain what makes the level more difficult or different from previous levels. Do you have new strategy ideas or rules? Include screen captures from the simulation to help explain.

    b. When you complete the level, capture the screen with your score and paste it below:

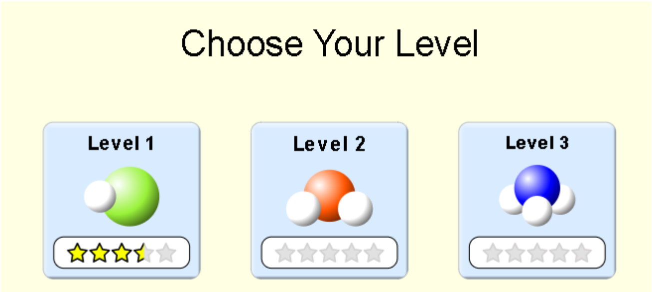
3. Play Level 3 of the game
    a. Explain what makes the level more difficult or different from previous levels. Do you have new strategy ideas or rules? Include screen captures from the simulation to help explain.

    b. When you get a wrong answer, how did the "Show Why" help you?

    c. When you complete the level, capture the screen with your score and paste it below:

Final Score:

After you play all levels of the game. Copy and paste your final results like this



Choose Your Level

III. Chemical Reactions Types

There are 3 major reactions some of which have sub types of chemical reactions:
All these types are considered to be in an aqueous medium where water is used as a solvent.

a) Precipitation Reactions: Also known as Double Replacement/Displacement Reactions
b) Acid – Base Reactions: Also known as Double Replacement/Displacement Reactions
c) Redox Reactions: There are several sub types for Redox Reactions:
    1. Single Replacement/Displacement Reactions
    2. Decomposition Reactions
    3. Combustion Reactions
    4. Combination (Synthesis) Reactions

Type 1. Precipitation Reactions:

Precipitation reactions are reactions by which the cations of one ionic compound will combine itself with another anion of another ionic compound. The intermolecular ionic forces of the anions and the cation yield a chemical compound which is settling at the bottom of the reaction as a solid that is called precipitate. This precipitate is water insoluble.

Example:

$AgNO_3(aq) + K_2Cr_2O_7(aq) \rightarrow \mathbf{Ag_2Cr_2O_7(s)} + KNO_3(aq)$

$\mathbf{Ag_2Cr_2O_7(s)}$ is a ruby red precipitate (solid) insoluble in water. The image below illustrates the $\mathbf{Ag_2Cr_2O_7}$ precipitate:

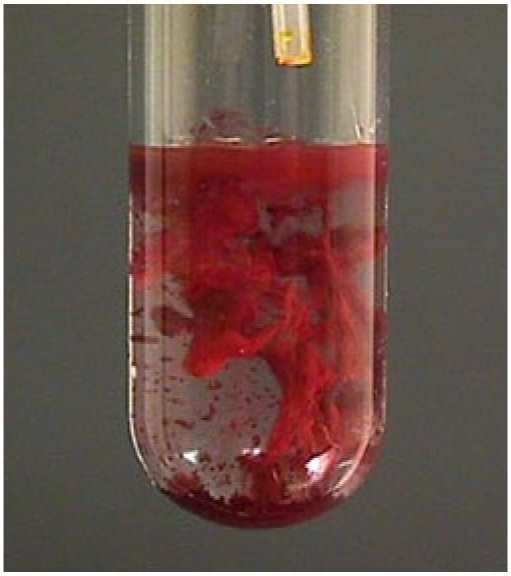


Figure 4.17 Precipitation Reaction
Reference: http://dept.harpercollege.edu/chemistry/chm/100/dgodambe/thedisk/chemrxn/r19.htm

One can predict the precipitation process by which the precipitate is produced. The solubility table is an excellent tool that predicts the formation of such precipitates.

Solubility Table:

The following are the solubility rules for common ionic solids. If there two rules appear to contradict each other, the preceding rule takes precedence.

1. Salts containing Group I elements (Li^+, Na^+, K^+, Cs^+, Rb^+) are soluble . There are few exceptions to this rule. Salts containing the ammonium ion (NH_4^+) are also soluble.
2. Salts containing nitrate ion (NO_3^-) are generally soluble.
3. Salts containing Cl^-, Br^-, or I^- are generally soluble. Important exceptions to this rule are halide salts of Ag^+, Pb^{2+}, and $(Hg_2)^{2+}$. Thus, AgCl, $PbBr_2$, and Hg_2Cl_2 are insoluble.
4. Most silver salts are insoluble. $AgNO_3$ and $Ag(C_2H_3O_2)$ are common soluble salts of silver; virtually all others are insoluble.
5. Most sulfate salts are soluble. Important exceptions to this rule include $CaSO_4$, $BaSO_4$, $PbSO_4$, Ag_2SO_4 and $SrSO_4$.
6. Most hydroxide salts are only slightly soluble. Hydroxide salts of Group I elements are soluble. Hydroxide salts of Group II elements (Ca, Sr, and Ba) are slightly soluble. Hydroxide salts of transition metals and Al^{3+} are insoluble. Thus, $Fe(OH)_3$, $Al(OH)_3$, $Co(OH)_2$ are not soluble.
7. Most sulfides of transition metals are highly insoluble, including CdS, FeS, ZnS, and Ag_2S. Arsenic, antimony, bismuth, and lead sulfides are also insoluble.
8. Carbonates are frequently insoluble. Group II carbonates ($CaCO_3$, $SrCO_3$, and $BaCO_3$) are insoluble, as are $FeCO_3$ and $PbCO_3$.
9. Chromates are frequently insoluble. Examples include $PbCrO_4$ and $BaCrO_4$.
10. Phosphates such as $Ca_3(PO_4)_2$ and Ag_3PO_4 are frequently insoluble.
11. Fluorides such as BaF_2, MgF_2, and PbF_2 are frequently insoluble.

Balancing Equations using **Solubility Rule:**

General approach:

a) Balance the molecular ionic chemical equation, the complete ionic equation and the net ionic equation.

b) With the help of the net ionic equation and the combination of the cations and the anions, one has to check ionic compound again the solubility table and determine whether this formed ionic compound is soluble and insoluble.

For very detailed solubility chart, one can use the periodic table solubility chart:

Net ionic equations

Ionic compounds are usually dissociated in aqueous solution; thus if we combine solutions of silver nitrate $AgNO_3$ and sodium chloride NaCl we are really combining four different species: the *cations* (positive ions) Ag+ and Na+ and the *anions* (negative ions) NO_3^- and Cl^-. It happens that when the ions Ag^+ and Cl^- are

brought together, they will combine to form an insoluble precipitate of silver chloride. The net equation for this reaction is
$Ag^+(aq) + Cl^-(aq) \rightarrow AgCl(s)$

Note that the ions NO_3^- and Cl^- are not directly involved in this reaction; the equation expresses only the *net change*, which is the removal of the silver and chloride ions from the solution to form an insoluble solid. the symbol (*aq*) signifies that the ions are in aqueous solution, and thus are *hydrated*, or attached to water molecules. The symbol (*s*) indicates that the substance AgCl exists as a solid. When a solid is formed in a reaction that takes place in solution, it is known as a *precipitate*. The formation of a precipitate is often indicated by underscoring.

Predicting the outcome when dissolved salts are mixed
From the above example involving silver chloride, it is clear that a meaningful net ionic equation can be written only if two ions combine to form an insoluble compound. In order to make this determination, it helps to know the solubility rules— which all students of chemistry were at one time required to memorize, but are nowadays usually obtained from tables such as the one shown below.

Balancing this molecular ionic chemical equation:

$2\ NaI(aq) + Pb(NO_3)_2(aq) \rightarrow PbI_2(s) + 2\ NaNO_3(aq)$

Complete ionic chemical equation:

Each aqueous ionic compound in the ionic chemical equation will be taken apart to its original ions, keeping all solids, liquids and gaseous compounds **untouched**:

$2\ NaI(aq) + Pb(NO_3)_2(aq) \rightarrow PbI_2(s) + 2\ NaNO_3(aq)$

The complete ionic chemical equation:

$2\ Na^+(aq) + 2\ I^-(aq) + Pb^{2+}(aq) + 2\ NO_3^-(aq) \rightarrow PbI_2(s) + 2\ Na^+(aq) + 2\ NO_3^-(aq)$

Net ionic chemical equation

The net ionic chemical equation will consider only ions react and produce the product. It eliminates the ions that appear at the same time at both reactants' as well as products' sides. Such ions are called: **Spectator ions**. They present in the reaction but they do not participate in actual chemical reaction which ends up producing the products.

$2\ Na^{+}(aq) + 2\ I^{-}(aq) + Pb^{2+}(aq) + 2\ NO_3^{-}(aq) \rightarrow PbI_2(s) + 2\ Na^{+}(aq) + 2\ NO_3^{-}(aq)$

In the above complete ionic chemical equation, the spectator ions are: $Na^{+}(aq)$ and $NO_3^{-}(aq)$.

By eliminating these spectator ions from both the reactants' and products' sides:

$\cancel{2\ Na^{+}(aq)} + 2\ I^{-}(aq) + Pb^{2+}(aq) + 2\ \cancel{NO_3^{-}(aq)} \rightarrow PbI_2(s) + 2\ \cancel{Na^{+}(aq)} + 2\ \cancel{NO_3^{-}(aq)}$

Net Ionic Chemical Equation:

$\mathbf{2\ I^{-}(aq) + Pb^{2+}(aq) \rightarrow PbI_2(s)}$

Example:

Complete molecular ionic chemical equation:

$\mathbf{KI(aq) + Pb(NO_3)_2(aq) \rightarrow PbI_2(s) + KNO_3(aq)}$

Complete ionic chemical equation:

$\mathbf{2\ K^{+}(aq) + 2\ I^{-}(aq) + Pb^{2+}(aq) + 2\ NO_3^{-}(aq) \rightarrow PbI_2(s) + 2\ K^{+}(aq) + 2\ NO_3^{-}(aq)}$

With $K^{+}(aq)$ and $NO_3^{-}(aq)$ are being the spectator ions.

Net ionic chemical equation:

$\mathbf{2\ I^{-}(aq) + Pb^{2+}(aq) \rightarrow PbI_2(s)}$

Anion (negative ion)	**Cation (positive ion)**	**Soluble?**
any anion	alkali metal ions (Li^{+}, Na^{+}, K^{+}, etc.)	yes
nitrate, NO_3^{-}	any cation	yes
acetate, CH_3COO^{-}	any cation except Ag^{+}	yes
halide ions Cl^{-}, Br^{-}, or I^{-}	Ag^{+}, Pb^{2+}, Hg_2^{2+}, Cu^{2+}	no

halide ions Cl^-, Br^-, or I^-	any other cation	yes
sulfate, SO_4^{2-}	Ca^{2+}, Sr^{2+}, Ba^{2+}, Ag^+, Pb^{2+}	no
sulfate, SO_4^{2-}	any other cation	yes
sulfide, S_2^-	alkali metal ions or NH_4^+	yes
sulfide, S_2^-	Be^{2+}, Mg^{2+}, Ca^{2+}, Sr^{2+}, Ba^{2+}, Ra^{2+}	yes
sulfide, S_2^-	any other cation	no
hydroxide, OH^-	alkali metal ions or NH_4^+	yes
hydroxide, OH^-	Sr^{2+}, Ba^{2+}, Ra^{2+}	slightly
hydroxide, OH^-	any other cation	no
phosphate, PO_4^{3-}, carbonate CO_3^{2-}	alkali metal ions or NH_4^+	yes
phosphate, PO_4^{3-}, carbonate CO_3^{2-}	any other cation	no

Problem Example 3: *net ionic equations*

Write net ionic equations for what happens when aqueous solutions of the following salts are combined:

a) $PbCl_2 + K_2SO_4$
b) $K_2CO_3 + Sr(NO_3)_2$
c) $AlCl_3 + CaSO_4$
d) $Na_3PO_4 + CaCl_2$

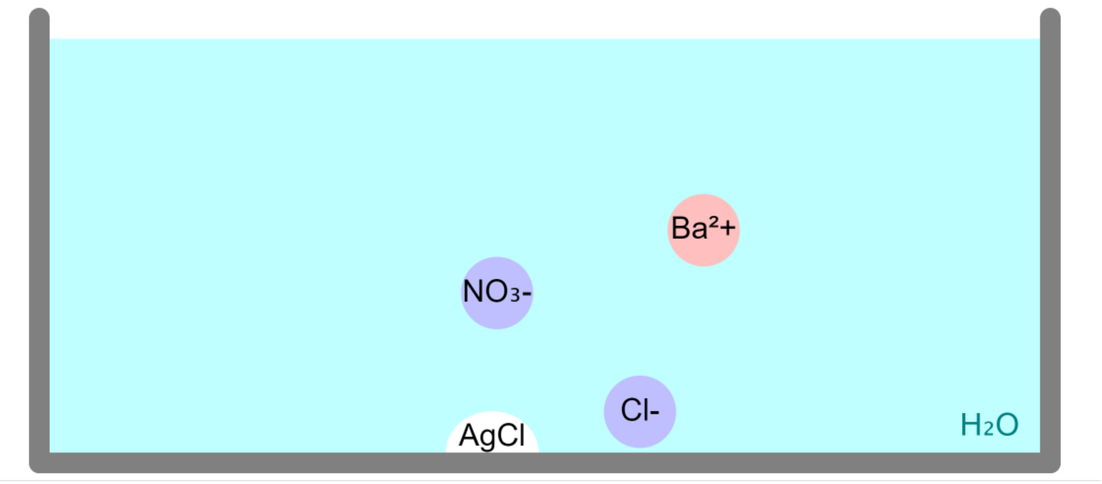
Solution: Use the solubility rules table(above) to find the insoluble combinations:

a)$Pb^{2+}(aq) + SO_4^{2-}(aq) \rightarrow PbSO4(s)$
b) $Sr^{2+}(aq) + CO_3^{2-}(aq) \rightarrow SrCO_3(s)$
c) no net reaction
d) $3\ Ca^{2+}(aq) + 2\ PO_4^{3-}(aq) \rightarrow 3\ Ca_3(PO_4)_2(s)$
(Note the need to balance the electric charges)

Precipitation Reaction:

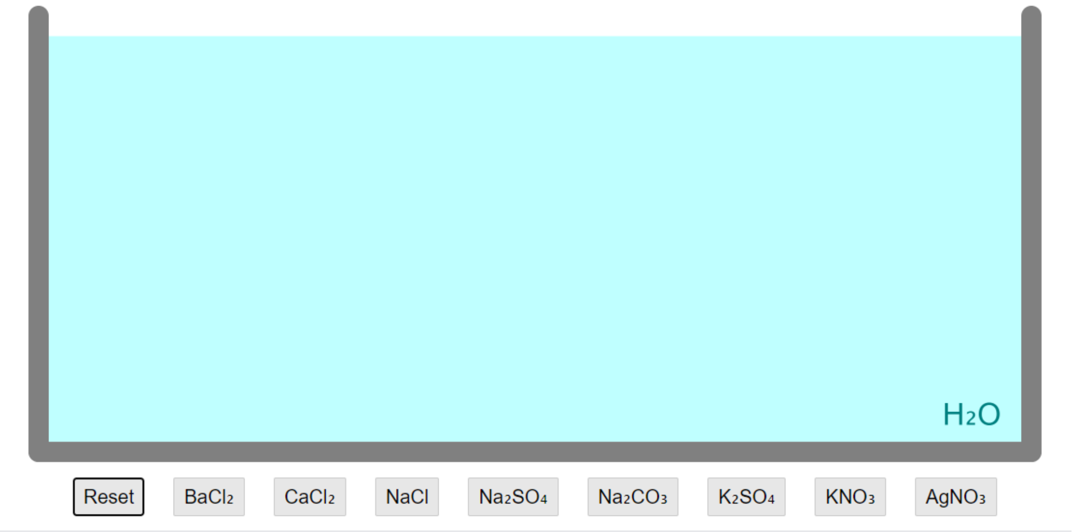
https://javalab.org/en/precipitation_reaction_en/

$AgNO_3(aq)$ + $BaCl_2(aq)$ → $AgCl(s)$ + $Ba(NO_3)_2(aq)$



AgCl is a solid and called a precipitate. It settles at the bottom of the reaction container.

Now try the combinations given in the simulation and fill in the table below:



Determine which one of these combination will make a reaction (Double Displacement/Replacement Reaction also called Precipitation Reaction). Just type Reaction in case there is a reaction. Use the Solubility table and information given above.

Compounds	$BaCl_2$	$CaCl_2$	NaCl	Na_2SO_4	Na_2CO_3	K_2SO_4	KNO_3	$AgNO_3$
$BaCl_2$	No Reaction							
$CaCl_2$		No Reaction						
NaCl			No Reaction					
Na_2SO_4				No Reaction				
Na_2CO_3					No Reaction			
K_2SO_4						No Reaction		
KNO_3							No Reaction	
$AgNO_3$								No Reaction

Type 2. Acid – Base Titrations:

An acid reacts with a base to in aqueous medium to produce salt and water. This reaction is called Acid – Base reaction or Acid – Base Neutralization or just Double Displacement/Replacement Reaction. A brief summary regarding acids and bases will be covered later. More details will follow in the later chapters.

Example:

HCl(aq) + NaOH(aq) → NaCl(aq) + H_2O(l) + Heat

HCl(aq) + H_2O(l) → H_3O^+(aq) + Cl^-(aq)

NaOH(aq) + H_2O(l) → Na^+(aq) + OH^-(aq) + H_2O(l)

The complete ionic chemical equation is:

H^+(aq) + Cl^-(aq) + Na^+(aq) + OH^-(aq) → Na^+(aq) + Cl^-(aq) + H_2O(l) + Heat

The net ionic chemical equation is: [Cl^-(aq) and Na^+(aq) spectator ions]

H^+(aq) + OH^-(aq) → H_2O(l) + Heat

The driving force for the acid – base reaction or neutralization is the formation of water by the reaction of the protons H^+ or correctly said the H_3O hydronium ions with hydroxide ions.

There are two types of acids according to their dissociation in water.

a) Strong acid: is an acid that dissociate completely in water
b) Weak acid: is an acid that dissociate partially in water

Strong acids are known to be 7:

Perchloric acid: $HClO_4$
Chloric acid: $HClO_3$
Hydrochloric acid: HCl
Hydroiodic acid: HI
Hydrobromic acid: HBr
Nitric acid: HNO_3
Sulfuric acid: H_2SO_4

All other acids inorganic and organic acids are considered to be weak.

Acetic Acid: CH_3COOH
Hydrofluoric acid: HF
Phosphoric acid: H_3PO_4
Oxalic acid: $H_2C_2O_4$
Carbonic acid: H_2CO_3

Fruits are very rich with weak acids:

Figure 4.18 Sources of Acids in Fruits

Weak acids are founds in Vegetables as well:
Reference: https://www.livestrong.com/article/260893-names-of-acids-in-fruits-vegetables-dairy-products/

Asparagus
Beans
Corn
Cucumbers
Garlic
Green beans
Greens (lettuce, kale, collards, spinach, etc.)
Onions
Peas
Pumpkins
Squash

There are two types of bases according to their dissociation in water.

a) Strong base: is a base that dissociate completely in water
b) Weak base: is a base that dissociate partially in water

Strong bases are known to be 2 types of group 1A and 2A in periodic table:

Sodium hydroxide: $NaOH$
Lithium hydroxide: $LiOH$
Potassium hydroxide: KOH
Cesium hydroxide: $CsOH$
Magnesium hydroxide: $Mg(OH)_2$
Calcium hydroxide: $Ca(OH)_2$
Strontium Hydroxide: $Sr(OH)_2$
Barium Hydroxide: $Ba(OH)_2$

All other bases inorganic and organic bases are considered to be weak.
Ammonium hydroxide: NH_4OH
Iron-III-hydroxide: $Fe(OH)_3$
Titanium-II-hydroxide: $Ti(OH)_2$
Aluminum hydroxide: $Al(OH)_3$
Pyridine: C_5H_5N
Aniline: $C_6H_5NH_2$
All amines are considered as weak bases such as methyl amine CH_3NH_2 etc…

Fruits and nuts are very rich with weak bases:


Figure 4.19 Nuts and dry fruits

Reference: https://nuts.com/healthy-eating/alkaline-diet

Reference: https://www.livestrong.com/article/494847-nuts-alkaline-forming/

The acid – base neutralization as mentioned yields salt and water:

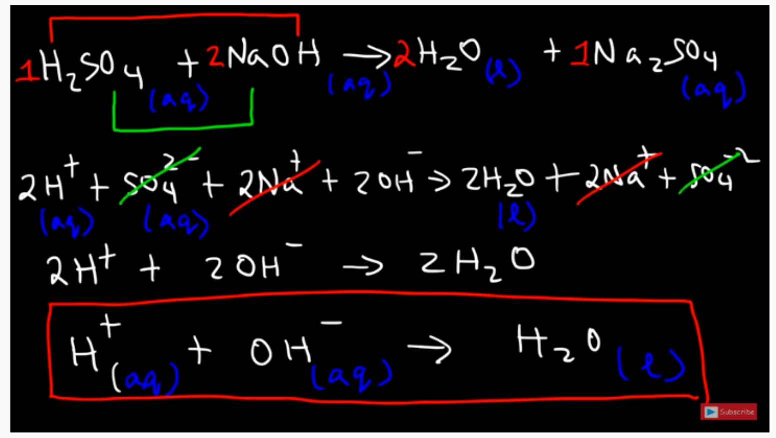
Examples:

$Fe(OH)_3(aq)$ + 3 $HNO_3(aq)$ → $Fe(NO_3)_3(aq)$ + 3 $H_2O(l)$ [water is produced as by product]
This type of reaction is considered neutralization reaction as well as double Replacement/Displacement Reaction.

$C_6H_5NH_2(aq)$ + $HCl(aq)$ → $C_6H_5NH_3^+ Cl^- (s)$

Aniline + Hydrochloric acid → anilinium chloride [No water is produced as by product]
This type of reaction is considered neutralization reaction as well as Combination Reaction.

The video below illustrates the acid – base neutralization in some details:



$$1H_2SO_{4\,(aq)} + 2NaOH_{(aq)} \rightarrow 2H_2O_{(l)} + 1Na_2SO_{4\,(aq)}$$

$$2H^+_{(aq)} + \cancel{SO_4^{2-}}_{(aq)} + \cancel{2Na^+} + 2OH^- \rightarrow 2H_2O_{(l)} + \cancel{2Na^+} + \cancel{SO_4^{-2}}$$

$$2H^+ + 2OH^- \rightarrow 2H_2O$$

$$\boxed{H^+_{(aq)} + OH^-_{(aq)} \rightarrow H_2O_{(l)}}$$

https://www.youtube.com/watch?v=UfTJrAPjeys

Type 3. Redox Reactions: There are several sub types for Redox Reactions:

1. **Single Replacement/Displacement Reactions**
2. **Decomposition Reactions**
3. **Combustion Reactions**
4. **Combination (Synthesis) Reactions**

The word "Redox" is made of a combination of two words: Red = Reduction and Ox = Oxidation. Therefore Redox reactions mean Reduction – Oxidation Reactions.

What is a Reduction? [Valence Electrons gaining]
A reduction is a process by which an element, molecule or compound accepts extra valence electrons from adjust atoms of another element or molecule or compound leading to the "Reduction" of oxidation number of that element, molecule or compound.

Oxidation number is the number of the charge that an atom, or molecule or compound can carry when they are found in solution as ions.

Oxidation Number Rules: [Assigning Oxidation Nubers]

1. Neutral atoms or molecules or compound have the oxidation number is zero. Examples: Fe, P and Na atoms are neutral and have the **oxidation number of zero.** Also, molecules such as O_2, N_2, Cl_2, NaCl, and Na_2CO_3 are neutral molecules and compounds have the **sum of oxidation numbers of zero**.
2. The oxidation number of the ions is equal to the charge that these ions carry. The **oxidation number of** Ca^{2+} ion is **+2**, Al^{3+} has the **oxidation of +3**, and P^{3-} has the **oxidation number of -3**, S^{2-} has the **oxidation number of -2**. NH_4^+ ammonium ion has the **oxidation number of +1**.
3. In general the **oxidation number of** hydrogen is **+1** when hydrogen is forming covalent bonds (combined itself with another none metal(s)). Examples: NH_3, HNO_3, C_2H_6
4. The **oxidation number of** hydrogen is **-1** when hydrogen is forming ionic bonds (combined itself with another metal(s)). Examples: KH, BaH_2, AlH_3 and $LiAlH_4$**.**
5. The metals in Group IA has the **oxidation number of +1**. Examples Na_3P and K_2S)
6. The metals in Group IA has the **oxidation number of +2**. Examples Ba_3P_2 and $Ba(HCO_3)_2$
7. Generally oxygen has the **oxidation number of -2**. Exceptions include molecules and polyatomic ions that contain O-O bonds, such as O_2, O_3 and H_2O_2, molecules and the O_2^{2-} ions.
8. Group VIIA elements have in general the **oxidation number of -1**. Examples $FeCl_3$, HF, and VI_3)

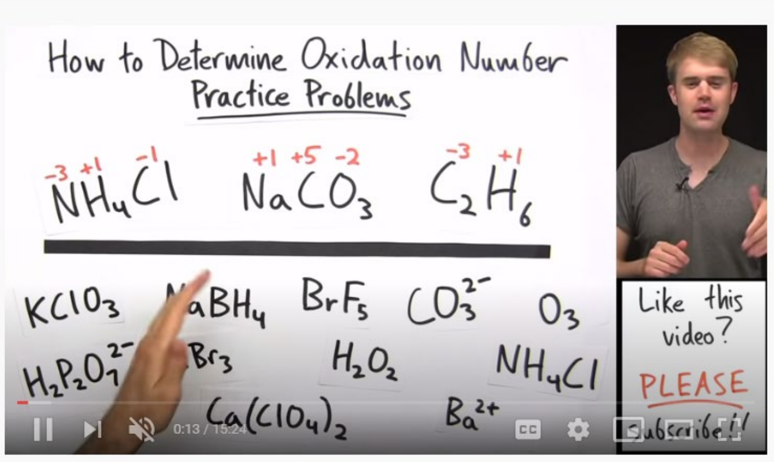
What is an Oxidation? [Valence Electrons losing]
An oxidation is a process by which an element, molecule or compound gives away some of their valence electrons to adjust atoms of another element or molecule or compound leading to the "Increase" of oxidation number of that element, molecule or compound.
Examples:

$Fe^0 \rightarrow Fe^{3+} + 3\,e^-$(oxidation: increase in charge (oxidation number)). This is an oxidation reaction.

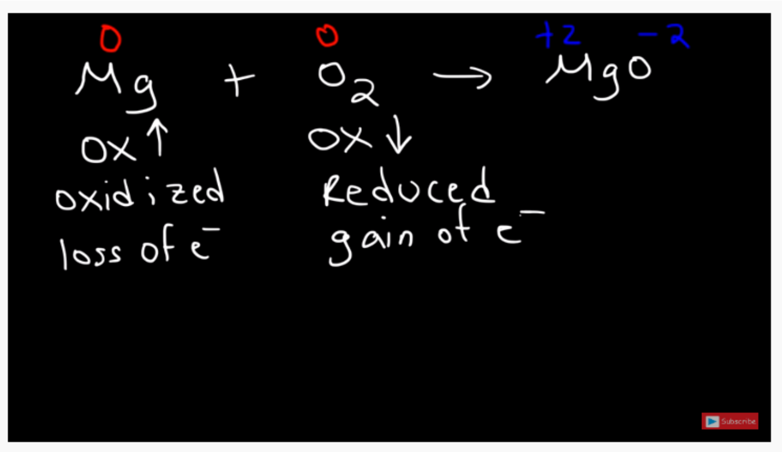
The redox reaction is made of 2 halves of reactions: the first half reaction is the oxidation reaction and the second half reaction is the reduction reaction. Both half reactions are interconnected and they occur at the same time.

Example of complete Redox reaction:
Na^0 → $Na^+ + e^-$ [first half reaction: oxidation reaction]
$e^- + Cl^0$ → Cl^- [second half reaction: reduction reaction]
$Na^0 + Cl^0$ → $Na^+ + Cl^-$ [Complete Redox Reaction]

The videos illustrate the redox reaction and the oxidation numbers applications:



https://www.youtube.com/watch?v=zpCy7KwqDO8



https://www.youtube.com/watch?v=dF5lB7gRtcA&t=7s

Oxidizing and Reducing agents:

$K^0 + Br^0$ → $K^+ + Br^-$

What does K do on Br?
K is forcing Br to be reduced. K is said to be **Reducing Agent.** K is providing the valence electrons to Br. K is reducing Br.

What does Br do on K?
Br is forcing K to be oxidized. Br is said to be **Oxidizing Agent.** Br is removing valence electrons from K. Br is oxidizing K.

Examples:

1. Assign **oxidation numbers** to each of the atoms in the following compounds:

Na_2CrO_4 Na = **+1** O = **-2** Cr = **+6**

$K_2Cr_2O_7$ K = **+1** O = **-2** Cr = **+6**

CO_2 O = **-2** C = **+4**

CH_4 H = **+1** C = **-4**

$HClO_4$ O = **-2** H = **+1** Cl = **+7**

MnO_2 O = **-2** Mn = **+4**

SO_3^{2-} O = **-2** S = **+4**

SF_4 F = **-1** S = **+4**

2. What is the range of oxidation states for carbon? -4 to +4

3. Which compound has C in a +4 state? CO_2

4. Which compound has C in a -4 state? CH_4

5. Nitrogen has 5 valence electrons (Group V). It can gain up to 3 electrons (-3), or lose up to 5 (+5) electrons. Fill in the missing names or formulas and assign an oxidation state to each of the following nitrogen containing compounds:

name	**formula**	**oxidation state of N**
ammonia	NH_3	**-3**
nitrogen	**N_2**	**0**
nitrite	**NO_2^-**	**+3**
nitrate	NO_3^-	**+5**
dinitrogen monoxide	**N_2O**	**+1**
nitrogen dioxide	NO_2	**+4**
hydroxylamine	NH_2OH	**-1**
nitrogen monoxide	**NO**	**+2**
hydrazine	N_2H_4	**-2**

6. During chemical reactions, the **oxidation state** of atoms can change. This occurs when compounds gain or lose electrons, or when the **bonds** to an atom change. This is illustrated by the reaction between nitrogen and hydrogen to make ammonia:

$$N_2(g) + 3\ H_2(g) \rightarrow 2\ NH_3(g)$$

Assign **oxidation numbers** to each of the atoms in this reaction.

N (in N_2) = **0** (in NH_3) = **-3**

H (in H_2) = **0** H (in NH_3) = **+1**

When an oxidation number **increases,** that species has been **oxidized**.

Which reactant undergoes an increase in its oxidation number? **H_2**

When an oxidation number **decreases,** that species has been **reduced**.

Which reactant undergoes a decrease in its oxidation number? **N_2**

The species that is oxidized is called the **reducing agent** because it gives up an electron, so that another species can gain an electron (be reduced).

What is the **reducing agent** in this reaction? **H_2**

The species that is reduced is called the **oxidizing agent** because it takes an electron away from another group, raising that group's oxidation number.

What is the **oxidizing agent** in this reaction? **N_2**

7. In each of the following reactions, assign **oxidation numbers** to all of the elements and identify the **oxidizing** and **reducing agents** and the **change in oxidation number**.

$4\ Fe + 3\ O_2 \rightarrow 2\ Fe_2O_3$

0 0 +3 -2

		change in oxidation number
oxidizing agent	**O_2**	**0 → -2**
reducing agent	**Fe**	**0 → +3**

$Cr_2O_7^{2-} + 2OH^- \rightarrow 2\ CrO_4^{2-} + H_2O$

+6 -2 -2 +1 +6 -2 +1 -2

		change in oxidation number
oxidizing agent	**no change in any oxidation numbers;**	
reducing agent	**not a redox reaction**	

$NH_4NO_2 \rightarrow N_2 + 2\ H_2O$ ***Think of this as NH_4^+ and NO_2^-**

-3 +1 +3 -2 0 +1 -2

		change in oxidation number
oxidizing agent	**NH_4NO_2**	
reducing agent	**NH_4NO_2**	***The nitrogens are in different states**

$P_4 + 10\ Cl_2 \rightarrow 4\ PCl_5$

0 0 +5 -1

		change in oxidation number
oxidizing agent	**Cl_2**	**0 → -1**
reducing agent	**P_4**	**0 → +5**

$2\ Cr^{3+} + H_2O + 6ClO_3^- \rightarrow Cr_2O_7^{2-} + 6ClO_2 + 2H^+$

+3 +1 -2 +5 -2 +6 -2 +4 -2 +1

		change in oxidation number
oxidizing agent	**ClO_3^-**	**+5 → +4**
reducing agent	**Cr^{3+}**	**+3 → +6**

SUPPLEMENTAL

****

Balancing Redox Reactions in Acidic Medium

Oxidation/Reduction (Redox) reactions can be balanced using the oxidation state changes, as seen in the previous example. However, there is an easier method, which involves breaking a redox reaction into two **half- reactions**. This is best shown by working an example.

Hydrobromic acid will react with permanganate to form elemental bromine and the manganese(II) ion. The unbalanced, net reaction is shown below,

$$Br^- + MnO_4^- \rightarrow Br_2 + Mn^{2+}$$

1. Break this into two **half-reactions**, one involving bromine and the other involving manganese.

Bromine half-reaction	Manganese half-reaction
$Br^- \rightarrow Br_2$	$MnO_4^- \rightarrow Mn^{2+}$

2. First balance the bromine half-reaction first.

   a) Balance the **bromine** atoms of the reaction

   _**2**__ Br^- → _**1**__ Br_2

   b) Now balance **charge** by adding **electrons** (e^-)

   _**2**__ Br^- → _**1**__ Br_2 **+ 2e⁻**

   This half-reaction is **producing**/~~**consuming**~~ **electrons**. This is an **oxidation**/~~**reduction**~~ half-reaction. Confirm this by assigning oxidation numbers to the bromine species.

   $Br^- = -1$ $Br_2 = 0$ (oxidation state increases; oxidation)

3. Next, balance the manganese half-reaction.

   a) Balance the **manganese** atoms of the half-reaction

   _**1**__ MnO_4^- → _**1**__ Mn^{2+}

   b) Next, balance **oxygen** by adding water molecules (**H_2O**)

   _**1**__ MnO_4^- → __**1**_ Mn^{2+} **+ 4H_2O**

c) Next, balance **hydrogen** by adding protons (**H^+**)

$8H^+$ + _1__ MnO_4^- → _1 Mn^{2+} **+ $4H_2O$**

___

d) Finally, balance **charge** by adding electrons (**e^-**).

$5e^-$ + $8H^+$ + _1__ MnO_4^- → _1__ Mn^{2+} **+ $4H_2O$**

This half-reaction is ~~**producing**~~/**consuming electrons**. This is a ~~**oxidation**~~/**reduction** half-reaction. Confirm this by assigning oxidation numbers to the manganese atoms.

MnO_4^- = +7 Mn^{2+} = +2 +7 → +2 is a reduction

Notice that the number of electrons equals the change in oxidation number.

4. Now put the two **half-reactions** together. **The number of electrons produced must equal the number of electrons consumed**.

$2 Br^-$ → Br_2 + **$2e^-$** **$5e^-$** + $8H^+$ + MnO_4^- → Mn^{2+} + $4H_2O$

multiply this half-reaction by _5 ____ multiply this half-reaction by _2 ___

_10_ Br^- → _5_ Br_2 + _10_ e^- _10_ e^- + _16_ H^+ + _2_ MnO_4^- → _2_ Mn^{2+} + _8_ H_2O

Add the two half-reactions, canceling out species that appear on both sides (including electrons) **10 e^- appear on both sides. Cancel those out to obtain**

$10\ Br^- + 16\ H^+ + 2\ MnO_4^- \rightarrow 2\ Mn^{2+} + 5\ Br_2 + 8\ H_2O$

Which compound is the **oxidizing agent**? **MnO_4^- (gets reduced)**

Which compound is the **reducing agent**? **Br^- (gets oxidized)**

Notice that there are protons (**H^+**) present in the reactants. This indicates that the reaction is carried out in an **acidic solution**.

Balancing Redox Reactions in Basic Medium

To carry this out in a **basic solution**, simply add enough hydroxide ions (**OH^-**) to each side of the equation to neutralize the protons. The product of the neutralization reaction will be water.

Add 16 OH^- to each side. On the left side, 16 H^+ + 16 OH^- = $16H_2O$

The overall balanced reaction under basic conditions is:

$$\underline{10}\ Br^- + \underline{2}\ MnO_4^- + \underline{16}\ H_2O \rightarrow \underline{5}\ Br_2 + \underline{2}\ Mn^{2+} + \underline{8}\ OH^- + 8\ H_2O$$

$$\underline{10}\ Br^- + \underline{2}\ MnO_4^- + \underline{8}\ H_2O \rightarrow \underline{5}\ Br_2 + \underline{2}\ Mn^{2+} + \underline{8}\ OH^-$$

Other Examples:

1. Balance the redox reaction between methanol and dichromate, which produces methanal and chromium (III), as shown below:

-2 +1 -2 +1 +6 -2 0 +1 -2 +3

$$\mathbf{CH_3OH + Cr_2O_7^{2-} \rightarrow CH_2O + Cr^{3+}}$$

First, separate this into two half-reactions

$CH_3OH \rightarrow CH_2O$ $Cr_2O_7^{-2} \rightarrow Cr^{+3}$

Then, balance the redox active species.

$CH_3OH \rightarrow CH_2O$ $Cr_2O_7^{-2} \rightarrow 2Cr^{+3}$

Then, balance oxygens with H_2O

$CH_3OH \rightarrow CH_2O$ $Cr_2O_7^{-2} \rightarrow 2Cr^{+3} + 7H_2O$

Balance hydrogen with H^+

$CH_3OH \rightarrow CH_2O + 2H^+$ $14H^+ + Cr_2O_7^{-2} \rightarrow 2Cr^{+3} + 7H_2O$

Balance charge with electrons.

$CH_3OH \rightarrow CH_2O + 2H^+ + 2e^-$ $6e^- + 14H^+ + Cr_2O_7^{-2} \rightarrow 2Cr^{+3} + 7H_2O$

Equalize the number of electrons lost and gained

2 total e^-; multiply by 3 to get 6 6 total e^-; multiply by 1 to get 6

Combine the two equations to get…

$$\mathbf{3CH_3OH + 6e^- + 14H^+ + Cr_2O_7^{-2} \rightarrow 3CH_2O + 6H^+ + 6e^- + 2Cr^{+3} + 7H_2O}$$

Simplify by canceling out all the electrons and $6H^+$ from each side… $3CH_3OH + 8H^+$ $+ Cr_2O_7^{-2} \rightarrow 3CH_2O + 2Cr^{+3} + 7H_2O$

This indicates that the reaction must be carried out in an **acidic** solution.

To carry it out in a **basic** solution, just add enough **OH^-** to neutralize the acid, **H^+ Add 8 OH^- to each side of the equation. On the left, the H^+ and OH^- form H_2O**

$3CH_3OH + 8H^+ + Cr_2O_7^{-2} + 8OH^- \rightarrow 3CH_2O + 2Cr^{+3} + 7H_2O + 8OH^-$
$3CH_3OH + 8H_2O + Cr_2O_7^{-2} \rightarrow 3CH_2O + 2Cr^{+3} + 7H_2O + 8OH^-$

Cancel out water molecules that appear on both sides (7 total)… $3CH_3OH +$ $H_2O + Cr_2O_7^{-2} \rightarrow 3CH_2O + 2Cr^{+3} + 8OH^-$

Balance the Redox chemical reactions:

2. $Cr_2O_{72}^{-} + Fe^{2+} \rightarrow Cr^{3+} + Fe^{3+}$

1) Balanced half-reactions:
$6e^- + 14H^+ + Cr_2O_7^{2-} \rightarrow 2Cr^{3+} + 7H_2O$
$Fe^{2+} \rightarrow Fe^{3+} + e^-$
2) Equalize the electrons:
$6e^- + 14H^+ + Cr_2O_7^{2-} \rightarrow 2Cr^{3+} + 7H_2O$
$6Fe^{2+} \rightarrow 6Fe^{3+} + 6e^-$ ← multiplied by a factor of 6
3) Add (and cancel) for the final answer:
$14H^+ + Cr_2O_7^{2-} + 6Fe^{2+} \rightarrow 2Cr^{3+} + 7H_2O + 6Fe^{3+}$
Note that the only thing that cancels are the six electrons.

3. $HNO_2 \rightarrow NO + NO_2$

1) The balanced half-reactions:
$e^- + H^+ + HNO_2 \rightarrow NO + H_2O$
$HNO_2 \rightarrow NO_2 + H^+ + e^-$
2) Add for the final answer:
$2HNO_2 \rightarrow NO + NO_2 + H_2O$
Note that the electrons were already balanced, so no need to multiply one or both half-reactions by a factor.
Comment #1: notice that this is no H^+ in the final answer, but please keep in mind that its presence is necessary for the reaction to proceed. In cases like this, the H^+ is acting in a catalytic manner; it is used up in one reaction and regenerated in another (in equal amount), consequently it does not appear in the final answer.
Comment #2: this type of a reaction is called a disproportionation. It is often found in redox situations, although not always. An important disproportionation reaction which does not involve redox is $2H_2O \rightarrow H_3O^+ + OH^-$. This reaction is of central importance in aqueous acid-base chemistry.

4. $H_2C_2O_4 + MnO_4^- \rightarrow CO_2 + Mn^{2+}$

1) The balanced half-reactions:
$H_2C_2O_4 \rightarrow 2CO_2 + 2H^+ + 2e^-$
$5e^- + 8H^+ + MnO_4^- \rightarrow Mn^{2+} + 4H_2O$
2) Equalize the electrons:
$5H_2C_2O_4 \rightarrow 10CO_2 + 10H^+ + 10e^-$ ← factor of 5

$10e^- + 16H^+ + 2MnO_4^- \rightarrow 2Mn^{2+} + 8H_2O \leftarrow$ factor of 2
3) The final answer (electrons and some hydrogen ion get cancelled):
$5H_2C_2O_4 + 6H^+ + 2MnO_4^- \rightarrow 10CO_2 + 2Mn^{2+} + 8H_2O$

5. $O_2 + As \rightarrow HAsO_2 + H_2O$

1) First a bit of discussion before the correct answer. The H_2O on the right side in the problem turns out to be a hint. This is because you need TWO half-reactions. For example, suppose the water wasn't in the equation and you saw this:
$O_2 + As \rightarrow HAsO_2$
You'd think "Oh, that's easy" and proceed to balance it like this:
$H^+ + O_2 + As \rightarrow HAsO_2$
Then, you'd "balance" the charge like this:
$e^- + H^+ + O_2 + As \rightarrow HAsO_2$
And that is wrong because there is an electron in the final answer. You cannot have electrons appear in the final answer of a redox reaction. (You can in a half-reaction, but remember half-reactions do not occur alone, they occur in reduction-oxidation pairs.)
2) Here are the correct half-reactions:
$4e^- + 4H^+ + O_2 \rightarrow 2H_2O$
$2H_2O + As \rightarrow HAsO_2 + 3H^+ + 3e^-$
3) In order to equalize the electrons, the first half-reaction is multiplied by a factor of 3 and the second by a factor of 4:
$12e^- + 12H^+ + 3O_2 \rightarrow 6H_2O$
$8H_2O + 4As \rightarrow 4HAsO_2 + 12H^+ + 12e^-$
4) The final answer:
$3O_2 + 2H_2O + 4As \rightarrow 4HAsO_2$
Notice that the H_2O winds up on the right-hand side of the equation.
By the way, try to balance
$O_2 + As \rightarrow HAsO_2$
Using H_2O on the left rather than H^+. That way leads to the correct answer without having to use half-reactions. There are some redox reactions where using half-reactions turns out to be "more" work, but there aren't that many.

6. $NO_3^- + I_2 \rightarrow IO_3^- + NO_2$

1) These are the balanced half-reactions:
$6H_2O + I_2 \rightarrow 2IO_3^- + 12H^+ + 10e^-$
$e^- + 2H^+ + NO_3^-$ ---> $NO_2 + H_2O$
2) Only the second half-reaction needs to be multiplied through by a factor:
$6H_2O + I_2 \rightarrow 2IO_3^- + 12H^+ + 10e^-$
$10e^- + 20H^+ + 10NO_3^- \rightarrow 10NO_2 + 10H_2O$
3) Adding the two half-reactions, but not eliminating anything except electrons:
$6H_2O + 20H^+ + I_2 + 10NO_3^- \rightarrow 2IO_3^- + 12H^+ + 10NO_2 + 10H_2O$
4) Remove some water and hydrogen ion for the final answer:
$8H^+ + I_2 + 10NO_3^- \rightarrow 2IO_3^- + 10NO_2 + 4H_2O$

7. $HBr + SO_4^{2-} \rightarrow SO_2 + Br_2$

1) Balanced half-reactions:
$2e^- + 4H^+ + SO_4^{2-} \rightarrow SO_2 + 2H_2O$
$2HBr \rightarrow Br_2 + 2H^+ + 2e^-$
2) The final answer (note that electrons were already equal):
$2H^+ + 2HBr + SO_4^{2-} \rightarrow SO_2 + Br_2 + 2H_2O$

8. $H_5IO_6 + Cr \rightarrow IO_3^- + Cr^{3+}$

1) The two half-reactions:
$2e^- + H^+ + H_5IO_6 \rightarrow IO_3^- + 3H_2O$
$Cr \rightarrow Cr^{3+} + 3e^-$
2) Multiply top half-reaction by 3, bottom by 2; the final answer:
$3H^+ + 3H_5IO_6 + 2Cr \rightarrow 2Cr^{3+} + 3IO_3^- + 9H_2O$

9. $Fe + HCl \rightarrow HFeCl_4 + H_2$
1) This problem poses interesting problems, especially with the Cl. The key to solving ths problem is to eliminate everything not directly involved in the redox. That means the H in $HFeCl_4$ as well as the Cl in it and HCl. When we do that, this is the unbalanced, ionic form we wind up with:
$Fe + H^+ \rightarrow Fe^{3+} + H_2$
2) The half-reactions (already balanced) are as follows:
$Fe \rightarrow Fe^{3+} + 3e^-$
$2e^- + 2H^+ \rightarrow H_2$
3) The final answer:
$2Fe + 6H^+ \rightarrow 2Fe^{3+} + 3H_2$
We will go back to the molecular equation with 8HCl. Six of the HCl molecules supply the $6H^+$ going to $3H_2$. The 7th and 8th HCl molecules supply the two H present in $2HFeCl_4$, as well as the 8 Cl needed in the two $HFeCl_4$ molecules.
$2Fe + 8HCl \rightarrow 2HFeCl_4 + 3H_2$

10. $NO_3^- + H_2O_2 \rightarrow NO + O_2$

1) The half-reactions (already balanced) are as follows:
$3e^- + 4H^+ + NO_3^- \rightarrow NO + 2H_2O$
$H_2O_2 \rightarrow O_2 + 2H^+ + 2e^-$
2) Multiply the top half-reaction by 2 and the bottom one by 3, add them and eliminate $6H^+$:
$2H^+ + 2NO_3^- + 3H_2O_2 \rightarrow 2NO + 4H_2O + 3O_2$
3) You can combine the hydrogen ion and the nitrate ion like this:
$2HNO_3 + 3H_2O_2 \rightarrow 2NO + 4H_2O + 3O_2$
This creates what is called a molecular equation.

11. $BrO_3^- + Fe^{2+} \rightarrow Br^- + Fe^{3+}$

1) These are the half-reactions:
$6e^- + 6H^+ + BrO_3^- \rightarrow Br^- + 3H_2O$
$Fe^{2+} \rightarrow Fe^{3+} + e^-$
2) Only the second half-reaction needs to be multiplied through by a factor, then we add the two half-reactions for the final answer:
$6H^+ + BrO_3^- + 6Fe^{2+} \rightarrow 6Fe^{3+} + Br^- + 3H_2O$

****

IV. Chemical Reactions Stoichiometry

Basic "chemical arithmetic"
A balanced chemical equation expresses the relative number of moles of each component (product or reactant), but because each formula in the equation implies a definite mass of the substance (its molar mass), the equation also implies that certain weight relations exist between the components. For example, the

equation describing the combustion of carbon monoxide to carbon dioxide

$2\ CO + O_2 \rightarrow 2\ CO_2$

The term *stoichiometry* can refer to any type of calculation that relates the quantities of reactants and products in a chemical reaction. Stoichiometry is essentially an expression of the principle that atoms are conserved in chemical change.

The term comes from the Greek words στοιχεῖον stoicheion "element" and μέτρον metron "measure"

implies the following relations:

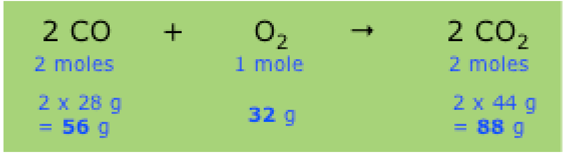


Figure 4.20 Mass in chemical reaction

The relative masses shown in the bottom line establish the *stoichiometry* of the reaction, that is, the relations between the masses of the various components. Since these masses vary in direct proportion to one another, we can define what amounts to a conversion factor (sometimes referred to as a *chemical factor*) that relates the mass of any one component to that of any other component.

The stoichiometry of chemical reactions is based on the mole ratios among the reactants and the products.

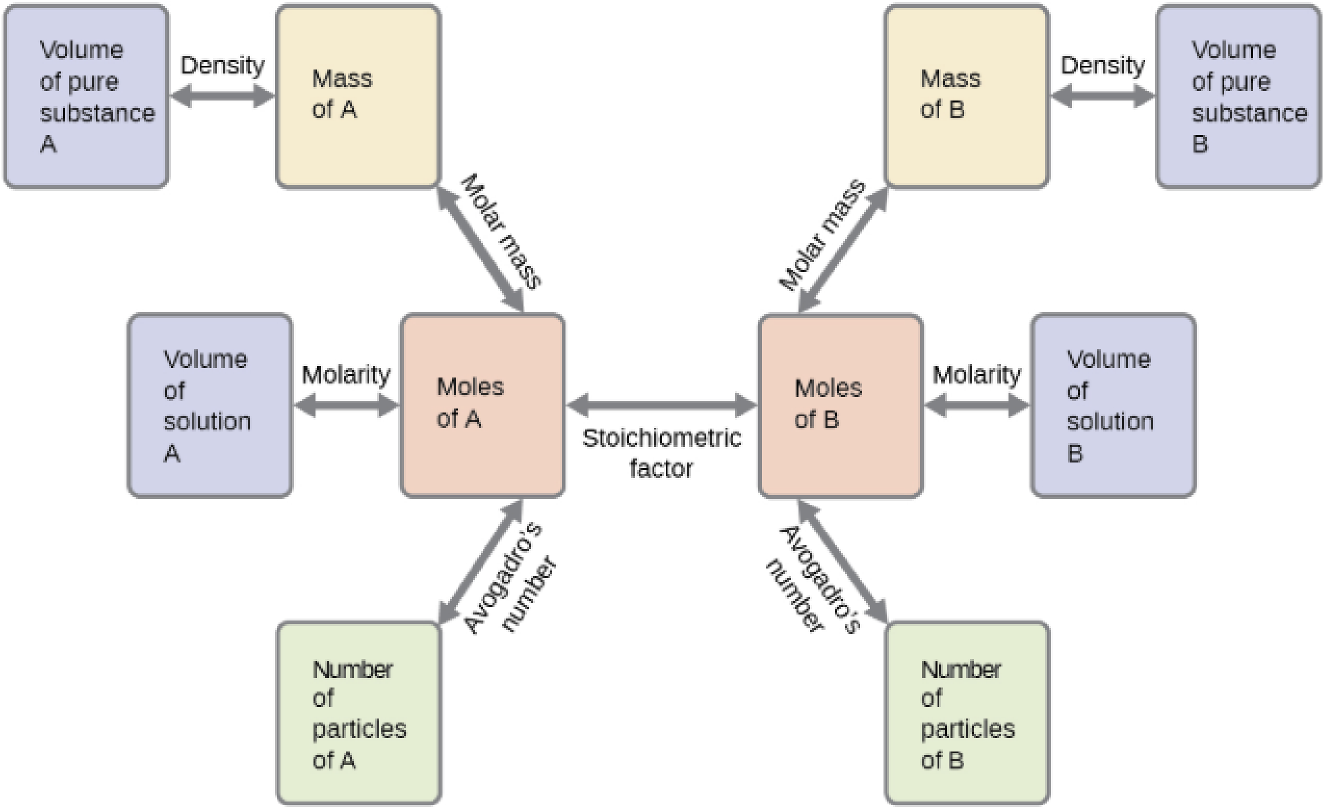
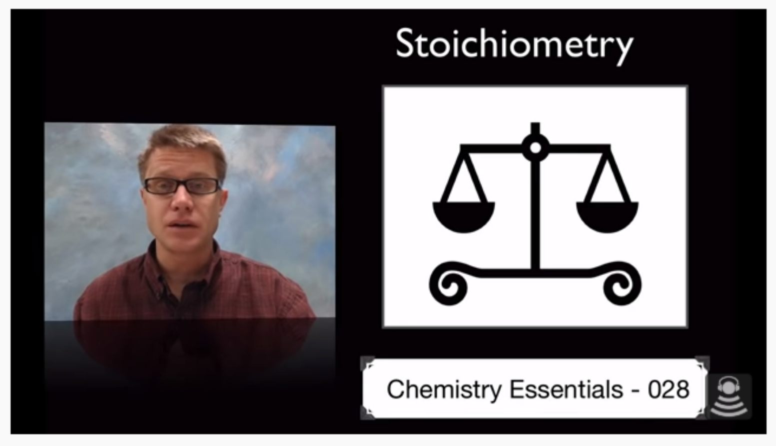


Figure 4.21 Concept map for Reaction Stoichiometry

Reference: https://pressbooks-dev.oer.hawaii.edu/chemistry/chapter/reaction-stoichiometry/

The video below illustrates the concept of stoichiometry:



https://www.youtube.com/watch?v=LQq203gyftA

Example:

The stoichiometry expresses the mole ratios among the reactants and products:

2 moles of $KClO_3$ / 2moles of KCl and
2 moles of $KClO_3$ / 3 moles O_2

We can translate this into: 2 moles of $KClO_3$ will produce 2 moles KCl as well as 3 moles O_2.

Examples:

Number of moles produced from certain amount of moles of one of reactants:

$$2\ KClO_3\quad 2\ KCl + 3\ O_2$$

a) How many moles of O2 will be formed from 1.65 moles of KClO3?

$$\begin{array}{l|l|l} 1.65 \text{ mol } KClO_3 & \underline{3} \text{ mol } O_2 & = \underline{2.48} \quad \text{mol } O_2 \\ \hline & \underline{2} \text{ mol } KClO_3 & \end{array}$$

b) How many moles of KClO3 are needed to make 3.50 moles of KCl?

$$\begin{array}{l|l|l} 3.50 \text{ mol } KCl & \underline{2} \text{ mol } KClO_3 & = \underline{3.50} \quad \text{mol } KClO_3 \\ \hline & \underline{2} \text{ mol } KCl & \end{array}$$

c) How many moles of KCl will be formed from 2.73 moles of KClO3?

= 2.73 mol KCl

2.73 moles $KClO_3$	2 mol KCl
	2 mol $KClO_3$

$2\ H_2O \rightarrow 2\ H_2 + O_2$

7. How many moles of O_2 are produced when 1.26 moles of H_2O is reacted?

1.26 mol H_2O	1 mol O_2	= .630 mol O_2
	2 mol H_2O	

How many moles of H_2O are needed to produce 55.7 moles of H_2?

55.7 mol H_2	2 mol H_2O	= 55.7 mol H_2O
	2 mol H_2	

8. If enough H_2O is reacted to produce 3.40 moles of H_2, then how may moles of O_2 must have been made? (a bit challenging, but just think about it and you can probably figure it out)

3.40 mol H_2	1 mol O_2	= 1.70 mol O_2
	2 mol H_2	

$$2\,KClO_3 \rightarrow 2\,KCl + 3\,O_2$$

9. How many **grams** of O_2 will be formed from 3.76 grams of $KClO_3$?

3.76g $KClO_3$	1 mol $KClO_3$	3 mol O_2	32.00 g O_2	= 1.47 g O_2
	122.55 g $KClO_3$	2 mol $KClO_3$	1 mol O_2	

10. How many **grams** of $KClO_3$ are needed to make 30.0 grams of KCl?

30.0 g KCl	1 mol KCl	2 mol $KClO_3$	122.55 g$KClO_3$	= 49.3 g $KClO_3$
	74.55 g KCl	2 mol KCl	1 mol $KClO_3$	

11. How many grams of KCl will be formed from 2.73 g of $KClO_3$?

2.73 g $KClO_3$	1 mol KCl O_3	2 mol KCl	74.55 g	= 1.66 g KCl
	122.55 g $KClO_3$	2 mol KCl O_3	1 mol KCl	

Examples:

Number of molecules produced from certain amount of moles of one of reactants:

Consider the reaction below:

$$N_2 + 3\,H_2 \leftrightarrow 2\,NH_3 + \text{Heat}$$

b) How many molecules of NH_3 produced if one has used 1.80 moles of H_2 is used.

b) Molecules of NH_3 = [1.80 ~~mole H_2~~] x [2 ~~mole of NH_3~~ / 3 ~~mole H_2~~] x [6.022 x 10^{23} molecules NH_3 / ~~mole H_2~~] = 7.23 x 10^{23} molecules NH_3

Examples:

Number of grams (mass) produced or reacted from or by certain amount of grams (mass) of one of reactants or products:

Consider the reaction below:
$ZnSO_4 + SrCl_2 \rightarrow SrSO_4 + ZnCl_2$

a) Calculate the mass of $SrCl_2$ is consumed when 55.0 g of $ZnCl_2$ is produced?
b) Calculate the mass of $SrSO_4$ is consumed when 88.5 g of $ZnSO_4$ is produced?

a) Mass of $SrCl_2$ = [55.0 ~~g of $ZnCl_2$~~] x [~~**mole $ZnCl_2$**~~ / 136.3 ~~g $ZnCl_2$~~] x [~~1 mol $SrCl_2$~~ / ~~1mol $ZnCl_2$~~] x [158.5 g $SrCl_2$ / ~~mol $SrCl_2$~~] = 63.958 g $SrCl_2$ = 64.0 g $SrCl_2$ (3 sig. figs)

$ZnCl_2$ molar mass = 136.3 g / mol
$SrCl_2$ molar mass = 158.5 g / mol

b) mass of $SrSO_4$ = [88.5 ~~**g of $ZnSO_4$**~~] x [~~**mol $ZnSO_4$**~~ / 161.5 ~~**g $ZnSO_4$**~~] x [1 ~~**mol $SrSO_4$**~~ / 1 ~~**mol $ZnSO_4$**~~] x [183.7 g $SrSO_4$ / ~~**mol $SrSO_4$**~~] = 100.66 g $SrSO_4$ = 0.101 x 10^3 g $SrSO_4$

$ZnSO_4$ molar mass = 161.5 g / mol
$SrSO_4$ molar mass = 183.7 g / mol

V. Yields of Reactions

The yield of the reaction depends on stoichiometric amounts of the reactant(s) present in the balanced chemical reaction.
Most chemical reactions that take place in the real world begin with more or less arbitrary amounts of the various reactants; we usually have to make a special effort if we want to ensure that stoichiometric amounts of the reactants are combined. This means that one or more reactant will usually be present in excess; there will be more present than can react, and some will remain after the reaction is over. At the same time, one reactant will be completely used up; we call this the limiting reactant because the amount of this substance present will control, or limit, the quantities of the other reactants that are consumed as well as the amounts of products produced.

The Limiting Reactant: is the reactant which will be consumed completely during the chemical reaction. The reaction will stop when all of the limiting reactant is consumed.
Excess Reactant: is the reactant that stays present when the reaction stops when the limiting reactant is completely consumed.
Theoretical Yield is a calculated yield of the product of the chemical reaction based on the limiting reactant calculated amount. It is pure calculation and there is no experiment involved in this calculation, therefore such yield is called theoretical yield.
Actual Yield is a calculated yield of the product based on an experiment that carried out in an actual chemistry laboratory.
Overall Yield is the percent ratio between the actual yield over the theoretical yield.
Limiting reactant problems are handled in the same way as ordinary stoichiometry problems with one additional preliminary step: you must first determine which of the reactants is limiting— that is, which one will be completely used up. To start you off, consider the following very simple example

The figure below illustrates the concept of limiting reactant as well the theoretical yield of reaction:

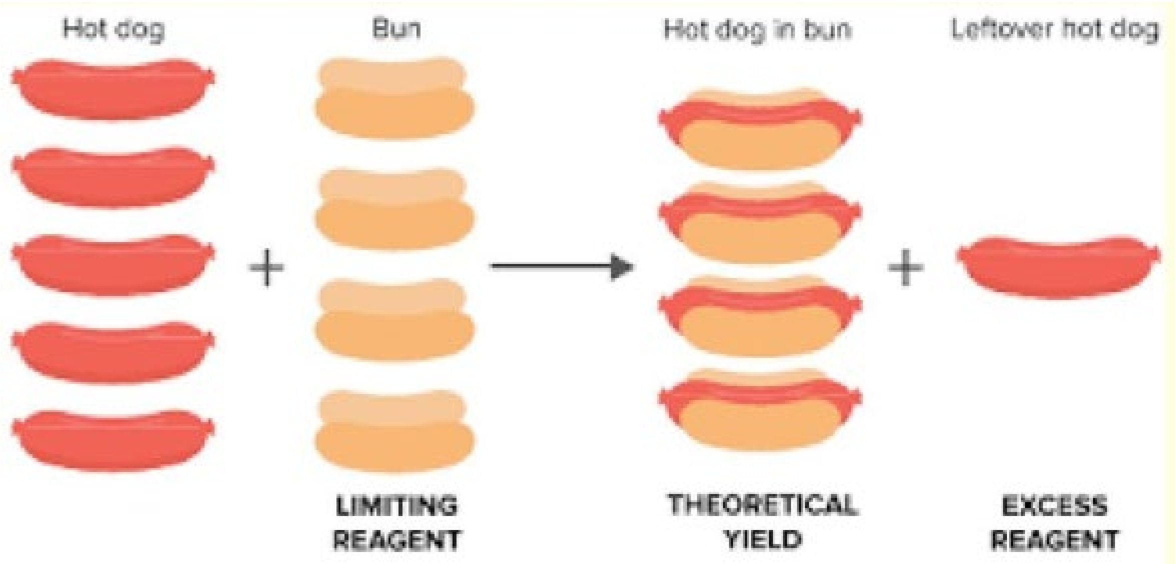
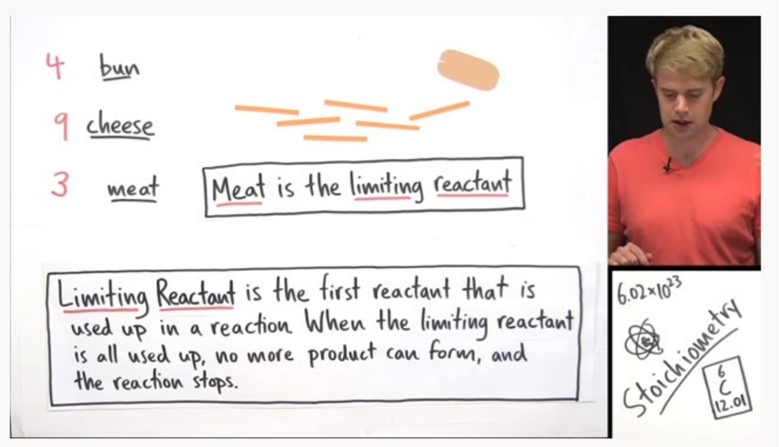


Figure 4.22 Limiting Reagent & Theoretical Yield

Reference: https://slideplayer.com/slide/12627403/

The videos below illustrate also the concept of limiting react and the percent yield:

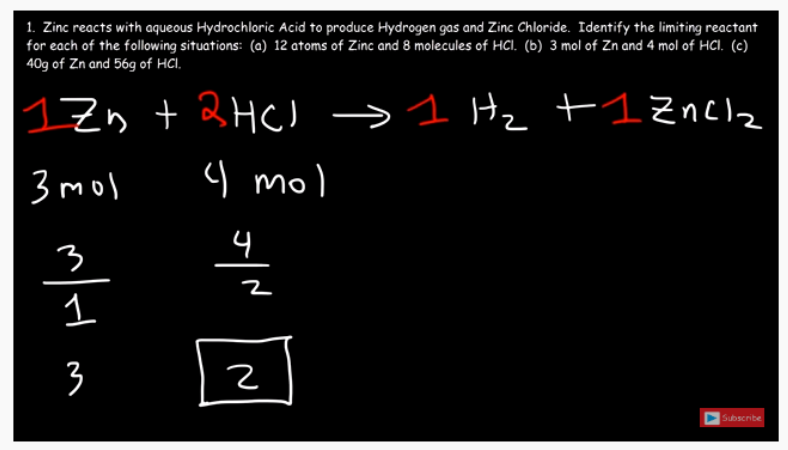


4 bun
9 cheese
3 meat

Meat is the limiting reactant

Limiting Reactant is the first reactant that is used up in a reaction When the limiting reactant is all used up, no more product can form, and the reaction stops.

https://www.youtube.com/watch?v=nZOVR8EMwRU



1. Zinc reacts with aqueous Hydrochloric Acid to produce Hydrogen gas and Zinc Chloride. Identify the limiting reactant for each of the following situations: (a) 12 atoms of Zinc and 8 molecules of HCl. (b) 3 mol of Zn and 4 mol of HCl. (c) 40g of Zn and 56g of HCl.

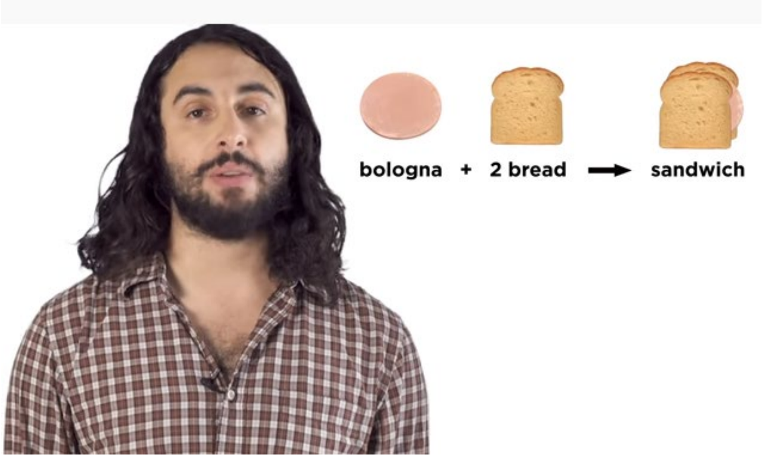
$$1Zn + 2HCl \rightarrow 1H_2 + 1ZnCl_2$$

3 mol 4 mol

$$\frac{3}{1} \qquad \frac{4}{2}$$

$$3 \qquad \boxed{2}$$

https://www.youtube.com/watch?v=IWtkhAv4RTo



https://www.youtube.com/watch?v=dodsvTfqWNc

Limiting reactants in everyday life
The concept of limiting reactants touches us all in our everyday lives — and as we will show in the second example below, even in the maintenance of life itself!

Aerobic and anaerobic respiration
Our bodies require a continual supply of energy in order to maintain neural activity, synthesize proteins and other essential biochemical components, replace cells, and to power muscular action. The "fuel" — the carrier of chemical energy — glucose, a simple sugar which is released as needed from the starch-like polymer glycogen, the form in which the energy we derive from food is stored.
Arterial blood carries dissolved glucose along with hemoglobin-bound dioxygen to individual cells which are the sites of glucose "combustion":

$C_6H_{12}O_6 + 6\ O_2 \rightarrow 6\ CO_2 + 6\ H_2O$

The net reaction and the quantity of energy released are the same as if the glucose were burned in the open air, but within the cells the reaction proceeds in a series of tiny steps which capture most of this energy for the body's use, liberating only a small fraction of it as thermal energy (heat).
Because this process utilizes oxygen from the air we breath, it is known as *aerobic respiration*. And as with any efficient combustion process, glucose is the limiting reactant here.

$C_6H_{12}O_6 \rightarrow 2\ CH_3CH(OH)COOH$

As you can see from this equation, glucose is only partially broken down (into *lactic acid*), and thus only part of its chemical energy is captured by the body.

There are numerous health benefits to aerobic exercise, including increased ability of the body to maintain an aerobic condition. But if you are into short-distance running (sprinting) or being pursued by a tiger, the reduced efficiency of anaerobic exercise may be a small price to pay.

Figure 4.23a Aerobic Exercise

Figure 4.23b

Percent Yield

It is often important to calculate percent yield in a chemical reaction to estimate the efficiency of a chemical reaction. Percent yield is defined as

Percent yield= (actual/theoretical)*100%. The actual yield is the amount of product in a chemical reaction, determined by weighing a product on a balance. Theoretical yield is a quantity calculated from a balanced chemical equation, using mole ratios and molar masses.

The theoretical yield is the maximum amount of product formed in a chemical reaction from the amount of reactants used.

When we perform stoichiometric calculations to determine the amount of product produced – that is a theoretical yield. But when we actually perform the experiment in a lab setting, we usually find we do not get as much product, we usually get a smaller actual yield due to human error or other experimental error.

To calculate the percent yield, the actual yield and theoretical yield are needed. You prepared cookie dough to make 5 dozen cookies. The phone rings and you answer. While talking, a sheet of 12 cookies burn and you have to throw them out. The rest of the cookies are okay. What is the percent yield of edible cookies?

Theoretical yield 60 cookies possible

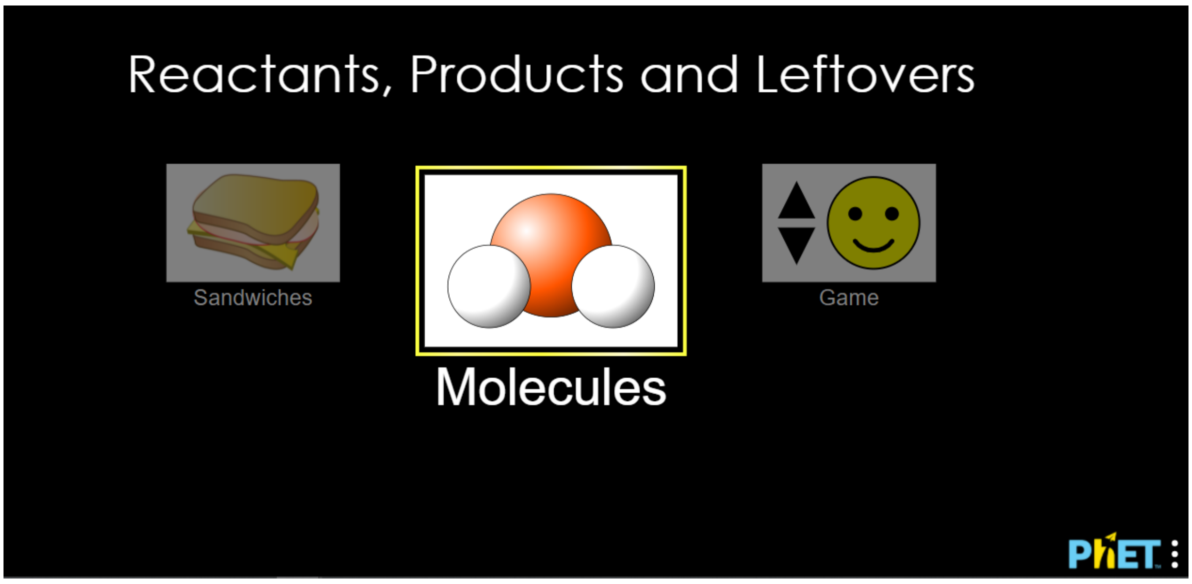
Actual yield 48 cookies to eat

Percent yield 48 cookies x 100 = 80% yield

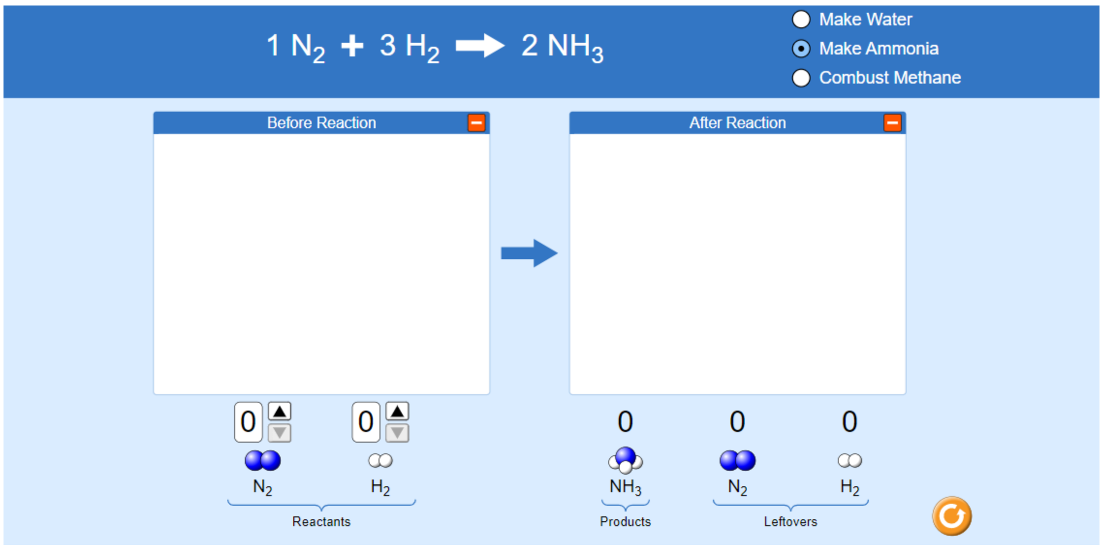
https://www.youtube.com/watch?v=CK2yK_JTUH4

The following simulation illustrates in detail about the leftover and excess reactant for any reaction.

https://phet.colorado.edu/sims/html/reactants-products-and-leftovers/latest/reactants-products-and-leftovers_en.html



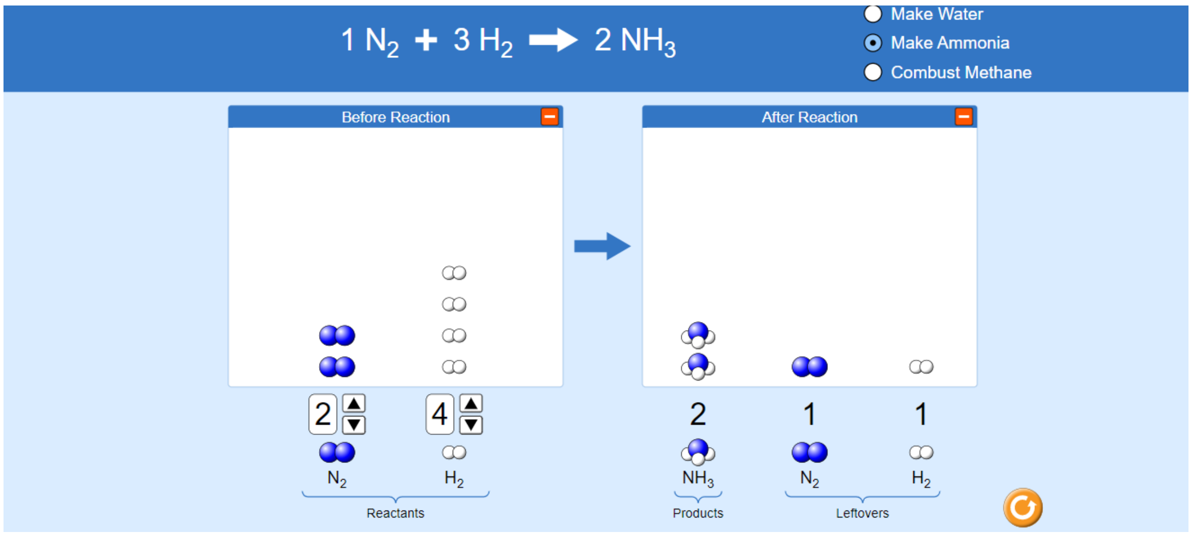
1.Go to the activity and click on the 2nd option "Molecules"
2. Choose the reaction "Making Ammonia. A screen like below should appear.



$1\ N_2 + 3\ H_2 \rightarrow 2\ NH_3$

○ Make Water
● Make Ammonia
○ Combust Methane

3. Try with 2 molecules of N_2 and 4 molecules of H_2.



$1\ N_2 + 3\ H_2 \rightarrow 2\ NH_3$

○ Make Water
● Make Ammonia
○ Combust Methane

4. How many molecules of NH3 are formed?

5. What is(are) the excess reactant(s)?

6. **Explain your results.**

Problem Example:
For the hypothetical reaction 3 A + 4 B → [products], determine which reactant will be completely consumed when we combine
a) equimolar quantities of A and B;
b) 0.57 mol of A and 0.68 mol of B.
Solution:

b) How many moles of B will react with .57 mol of A? The answer will be (4/3 × 0.57 mol). If this comes to less than 0.68 mol, then B will be the limiting reactant, and you must continue the problem on the basis of the amount of B present. If the limiting reactant is A, then all 0.57 mol of A will react, leaving some of the B in excess. Work it out!

Practice Problem#1: $CO + 2\ H_2 \rightarrow CH_3OH$

If 12.0 g H_2 and 74.5 g CO are used determine the limiting reactant.

Number of moles of the product CH_3OH based on CO as reactant = [74.5 ~~g CO~~] x [~~mol CO~~ / 28.0 ~~g CO~~] x [1 mol CH_3OH / 1 ~~mol CO~~] = **2.66 moles of CH_3OH**

[Note: molar mass of CO is used to be 28.0 g/mol]

Number of moles of the product CH_3OH based on H_2 as reactant = [12.0 ~~g H_2~~] x [~~mol H_2~~ / 2.00 ~~g H_2~~] x [1 mol CH_3OH / 2 ~~mol H_2~~] = **3.00 moles of CH_3OH**

[Note: molar mass of H_2 is used to be 2.00 g/mol]

Since 2.66 moles is smaller than 3.00 → CO is the limiting reactant and H_2 is said to be the excess reactant.

Now we can determine (calculate) the theoretical yield based on the limiting reactant **CO**

Theoretical yield = [2.66 ~~mol CH_3OH]~~ x [32.0 g CH_3OH / ~~mol CH_3OH~~] = **85.1 g CH_3OH**

[Note: molar mass of CH_3OH is used to be 32.0 g/mol]

Example:

Limiting Reactants, Theoretical Yield, Actual Yield and the Overall Yield:

C_3H_8 + 5 O_2 → 3 CO_2 + 4 H_2O

If 0.550 g C_3H_8 is reacting with 0.550 g O_2. Calculate:

a) The amount moles of CO_2 produced based on the limiting reactant
b) Theoretical yield (based on the limiting reactant)
c) The overall yield if the actual yield of is 0.550 g CO_2
d) The % error of the yield

a) The amount of CO_2 produced based on the limiting reactant

Number of CO_2 moles based on C_3H_8 = [0.550 ~~g C_3H_8~~] x [1 ~~mol C_3H_8~~ / 44.0 ~~g C_3H_8~~] x [3 mol CO_2 / 1 ~~mol C_3H_8~~] = **0.0375 moles CO_2**

[Note that molar mass of C_3H_8 is used to be 44.0 g/mol]
[Note that molar mass of CO_2 is used to be 44.0 g/mol]
[Note that molar mass of O_2 is used to be 32.0 g/mol]

Number of CO_2 moles based on O_2 = [0.550 ~~g O_2~~] x [~~mol O_2~~ / 32.0 ~~g O_2~~] x [3 mol CO_2 / 5 ~~mol O~~$_2$] = **0.0103 moles CO_2**

0.103 moles are less than 0.0375 moles. Therefore, O_2 is the limiting reactant.

b) Theoretical yield (based on the limiting reactant)

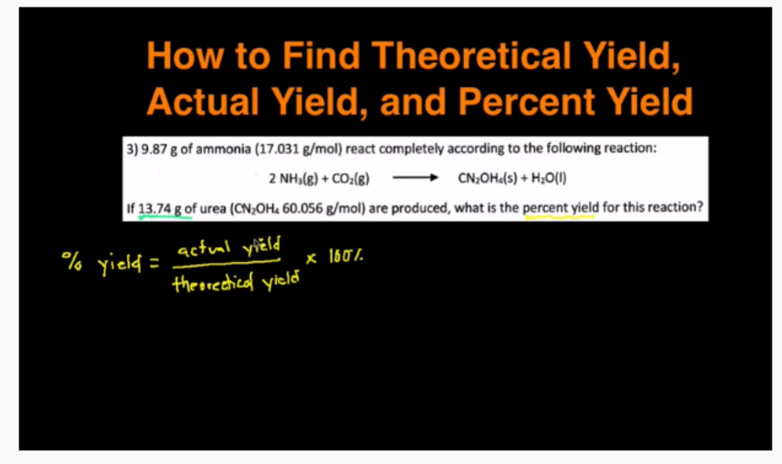
Theoretical yield of CO_2 based on the limiting reactant = [0.0103 mol CO_2] x [44.0 g CO_2 / mol CO_2] = **0.572 g CO_2**

c) The overall yield if the actual yield of is 0.550 g CO_2

The overall yield = [Actual Yield / Theoretical Yield] x 100%
The overall yield = [0.550 g CO_2 / 0.572 g CO_2] x 100% = **96.2 %**

d) **The % error of the yield = | {[Theoretical Yield – Actual Yield] / [Theoretical Yield]} | x 100%**
The % error of the yield = | {[0.572 g – 0.550 g] / [0.572 g]} | x 100% = **3.85 %**

The videos below show more examples for the actual yield, theoretical yield and the percent yield:



How to Find Theoretical Yield, Actual Yield, and Percent Yield

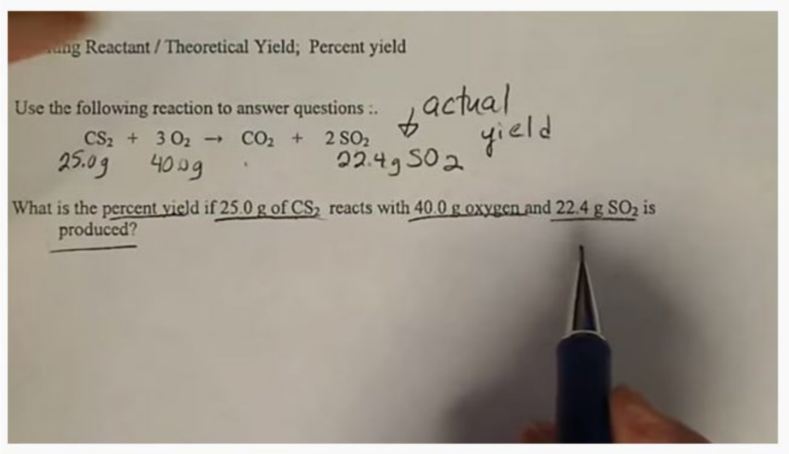
3) 9.87 g of ammonia (17.031 g/mol) react completely according to the following reaction:

$2\ NH_3(g) + CO_2(g) \longrightarrow CN_2OH_4(s) + H_2O(l)$

If 13.74 g of urea (CN_2OH_4 60.056 g/mol) are produced, what is the percent yield for this reaction?

$\% \text{ yield} = \frac{\text{actual yield}}{\text{theoretical yield}} \times 100\%$

https://www.youtube.com/watch?v=s8hva1fUo0Y



ing Reactant / Theoretical Yield; Percent yield

Use the following reaction to answer questions :.

$CS_2 + 3\ O_2 \rightarrow CO_2 + 2\ SO_2$

What is the percent yield if 25.0 g of CS_2 reacts with 40.0 g oxygen and 22.4 g SO_2 is produced?

https://www.youtube.com/watch?v=41KsCvYJDoI

VI. Quantitative Chemical Analysis

Several physical methods can be included in the quantitative chemical analysis.
Such physical methods include precipitation, neutralization, oxidation, or, in general, the formation of a new product. The major types of strictly chemical methods are known as gravimetric analysis and volumetric, or titrimetric analysis. Some other physical methods include also measurement of some physical property such as density, refractive index, absorption or polarization of light, electromotive force, magnetic susceptibility.

Some Physical Methods:

Titration:

A method by which a compound with unknown concentration is determined by a neutralization reaction with another compound that has known concentration. Titration is also known as **neutralization reaction** of acid and base.

In the 18th century, the strength (actually the concentration) of vinegar samples was determined by noting the amount of potassium carbonate, K2CO3, which had to be added, a little at a time, before bubbling ceased. The greater the weight of potassium carbonate added to reach the point where the bubbling ended, the more concentrated the vinegar. We now know that the effervescence that occurred during this process was due to reaction with acetic acid, CH_3CO_2H, the compound primarily responsible for the odor and taste of vinegar. Acetic acid reacts with potassium carbonate according to the following equation

$2CH_3CO_2H(aq) + K_2CO_3(s) \longrightarrow 2CH_3CO_2K(aq) + CO_2(g) + H_2O(l)$

The bubbling was due to the production of CO2. The test of vinegar with potassium carbonate is one type of quantitative analysis—the determination of the amount or concentration of a substance in a sample. In the analysis of vinegar, the concentration of the solute (acetic acid) was determined from the amount of reactant that combined with the solute present in a known volume of the solution.

The equivalence point of a titration may be detected visually if a distinct change in the appearance of the sample solution accompanies the completion of the reaction. The halt of bubble formation in the classic vinegar analysis is one such example, though, more commonly, special dyes called indicators are added to the sample solutions to impart a change in color at or very near the equivalence point of the titration.

Equivalence points may also be detected by measuring some solution property that changes in a predictable way during the course of the titration. Regardless of the approach taken to detect a titration's equivalence point, the volume of titrant actually measured is called the end point.

Properly designed titration methods typically ensure that the difference between the equivalence and end points is negligible. Though any type of chemical reaction may serve as the basis for a titration analysis, the three described in this chapter (precipitation, acid-base, and redox) are most common. Additional details regarding titration analysis are provided in the chapter on acid-base equilibria.

The setup of the titration is given below:

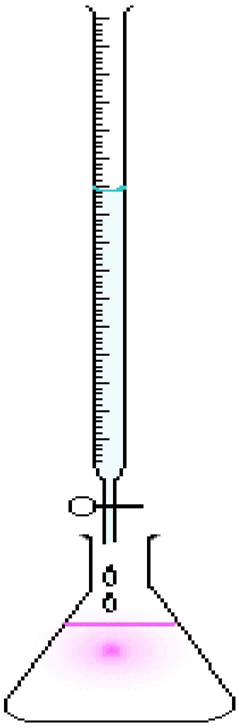


Figure 4.24 Titration Set up

Ref: www.commons.wikimedia.com

Figure 4.25 Titraion Lab Experiment
Reference: www.flickr.com

The buret holds chemical compound called titrant which has known concentration. The Erlenmeyer flask holds the unknown concentration of the compound which is known as analyte or titrant.

Two points are very important in the titration:

End point: A point by which the indicator in the analyte solution changes its color by an extra drop added of the titrant inside the buret.

Equivalent point: A point by which number of moles of the titrant solution compound inside the buret equals the number of moles of the analyte solution compound inside in Erlenmeyer flask.

The figure below shows the difference between the end point and equivalent point of the titration of HCl with NaOH.

https://www.khanacademy.org/test-prep/mcat/chemical-processes/titrations-and-solubility-equilibria/a/acid-base-titration-curves

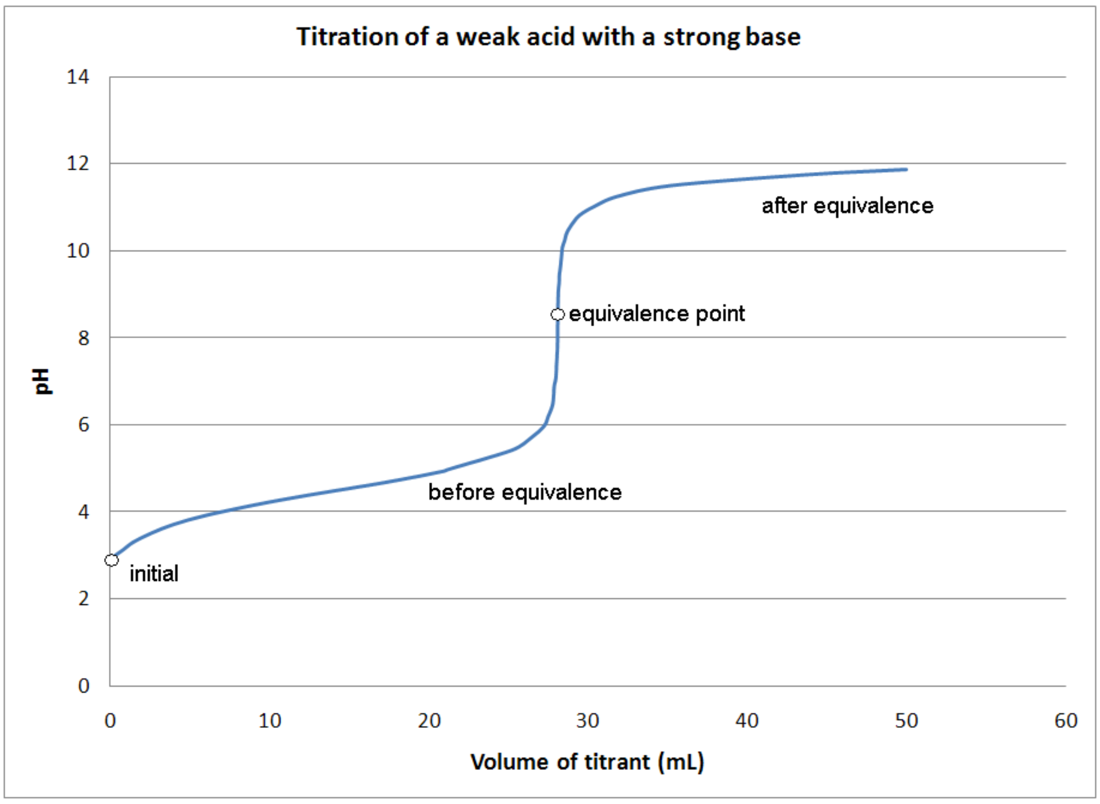


Figure 4.26 Equivalence point & End Point

Ref: Wikimedia commons

A typical setup of the titration is given below:

https://www.khanacademy.org/test–prep/mcat/chemical–processes/titrations–and–solubility–equilibria/a/acid–base–titration–curves

A You Tube video goes over the titration procedure in details:

Note that: the end point comes always after the equivalent point. One drop of the titrant signals the color change.

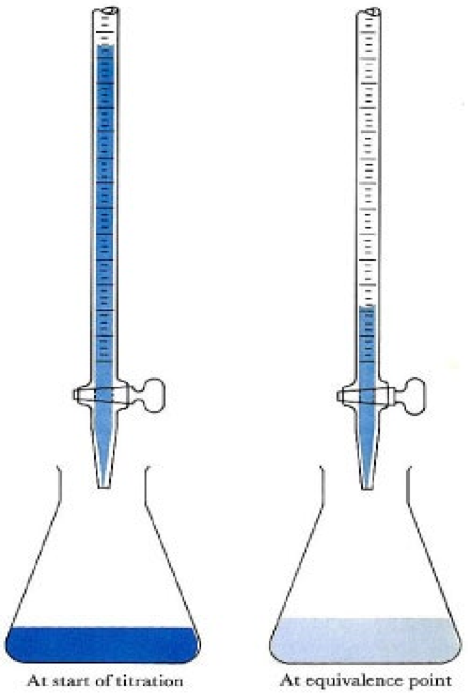


Figure 4.27 End point color change

Ref: commons.wikimedia.org/

Numerical problems are solved to find unknown concentration or volume of Acid/Base in neutralization reaction using titration data.

Example:

Practice Problem#1: The end point in a titration of a 50.00-mL sample of aqueous HCl was reached by addition of 35.23 mL of 0.250 M NaOH titrant. The titration reaction is: HCl(aq) + NaOH(aq) ⟶ NaCl(aq) + H2 O(l) What is the molarity of the HCl?

Solution As for all reaction stoichiometry calculations, the key issue is the relation between the molar amounts of the chemical species of interest as depicted in the balanced chemical equation. The approach outlined in previous modules of this chapter is followed, with additional considerations required, since the amounts of reactants provided and requested are expressed as solution concentrations.

The molar amount of HCl is calculated to be:

$$35.23\ \text{mL NaOH} \times \frac{1\ \text{L NaOH}}{1000\ \text{ml NaOH}} \times \frac{0.250\ \text{mol}}{1\ \text{L}} \times \frac{1\ \text{mol HCl}}{1\ \text{mol NaOH}} = 8.81 \times 10{-}3\ \text{mol HCl}$$

Using the provided volume of HCl solution and the definition of molarity, the HCl concentration is: M = mol HCl L solution M $= \dfrac{8.81 \times 10{-}3\ \text{mol HCl}}{50.00\ \text{mL} \times 1\ \text{L}/1000\ \text{mL M}}$

= 0.176 M

Note: For these types of titration calculations, it is convenient to recognize that solution molarity is also equal to the number of millimoles of solute per milliliter of solution: M = mol solute L solution × 103 mmol mol 103 mL L = mmol solute mL solution Using this version of the molarity unit will shorten the calculation by eliminating two conversion factors: 35.23 mL NaOH × 0.250 mmol NaOH mL NaOH × $\dfrac{1\ \text{mmol HCl}}{1\ \text{mmol NaOH}}$ × 50.00 mL solution = 0.176 M HCl

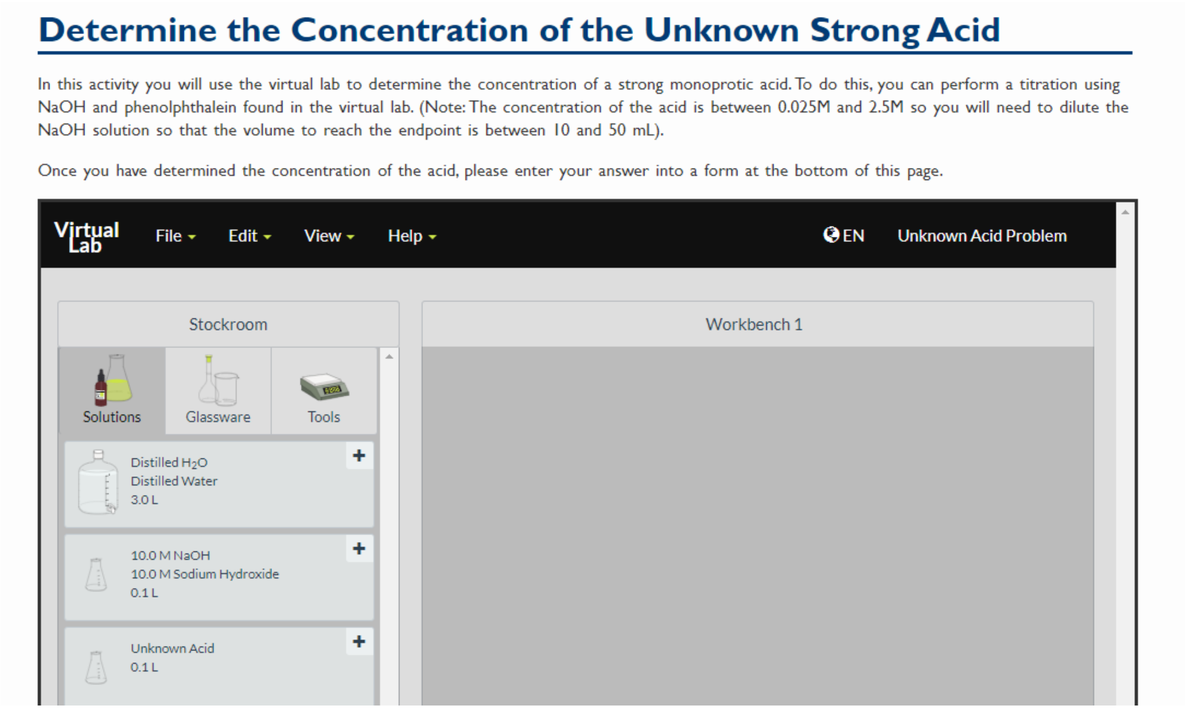
Practice Problem#2: 2 KOH + H_2SO_4 → K_2SO_4 + 2 H_2O

If 35.0 mL of 0.150 M KOH are used to neutralize 35.0 mL of H_2SO_4. Calculate the molarity of H_2SO_4.

Molarity of H_2SO_4 = [0.0350 ~~**L KOH**~~] x [0.150 **mol KOH** / ~~**L KOH]**~~ x [1 mol H_2SO_4 / 2 **mol KOH**] x [1 / 0.035 L H_2SO_4] = **0.075 mol H_2SO_4 / L H_2SO_4 = 0.075 M = 0.075 molar**

Try this ACID BASE VIRTUAL LAB on https://.chemcollective.org

http://chemcollective.org/activities/autograded/124



Determine the Concentration of the Unknown Strong Acid

In this activity you will use the virtual lab to determine the concentration of a strong monoprotic acid. To do this, you can perform a titration using NaOH and phenolphthalein found in the virtual lab. (Note: The concentration of the acid is between 0.025M and 2.5M so you will need to dilute the NaOH solution so that the volume to reach the endpoint is between 10 and 50 mL).

Once you have determined the concentration of the acid, please enter your answer into a form at the bottom of this page.

Activity: Set up the lab and find the concentration of unknown monoprotic acid in this virtual lab.

Gravimetry:

Gravimetry is a physical method by which an ion or molecule or a compound is isolated by precipitation reaction and then the ion or molecule or compound amount (concentration) will be determined

- What is the concentration of the analyte in a solution?
- How pure is our sample?

The sample here could be a solid or in solution. There are two common types of gravimetric analysis. Both involve changing the phase of the analyte to separate it from the rest of a mixture, resulting in a change in mass. You might hear either or both of these methods being called gravimetric analysis as well as the more descriptive names below.

Figure 4.28 Drawing of Alice from Lewis Carroll's "Alice in Wonderland" holding a brown bottle labeled, "Drink Me."

Ref: www.khanacademy.org/

It is generally not recommended to drink a mystery liquid! Maybe Alice could have used gravimetric analysis to figure out what is in the bottle. How might she check for the presence of soluble silver salts? Image of Alice *from Wikimedia Commons,* public domain *Volatilization gravimetry* involves separating components of our mixture by heating or chemically decomposing the sample. The heating or chemical decomposition separates out any volatile compounds, which results in a change in mass that we can measure. We will go through a detailed example of volatilization gravimetry in the next section of this article! *Precipitation gravimetry* uses a precipitation reaction to separate one or more parts of a solution by incorporating it into a solid. The phase change occurs since the analyte starts in the solution phase and then reacts to form a solid precipitate. The solid can be separated from the liquid components by filtration. The mass of the solid can be used to calculate the amount or concentration of the ionic compounds in solution.
In this article, we will go through an example of using volatilization gravimetric in a chemistry lab setting. We will also discuss some of the things that might go wrong during a gravimetric analysis experiment and how that might affect our results.

Bad news! We have just been informed by our inept lab assistant, Igor, that he may have accidentally contaminated a bottle of the metal hydrate.

$BaCl_2 \cdot 2H_2O$ with an unknown amount of KCl. In order to find the purity of BaCl2·2H2O of the metal hydrate mixture to remove water from the sample. After heating, the sample has a reduced mass of 9.14 g,

What is the mass percent of $BaCl_2.2HO$ **in the original mixture?**
Gravimetric analysis problems are simply stoichiometry problems with a few extra steps. Hopefully you will remember that in order to do any stoichiom$_2$etric calculations, we need

the coefficients from the balanced chemical equation.
[Why don't we include KCl in the equation?]
Let's go through the calculation step-by-step.
Step #1: Calculate change in sample mass
We can find the amount of water lost during the heating process by calculating the change in mass for our sample.
Mass of H2O=Initial sample mass−Final sample mass=9.51g−9.14g=0.37g H_2O

Step #2. Convert mass of evaporated water to moles
In order to convert the amount of water lost using the mole ratio, we will need to convert the mass of evaporated water to moles. We can do this conversion using the molecular weight of water, 18.02 g/mol

$$0.37\ g\ H_2O * \frac{1\ mol\ H_2O}{18.02\ g\ H_2O} = 0.0205\ mols$$

Step #3. Convert moles of water to moles of $BaCl_2.2H_2O$

using the mole ratio from the balanced reaction.

$$0..0205\ mols\ of\ H_2O * \frac{1mol\ BaCl_2.\ 2H_2O}{2\ mols\ H_2O}$$

$$= 0.0103\ mols\ of\ BaCl_2.2H_2O$$

Step #4. Convert moles of $BaCl_2.2H_2O$ to mass in Grams.

Using the molar mass of $BaCl_2.2H_2O$:

$$0.0103\ mols\ of\ BaCl_2.2H2O * \frac{244.47\ g}{1\ mol\ \ BaCl_2.2H_2O}$$

Step #5. Calculate mass percent of $BaCl_2.2H_2O$ in the original sample

In the original sample the mass percent can be calculated using the ratio of the mass from **Step** #4 and the original sample mass.
Mass% BaCl2·2H2O=2.51gBaCl2·2H2O
In 9.51g of mixture×100%=26.4%BaCl2·2H2O (No thanks to Igor!)

SUPPLEMENTAL

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Shortcut: We could also combine #2 to #4 into a single calculation (with the caveat
We just successfully used gravimetric analysis to calculate the purity of a mixture, hooray! However, sometimes when you are in lab, things might not go quite so smoothly. Things that could go wrong include:

Stoichiometry errors, such as not balancing the equation for the dehydration

Lab errors, such as not giving the water enough time to evaporate or forgetting to tare a piece of glassware
What would happen to our answer for the above situations?
Situation #1: We forgot to balance the equation

Concept check: What mass of metal hydrate would we calculate in situation #1?
The moral of this story? Double check that all equations are properly balanced!
Situation #2: We ran out of time and not all the water evaporated

Figure 4.29 Anhydrous Copper sulfate crystals on watch glass

Hand holding watchglass with white anhydrous copper(II) sulfate, and hydrated copper(II) sulfate, which appears as a sky blue spot in the middle of the white powder after water was added.

In some cases, the color differs between the metal hydrate and the anhydrous compound. For example, anhydrous copper(II) sulfate is a white solid that turns bright sky blue when it is hydrated. In such cases, you could use the color change as well as the mass to monitor the dehydration process.

In the second situation, we did not fully dehydrate our sample. This could happen for a lot of reasons, unfortunately. For example, we could run out of time, the heat could be set too low, or maybe we just took the sample off the heat before it was done by mistake. How does that affect our calculations?

In this situation, the difference in mass we calculate in **Step**#1 will be *lower than it should be*, so we will have correspondingly fewer moles of water in **Step #2**. That will result in calculating a *lower* percent mass of $BaCl2$ compared to fully dehydrating the sample. In the end, we will end up underestimating the purity of the metal hydrate.

Chemists usually try to avoid situation #2 by *drying to constant mass*. That means monitoring the change in mass during the drying period until you no longer observe any further change in mass (which also depends on the accuracy of your lab balance). When you first start heating your sample, you might expect to see a significant mass decrease as water is lost. As you continue to heat the sample, the change in mass gets smaller since there is less water left in the sample to evaporate. At some point, there won't be enough water left to make a significant change in mass, so the measured mass will stay approximately constant over multiple measurements. At that point, you can hopefully assume your sample is dry!

Lab tip: Surface area is always a factor when removing volatiles from a sample. Having a higher surface area will increase the rate of evaporation. You can increase the surface area of the sample by spreading your sample as thinly as possible on the heating surface or breaking up any larger chunks of solid, since moisture can get trapped inside the chunks.

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Summary

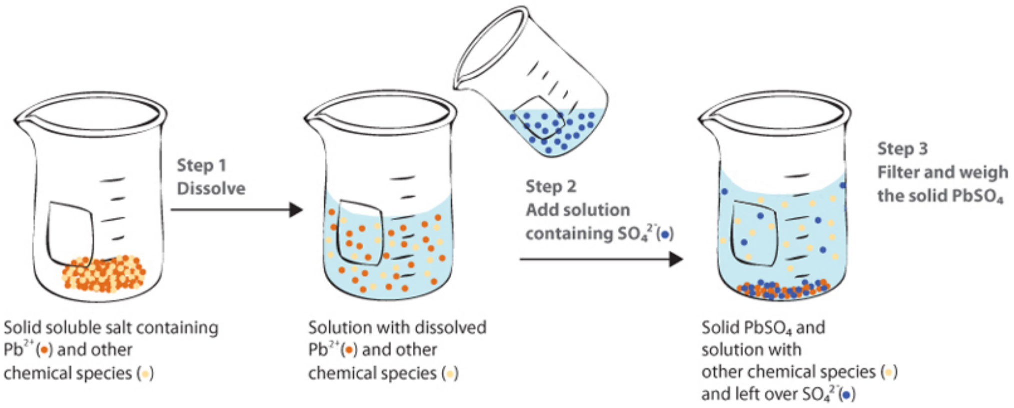
Gravimetric analysis is a class of lab techniques that uses changes in mass to calculate the amount or concentration of an analyte. One type of gravimetric analysis is called volatilization gravimetry, which measures the change in mass after removing volatile compounds. An example of volatilization gravimetry would be using the change in mass after heating to calculate the amount or purity of a metal hydrate. Some useful tips for gravimetric analysis experiments and calculations are:

- Double check stoichiometry and make sure equations are balanced.
- When removing volatiles from a sample, make sure to dry to constant mass.
- Always tare your glassware!
  https://www.khanacademy.org/science/ap-chemistry/stoichiometry-and-molecular-composition-ap/limiting-reagent-stoichiometry-ap/a/gravimetric-analysis

Another Example: Precipitation Gravimetry

The amount of lead ions Pb^{2+} present in a water can present a health risk. One has to design an experiment to check the presence of lead ions and then determine its amount in water by gravimetric method using the precipitation reaction.

The figure below explains this type of method:



Ref. 4.30 Steps for precipitation Gravimetry

Reference: http://www.chemcollective.org/chem/ubc/exp01/index.php

The filtration is carried out using vacuum filtration as shown below:

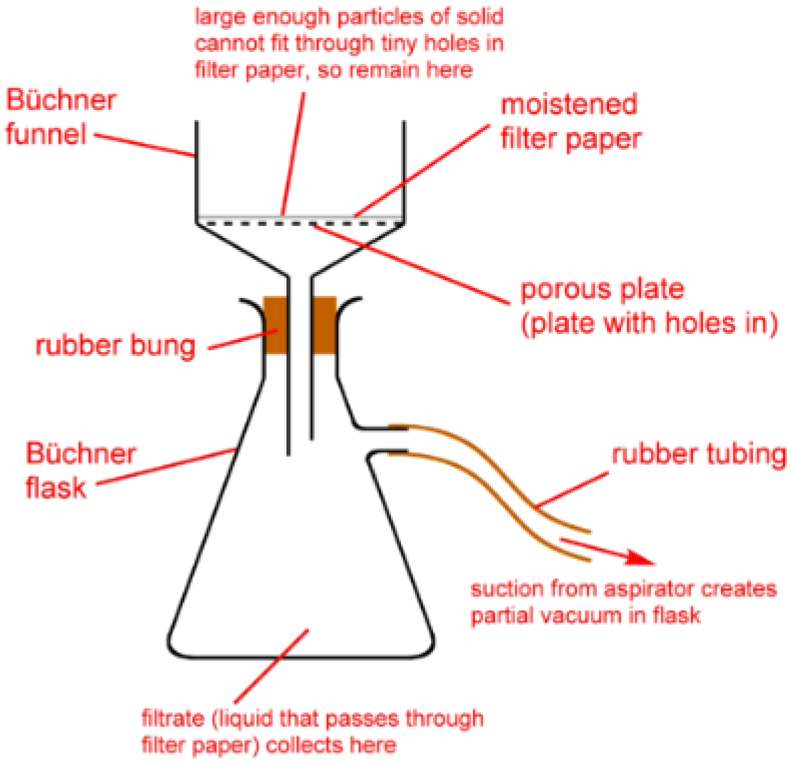


Figure 4.31 Vaccuum Filtration Set up
Reference:
https://chem.libretexts.org/Bookshelves/Ancillary_Materials/Demos_Techniques_and_Experiments/General_Lab_Techniques/Vacuum_Filtration

Example:

A 0.955 g solid mixture containing K_2SO_4 is dissolved in water and treated with an excess of Ba $(NO_3)_2$,
resulting in the precipitation of 0.850 g of $BaSO_4$.

What is the concentration (mass percent) of K_2SO_4 in the mixture?

Ba $(NO_3)_2$ is the excess reagent
K_2SO_4 is the limiting reactant

Amount of K_2SO_4 based on the product $BaSO_4$ =

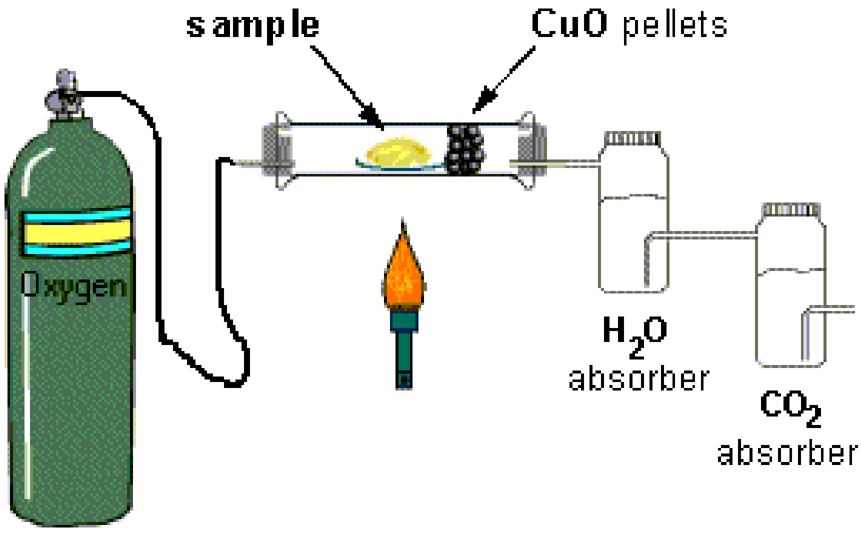
[0.850 ~~g $BaSO_4$~~] x [1 ~~mol $BaSO_4$~~ / 233.38 ~~g $BaSO_4$~~] x [1 ~~mol K_2SO_4~~ / 1 ~~mol $BaSO_4$~~] x [174.259 g K_2SO_4 / ~~mol K_2SO_4~~] = **0.635 g K_2SO_4**

[Note: molar mass of $BaSO_4$ = 233.38 g / mol]
[Note: molar mass of K_2SO_4] = 174.259 g / mol]

The % of K_2SO_4 = [0.635 g K_2SO_4 / 0.955 g mixture] x 100% = **66.5 %**

Combustion Analysis:

Combustion analysis is a method used in both organic chemistry and analytical chemistry to determine the elemental composition (i.e. the empirical formula) of a pure organic compound by combustion reaction of the sample and the products of this combustion will be quantitative analyzed.



sample

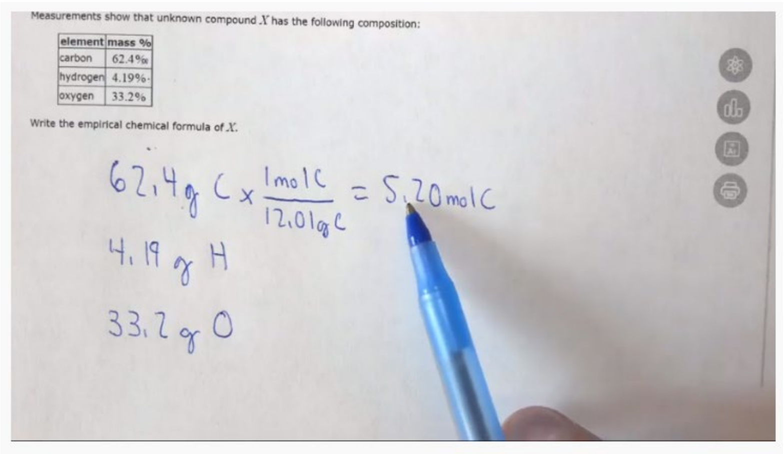
Figure 4.31 Combustion Analysis Set up
Reference: http://www.chem.wilkes.edu/~mencer/combustion/combust_app.htm

The combustion reaction is carried out under the excess of oxygen. Oxygen is passed through a closed tube which is heated. The carbon and hydrogen present in the sample are converted into carbon dioxide CO_2 and water H_2O. The excess O_2 helps to push through the products through the tube. Inside the tube, the products pass through copper-II-oxide, CuO solid. CuO is acting as a catalyst (similar to Nick, Platinum and Palladium compounds act as catalysts in the catalytic converter in the vehicles). CuO catalyzes the conversion of any leftover traces of carbon and hydrogen and into CO_2 and H_2O accordingly.

H_2O is collected in an absorber filled with magnesium perchlorate, $Mg(ClO_4)_2$. The change in mass of this absorber is followed and observed. The mass change is equal to the mass of water produced during the combustion reaction.
CO_2 is collected in a separate absorber filled with sodium hydroxide, NaOH. The change in mass of this absorber is equal to the mass of carbon dioxide produced during the combustion process.

Nitrogen and oxygen (N or O) masses if present can be determined by the difference between the mass of combusted sample and the sum of the masses of the carbon in the carbon dioxide and hydrogen in the water (the masses of the C and H are found using stoichiometric calculations).

The video below illustrates the elemental analysis of a compound:



Measurements show that unknown compound X has the following composition:

element	mass %
carbon	62.4%
hydrogen	4.19%
oxygen	33.2%

Write the empirical chemical formula of X.

$62.4\,g\ C \times \frac{1\,mol\ C}{12.01\,g\ C} = 5.20\,mol\ C$

$4.19\,g\ H$

$33.2\,g\ O$

https://www.youtube.com/watch?v=WC3mzs2S6aQ

Example:

Elemental analysis of an organic compound using the combustion reaction reveals the

results below:
$2.6406 \text{ g } CO_2$
$0.5400 \text{ g } H_2O$
The molecular formula is to be determined if the molar mass of this organic compound is 78.11 g/mol

The combustion reaction is given below:

$$C_xH_y \quad + (\text{excess}) \quad O_2 \quad \rightarrow \quad (x)\ CO_2 \quad + \quad (y/2)\ H_2O$$

CO_2 grams are converted into mol C (x)
H_2O grams are converted into mol H (y)

$$2.6406 \text{ g } CO_2 \times \frac{1 \text{ mol } CO_2}{44.01 \text{ g } CO_2} \times \frac{1 \text{ mol C}}{1 \text{ mol } CO_2} = 0.06000 \text{ mol C}$$

$$0.5400 \text{ g } H_2O \times \frac{1 \text{ mol } H_2O}{18.00 \text{ g } H_2O} \times \frac{2 \text{ mol H}}{1 \text{ mol } H_2O} = 0.06000 \text{ mol H}$$

The empirical formula is **CH**

The empirical formula has the molar mass = CH = 12.0 g/mole + 1.00 g/mol = 13.0 g/mole
The molar mass of the organic compound = 78.11 g/mole

The empirical formula unit = [molar mass of the compound] / [molar mass of empirical formula]

[The empirical formula unit] = [78.11 g/mole] / [13.0 g/mole] = 6 units

The molecular formula = 6 x CH = C_6H_6
One can confirm the result by calculating the molar mass of C_6H_6 which is then calculated to be 78.0 g/ mole.

End of Chapter Questions:

Balancing Chemical Equation:

1) _$Mg(OH)_2$ + _ **2**_ HCl → ______$MgCl_2$ + _ **2**_ H_2O

Double replacement

2) _Na_2CO_3 + _ **2**_ HCl → __**2**_ $NaCl$ +______H_2CO_3
Double replacement

3) ___NH_4NO_2 → ___N_2 + _ **2**_ H_2O
Decomposition

4) _**2**_ N_2 + __**5**_ O_2 → __**2**_ N_2O_5

Synthesis

5) _$MgCO_3$ →________MgO +____CO_2

Decomposition

6) __**2**_ KBr +_____Cl_2 → __**2**_ KCl +___Br_2

Single replacement

7) _Zn +_________$CuSO_4$ →_____Cu +_____$ZnSO_4$

Single replacement

8) __**4**_ P + __**3**_ O_2 →_____P_4O_6

Synthesis

9) _$SrBr_2$ +_________$(NH_4)_2CO_3$ →____$SrCO_3$ + _ **2**_ NH_4Br

Double replacement

10) __**2**_ $AgNO_3$ +_____$(NH_4)_2CrO_4$ →____Ag_2CrO_4 + _ **2**_ NH_4NO_3

Double replacement
11) __**2**_ K + _ **2**_ H_2O → __**2**_ KOH +___H_2

Single replacement

12) __2_ Al + _ 3_ $Pb(NO_3)_2$ → __2_ $Al(NO_3)_3$ + _ 3_ Pb

Single replacement

13) __3_ Fe + _ 2_ O_2 →_____Fe_3O_4

Synthesis

14) __4_ Li +______O_2 → _ 2_ Li_2O

Synthesis

15) _$ZnCl_2$ + _ 2_ KOH →_______$Zn(OH)_2$ +_ 2_ KCl

Double replacement

16) _Fe_3O_4 + _ 4_ H_2 → __ 3_ Fe +_ 4_ H_2O

Single replacement

17) _$Pb(NO_3)_2$ →________Pb + _ 2_ NO_2 +____O_2

Decomposition

18) __2_ H_2O → __2_ H_2 +____O_2

Decomposition

19) __3_ Mg +______N_2 →_____Mg_3N_2

Synthesis

Net Ionic Equation

1. $2NaCl(aq)$ + $Pb(NO_3)_2(aq)$ → $PbCl_2(s)$ + $2NaNO_3(aq)$

Ionic Equation: $2Na^+(aq)$ + $2Cl^-(aq)$ + $Pb^{2+}(aq)$ + $2NO_3^-(aq)$ →
$PbCl_2(s)$ + $2Na^+(aq)$ + $2NO_3^-(aq)$
Net Ionic Equation: $2Cl^-(aq)$ + $Pb^{2+}(aq)$ → $PbCl_2(s)$

2. $Na_2CO_3(aq)$ + $FeCl_2(aq)$ → $FeCO_3(s)$ + $2NaCl(aq)$

Ionic Equation: $2Na^+(aq)$ + $CO_3^{2-}(aq)$ + $Fe^{2+}(aq)$+ $2Cl^-(aq)$ →
$FeCO_3(s)$ + $2Na^+(aq)$ + $2Cl^-(aq)$
Net Ionic Equation:: $CO_3^{2-}(aq)$ + $Fe^{2+}(aq)$ → $FeCO_3(s)$

3. $Mg(OH)_2(aq)$ + $2HCl(aq)$ → $MgCl_2(aq)$ + $2H_2O(l)$
Ionic Equation: $Mg^{2+}(aq)$ + $2OH^-(aq)$ + $2H^+(aq)$ + $2Cl^-(aq)$ →
$Mg^{2+}(aq)$ + $2Cl^-(aq)$ + $2H_2O(l)$
Net Ionic Equation:: $2OH^-(aq)$ + $2H^+(aq)$ → $2H_2O(l)$

$OH^-(aq)$ + $H^+(aq)$ → $H_2O(l))$

4. $K_2(C_rO_4)(aq)$ + $CaCl_2(aq)$ → $2KCl(aq)$ + $Ca(C_rO_4)(aq)$
Ionic Equation: $2K^+(aq)$ + $C_2O_4^{2-}(aq)$ + $Ca^{2+}(aq)$+ $2Cl^-(aq)$ → $2K^+(aq)$ +
$2Cl^-(aq)$ + Ca^{2+} + $C_2O_4^{2-}$
Net Ionic Equation:: NA all spectator ions

5. $2(NH_4)_3PO_4(aq)$ + $3Zn(NO_3)_2(aq)$ → $6NH_4NO_3(aq)$ + $Zn_3(PO_4)_2(s)$
Ionic Equation: $6NH_4^+(aq)$ + $2PO_4^{3-}(aq)$ + $3Zn^{2+}(aq)$ + $6NO_3^-(aq)$ → $6NH_4^+(aq)$ + $6NO_3^-(aq)$ + $Zn_3(PO_4)_2(s)$
NIE: $2PO_4^{3-}(aq)$ + $3Zn^{2+}(aq)$ → $Zn_3(PO_4)_2(s)$

6. $2LiOH(aq)$ + $BaCl_2(aq)$ → $2LiCl(aq)$ + $Ba(OH)_2(aq)$
Ionic Equation: $2Li^+(aq)$ + $2OH^-(aq)$ + $Ba^{2+}(aq)$ + $2Cl^-(aq)$ →
$2Li^+(aq)$ + $2Cl^-(aq)$ + Ba^{2+} + 2 OH^-
Net Ionic Equation:: Na all spectator ions

7. $Na_2CO_3(aq)$ + $2HCl(aq)$ → $2NaCl(aq)$ + $CO_2(g)$ + $H_2O(l)$
Ionic Equation: $2Na^+(aq)$ + $CO_3^{2-}(aq)$ + $2H^+(aq)$ + $2Cl^-(aq)$ →
$2Na^+(aq)$ + $2Cl^-(aq)$ + $CO_2(g)$ + $H_2O(l)$
Net Ionic Equation:: $CO_3^{2-}(aq)$ + $2H^+(aq)$ → $CO_2(g)$ + $H_2O(l)$

8. $Mg(NO_3)_2(aq)$ + $Na_2CrO_4(aq)$ → $2NaNO_3(aq)$ + $MgCrO_4(s)$
Ionic Equation: $Mg^{2+}(aq)$ + $2NO_3^-(aq)$ + $2Na^+(aq)$ + $CrO_4^{2-}(aq)$ → $2Na^+(aq)$ + $2NO_3^-(aq)$ + $MgCrO_4(s)$
Net Ionic Equation:: $Mg^{2+}(aq)$ + $CrO_4^{2-}(aq)$ → $MgCrO_4(s)$

9. $2FeCl_3(aq)$ + $3Mg(s)$ → $3MgCl_2(aq)$ + $2Fe(s)$

Ionic Equation: $2Fe^{3+}(aq)$ + $6Cl^-(aq)$ + $3Mg(s)$ → $3Mg^{2+}(aq)$ +
$6Cl^-(aq)$ + $2Fe(s)$

Net Ionic Equation:: $2Fe^{3+}(aq)$ + $3Mg(s)$ → $3Mg^{2+}(aq)$ +
$2Fe(s)$

10. $BaBr_2(aq)$ + $Na_2SO_4(aq)$ → $BaSO_4(s)$ + $2NaBr(aq)$
Ionic Equation: $Ba^{2+}(aq)$ + $2Br^-(aq)$+ $2Na^+(aq)$ + $SO_4^{2-}(aq)$ →
$BaSO_4(s)$ + $2Na^+(aq)$ + $2Br^-(aq)$
Net Ionic Equation:: $Ba^{2+}(aq)$ + $SO_4^{2-}(aq)$ → $BaSO_4(s)$

11. $2AgNO_3(aq)$ + $MgI_2(aq)$ → $2AgI(s)$ + $Mg(NO_3)_2(aq)$
Ionic Equation: $2Ag^+(aq)$ + $2NO_3^-(aq)$ + $Mg^{2+}(aq)$ + $2I^-(aq)$ →
$2AgI(s)$ + $Mg^{2+}(aq)$ + $2NO_3^-(aq)$
Net Ionic Equation:: $2Ag^+(aq)$ + $2I^-(aq)$ → $2AgI(s)$

Or $Ag^+(aq)$ + $I^-(aq)$ → $AgI(s))$

12. $3(NH_4)_2C_rO_4(aq)$+ $2Al(ClO_4)_3(aq)$ → $Al_2(C_rO_4)_3(s)$ + $6NH_4ClO_4(aq)$

Ionic Equation: $6NH_4^+(aq)$ + $3C_rO_4^{2-}(aq)$ + $2Al^{3+}(aq)$ + $6ClO_4^-(aq)$ → $6NH_4^+(aq)$ +
$6ClO_4^-(aq)$ + $Al_2(C_rO_4)_3(s)$

Net Ionic Equation:: $3C_2O_4^{2-}(aq)$ + $2Al^{3+}(aq)$ → $Al_2(C_rO_4)_3(s)$

13. $Ni(NO_3)_2(aq)$ + $2NaOH(aq)$ → $Ni(OH)_2(s)$ + $2NaNO_3(aq)$

Ionic Equation: $Ni^{2+}(aq)$ + $2NO_3^-(aq)$ + $2Na^+(aq)$ + $2OH^-(aq)$ →
$Ni(OH)_2(s)$ + $2Na^+(aq)$ + $2NO_3^-(aq)$

Net Ionic Equation:: $Ni^{2+}(aq)$ + $2OH^-(aq)$ → $Ni(OH)_2(s)$

14. $2HBr(aq)$ + $Pb(ClO_4)_2(aq)$ → $2HClO_4(aq)$ + $PbBr_2(s)$

Ionic Equation: $2H^+(aq)$ + $2Br^-(aq)$ + $Pb^{2+}(aq)$ + $2ClO_4^-(aq)$
→ $2H^+(aq)$ + $2ClO_4^-(aq)$ + $PbBr_2(s)$

Net Ionic Equation:: $2Br^-(aq)$+ $Pb^{2+}(aq)$ → $PbBr_2(s)$

15. $2KF(aq)$ + $Mg(NO_3)_2(aq)$ → $2KNO_3(aq)$ + $MgF_2(s)$

Ionic Equation: $2K^+(aq)$ + $2F^-(aq)$ + $Mg^{2+}(aq)$ + $2NO_3^-(aq)$ →
$2K^+(aq)$ + $2NO_3^-(aq)$ + $MgF_2(s)$

Net Ionic Equation:: $2F^-(aq)$ + $Mg^{2+}(aq)$ → $MgF_2(s)$

16. $2Na_3PO_4(aq) + 3Ni(ClO_4)_2(aq) \rightarrow 6NaClO_4(aq) + Ni_3(PO_4)_2(s)$

Ionic Equation: $6Na^+(aq) \quad 2PO_4^{3-}(aq) + 3Ni^{2+}(aq) + 6ClO_4^-(aq) \rightarrow$
$6Na^+(aq) + 6ClO_4^-(aq) + Ni_3(PO_4)_2(s)$

Net Ionic Equation: $2PO_4^{3-}(aq) + 3Ni^{2+}(aq) \rightarrow Ni_3(PO_4)_2(s)$

17. $CuCl_2(aq) + 2AgC_2H_3O_2(aq) \rightarrow Cu(C_2H_3O_2)_2(aq) + 2AgCl(s)$

Ionic Equation: $Cu^{2+}(aq) + 2Cl^-(aq) + 2Ag^+(aq) + 2C_2H_3O_2^-(aq) \rightarrow$
$Cu^{2+}(aq) + 2C_2H_3O_2^-(aq) + 2AgCl(s)$

Net Ionic Equation: $Cl^-(aq) + Ag^+(aq) \rightarrow AgCl(s)$

Oxidation Reduction:

1. Determine the oxidation number of the elements in each of the following compounds:

   a. H_2CO_3
   H: +1, O: -2, C: +4

   b. N_2
   N: 0

   c. $Zn(OH)_4^{2-}$
   Zn: 2+, H: +1, O: -2

   d. NO_2^-
   N: +3, O: -2

   e. LiH
   Li: +1, H: -1

   f. Fe_3O_4
   Fe: +8/3, O: -2

2. Identify the species being oxidized and reduced in each of the following reactions:

   a. $Cr^+ + Sn^{4+} \longrightarrow Cr^{3+} + Sn^{2+}$
   Cr^+: oxidized, Sn^{4+}: reduced

   b. $3\ Hg^{2+} + 2\ Fe\ (s) \longrightarrow 3\ Hg_2 + 2\ Fe^{3+}$
   Hg^{2+}: reduced, Fe: oxidized

   c. $2\ As\ (s) + 3\ Cl_2\ (g) \longrightarrow 2\ AsCl_3$
   As: oxidized, Cl_2: reduced

3. Would you use an oxidizing agent or reducing agent in order for the following reactions to occur?

   a. $ClO_3^- \longrightarrow ClO_2$ **reducing agent**

b. $SO_4^{2-} \rightarrow S^{2-}$ **reducing agent**

c. $Mn^{2+} \rightarrow MnO_2$ **oxidizing agent**

d. $Zn \rightarrow ZnCl_2$ **oxidizing agent**

4. Write balanced equations for the following redox reactions:

a. **2** $NaBr + Cl_2 \rightarrow$ **2** $NaCl + Br_2$

b. $Fe_2O_3 +$ **3** $CO \rightarrow$ **2** $Fe +$ **3** CO_2 in acidic solution

c. **5** $CO + I_2O_5 \rightarrow$ **5** $CO_2 + I_2$ in basic solution

5. Write balanced equations for the following reactions:

a. $Cr(OH)_3 + Br_2 \rightarrow CrO_4^{2-} + Br^-$ in basic solution

$10\ OH^- + 2\ Cr(OH)_3 + 3\ Br_2 \rightarrow 2\ CrO_4^{2-} + 8\ H_2O + 6\ Br^-$

b. $O_2 + Sb \rightarrow H_2O_2 + SbO_2^-$ in basic solution

$2\ OH^- + 2\ Sb + 3\ O_2 + 2\ H_2O \rightarrow 2\ SbO_2^- + 3\ H_2O_2$

c. $HCOOH + MnO_4^- \rightarrow CO_2 + Mn^{2+}$ in acidic solution

$6\ H^+ + 2\ MnO_4^- + 5\ HCOOH \rightarrow 2\ Mn^{2+} + 8\ H_2O + 5\ CO_2$

d. $ClO_2^- \rightarrow ClO_2 + Cl^-$ in acidic solution

$5\ ClO_2^- + 4\ H^+ \rightarrow 4\ ClO_2 + Cl^- + 2\ H_2O$

6. Write the balanced half reactions of the following reactions:

a. $NiO_2 + 2\ H_2O + Fe \rightarrow Ni(OH)_2 + Fe(OH)_2$ in basic solution

$2\ H_2O + NiO_2 + 2\ e^- \rightarrow Ni(OH)_2 + 2\ OH^-$

$2\ OH^- + Fe \rightarrow Fe(OH)_2 + 2\ e^-$

b. $CO_2 + 2\ NH_2OH \rightarrow CO + N_2 + 3\ H_2O$ in basic solution

$CO_2 + H_2O + 2\ e^- \rightarrow CO + 2\ OH^-$

$2\ OH^- + 2\ NH_2OH \rightarrow N_2 + 2\ e^- + 4\ H_2O$

c. $2\ H^+ + H_2O_2 + 2\ Fe^{2+} \rightarrow 2\ Fe^{3+} + 2\ H_2O$ in acidic solution

$H_2O_2 + 2\ e^- + 2\ H^+ \rightarrow 2\ H_2O$

$Fe^{2+} \rightarrow Fe^{3+} + e^-$

d. $H^+ + 2\ H_2O + 2\ MnO_4^- + 5\ SO_2 \rightarrow 2\ Mn^{2+} + 5\ HSO_4^-$ in acidic solution

$8\ H^+ + MnO_4^- + 5\ e^- \rightarrow Mn^{2+} + 4\ H_2O$

$SO_2 + 2\ H_2O \rightarrow HSO_4^- + 3\ H^+ + 2\ e^-$

Balancing Redox Reaction in acidic medium:

Balance each redox reaction in <u>Acidic</u> solution:

$Mn^{2+} + BiO_3^{-} \rightarrow MnO_4^{-} + Bi^{3+}$

$14\ H^{+} + 2\ Mn^{2+} + 5\ BiO_3^{-} \rightarrow 2\ MnO_4^{-} + 5\ Bi^{3+} + 7\ H_2O$

$MnO_4^{-} + S_2O_3^{2-} \rightarrow S_4O_6^{2-} + Mn^{2+}$

$16\ H^{+} + 2\ MnO_4^{-} + 10\ S_2O_3^{2-} \rightarrow 2\ Mn^{2+} + 8\ H_2O + 5\ S_4O_6^{2-}$

$P + Cu^{2+} \rightarrow Cu + H_2PO_4^{-}$

$8\ H_2O + 2\ P + 5\ Cu^{2+} \rightarrow 2\ H_2PO_4^{-} + 12\ H^{+} + 5\ Cu$

$PH_3 + I_2 \rightarrow H_3PO_2^{-} + I^{-}$

$4\ H_2O + 2\ PH_3 + 3\ I_2 \rightarrow 2\ H_3PO_2^{-} + 8\ H^{+} + 6\ I^{-}$

$NO_2 \rightarrow NO_3^{-} + NO$

$H_2O + 3\ NO_2 \rightarrow 2\ NO_3^{-} + NO + 2\ H^{+}$

Balance each redox reaction in <u>Basic</u> solution:

$MnO_4^{-} + C_2O_4^{2-} \rightarrow MnO_2 + CO_2$

$4\ H_2O + 2\ MnO_4^{-} + 3\ C_2O_4^{2-} \rightarrow 2\ MnO_2 + 8\ OH^{-} + 6\ CO_2$

$ClO_2 \rightarrow ClO_2^{-} + ClO_3^{-}$

$2\ OH^{-} + 2\ ClO_2 \rightarrow ClO_2^{-} + ClO_3^{-} + H_2O$

$Cu(NH_3)_4{}^{2+} + S_2O_4{}^{2-} \rightarrow SO_3{}^{2-} + Cu + NH_3$

$Cu(NH_3)_4{}^{2+} + S_2O_4{}^{2-} + 4\ OH^- \rightarrow Cu + 4NH_3 + 2\ SO_3{}^{2-}$

$Zn + NO_3{}^- \rightarrow Zn(OH)_4{}^{2-} + NH_3$

$6\ H_2O + NO_3{}^- + 7\ OH^- + 4\ Zn \rightarrow NH_3 + 4\ Zn(OH)_4{}^{2-}$

$6\ H_2O + NO_3{}^- + 7\ OH^- + 4\ Zn \rightarrow NH_3 + 4\ Zn(OH)_4{}^{2-}$

$6\ H_2O + NO_3{}^- + 7\ OH^- + 4\ Zn \rightarrow NH_3 + 4\ Zn(OH)_4{}^{2-}$

$Zn \rightarrow Zn(OH)_4{}^{2-} + H_2$

$2\ OH^- + Zn + 2\ H_2O \rightarrow Zn(OH)_4{}^{2-} + H_2$

$Al + OH^- \rightarrow AlO_2{}^- + H_2$

$2\ Al + 2\ H_2O + 2\ OH^- \rightarrow 2\ AlO_2{}^- + 3\ H_2$

Limiting Reactant, Percent Yield, mole Stoichiometry:

1. Combustion of analysis of 0.800 grams of an unknown hydrocarbon yields 2.613 g and 0.778 g H_2O. What is the percent composition of hydrocarbon?

a) 66.6% C; 33.4% H
b) 82.3% C; 17.7% H
c) 89.1% C; 10.9% H
d) 92.4% C; 7.60% H
e) not enough information given to solve the problem

Answer: C

2. Sodium metal and water react to form sodium hydroxide and hydrogen gas. What mass of Na will react with excess water to produce 15 g NaOH?

$2\,Na(s) + 2\,H_2O \rightarrow H_2(g) + 2NaOH(aq)$

a) 4.3 g
b) 5.4 g
c) 8.6 g
d) 11 g
e) 26 g

Answer: C

3. In the reaction below, which substances are dissolved in water?

$Cu(s) + H_2SO_4 \rightarrow CuSO_4 + H_2(g)$

a) H_2SO_4 and $CuSO_4$
b) Cu and $CuSO_4$
c) Cu
d) H_2 and H_2SO_4
e) H_2 and Cu

Answer: A

4. In the reaction given below, if 12 moles of aluminum oxide are consumed, how many moles of oxygen gas are produced?

$2\,Al_2O_3 \rightarrow 4\,Al + 3\,O_2$

a) 3
b) 4
c) 6
d) 12
e) 18

Answer: E

5. In the reaction below, 8.0 g of H_2 react with 9.0 g O_2. Which of the following statements is true?

$2 H_2 + O_2 \rightarrow 2 H_2O$

a) The equation is not balanced
b) The H_2 is the limiting reactant
c) The O_2 is the limiting reactant
d) 2.0 moles of H_2O would be produced
e) 26 grams of H_2O would be produced

Answer: C

7. How many grams of MgI_2 are produced by the reaction of 25.0 g of Mg with 25.0 g of I_2?

$Mg + I_2 \rightarrow MgI_2$

a) 9.20 g
b) 18.4 g
c) 27.4 g
d) 49.0 g
e) 195 g

Answer: C

8. If 70.9 g of chlorine reacts with sufficient cesium to produce cesium chloride, what is the theoretical yield?

$2 Cs + Cl_2 \rightarrow 2 CsCl$

a) 70.9 g
b) 132.9 g
c) 146 g
d) 337 g
e) 285 g

Answer: D

9. Which compound will not dissolve in water in large amounts?

a) KNO_3
b) NH_4Cl
c) $Ca(OH)_2$
d) AgCl
e) Ag_2SO_4

Answer: D

10. Which compound will dissolve in water in large amounts?

a) AgCl
b) $Al(OH)_3$
c) Na_2SO_4
d) Na_2SO_4
e) MgS

Answer: C

11. In the reaction 2 CO(g) + O_2(g) → $2CO_2$(g), what is the ratio of moles of oxygen used to moles of CO_2 produced?

a) 1:1
b) 2:1
c) 1:2
d) 2:2

Answer: C

12. Which of the following is true about the total number of reactants and the total number of products in the reaction shown below?

C_5H_{12}(l) + 8 O_2(g) → 5 CO_2(g) + 6 H_2(g)

a) 9 moles of reactants chemically change into 11 moles f product
b) 9 grams of reactants chemically change into 11 grams of product
c) 9 liters of reactants chemically change into 11 liters of product
d) 9 atoms of reactants chemically change into 11 of product

Answer: A

13. Which of the following is an **INCORRECT** interpretation of the balanced equation shown below?

2S(s) + 3O_2 (g) → 2SO(g)

a) 2 atoms S + 3 molecules O_2 → 2 molecules SO_3
b) 2 g S + 3 g O_2 → 2 g SO_3
c) 2 mol S + 3 mol O_2 → 2 mole SO_3
d) None of the above

Answer: B

14. Hydrogen gas can be produced by reacting aluminum with sulfuric acid. How many moles of sulfuric acid are needed to completely react with 15.0 mol aluminum?
2 Al(s) + 3 H_2SO_4 → $Al_2(SO_4)_3$(aq) + 3 H_2(g)

a) 0.100 mol
b) 10.0 mol
c) 15.0 mol
d) 22.5 mol

Answer: D

15. The equation below shows the decomposition of lead nitrate. How many grams of oxygen are produced when 11.5 g NO_2 is formed?
2 $Pb(NO_3)_2$(s) → 2 PbO(s) + 4 NO_2(g) + O_2(g)

a) 1.00 g
b) 2.00 g

c) 2.88 g
d) 32.0 g

Answer: B

16. Which of the following is NOT true yield?

a) The value of the actual yield must be given in order for the percent yield to calculated
b) The percent yield is the ratio of the actual yield to the theoretical yield
c) The actual yield may be different from the theoretical yield because reactions do not always go to completion
d) The actual yield may be different from the theoretical yield because insufficient limiting reagent was used

Answer: D

17. Which of the following is NOT a reason why actual yield less than theoretical yield?

a) Impure reactants present
b) Competing side reaction
c) Loss of products during purification
d) Conservation of mass

Answer: D

18. Lead nitrate can be decomposed by heating. What is the percent yield of the decomposition reaction if 9.9 g of $Pb(NO_3)_2$ are heated to give 5.5 g of PbO?

$2\ Pb(NO_3)_2\ (s) \rightarrow 2\ PbO(s) + 4\ NO_2(g) + O_2(g)$

a) 44%
b) 56%
c) 67%
d) 82%

Answer: D

19. In a particular reaction between copper metal and silver nitrate, 12.7 g Cu produced 38.1 g. What is the percent yield of silver in this reaction?

$Cu(s) + AgNO_3(aq) \rightarrow Cu(NO_3)_2 + 2\ Ag$

a) 56.7%
b) 77.3%
c) 88.2%
d) 176%

Answer: C

20. Which conversion factor do you use first to calculate the number of grams of CO produced by the reaction of 50.6 g of CH_4 with O_2? The equation for the complete combustion of methane is:
$CH_4(g) + 2\ O_2(g) \rightarrow CO_2(g) + 2\ H_2O(l)$

a) 1 mol CH_4 / 16.0 g CH_4
b) 2 mol O_2 / 1 mol CO_2
c) 16.0g CH_4 / mol CO_2
d) 44.0 g CO_2 / 2 mol CO_2

Answer: A

Acid – Base Titration

1. Consider the acid – base reaction below:

$$H_2SO_4 \quad + \quad NaOH \quad \rightarrow \quad Na_2SO_4 \quad + \quad H_2O$$

If it takes 27.4 mL of 0.768 M NaOH to titrate 16.7 mL of H_2SO_4, what is the concentration of the H_2SO_4 solution?

a) 0.530 M
b) 0.630 M
c) 0.440 M
d) 0.330 M

Answer: B

2. Consider the acid – base reaction below:

$$NaOH \; + \; HCl \; \rightarrow H_2O \; + \; NaCl$$

If 24.5 mL of HCl solution is needed to titrate 33.0 mL of a 0.112 M NaOH, what is the concentration of the HCl solution?

a) 0.151 M
b) 0.250 M
c) 0.384 M
d) 0.865 M

Answer: A

3. Consider the acid – base reaction below:

$$Ba(OH)_2 \; + \; HClO_4 \; \rightarrow \; Ba(ClO_4)_2 \; + \; H_2O$$

How many mL of 1.2 M $HClO_4$ is needed to neutralize 5.8 mL of a 0.44 M $Ba(OH)_2$solution?

a) 5.3 mL of 1.2 $HClO_4$
b) 6.3 mL of 1.2 $HClO_4$
c) 7.3 mL of 1.2 $HClO_4$
d) 4.3 mL of 1.2 $HClO_4$

Answer: D

4. How many liters of 0.100 M HCl would be required to react completely
with 5.00 grams of calcium hydroxide?

$Ca(OH)_2(s) + 2\ HCl(aq) \rightarrow CaCl_2(aq) + 2\ H_2O(l)$

a) 1.25 L

b) 1.35 L
c) 1.15 L
d) 1.05 L

Answer B

2. If I combined 15.0 grams of calcium hydroxide with 75.0 mL of 0.500 M HCl, how many grams of calcium chloride would be formed?

a) 1.50 g
b) 3.15 g
c) 4.50 g
d) 2.08 g

Answer: D

3. How many grams of the excess reagent will be left over after the reaction

$Ca(OH)_2(s) + 2\ HCl(aq) \rightarrow\ CaCl_2(aq) + 2\ H_2O(l)$

If I combined 15.0 grams of calcium hydroxide with 75.0 mL of 0.500 M HCl, how many grams of calcium chloride would be formed?

a) 12.5 grams of $Ca(OH)_2$
b) 11.8 grams of $Ca(OH)_2$
c) 13.6 grams of $Ca(OH)_2$
d) 10.7 grams of $Ca(OH)_2$

Answer: A

4. What volume (mL) of 0.500 M $Cr_2(SO_4)_3$ solution is needed to react completely with 300. mL of 0.400 M $BaCl_2$?

a) 75.0 mL
b) 85.0 mL
c) 80.0 mL
d) 89.0 mL

Answer: C

5. 50.0 mL of 0.10 M silver nitrate is added to 50.0 mL of 0.20 M calcium chloride. A white precipitate forms. After the reaction is complete, calculate the concentration of Cl^- ions remaining in solution.

a) 0.15 M
b) 0.25 M
c) 0.05 M
d) 0.45 M

Answer: C

6. A 0.307 g sample of an unknown triprotic acid is titrated to the equivalence point using 35.2 mL of 0.106 M NaOH. Calculate the molar mass of the acid.

   $H_3A + 3\ NaOH \rightarrow Na_3A + 3\ H_2O$

   a) 227 g/mol
   b) 237 g/mol
   c) 247 g/mol
   d) 257 g/mol

   Answer: C

7. Given: $2\ MnO_4^- + 5\ H_2O_2 + 6\ H^+ \rightarrow 2\ Mn^{2+} + 8\ H_2O + 5\ O_2$

   What volume of a 0.150 M $KMnO_4$ solution would be needed to titrate 75.0 mL of a 0.150 M H_2O_2 solution?

   a) 40.0 mL
   b) 30.0 mL
   c) 20.0 mL
   d) 10.0 mL

   Answer: B

Gravimetric Analysis

1. In the reaction $CaCO_3 + 2HNO_3 \rightarrow Ca(NO_3)_2 + CO_2 + H_2O$, how many milliliters of 0.1015 M HNO_3 are required to react with 0.9857 grams of $CaCO_3$?

   a) 0.1940 mL
   b) 97.04 mL
   c) 194.1 mL
   d) 200.5 mL

   Answer: C

2. In an experiment, an average of 67.0 ml of 0.468 mol/L magnesium hydroxide ($Mg(OH)_2$) is required to titrate 50.0 ml of the acid in order to reach the endpoint. The neutralization reaction is:

   $2CH_3COOH\ (aq) + Mg(OH)_2\ (aq) \rightarrow Mg(CH_3COO)_2\ (aq) + 2H_2O\ (l)$

   The concentration of acetic acid (CH_3COOH) is

   a) 0.627 mol/L
   b) 1.25 mol/L
   c) 0.314 mol/L.
   d) 0893 mol/L

   Answer: B

3. Which statement concerning titrations is incorrect?

   a) The titration error can be accounted for by running a blank titration.
   b) The titrant is a primary standard after standardization.
   c) The endpoint and equivalence point are not the same.
   d) None of the above

   Answer: B

4. The end point of a titration is defined as
   a) the equivalence point of the titration.
   b) the actual measured volume of titrant required to complete a titration.
   c) the volume associated with actual stoichiometric quantity of titrant required to complete a titration.
   d) None of the above

   Answer: B

5. Iron in the +2 oxidation state reacts with potassium dichromate to produce Fe^{3+} and Cr^{3+} according to the equation $6Fe^{2+} + Cr_2O_7^{2-} + 14H^+ \rightarrow 6Fe^{3+} + 2Cr^{3+} + 7H_2O$. How many milliliters of 0.1658 M $K_2Cr_2O_7$ are required to titrate 200.0 mL of 0.2500 M Fe^{2+} solution?
   a) 50.26 mL
   b) 301.6 mL
   c) 8.290 mL
   d) 7.56 mL

   Answer: A

6. A 0.42 gram sample of acetylsalicylic acid ($C_9H_8O_4$, aspirin) is crushed and dissolved in water. The sample is titrated with 0.160 M sodium hydroxide. The titration required an average volume of 12.50 ml of sodium hydroxide to reach the endpoint.
The purity of the sample

a) 60%
b) 95%
c) 86%
d) 75%

Answer: C

7. To obtain a precipitate that is useful for gravimetric analysis, the analyst tries to obtain conditions to encourage crystal growth, as opposed to the formation of a colloid. Which of the following statements aids in the formation of a crystalline precipitate?

a) The solution is kept cool to slow down the movement of ions to allow crystals to form.
b) The solutions are made as dilute as practical to allow crystals to form slowly.
c) The solutions are mixed rapidly to allow the appropriate ions to make contact without interference of other materials.
d) None of the above

Answer: B

8. A sample containing 0.2784 grams of sodium chloride (NaCl) and 0.5486 grams of magnesium chloride ($MgCl_2$). The chloride in the sample was precipitated by the addition of 47.8 mL of a silver nitrate solution. What is the concentration of the silver nitrate solution?

a) 0.341M $AgNO_3$
b) 0.220 M $AgNO_3$
c) 0.00341 M $AgNO_3$
d) 0.0035 M $AgNO_3$

Answer: A

9. A sample of ore containing manganese weighed 1.2354 grams. This sample was heated in a solution of nitric acid, which dissolved the manganese producing manganese(III) nitrate [$Mn(NO_3)_3$]. The acidity of the solution was adjusted, and hydrogen sulfide gas was bubbled into the solution producing 0.2876 grams of manganese(III) sulfide [Mn_2S_3]. What is the percentage of manganese in the original sample?

a) 12.41% Mn
b) 6.19% Mn
c) 3.09% Mn
d) 2.34% Mn

Answer: A

10. A sample containing Al_2O_3 and $Na_2Cr_2O_7 \cdot 2H_2O$ was brought into the laboratory for analysis. The analyst heated a 2.2846 gram sample of this material to 100 °C for one hour, at which time only Al_2O_3 and $Na_2Cr_2O_7$ remained. This mixture was found to weigh 2.2312 grams. Calculate the percent chromium in the sample.

a) 6.746% Cr
b) 13.50% Cr
c) 16.97 % Cr
d) 12.56% Cr

Answer: A

11. In the combustion of phthalic acid [$C_6H_4(COOH)_2$], how many moles of water are produced per mole of phthalic acid burned?

a) 6 mol H_2O
b) 3 mol H_2O
c) 4 mol H_2O
d) 2 mol H_2O

Answer: B

12. In gravimetric analysis, the ideal product should be

a) very pure, soluble, and should possess a known composition.
b) very pure, insoluble, easily filterable, and should possess an unknown composition.
c) very pure, insoluble, easily filterable, and should possess a known composition.
d) None of the above

Answer: C

13. In gravimetric analysis,

a) the mass of a solution is used to calculate the quantity of the original analyte.
b) the mass of a product is used to calculate the quantity of the original analyte.
c) the mass of a product is used to calculate the quantity of the impurity.
d) None of the above

Answer: B

Combustion Analysis:

1. A hydrocarbon fuel is fully combusted with 18.214 g of oxygen to yield 23.118 g of carbon dioxide and 4.729 g of water. The calculated empirical formula of the hydrocarbon is:

a) C_4H_3
b) C_3H_7
c) CH
d) C_2H_3

Answer: C

2. After combustion with excess oxygen, a 12.501 g of a petroleum compound produced 38.196 g of carbon dioxide and 18.752 of water. A previous analysis determined that the compound does not contain oxygen. What is the empirical formula of the compound?

a) C_2H_7
b) C_3H_9
c) C_4H_{10}
d) C_5H_{12}

Answer: D

3. In the course of the combustion analysis of an unknown compound containing only carbon, hydrogen H_2, and nitrogen N_2, 12.923 g of carbon dioxide CO_2 and 6.608 g of water were measured. Treatment of the nitrogen with H_2 gas resulted in 2.501 g NH_3. The complete combustion of 11.014 g of the compound needed 10.573 g of oxygen. What the compound's empirical formula?

a) $C_2H_7N_3$
b) $C_3H_7N_5$
c) C_2H_5N
d) $C_5H_3N_7$

Answer: C

4. 12.915 g of a biochemical substance containing only carbon C, hydrogen H_2, and oxygen O_2 was burned in an atmosphere of excess oxygen. Subsequent analysis of the gaseous result yielded 18.942 g carbon dioxide and 7.749 g of water. What is the empirical formula of the substance?

a) CH_2O
b) C_2H_3O
c) C_3H_4O
d) C_5H_3O

Answer: A

5. 33.658 g of oxygen O_2 was used to completely react with a sample of a hydrocarbon in a combustion reaction. The reaction products were 33.057 g of carbon dioxide and 10.816 g of water. What is the empirical formula of the compound?

a) C_3H_4
b) C_5H_8
c) CH
d) CH_3

Answer: B

Chapter 5: Thermochemistry Concepts

Key Concepts

I. Historical Background of Thermochemistry Concepts
II. Basic Concept of Energy
III. Calorimetry Concept
IV. Enthalpy and the First Law of Thermodynamics
V. Application

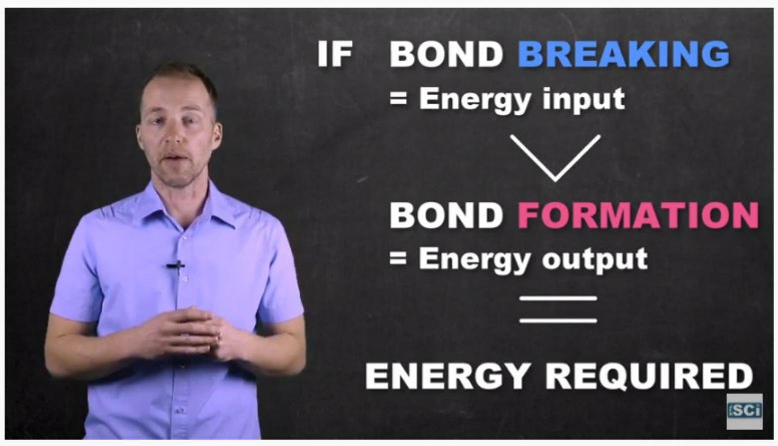
I. Historical Background of Thermochemistry Concepts

Thermochemistry is a branch of thermodynamic. The word thermodynamics came from the Greek who gave the thermodynamics word a meaning of heat power. Thermodynamics applications are around us in science and engineering in particular.
The thermodynamics concepts were developed in the period of 17th century (around 1780) by two French men, one of whom was a chemist (Antoine Laurent Lavoisier) and the other was a mathematician (Pierre Simon de Laplace). Both had realized experimentally that the heat produced in a forward reaction chemical reaction was absorbed by the reverse chemical reaction.

Example: $N_2(g) + 3\,H_2 \leftrightarrow 2\,NH_3(g) + \text{heat}$

The chemical equilibrium above is called a system which also include everything belongs to this chemical equilibrium such as reaction container amount of reactants and products. Anything outside this system is called the surrounding. Both the system (chemical reaction) and the surrounding make the universe around us.

The concepts of thermochemistry is given in a video introduction:



https://www.youtube.com/watch?v=_zXPQYRTrYw

II. Basic Concept of Energy

The concept that we call energy was very slow to develop; it took more than a hundred years just to get people to agree on the definitions of many of the terms we use to describe energy and the interconversion between its various forms. But even now, most people have some difficulty in explaining what it is; somehow, the definition we all learned in elementary science ("the capacity to do work") seems less than adequate to convey its meaning.

Although the term "energy" was not used in science prior to 1802, it had long been suggested that certain properties related to the motions of objects exhibit an endurance which is incorporated into the modern concept of "conservation of energy". René Descartes (1596-1650) stated it explicitly: When God created the world, He "caused some of its parts to push others and to transfer their motions to others..." and thus "He conserves motion".*
In the 17th Century, the great mathematician Gottfried Leibniz (1646-1716) suggested the distinction between vis viva ("live force") and vis mortua ("dead force"), which later became known as kinetic energy (1829) and potential energy (1853).

Kinetic energy and potential energy

https://www.youtube.com/watch?v=OpxGp2P48kI

Whatever energy may be, there are basically two kinds.
Kinetic energy is associated with the motion of an object, and its direct consequences are part of everyone's daily experience; the faster the ball you catch in your hand, and the heavier it is, the more you feel it. Quantitatively, a body with a mass m and moving at a velocity v possesses the kinetic energy *mv*2/2.
Problem Example 1
A rifle shoots a 4.25 g bullet at a velocity of 965 m s–1. What is its kinetic energy?
Solution: The only additional information you need here is that
1 J = 1 kg m2 s–2:
KE = ½ × (.00425 kg) (965 m s–1)2 = 1980 J

Potential energy is energy a body has by virtue of its location. But there is more: the body must be subject to a "restoring force" of some kind that tends to move it to a location of lower potential energy. Think of an arrow that is subjected to the force from a stretched bowstring; the more tightly the arrow is pulled back against the string, the more potential energy it has.

More generally, the restoring force comes from what we call a force field— a gravitational, electrostatic, or magnetic field. We observe the consequences of gravitational potential energy all the time, such as when we walk, but seldom give it any thought.

If an object of mass *m* is raised off the floor to a height *h*, its potential energy increases by *mgh*, where *g* is a proportionality constant known as the *acceleration of gravity*; its value at the earth's surface is 9.8 m s^{-2}.

Problem Example 2

Find the change in potential energy of a 2.6 kg textbook that falls from the 66-cm height of a table top onto the floor.

Solution: PE = m g h = (2.6 kg)(9.8 m s^{-2})(0.66 m) = 16.8 kg m^2 s^{-2} = 16.8 J

Similarly, the potential energy of a particle having an electric charge *q* depends on its location in an electrostatic field.

"Chemical energy"

Electrostatic potential energy plays a major role in chemistry; the potential energies of electrons in the force field created by atomic nuclei lie at the heart of the chemical behavior of atoms and molecules. "Chemical energy" usually refers to the energy that is stored in the chemical bonds of molecules. These bonds form when electrons are able to respond to the force fields created by two or more atomic nuclei, so they can be regarded as manifestations of electrostatic potential energy. In an exothermic chemical reaction, the electrons and nuclei within the reactants undergo rearrangment into products possessing lower energies, and the difference is released to the environment in the form of heat.

Interconversion of potential and kinetic energy

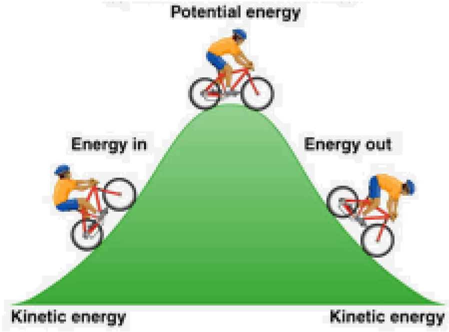
Transitions between potential and kinetic energy are such an intimate part of our daily lives that we hardly give them a thought. It happens in walking as the body moves up and down.

Figure 5.1

Our bodies utilize the chemical energy in glucose to keep us warm and to move our muscles. In fact, life itself depends on the conversion of chemical energy to other forms.

Energy is conserved: it can neither be created nor destroyed. So when you go uphill, your kinetic energy is transformed into potential energy, which gets changed back into kinetic energy as you coast down the other side. And where did the kinetic energy you expended in peddling uphill come from? By conversion of some of the chemical potential energy in your breakfast cereal.

When you drop a book onto the floor, its potential energy is transformed into kinetic energy. When it strikes the floor, this transformation is complete. What happens to the energy then? The kinetic energy that at the moment of impact was formerly situated exclusively in the moving book, now becomes shared between the book and the floor, and in the form of randomized thermal motions of the molecular units of which they are made; we can observe this effect as a rise in temperature.



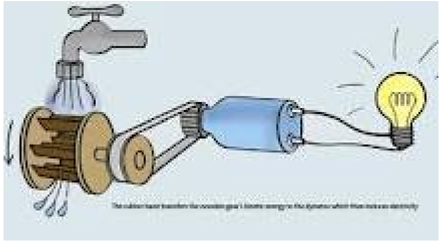


Figure 5.3 Energy Conversions

Figure 5.2 Interconversion between Potential & Kinetic Energy

Much of the potential energy of falling water can be captured by a water wheel or other device that transforms the kinetic energy of the exit water into kinetic energy. The output of a hydroelectric power is directly proportional to its height above the level of the generator turbines in the valley below. At this point, the kinetic energy of the exit water is transferred to that of the turbine, most of which (up to 90 percent in the largest installations) is then converted into electrical energy.
Will the temperature of the water at the bottom of a water fall be greater than that at the top? James Joule himself predicted that it would be. It has been calculated that at Niagra falls, that complete conversion of the potential energy of 1 kg of water at the top into kinetic energy when it hits the plunge pool 58 meters below will result in a temperature increase of about 0.14 C°. (But there are lots of complications. For example, some of the water breaks up into tiny droplets as it falls, and water evaporates from droplets quite rapidly, producing a cooling effect.)
Chemical energy can also be converted, at least partially, into electrical energy: this is what happens in a battery. If a highly exothermic reaction also produces gaseous products, the latter may expand so rapidly that the result is an explosion — a net conversion of chemical energy into kinetic energy (including sound).

Figure 5.4 Conversion of Chemical Energy into other Energy

Thermal energy
Kinetic energy is associated with motion, but in two different ways. For a macroscopic object such as a book or a ball, or a parcel of flowing water, it is simply given by ½ $mv2$.
But as we mentioned above, when an object is dropped onto the floor, or when an exothermic chemical reaction heats surrounding matter, the kinetic energy gets dispersed into the molecular units in the environment. This "microscopic" form of kinetic energy, unlike that of a speeding bullet, is completely random in the kinds of motions it exhibits and in its direction. We refer to this

as "thermalized" kinetic energy, or more commonly simply as *thermal energy*. We observe the effects of this as a rise in the temperature of the surroundings. The temperature of a body is direct measure of the quantity of thermal energy is contains.

Conversion of thermal energy to heat is never completely recoverable

Once kinetic energy is thermalized, only a portion of it can be converted back into potential energy. The remainder simply gets dispersed and diluted into the environment, and is effectively lost.

To summarize, then:

- Potential energy can be converted entirely into kinetic energy..
- Potential energy can also be converted, with varying degrees of efficiency,into electrical energy.
- The kinetic energy of macroscopic objects can be transferred between objects (barring the effects of friction).
- Once kinetic energy becomes thermalized, only a portion of it can be converted back into either potential energy or be concentrated back into the kinetic energy of a macroscopic. This limitation, which has nothing to do with technology but is a fundamental property of nature, is the subject of the second law of thermodynamics.
- A device that is intended to accomplish the partial transformation of thermal energy into organized kinetic energy is known as a *heat engine*.

How molecules take up thermal energy

As noted above, the *heat capacity* of a substance is a measure of how sensitively its temperature is affected by a change in heat content; the greater the heat capacity, the less effect a given flow of heat q will have on the temperature.

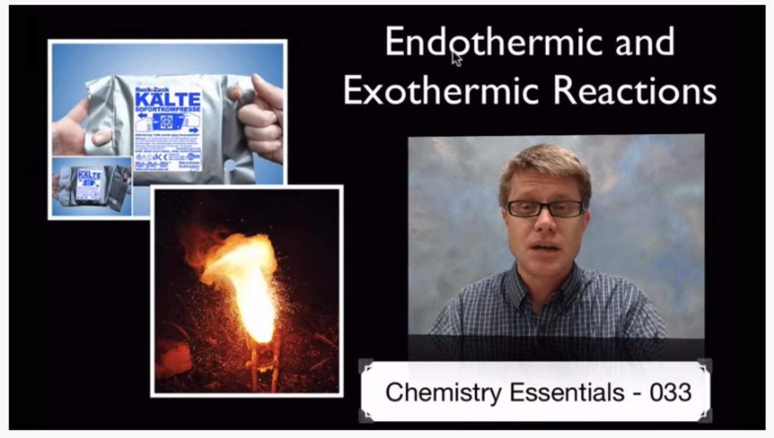
Remember: thermal energy is randomized translational kinetic energy. We also pointed out that *temperature* is a measure of the average kinetic energy due to *translational motions* of molecules. If vibrational or rotational motions are also active, these will also accept thermal energy and reduce the amount that goes into translational motions. Because the temperature depends only on the latter, the effect of the other kinds of motions will be to reduce the dependence of the internal energy on the temperature, thus raising the *heat capacity* of a substance.

Chemical reactions can give heat (thermal energy) to the surrounding during the process of the reactions and said to be **exothermic** chemical reactions. Also chemical reactions need to take in heat from the surrounding for these reactions to progress. Such chemical reactions are said to be **endothermic** chemical reactions.

In general, “**exo**” in Greek means outside and “**endo**” in Greek means inside.

Energy can be utilized from these chemical reactions changes in many applications in the industry and some other applications around us.

The videos below illustrate the exothermic versus endo thermic chemical reactions changes:



https://www.youtube.com/watch?v=L-G7pLufXAo

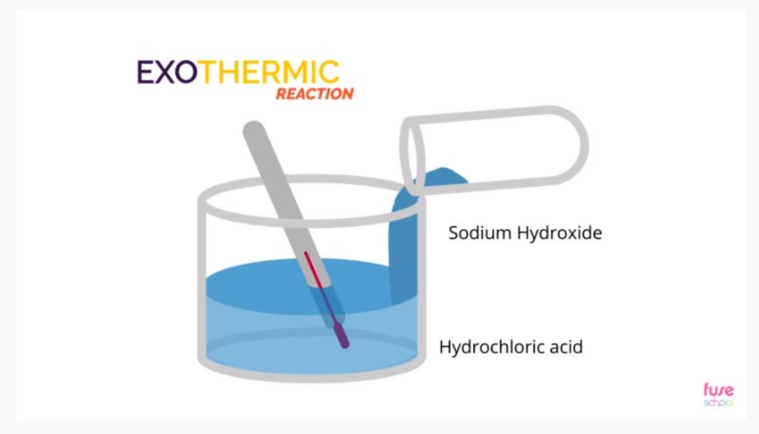
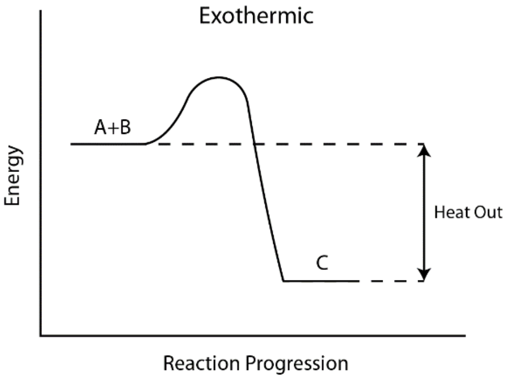
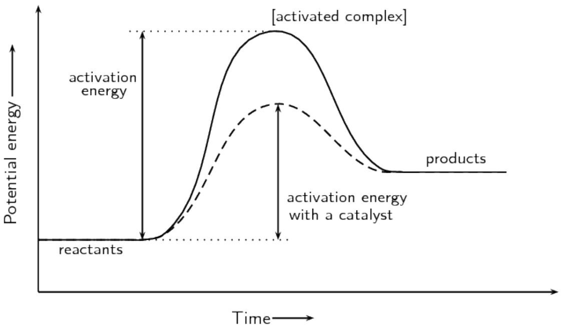


Figure 5.5 Exothermic Reaction
https://www.youtube.com/watch?v=eJXL0IrbtqE

Exothermic and Endothermic Curves:

The chemical reactions changes of exothermic and endothermic reactions can be observed and followed through the curves of exothermic and endothermic reactions as shown below:





Exothermic Reaction **Endothermic Reaction**

Figure 5.6 Energy Diagram for Exo and Endothermic Reaction
Reference: https://commons.wikimedia.org/

The types of energies in the curves (potential energy and activation energy) will be discussed later. In general, in the exothermic chemical reaction or change, energy will be **released** (given away) and in the endothermic chemical reaction or change, energy will be **absorbed** (taken in).

Writing Exothermic and Endothermic Reactions Equations:

Exothermic and Endothermic chemical reactions equations can be written in **three** ways:

Examples:

1. Using the word "Heat".

Exothermic Equation Example:

$C(s) + O_2(g) \rightarrow CO_2(g) + \text{Heat}$

Endothermic Equation Example:

$\text{Heat} + C(s) + H_2O(g) \rightarrow H_2(g) + CO(g)$

2. Using a value instead of the "Heat"

Exothermic Equation Example:

$C(s) + O_2(g) \rightarrow CO_2(g) + 393 \text{ kJ/mole}$
Endothermic Equation Example:

$131 \text{ kJ/mole} + C(s) + H_2O(g) \rightarrow H_2(g) + CO(g)$

3. Using the "Enthalpy Symbol" with negative or positive values to replace the word heat

Exothermic Equation Example:

$C(s) + O_2(g) \rightarrow CO_2(g) \quad \Delta H = - 393 \text{ kJ/mole}$ [Exothermic: Negative Value]

Endothermic Equation Example:

$\text{Heat} + C(s) + H_2O(g) \rightarrow H_2(g) + CO(g) \quad \Delta H = + 131 \text{ kJ/mole}$ [Endothermic: Positive Value]

The term “Enthalpy” will be discussed later.

Exothermic and Endothermic applications examples from around us:

Cold (Ice) pack (endothermic chemical reaction)
Hot pack (exothermic chemical reaction)

Cold (Ice) pack (endothermic chemical reaction)

Figure 5.7 Cold Pack
Ref: www.openstax.org/

Ammonium sold is put inside a large sealed plastic bag. Inside this plastic bag there is another small bag that is sealed and has water in it. As soon as the water containing small bag is punched through, water comes out and start dissolving ammonium nitrate and heat is taken in from the surroundings and the plastic bag will be cold and the reaction is said to be endothermic.
Cold or ice pack is used to cool down pain due to injuries.

The endothermic chemical reaction is given below:

Heat + $NH_4NO_3(s)$ + $H_2O(l)$ ↔ $NH_4(aq)$ + $NO_3^-(aq)$ + $H_2O(l)$ or
25.7 kJ/mole + $NH_4NO_3(s)$ + $H_2O(l)$ ↔ $NH_4(aq)$ + $NO_3^-(aq)$ + $H_2O(l)$ or
$NH_4NO_3(s)$ + $H_2O(l)$ ↔ $NH_4(aq)$ + $NO_3^-(aq)$ + $H_2O(l)$ $\Delta H = +$
25.7 kJ/mole

Hot pack (exothermic chemical reaction)

Calcium chloride is put inside a large sealed plastic bag. Inside this plastic bag there is another small bag that is sealed and has water in it. As soon as the water containing small bag is punched through, water comes out and start dissolving Calcium chloride and heat is given away from the reaction system to the surroundings and the plastic bag will be warmed up and the reaction is said to be exothermic.

Hot pack is used to warm up the surrounding especially it is used in the camping in the winter times.

The exothermic chemical reaction is given below:

$CaCl_2(s) + H_2O(l) \leftrightarrow Ca^{2+}(aq) + 2\ Cl^-(aq) + H_2O(l) + \text{Heat}$ or
$CaCl_2(s) + H_2O(l) \leftrightarrow Ca^{2+}(aq) + 2\ Cl^-(aq) + H_2O(l) + 82.8\ \text{kJ/mole}$ or
$CaCl_2(s) + H_2O(l) \leftrightarrow Ca^{2+}(aq) + 2\ Cl^-(aq) + H_2O(l) \quad \Delta H = -82.8\ \text{kJ/mole}$

Figure 5.8 Hot Pack
Ref: www.openstax.org/

Reference: https://www.youtube.com/watch?v=leonysaMIRo

Heat, Temperature and Thermal Energy:

Heat:

A term is used to describe the transfer the thermal energy between molecules within a system. Heat measures how thermal energy flows, moves or transfer.
It is measured in different systems as follows:
English System: Heat measured in British Thermal Unit (BTU)
Metric System: Calories (cal)
International System (SI): Joules (J)
Note that 1 calorie = 4.184 Joules

Most of our heat in our solar system is taken from the sun (about 90%).

Temperature:

A tool is used to measure the heat. It is measured in different systems as follows:
English System: Fahrenheit (^oF)
Metric System: Centigrade Celsius (^oC)
International System (SI): Kelvin (K)

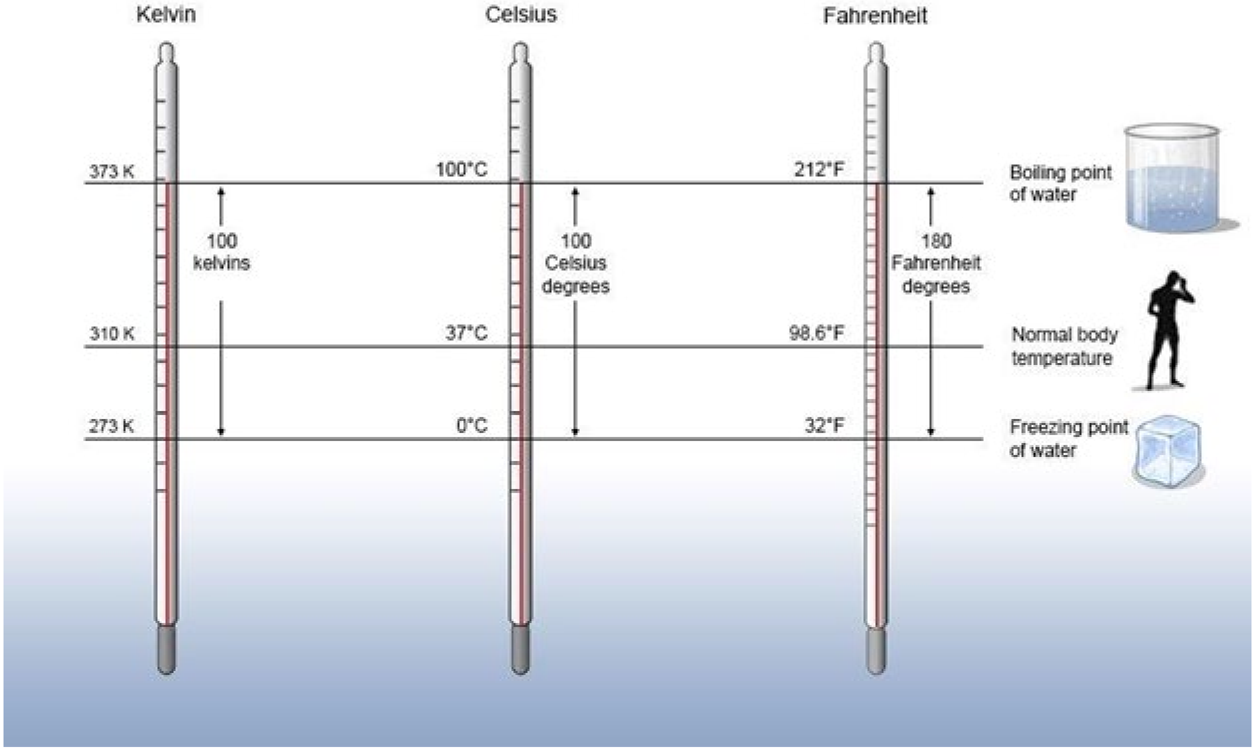
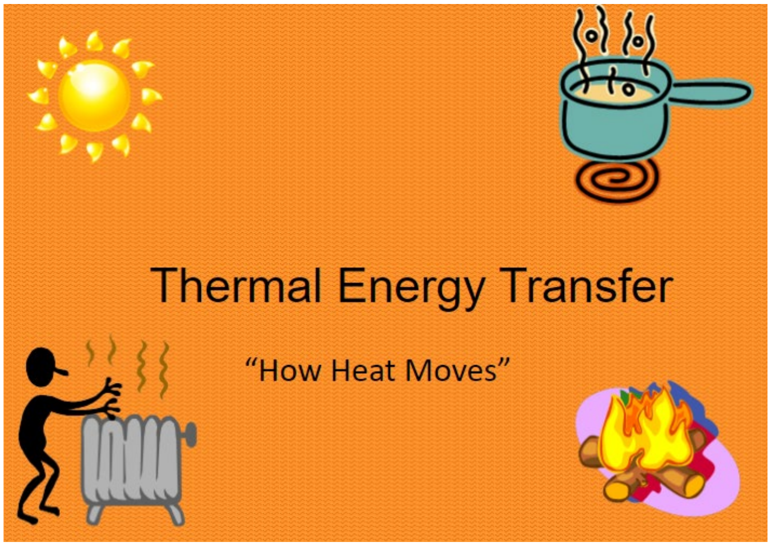


Figure 5.9 Different Scales of Temperature
Reference: https://commons.wikimedia.org/

Thermal Energy:

It is the energy contained within a system and associated with the random motion of atoms and molecules in that system. Such energy is called kinetic energy.

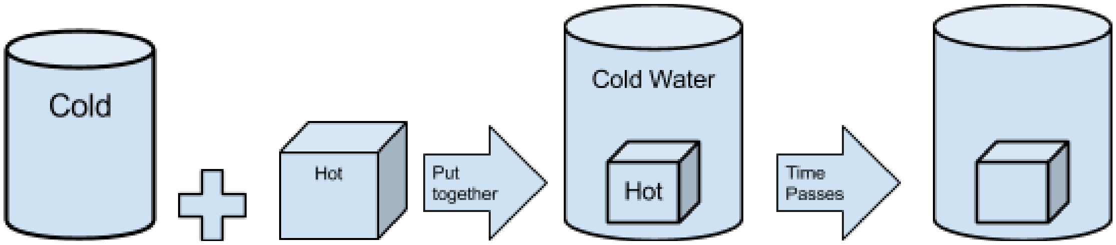
The figure below illustrates the thermal energy concept:



Reference: https://slideplayer.com/slide/8214047/

Heat Transfer:

Heat transfers from hot to cold and never reverse.



The figure above shows this move:

Figure 5.10 Heat & Temperature
Reference: https://phet.colrado.edu

Hot matter expands while cold matter shrinks:

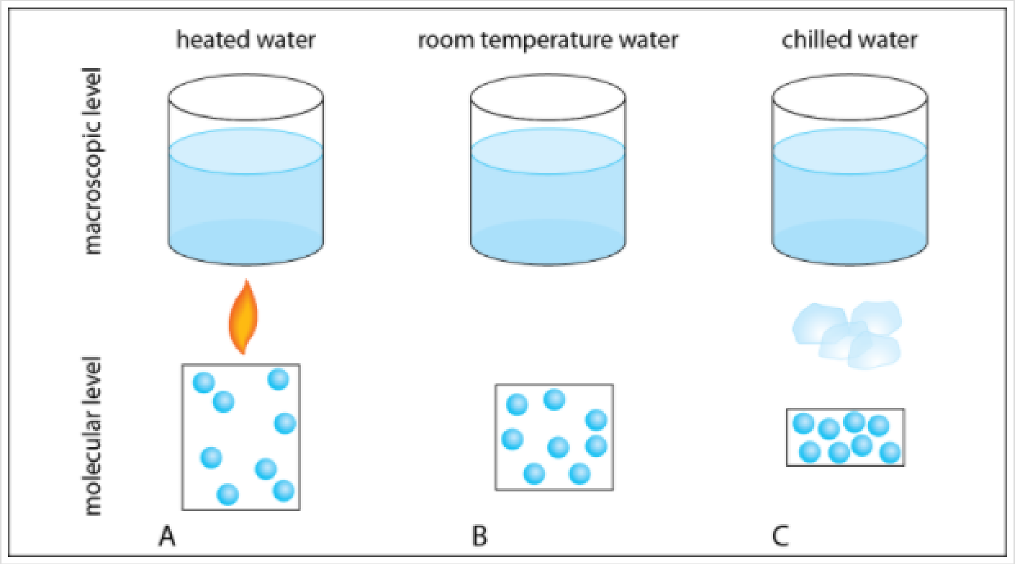


Figure 5.11 Kinetic energy & Temperature

Reference: https://manoa.hawaii.edu/exploringourfluidearth/physical/density-effects/density-temperature-and-salinity/weird-science-macroscopic-changes-liquid-water-volume

The heat transfers from hotter matter to colder matter and at the end of the transfer both matters will attain an equilibrium temperature which is the same for both matters.

The figure below illustrates this phenomena:

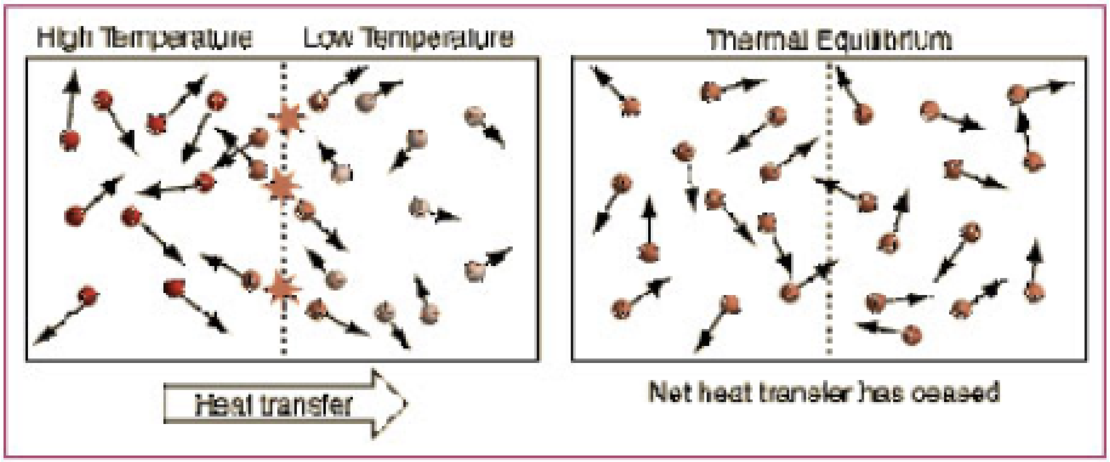


Figure 5.12 Thermal energy Transfer
Reference: https://legacy.etap.org/demo/chem5/instruction5tutor.html

Now we can introduced the concept of heat change and transfer measurements. The heat capacity C of a matter is defined as the heat (energy) q absorbed or released when this matter is exposed to a temperature change ΔT of 1 ^oC or 1 K (Kelvin).

$$C = q / \Delta T$$

Heat capacity C is an **extensive property** of the matter, which means it depends on the amount of the matter.
For example: The heat capacity of 250.0 grams of Iron metal is 10 times higher than the heat capacity of 25.0 grams of the same of Iron.
We expand the formula further by looking at concept of the **specific heat** and the **molar heat capacity** of a matter which is defined as follows:

Specific Heat:

$$c = q / m \Delta T \qquad \text{and} \qquad q = m c \Delta T$$

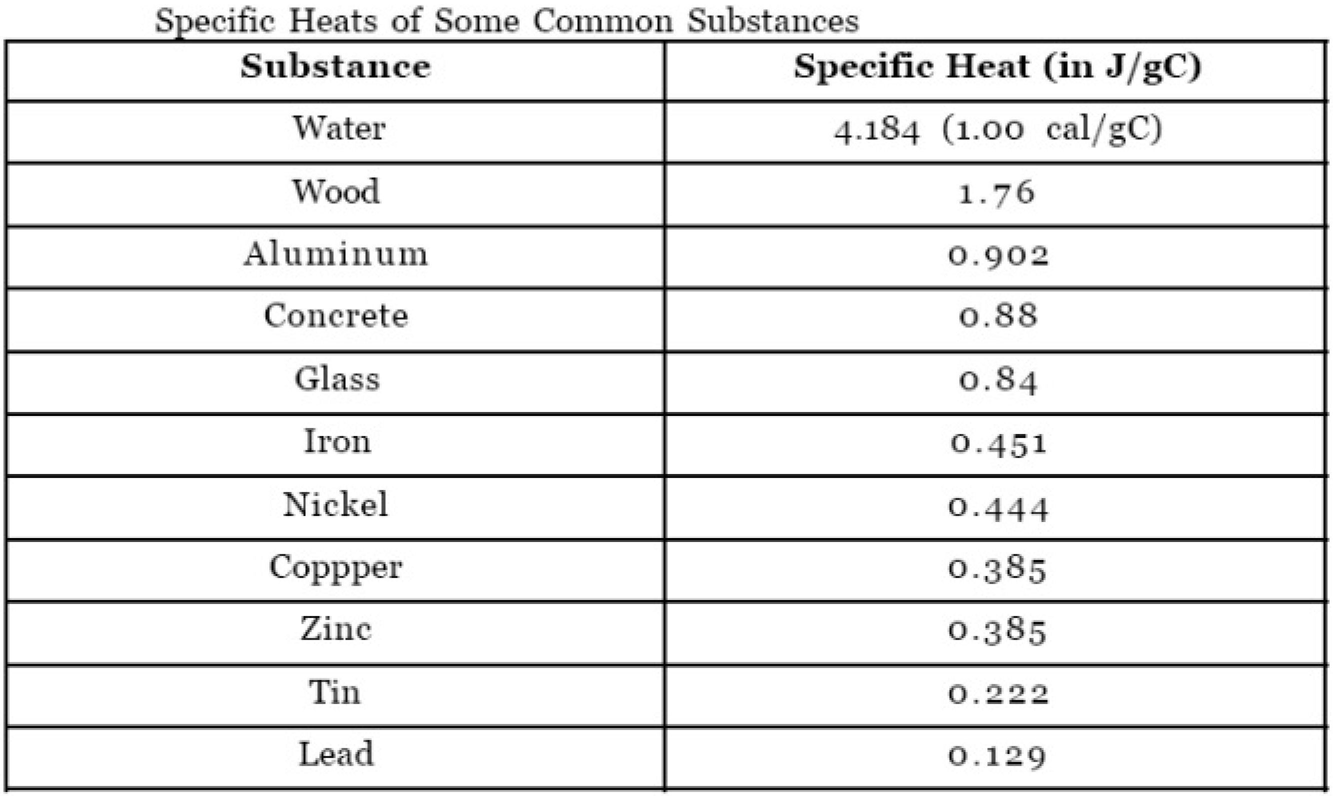
Where:

c = specific heat
q = heat
ΔT = temperature change
m = mass of the matter

The specific heat c is defined as the amount of energy needed to raise the temperature of 1.0 gram of a matter 1.0 degree (1.0 ^oC or 1 K). The unit of the specific heat is cal / g x ^oC or 4.184 J / g x ^oC. The specific heat is an intensive property of the matter which means it does not depend on the amount of the matter.

Example: the specific heat of 100.0 grams aluminum metal is equal to the specific heat of 10.0 grams of the same aluminum metal which is in both cases 0.2156 cal / g x ^{o}C or 0.902 J / g x ^{o}C

Example of the Specific Heats for some substances is given below:



Specific Heats of Some Common Substances

Substance	Specific Heat (in J/gC)
Water	4.184 (1.00 cal/gC)
Wood	1.76
Aluminum	0.902
Concrete	0.88
Glass	0.84
Iron	0.451
Nickel	0.444
Coppper	0.385
Zinc	0.385
Tin	0.222
Lead	0.129

Reference: file:///C:/Users/matteya/Downloads/Metal%20HeatLAB.pdf

Molar Heat Capacity:

From its name "molar", one will think that the mole of matter is involved. This is true and molar heat capacity is defined as:

$\mathbf{C_n = q / n \Delta T}$ **and** $\mathbf{q = n c_n \Delta T}$

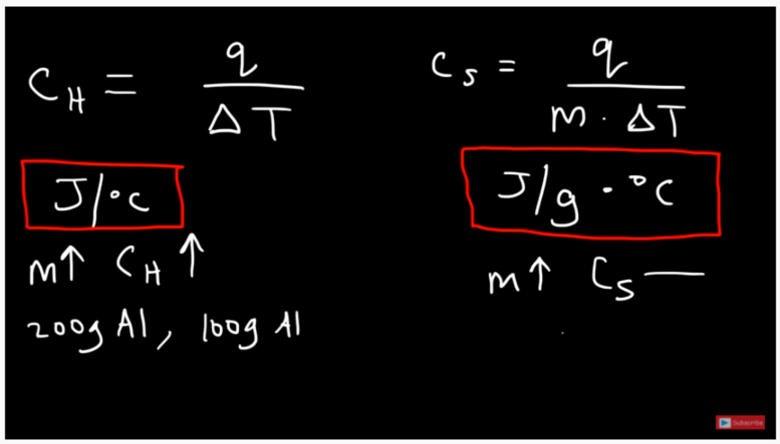
Where:

$\mathbf{C_n}$ = molar heat capacity
q = heat
ΔT = temperature change
n = number of moles of the matter

The molar heat capacity c_n is defined as the amount of energy needed to raise the temperature of 1.0 mole of a matter 1.0 degree (1.0 ^{o}C or 1 K). The unit of the molar heat is cal / mole x ^{o}C or 4.184 J / mole x ^{o}C.

The molar heat is an intensive property of the matter which means it does not depend on the amount of the matter.
Example: the molar heat of 100.0 moles aluminum metal is equal to the molar heat of 10.0 moles of the same aluminum metal which is in both cases 5.808 cal / mole x °C or 24.3 J / mole x °C

The videos below explain the terms of heat capacity, the specific heat of capacity and the molar heat capacity:



$C_H = \frac{q}{\Delta T}$

$\boxed{J/°C}$

m↑ C_H ↑

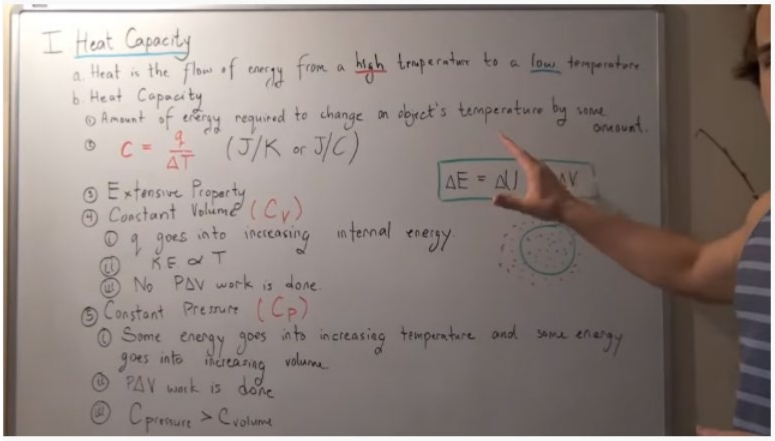
200g Al, 100g Al

$C_s = \frac{q}{m \cdot \Delta T}$

$\boxed{J/g \cdot °C}$

m↑ C_s —

https://www.youtube.com/watch?v=IoHXMaiwT80



I Heat Capacity

a. Heat is the flow of energy from a high temperature to a low temperature

b. Heat Capacity

① Amount of energy required to change an object's temperature by some amount.

② $C = \frac{q}{\Delta T}$ (J/K or J/C)

③ Extensive Property

④ Constant Volume (C_V)

(i) q goes into increasing internal energy

(ii) KE ∝ T

(iii) No PΔV work is done.

⑤ Constant Pressure (C_P)

(i) Some energy goes into increasing temperature and some energy goes into increasing volume

(ii) PΔV work is done

(iii) $C_{pressure} > C_{volume}$

https://www.youtube.com/watch?v=utyMTIPTumM

Heat Calculations Examples

1. How much heat in kilojoules has to be removed from 250.0 g of water to lower its temperature from 55.0 °C to 25.0 °C?

$$c = q / m\Delta T$$

c = specific heat of water = 1 cal /g x ^{o}C = 4.184 J / g x ^{o}C

q = m c ΔT = [250.0 g x 4.184 J /g x ^{o}C] x [55.0 – 25.0] ^{o}C = 31380 J = 31.380 kJ = 31.4 kJ

2. Calculate the mass of water that gives heat of 585.0 kilojoules when its temperature is decreased from 83.50 ^{o}C to 13.50 ^{o}C?

c = q / m ΔT

m = q/ c ΔT

c = specific heat of water = 1 cal /g x ^{o}C = 4.184 J / g x ^{o}C

m = [585.0 x 10^{3} J] / [4.184 J /g x ^{o}C] x [70.00 ^{o}C] = 1997 g

3. 25.0 g of mercury is heated from 25°C to 155°C, and absorbs 455 Joules of heat in the process. Calculate the specific heat capacity of mercury

c = q / m ΔT

c = [455 J] / [25.0 g] x[155 – 25] ^{o}C = 0.14 J / g x ^{o}C

4. What is the specific heat capacity of silver metal if 55.00 g of the metal absorbs 47.3 **calories** of heat and the temperature rises 15.0°C?
c = q / m ΔT

c = [47.3 cal] / [55.00 g] x [15.0 ^{o}C] = 0.0573 cal / g x ^{o}C

5. If a sample of chloroform is initially at 25.0 °C, what is its final temperature if 150.0 g of chloroform absorbs 1.00 kilojoules of heat, and the specific heat of chloroform is 0.960 J / g x °C?

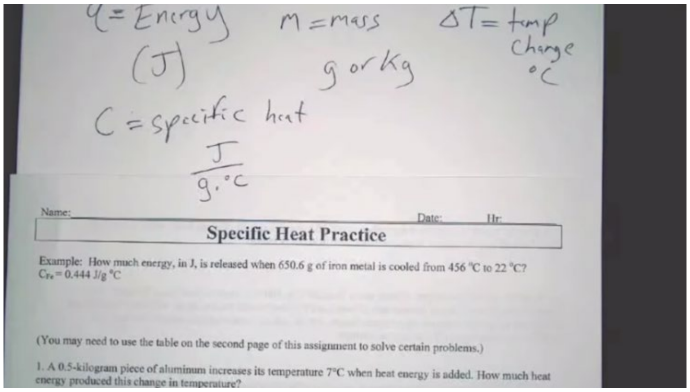
c = q / m ΔT

ΔT = q / m x c

ΔT = [1.00 x 10^{3} J] / [150.0 g] x [0.960 J / g x °C] = 6.944 °C

ΔT = T(final) - T(initial) = 6.044 °C = T(final) - 25.0 °C = 31.9 °C

The video below goes over some examples:



q = Energy (J)

m = mass g or kg

ΔT = temp Change °C

C = specific heat $\frac{J}{g \cdot °C}$

Name: Date: Hr:

Specific Heat Practice

Example: How much energy, in J, is released when 650.6 g of iron metal is cooled from 456 °C to 22 °C? C_{Fe} = 0.444 J/g °C

(You may need to use the table on the second page of this assignment to solve certain problems.)

1. A 0.5-kilogram piece of aluminum increases its temperature 7°C when heat energy is added. How much heat energy produced this change in temperature?

Reference: https://www.youtube.com/watch?v=4RkDJDDnIss

III. Calorimetry Concept

Calorimetry

Calorimetry is a method by which heat transfer into and out the system during the chemical reactions (combustion reactions for example) is measured. In this process the heat transfer is calibrated with the calibrated object. The temperature change in the process is used to calculate the heat transferred. This calculation needs to be specific based on surrounding and system definitions.
System: the chemical compound which is undergoing chemical reaction.
Surrounding: the calorimeter with ALL its components including the equipment that measures the heat.

Calorimeter:

Calorimeter is a tool or equipment used to measure the heat absorbed (endothermic: temperature will decrease) or given away by (exothermic: temperature will increase) during a chemical reaction. There are five types of calorimeters in use:

There are 2 major types of calorimeters:

1. **Adiabatic Calorimeters**
2. **Reactions Calorimeters**

1. Adiabatic Calorimeters:

These types of Calorimeters are used to measure the enthalpy change in a system, during physical processes such as crystallization, mixing, dilution etc. These calorimeters do not exchange heat with the surround and function at zero heat exchange conditions also known as adiabatic conditions.
The video below illustrates the function of the adiabatic calorimeter:

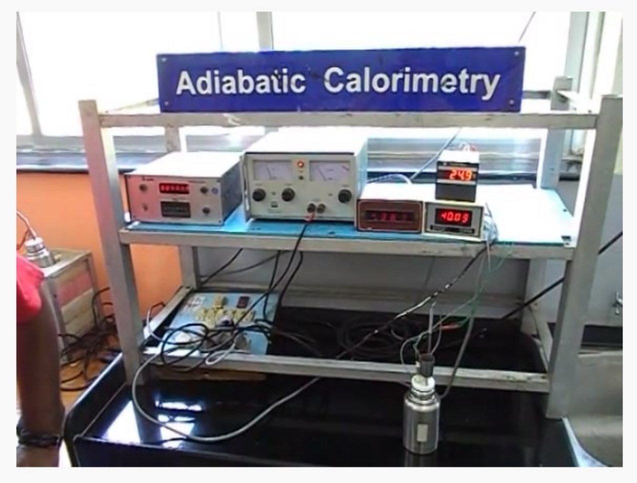


Figure 5.13 Adiabatic Calorimeter

Reference: https://www.youtube.com/watch?v=44X1z0_snIY

2. **Reactions Calorimeters**

There are several reactions calorimeter available in the market and in the universities and colleges

These calorimeters measure the heat exchange or transfer in exothermic and endothermic reactions. The reactions calorimeters can measure chemical or physical reactions or changes.

Types of Reactions Calorimeters:

4 types of reactions calorimeters are available

Heat-flow,

Heat-balance,

Constant flux

Power compensation

Detailed functionalities regarding these types can be read at:
https://www.azosensors.com/article.aspx?ArticleID=798#:~:text=There%20are%20traditionally%20four%20types,is%20occurring%20during%20the%20reaction.

Heat Flow Calorimeters examples are given below:

A. Foam Cup Calorimeter:

This type of calorimeter is used mostly at undergraduate physics and chemistry labs because it cheap and easy to use and has reasonable % error (but not very accurate). The two figures below show the setup of this foam cup calorimeter.

Inside the thermometer is specific amount of water with specific volume (using the density of water this volume is converted into mass of water). A weighed metal of liquid solution is warmed up to 50^{o}C to 60^{o}C and then immediately transferred into the foam cup (calorimeter) and the temperature is followed till there is no rise in the temperature and an equilibrium temperature of the system is attained.

Foam cup calorimeter

Figure 5.14 Styrofoam Cup Calometer

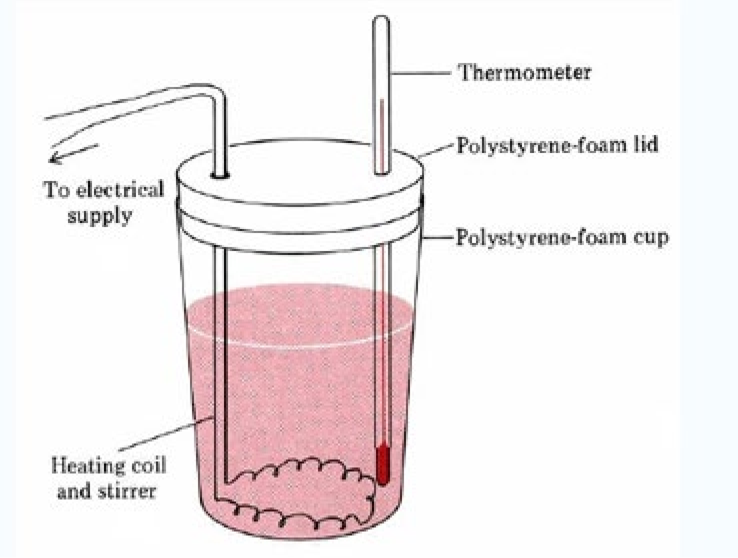


Figure 5.15 Coffee Cup Calorimeter Diagram

Figure 1
Reference: https://commons.wikimedia.org/wiki/File:Coffee_cup_calorimeter_pic.jpg
Figure 2
Reference:http://wiki.chemprime.chemeddl.org/articles/a/_/c/File~A_Coffee_Cup_Calorimeter_.jpg_6993.html

B. Bomb Calorimeter:

This type of calorimeter is used in commercial applications as well as in research labs at the universities and special institutes. Bomb calorimeter is used to measure the heat of combustion reaction. It uses stainless steel combustion reaction chamber with the presence of oxygen. Immediately after the combustion reaction occurs which is assisted with an electrical current goes through the samples to ignite for few seconds, the heat is transferred to the water which is contained in outer sealed mantel of the combustion chapter. The heat will warm up the water and the temperature is monitored and recorded and the heat of the combustion is calculated.

Bomb Calorimeter

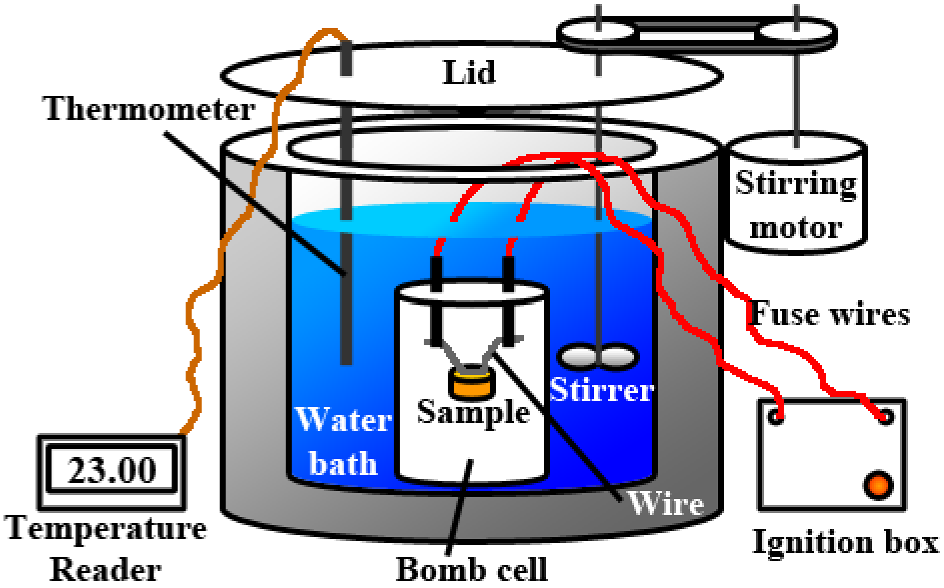
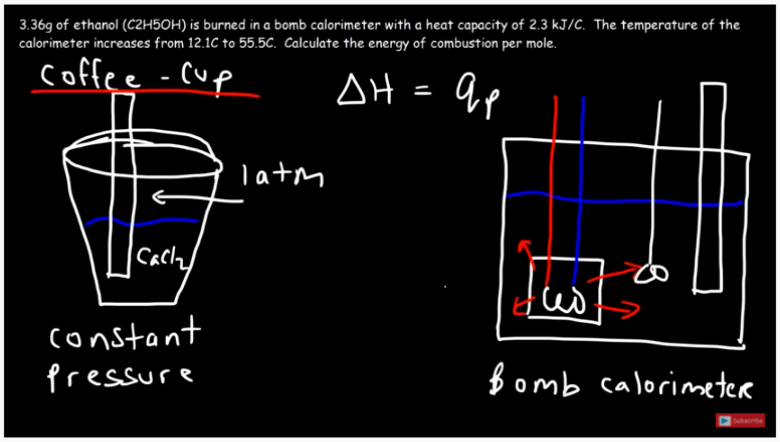
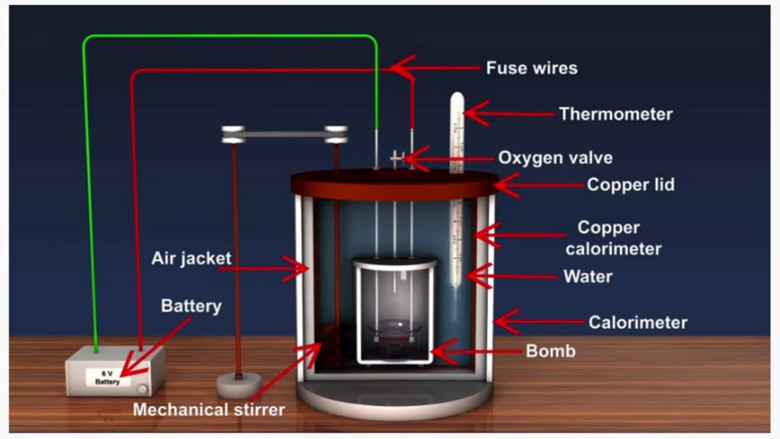


Figure 5.16 Bomb Calorimeter
Reference: https://commons.wikimedia.org/wiki/File:Bomb_Calorimeter_Diagram.png

The videos below illustrates the bomb calorimeter concept:


3.36g of ethanol (C2H5OH) is burned in a bomb calorimeter with a heat capacity of 2.3 kJ/C. The temperature of the calorimeter increases from 12.1C to 55.5C. Calculate the energy of combustion per mole.

https://www.youtube.com/watch?v=F2cMvNDRqQA

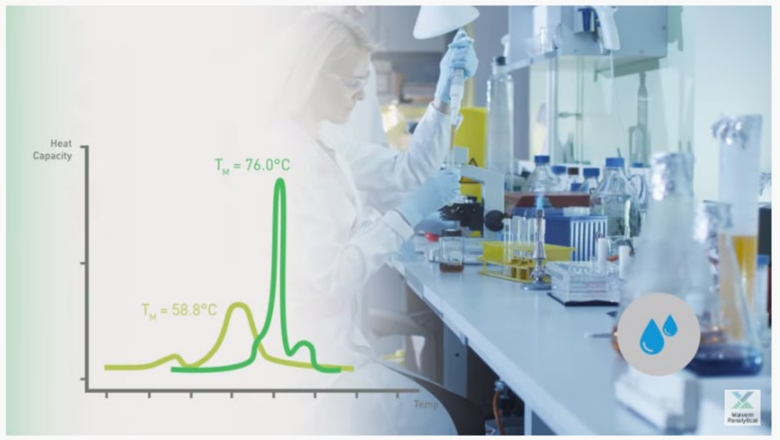


Reference: https://www.youtube.com/watch?v=wwJG2JVg6qM

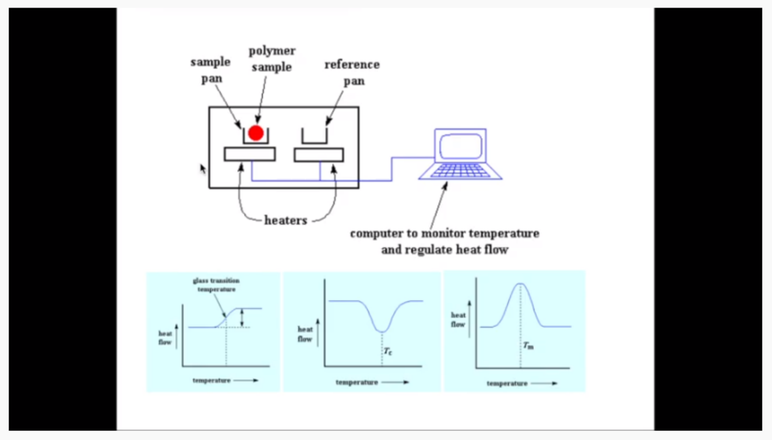
C. Differential Scanning Calorimeter:

This type of calorimeter is used to test the physical properties of plastics, polymers, monomers and elastomers. This calorimeter deals with the thermal analysis technique in the research and quality control. The calorimeter monitors the product analysis at different range of temperatures and heat changes which facilitates the study of the chemical properties of the sample within its heat capacity.

The videos below illustrate the concept of the Differential Scanning Calorimeter:



https://www.youtube.com/watch?v=2CU3uvjKXlk



https://www.youtube.com/watch?v=yI0NgffmLeI

D. Solution Calorimeter:

This type of calorimeter is used to measure the heat of solution of dissolving a solid compound in in a liquid solution. Also the heat of solution can be called the heat of dilution when dissolving a liquid solution in another liquid solution.

The videos below illustrate the concept of the Solution Calorimeter:

Figure 5.18 Solution Calorimeter

https://www.youtube.com/watch?v=HnYZh69HJqU

https://www.youtube.com/watch?v=dpmr0665FFA

The **ice calorimeter** is an important tool for measuring the heat capacities of liquids and solids, as well as the heats of certain reactions. This simple yet ingenious apparatus is essentially a device for measuring the change in volume due to melting of ice. To measure a heat capacity, a warm sample is placed in the inner compartment, which is surrounded by a mixture of ice and water.

The heat withdrawn from the sample as it cools causes some of the ice to melt. Since ice is less dense than water, the volume of water in the insulated chamber decreases. This causes an equivalent volume of mercury to be sucked into the inner reservoir from the outside container. The loss in weight of this container gives the decrease in volume of the water, and thus the mass of ice melted. This, combined with the heat of fusion of ice, gives the quantity of heat lost by the sample as it cools to 0°C.

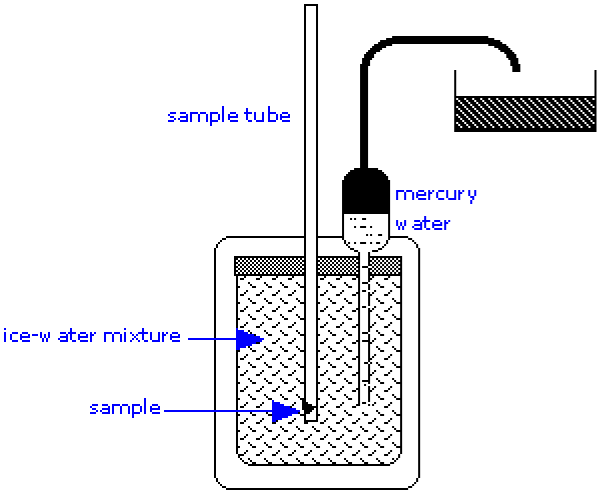


Figure 5.19 Ice Calorimeter

The Heat of Solution, Heat of Dilution and Heat Neutralization as well as Specific Heat Calculations using Heat Flow Calorimeters:

The temperature is followed till there is no rise in the temperature and an equilibrium temperature of the system is attained.
Then general formula is: (at thermal equilibrium at the end of reaction or solution or dilution).

q(compound A) + q(compound B) = 0

q(compound A) = - q(compound B)

-Heat is lost by compound A = Heat is gained by compound B

The heat flow is from A → B

Examples:

Heat transfer or exchange between two substances (similar to the foam cup calorimeter).

1. A piece of metal weighing 59.047 g was heated to 100.0 °C and then put it into 100.0 mL of water (initially at 23.7 °C). The metal and water were allowed to come to an equilibrium temperature, determined to be 27.8 °C. Assuming no heat lost to the environment, calculate the specific heat of the metal.

-Heat is lost by the metal = Heat is gained by water

-mass$_{(metal)}$ x c$_{(metal)}$ x ΔT$_{(metal)}$ = mass$_{(water)}$ x c$_{(water)}$ x ΔT$_{(water)}$

-[59.047 g] x c$_{(metal)}$ x [100 ^{o}C – 27.8 ^{o}C] = [100.0 mL x 1.00 g / mL] x [4.184 J / (g x ^{o}C)] x [27.8 ^{o}C – 23.7 ^{o}C]

[59.047 g] x c$_{(metal)}$ x [100 ^{o}C – 27.8 ^{o}C] = 1713.8 J
c$_{(metal)}$ = [1713.8 J] / { [59.047 g] x [100 ^{o}C – 27.8 ^{o}C] } = **0.402 J/g x ^{o}C**

2. In a coffee-cup calorimeter, 100.0 g of H_2O and 100.0 mL of HCl are mixed. The HCl had an initial temperature of 44.6 ^{o}C and the water was originally at 24.6 ^{o}C. After the reaction, the temperature of both substances is 31.3 ^{o}C.

A) Was the reaction exothermic or endothermic? Explain.

For the water- endothermic. The temperature increased from 24.6 ^{o}C to 31.3 ^{o}C indicating energy was absorbed by the water.
For the HCl- exothermic. The temperature decreased from 44.6 ^{o}C to 31.3 ^{o}C indicating energy was released by the HCl.

B) Calculate how much heat the water lost or gained.

q$_{(water)}$ = mass$_{(water)}$ x c$_{(water)}$ x ΔT$_{(water)}$ = [100.0 g] x [4.184 J / (g x ^{o}C)] x [31.3 ^{o}C – 24.6 ^{o}C] =

q$_{(water)}$ = 2803.3 J = **2.80 x 10^{3} J = 2.80 kJ**

3. What is the final temperature after 840.0 Joules is absorbed by 10.0g of water at 25.0°C?

$q_{(water)} = mass_{(water)}$ x $c_{(water)}$ x $\Delta T_{(water)}$
840.0 J = [10.0 g] x [4.184 J / (g x °C)] x $\Delta T_{(water)}$
$\Delta T_{(water)}$ = [[840.0 J] / { [10.0 g] x [4.184 J / (g x °C)] = 20.1 °C
$T_{(Final)}$ = 25.0 + 20.1 = **45.1 °C**

4. A 0.88 g gummy bear is burned in a bomb calorimeter. The temperature started at 21.5 °C and leveled off at 24.2 °C. The manufacturer of the bomb calorimeter determined the heat capacity of the calorimeter to be 11.4 kJ/°C. Calculate the heat of combustion per gram of gummy bear.

q = $c_{(calorimeter)}$ ΔT = [11.4 kJ/°C] x [24.2-21.5 °C] = [11.4 kJ/°C)(2.7 °C] = 30.78 kJ
(30.78 kJ) / (0.88 g) = **34.98 kJ / g**

5. A piece of metal weighing 85.5 g was heated to 100.0 °C and then put it into 100.0 mL of water (initially at 23.7 °C). The metal and water were allowed to come to an equilibrium temperature, calculate this final temperature (the equilibrium temperature) if the specific heat of the piece of the metal is 0.350 J / (g x °C)

-Heat is lost by the metal = Heat is gained by water
-$mass_{(metal)}$ x $c_{(metal)}$ x $\Delta T_{(metal)}$ = $mass_{(water)}$ x $c_{(water)}$ x $\Delta T_{(water)}$
[85.5 g] x [0.350 J / (g x °C)] x [$T_{(final)} - T_{(initial\ metal)}$] = - [100.0 mL x 1.00 (g / mL)] x [4.184 J / (g x °C)] x [$T_{(final)} - T_{(initial\ water)}$]

[29.925 / °C] x [$T_{(final)}$ – 100.0 °C] = - [418.4 / °C] x [$T_{(final)}$ – 23.7 °C]
29.925 $T_{(final)}$ - 2992.5 = - 418.4 $T_{(final)}$ + 23.7]
29.925 $T_{(final)}$ + 418.4 $T_{(final)}$ = 23.7 + 2992.5 = 3016.2
448.325 $T_{(final)}$ = 3016.2
$T_{(final)}$ = [3016.2 / 448.325] = 6.7277 °C = **6.73 °C**

6. A 0.258 g piece of potassium nitrate solid is placed into water inside of a coffee cup calorimeter resulting in a vigorous reaction. Assume a total volume of 100 mL for the resulting solution. The temperature of the solution changes from 22 °C to 25.1 °C due to the reaction. How much heat is generated per gram of potassium for this reaction? Assume the density of the solution after the reaction is the density of water and that the heat capacity of the solution and reaction vessel is only due to the water that has a specific heat of 4.184 J/ (g x °C).

-Heat is lost by the metal = Heat is gained by water

q = m x $c_{(solution)}$ x $\Delta T_{(solution)}$ = [100 g] x [(4.184 J/g-°C)] x [25.1 °C - 22 °C] = 1297 J
q = m x $c_{(solution)}$ x $\Delta T_{(solution)}$ = [100 g] x [(4.184 J/g-°C)] x [3.1 °C]
q = (1297 J)/(0.258 g) = **5027 J/ g**

7. 25.0 mL of 0.15 M HCl is neutralized with 30.0 mL of 0.25 M inside a foam cup calorimeter.

Both acid and base were initially at 23.5 °C when they were added to the foam cup calorimeter. The final temperature recorded for this neutralization is 26.5 °C. Calculate the heat of neutralization reaction.

$HCl(aq) + NaOH(aq) \longrightarrow NaCl(aq) + H_2O(l)$

The heat taken by the solution = -heat given off by reaction

$$-q_{(solution)} = q_{(reaction)} = q_{(neutralization)}$$

$$q_{(solution)} = m \times c_{(solution)} \times \Delta T$$

a. Assume that the specific heat of reaction equals the specific heat of water (water is the solvent for both acid and base).
b. Furthermore, the density of the solution is assumed to be the density of water 1.00 g / mL

The total volume of the solution = Volume of HCl + Volume of NaOH = 25.0 mL + 30.0 mL = 55.0 mL

c. Mass of solution = [55.0 mL x 1.00 g / mL] = 55.0 g
d. ΔT = [26.5 °C – 23.5 °C] = 3.0 °C

$q_{(solution)} = q_{(neutralization)}$ = [55.0 g] x [[4.184 J/ (g x °C)] x [3.0 °C] = 690.36 J = **690 J**

8. A 1.5 kg block of Ni at 100 °C is placed into 500 mL of water that has a temperature of 21 °C. What is the final temperature assuming the specific heat of Ni is 0.44 J/g-°C and the specific heat of water is 4.184 J/g-°C. Hint: the total heat lost is equal to the total heat gained

Heat is lost by the Ni metal = - Heat is gained by water

$q_{(metal)} = - q_{(water)}$

[1500 g Ni] x [0.44 J / g x °C] x [100 °C - T_f] = [500 mL x 1g/1mL] x [4.184 J / g x °C] x [T_f - 21 °C]

Re-arranging:

T_f = 40 °C

9. 25.6 g of ethanol was combusted in a bomb calorimeter and the heat obtained is that has a heat of 6.53 kJ . The initial temperature of the combustion was at 24.0 °C. Find its final temperature.

$C_2H_5OH + 3\ O_2 \longrightarrow 2\ CO_2 + 3\ H_2O$

-Heat is lost by the Ni metal = Heat is gained by water

$-q_{(ethanol)} = q_{(water)} = q_{(heat\ of\ reaction)} = q_{(combustion)} = m \times c_{(ethanol)} \times \Delta T$

Assuming the specific heat is equal to heat of water = 4.184 J / g x °C

6.53 kJ = 6.53 x 1000 J = - [25.6 g] x [4.184 J / g x °C] x [$T_{(final)}$ - $T_{(initial)}$]

6.53 kJ = 6.53 x 1000 J = - [107 J / °C] x [[$T_{(final)}$ - 24.0 °C]

6.53 x 1000 J = [(107 J / °C)] $T_{(final)}$ + 2568 J = (107 J / °C) $T_{(final)}$ + 2568 J

6.53 x 1000 J - 2568 J = [(107 J / °C)] $T_{(final}$

3962 J = (107 J / / °C) $T_{(final)}$

$T_{(final)}$ = 37.0 °C

10. When a 100. g sample of methane, CH_4, is burned in a bomb calorimeter the temperature changes from 21.0 °C to 31.0 °C and 2200. J of heat is given off. What is the specific heat of methane?

$q_{(combustion)} = m \text{ x } c \text{ x } \Delta T$

$c = q_{(combustion)} \ / \ m \text{ x } \Delta T = [2200 \text{ J}] \text{ x } / \ [100. \text{ g x } 10.0 \text{ °C}]$
Specific heat = $q_{(combustion)} \ / \ m \text{ x } \Delta T$ = [2200. J / °C] x / [100. g] = **2.20 J / g x °C**

11. When 3.12 g of glucose, $C_6H_{12}O_6$, is burned in a bomb calorimeter, the temperature of the calorimeter increases from 23.8 °C to 35.6 °C. The calorimeter contains 775 g of water, and the bomb itself has a heat capacity of 893 J/°C. How much heat was produced by the combustion of the glucose sample?

The heat produced by the reaction is absorbed by the water and the bomb:
qrxn = −(qwater + qbomb)

qwater = [775 g] x [(4.184 J / g x °C)] x [35.6 °C – 23.8 °C] = 38262.68 J
qbomb = [893 J / °C] x [35.6 °C – 23.8 °C] = 10537.4 J

Add both (qwater + qbomb) = 48.8 J
This reaction released 48.8 kJ of heat when 3.12 g of glucose was burned.

The following activity has been taken from Chemcollective.org

http://chemcollective.org/activities/autograded/115

Activity:

Coffee

During the summer after your first year at Carnegie Mellon, you are lucky enough to get a job making coffee at Starbucks, but you tell your parents and friends that you have secured a lucrative position as a "java engineer." An eccentric chemistry professor (not mentioning any names) stops in every day and orders 250ml of Sumatran coffee at precisely 75.0°C. You then need to add enough milk at 5.00°C to drop the temperature of the coffee, initially at 80.0°C, to the ordered temperature.

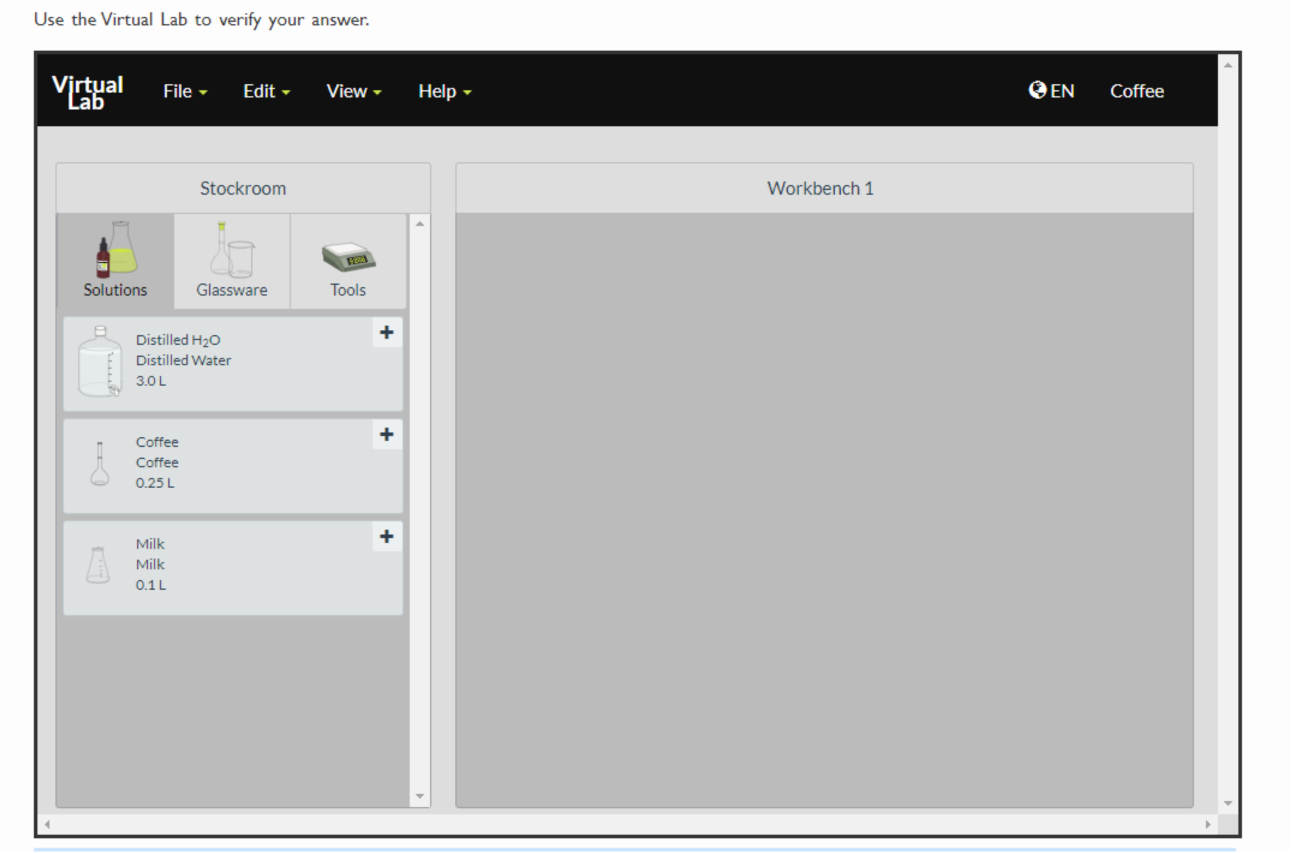
Calculate the amount of milk (in ml) you must add to reach this temperature. Show all your work in the provided spaces.

In order to simplify the calculations, you will start by assuming that milk and coffee have the specific heat and density as if water. In the following parts, you will remove these simplifications. Solve now this problem assuming the density is 1.000 g/ml for milk and coffee and their specific heat capacity is 4.184 J/(g °C).

Hint: the coffee is in an insulated travel mug, so no heat escapes. To insulate a piece of glassware in Virtual Lab, Mac-users should command-click (or open-apple click) on the beaker or flask;

Windows users should right click on the beaker or flask. From the menu that appears choose “Thermal Properties.” Check the box labeled “insulated from surroundings.” The temperature of the solution in that beaker or flask will remain constant.

Use the Virtual Lab to verify your answer.



Use the Virtual Lab to verify your answer.

IV. First Law of Thermodynamics & Enthalpy

First Law of Thermodynamics

Heat & Work

Heat and work are both measured in energy units, so they must both represent energy. How do they differ from each other, and from just plain “energy” itself?
Heat and work are processes and cannot be stored

In our daily language, we often say that "this object contains a lot of heat", but this kind of talk is a no-no in thermodynamics! It's ok to say that the object is "hot", meaning that its temperature is high.

The term "heat" has a special meaning in thermodynamics: it is a process in which a body (the contents of a tea kettle, for example) acquires or loses energy as a direct consequence of its having a different temperature than its surroundings (the rest of the world).

Figure 5.20 Transfer of Heat

Thermal energy can only flow from a higher temperature to a lower temperature. It is this flow that constitutes "heat".
Use of the term "flow" of heat recalls the 18th-century notion that heat is an actual substance called "caloric" that could flow like a liquid.
Heat is the transfer of energy by conduction or radiation
Transfer of thermal energy can be accomplished by bringing two bodies into physical contact (the kettle on top of the stove, or through an electric heating element inside the kettle). Another mechanism of thermal energy transfer is by radiation; a hot object will convey energy to any body in sight of it via electromagnetic radiation in the infrared part of the spectrum. In many cases, a combination of modes will be active:
Thus when you place a can of beer in the refrigerator, both processes are operative: the can radiates heat to the cold surfaces around it, and absorbs it by direct conduction from the ambient air.

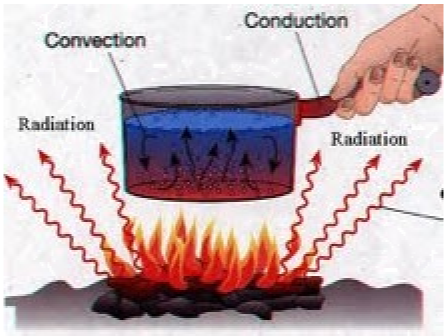


Figure 5.21 Different Methods of Heat Transfer

So what is work?
Work refers to the transfer of energy some means that does not depend on temperature difference.

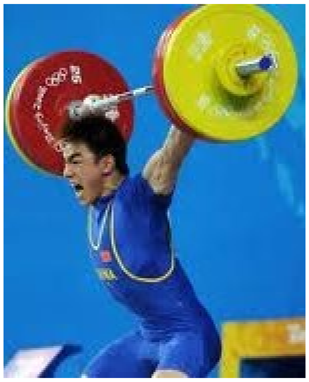


Figure 5.22 Work Done by system

Work, like energy, can take various forms, the most familiar being mechanical and electrical. Mechanical work arises when an object moves a distance Δx against an opposing force f: $w = f\Delta x$ N-m; 1 N-m = 1 J.
[image from Ben Wiens Energy site]

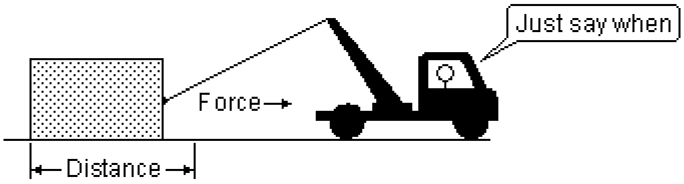


Figure 5.23 Work Done by Force

Electrical work is done when a body having a charge q moves through a potential difference ΔV. Work, like heat, exists only when energy is being transferred.
When two bodies are placed in thermal contact and energy flows from the warmer body to the cooler one,we call the process "heat". A transfer of energy to or from a system by any means other than heat is called "work".

Heat can only partially be converted into work
Work can be completely converted into heat (by friction, for example), but heat can only be partially converted to work. Conversion of heat into work is accomplished by means of a *heat engine*, the most common example of which is an ordinary gasoline engine. The science of thermodynamics developed out of the need to understand the limitations of steam-driven heat engines at the beginning of the Industrial Age. A fundamental law of Nature, the Second Law of Thermodynamics, states that the complete conversion of heat into work is impossible. Something to think about when you purchase fuel for your car!

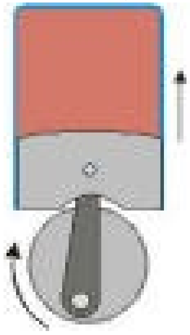


Figure 5.24 Piston

Thermodynamic View of the World

In thermodynamics, we must be very precise in our use of certain words. The two most important of these are system and surroundings. A *thermodynamic system* is that part of the world to which we are directing our attention. Everything that is not a part of the system constitutes the *surroundings.* The system and surroundings are separated by a *boundary*. If our system is one mole of a gas in a container, then the boundary is simply the inner wall of the container itself. The boundary need not be a physical barrier; for example, if our system is a factory or a forest, then the boundary can be wherever we wish to define it. We can even focus our attention on the dissolved ions in an aqueous solution of a salt, leaving the water molecules as part of the surroundings. The single property that the boundary must have is that it be clearly defined, so we can unambiguously say whether a given part of the world is in our system or in the surroundings.

If matter is not able to pass across the boundary, then the system is said to be *closed*; otherwise, it is *open*. A closed system may still exchange energy with the surroundings unless the system is an *isolated* one, in which case neither matter nor energy can pass across the boundary. The tea in a closed Thermos bottle approximates a closed system over a short time interval.

Properties and the state of a system

The *properties* of a system are those quantities such as the pressure, volume, temperature, and its composition, which are in principle measurable and capable of assuming definite values. There are of course many properties other than those mentioned above; the density and thermal conductivity are two examples. However, the pressure, volume, and temperature have special significance because they determine the values of all the other properties; they are therefore known as *state properties* because if their values are known then the system is in a definite *state*.

Change of state: the meaning of Δ

In dealing with thermodynamics, we must be able to unambiguously define the change in the state of a system when it undergoes some process. This is done by specifying changes in the values of the different state properties using the symbol Δ (*delta*) as illustrated here for a change in the volume:
$\Delta V = \mathrm{Vfinal} - \mathrm{Vinitial}(1-1)$
We can compute similar delta-values for changes in P, V, ni (the number of moles of component i), and the other state properties we will meet later.

2 Internal energy and the First Law

Internal energy is simply the totality of all forms of kinetic and potential energy of the system. Thermodynamics makes no distinction between these two forms of energy and it does not assume the existence of atoms and molecules. But since we are studying thermodynamics in the context of chemistry, we can allow ourselves to depart from "pure" thermodynamics enough to point out that the internal energy is the sum of the kinetic energy of motion of the molecules, and the potential energy represented by the chemical bonds between the atoms and any other intermolecular forces that may be operative.

Khan Academy : 1st law of Thermo, 11:26 min
https://www.youtube.com/watch?v=NyOYW07-L5g

How can we know how much internal energy a system possesses? The answer is that we cannot, at least not on an absolute basis; all scales of energy are arbitrary. The best we can do is measure changes in energy. However, we are perfectly free to define zero energy as the energy of the system in some arbitrary *reference state*, and then say that the internal energy of the system in any other state is the difference between the energies of the system in these two different states.

The first law of thermodynamics states that the energy cannot be created or destroyed under any conditions. Furthermore, the energy is converted from one form to another, i.e. the conversion between heat **q,** work **w** and the internal energy **U.**

The first law of thermodynamics can be summarized in the formula below:

$$\Delta U = q + w$$

Where:

ΔU = total internal energy change of the system
q = heat exchanged between the system and its surrounding
w = the work done by or on the system

Furthermore, work w is equal = negative value of the external pressure **P** on the system X change in volume **Δ V:**

$$w = - p \Delta V$$

replacing w in the equation of the first law of thermodynamic on obtains:

$$\Delta U = q - p \Delta V$$

The internal energy of the system will:

Decrease: in case the system gives off heat or does work on the surrounding
Increase: in case the system taking in heat from the surrounding or surrounding does work on the system

Also,

If Tsystem > Tsurroundings then the heat flows from the system to the surroundings

$q < 0$.

This is an **exothermic system: Heat is given to the surroundings by the system.**

If Tsystem < Tsurroundings then the heat flows from the surroundings to the system

$q > 0$.

This is an **endothermic system: Heat is taken by the system from the surroundings**

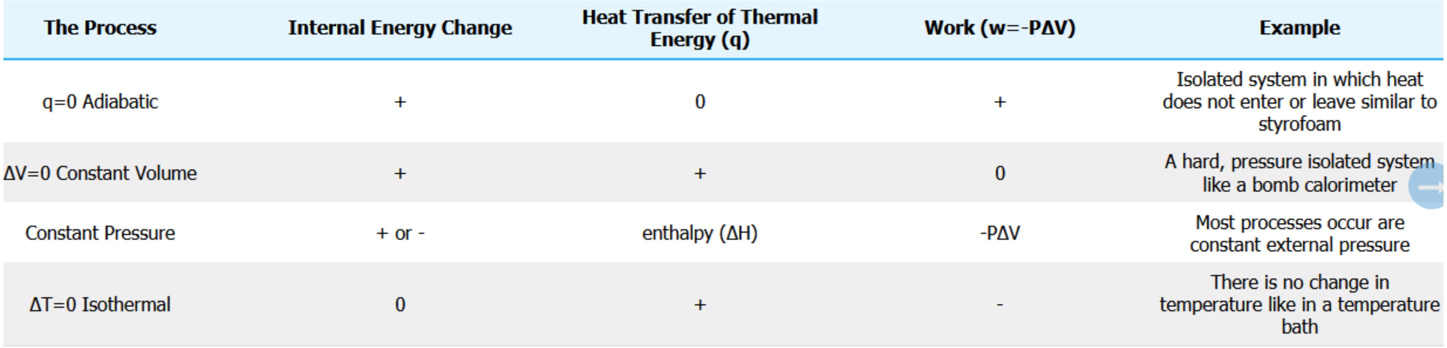
Since the first law of thermodynamics states that the energy cannot be created of destroyed the, then the change of the internal energy is always equaling zero:

Thus, if the energy is lost by the system, the surrounding then absorbs this lost energy.
If the energy in absorbed onto the system (energy is gained), then the energy is given from the surrounding to the system.

$$\Delta U\text{system} + \Delta U\text{surroundings} = 0$$

$$\Delta U\text{system} = - \Delta U\text{surroundings}$$

The table below illustrates some examples of the interaction between the q and w as well as the surrounding:



The Process	Internal Energy Change	Heat Transfer of Thermal Energy (q)	Work (w=-PΔV)	Example
q=0 Adiabatic	+	0	+	Isolated system in which heat does not enter or leave similar to styrofoam
ΔV=0 Constant Volume	+	+	0	A hard, pressure isolated system like a bomb calorimeter
Constant Pressure	+ or -	enthalpy (ΔH)	-PΔV	Most processes occur are constant external pressure
ΔT=0 Isothermal	0	+	-	There is no change in temperature like in a temperature bath

Reference:
https://chem.libretexts.org/Bookshelves/Physical_and_Theoretical_Chemistry_Textbook_Maps/Supplemental_Modules_(Physical_and_Theoretical_Chemistry)/Thermodynamics/The_Four_Laws_of_Thermodynamics/First_Law_of_Thermodynamics

Example:

NH_3 gas is placed in a system with constant pressure. If the surrounding around the system loses 75 J of heat and does 555 J of work onto the system, what is the internal energy of the system?

Using the first law of thermodynamics formula:

$$\Delta U = q + w$$

Since the surrounding loses heat which gained by the system → q is positive
Since the surrounding does work on the system → w is positive

Thus, both q and w are positive:

$$\Delta U = 75\text{ J} + 555\text{ J} = 630\text{ J}$$

Example:

A system has constant volume ($\Delta V = 0$) and the heat around the system increases by 86 J.

a) What is the sign for heat (q) for the system?
b) What is ΔU equal to?
c) What is the value of internal energy of the system in Joules?

Since the system is under constant volume ($\Delta V = 0$), then the work will equal zero:

$\mathbf{w = - p \, \Delta V}$

since $\Delta V = 0$

$\mathbf{w = - p \times (0) = 0}$

and since the surrounding heat is increased by 86 J, then

$\mathbf{\Delta U = q + w = q + 0 = q}$

a) What is the sign for heat (q) for the system?

q will be negative: Heat is lost by the system and gained by the surrounding. q is less than zero.

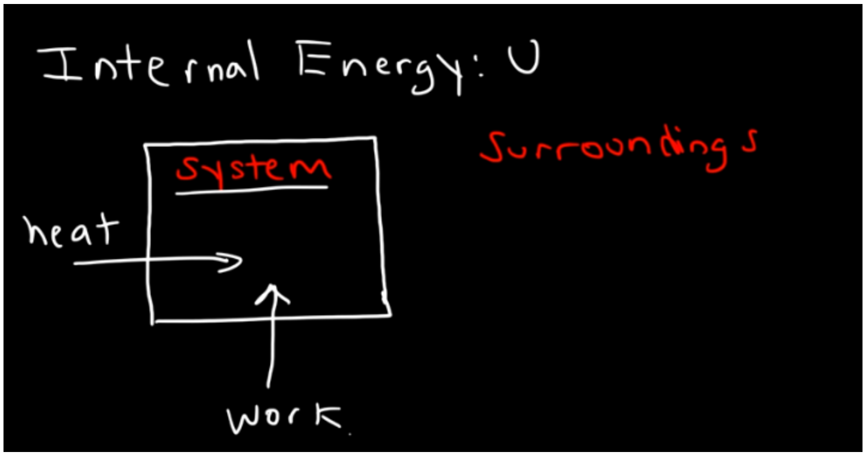
b) What is ΔU equal to?

$\mathbf{\Delta U = q + w = q + 0 = q}$

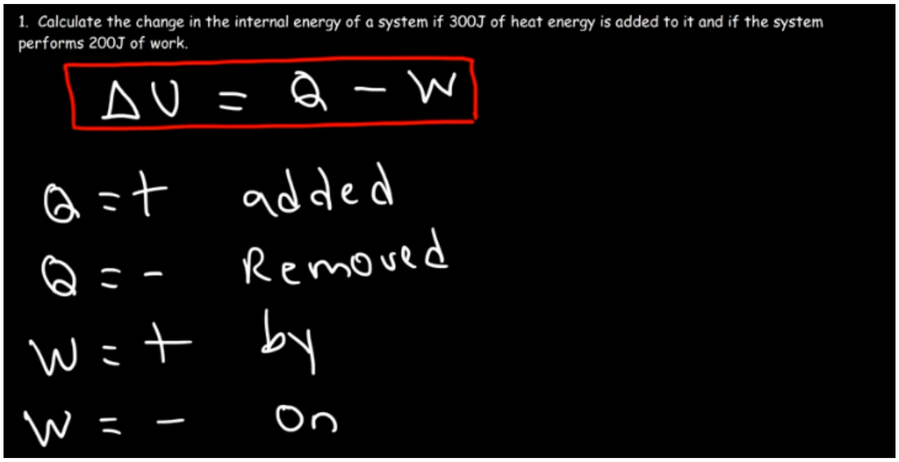
c) What is the value of internal energy of the system in Joules?

$\mathbf{\Delta U = q + w = q + 0 = q = - 86 \, J}$

The videos below illustrate some examples as well:



https://www.youtube.com/watch?v=NyOYW07-L5g



1. Calculate the change in the internal energy of a system if 300J of heat energy is added to it and if the system performs 200J of work.

$$\boxed{\Delta U = Q - W}$$

Q = + added

Q = − Removed

W = + by

W = − On

https://www.youtube.com/watch?v=7Siv2NNCFag

When the heat is absorbed or gained under the condition of constant pressure, then the change of the heat is called enthalpy. The enthalpy (H) is under the constant pressure condition will equal to the sum of the internal energy (U) and the product of pressure and volume (PV).

$H = U + PV$

The change in enthalpy ΔH will equal the change in the internal energy and the volume.

$\Delta H = \Delta U + P \Delta V$ [Pressure P is constant].

The internal energy (U) of a system is recognized as the random, unorganized motion of molecules. The total internal energy in a system includes potential and kinetic energy. It is the sum of all the microscopic energies such as: translational kinetic energy, vibrational and rotational kinetic energy etc.

.During a system change, its internal energy will change and the internal energy can be transferred from the system to the surrounding.

Energy is transferred **into** the system when the system is gaining energy (heat) q from the surrounding or when the surrounding is doing work (w) on the system.
Energy is transferred out of the system (given off) when the system is losing energy (heat) q to the surrounding or when the system is doing work (w) on the surrounding.

$P \Delta V$ represents the work (w) with the ΔV is positive. Then the $P \Delta V$ term will equal:

$P \Delta V = - w$

By substitution, the enthalpy change ΔH then equals:

$\Delta H = \Delta U + P \Delta V = \Delta U - w$

The molar enthalpy ΔHm is defined as the enthalpy change per a mole of substance.
.Enthalpy is a state function which does not depend on the path of the change. It is an extensive property that depends on mass of the system. If the system moves from one state to another state, the enthalpy change is independent of the path between the two states of the system.

The combustion reaction of methane will yield 802.3 kJ/mol

$CH_4 + O_2 \rightarrow CO_2 + 2\ H_2O \quad \Delta H = - 802.3$ kJ/mol [for 1 mole]

If 2 moles of CH_4 are used then:

$2\ CH_4 + 2\ O_2 \rightarrow 2\ CO_2 + 4\ H_2O \quad \Delta H = - 2 \times 802.3$ kJ/mol [for 2 mole]

The thermochemical equation for the 2 moles of CH_4 combustion:

$2\ CH_4 + 2\ O_2 \longrightarrow 2\ CO_2 + 4\ H_2O \quad \Delta H = - 1604.6$ kJ/mol

Example:

When 1.50 g Mg(*s*) reacts with 50.0 mL of 0.850 M HCl(*aq*), 5.15 kJ of heat are produced. Determine the enthalpy change per mole of magnesium reacting for the reaction and write the complete thermochemical equation:

$Mg(s) + 2\ HCl(aq) \longrightarrow MgCl_2(aq) + H_2(g)$

Number of moles of Mg = (1.50 g) / (24.3 g Mg /mole) = 0.0617 moles

ΔH = 1 mole Mg x [5.15 kJ / 0.0617 moles] = - 83.5 kJ / mole [Heat is produced]

The thermochemical equation:

$Mg(s) + 2\ HCl(aq) \longrightarrow MgCl_2(aq) + H_2(g) \qquad \Delta H = - 83.5$ kJ / mole

The heat absorbed or gained will equal $\Delta H = q$ if there is no expansion work on the system and the pressure P is constant.

With the help of formula $\Delta H = q$, the process of exothermic or endothermic processes will be determined.
In other words:
By the endothermic process: the system is gaining heat from the surrounding and q will be greater than zero and ΔH will be greater than zero as well.
By the exothermic process: the system is giving off heat to the surrounding and q will be less than zero and ΔH will be less than zero as well.

Effect of the temperature on the enthalpy:

When temperature increases, the molecular interactions increase the internal energy of the system as well as the enthalpy of the system.

$c = q / \Delta T$

At the constant pressure:

$c_p = [\Delta H / \Delta T]_p$ The subscript indicates the constant pressure condition.

Enthalpy of phase changes

A plot of the enthalpy of a system as a function of its temperature is called an ***enthalpy diagram***. The slope of the line is given by *Cp*. The enthalpy diagram of a pure substance such as water shows that this plot is not uniform, but is interrupted by sharp breaks at which the value of *Cp* is apparently infinite, meaning that the substance can absorb or lose heat without undergoing any change in temperature at all. This, of course, is exactly what happens when a substance undergoes a phase change; you already know that the temperature the water boiling in a kettle can never exceed 100 until all the liquid has evaporated, at which point the temperature of the steam will rise as more heat flows into the system.

A plot of the enthalpy of carbon tetrachloride as a function of its temperature provides a concise view of its thermal behavior. The slope of the line is given by the heat capacity Cp. All H-vs.-C plots show sharp breaks at which the value of Cp is apparently infinite, meaning that the substance can absorb or lose heat without undergoing any change in temperature at all. This, of course, is exactly what happens when a substance undergoes a phase change; you already know that the temperature of the water boiling in a kettle can never exceed 100°C until all the liquid has evaporated, at which point the temperature (of the steam) will rise as more heat flows into the system.
The lowest-temperature discontinuity on the CCl4 diagram corresponds to a solid-solid phase transition associated with a rearrangement of molecules in the crystalline solid.

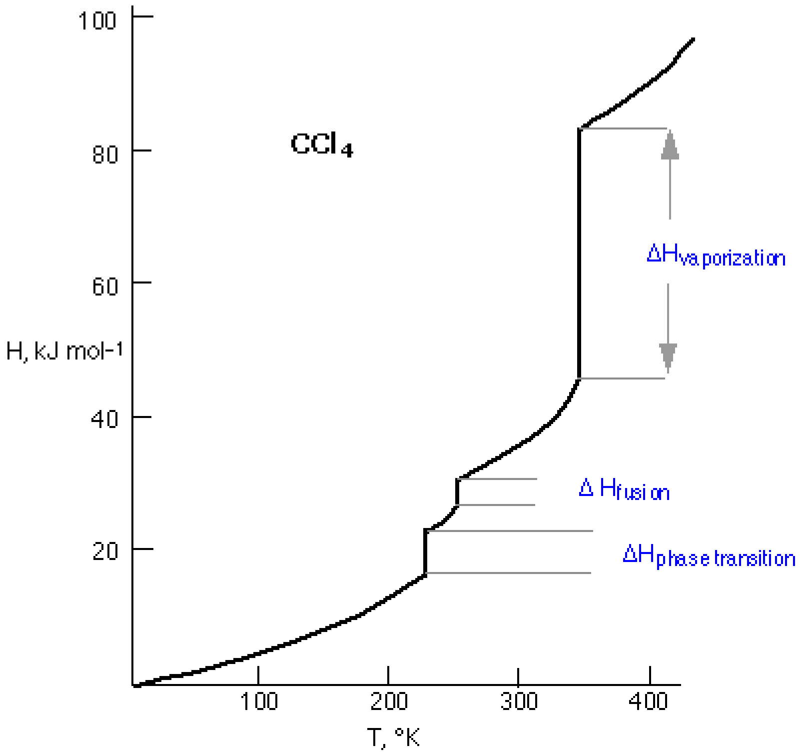
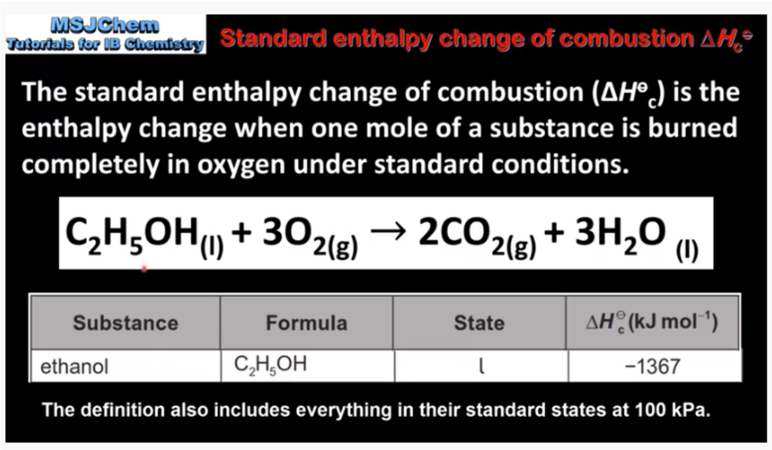


Figure 5.25 Enthalpy Diagram of CCl_4
Ref: https://www.chem1.com/acad/webtext/energetics/CE-2.html

Standard Enthalpy:

A standard state is defined by IUPAC as standard state by which the system has the pressure of 1 bar (0.987 atm) and in general 1 atm is adopted and 1 M (molar) concentrations of the reactants. The standard Δ H is given the superscript "o".
The symbol of the standard enthalpy is ΔH^o
There is no standard temperature but usually the temperature used and considered is 298.15 K.
Δ H with the superscript "o" indicates the enthalpy under no standard conditions.

The videos below illustrate the concept of the standard enthalpy and the standard enthalpy of combustion:



Standard enthalpy change of combustion $\Delta H_c^\ominus$

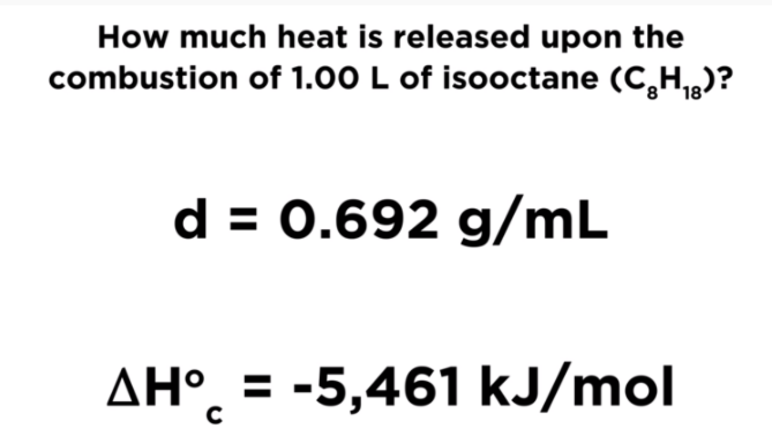
The standard enthalpy change of combustion (ΔH^o_c) is the enthalpy change when one mole of a substance is burned completely in oxygen under standard conditions.

$$C_2H_5OH_{(l)} + 3O_{2(g)} \rightarrow 2CO_{2(g)} + 3H_2O_{(l)}$$

Substance	Formula	State	$\Delta H_c^\ominus$ (kJ mol^{-1})
ethanol	C_2H_5OH	l	−1367

The definition also includes everything in their standard states at 100 kPa.

Reference: https://www.youtube.com/watch?v=wZYOGgc25yQ



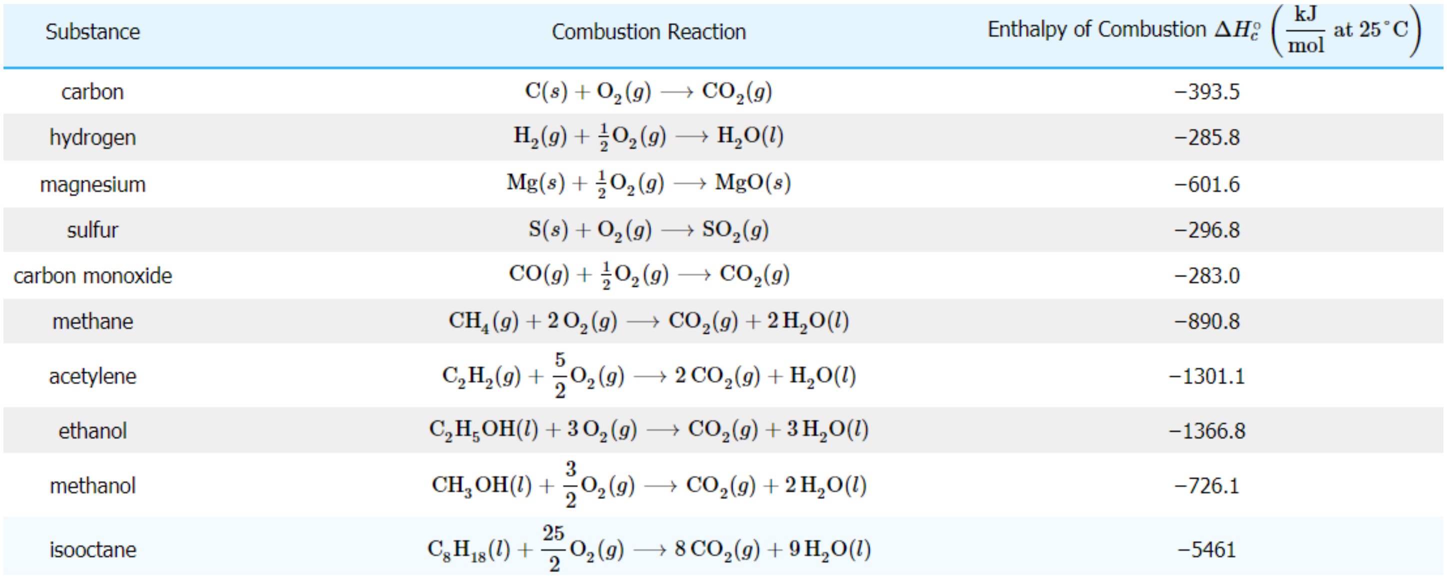
How much heat is released upon the combustion of 1.00 L of isooctane (C_8H_{18})?

$d = 0.692$ g/mL

$\Delta H°_c = -5,461$ kJ/mol

Reference: https://www.youtube.com/watch?v=RI7xCYBmDqQ

The table below shows the standard enthalpy of the combustions:



Substance	Combustion Reaction	Enthalpy of Combustion $\Delta H_c^\circ \left(\frac{\text{kJ}}{\text{mol}} \text{ at } 25^\circ\text{C}\right)$
carbon	$C(s) + O_2(g) \longrightarrow CO_2(g)$	−393.5
hydrogen	$H_2(g) + \frac{1}{2}O_2(g) \longrightarrow H_2O(l)$	−285.8
magnesium	$Mg(s) + \frac{1}{2}O_2(g) \longrightarrow MgO(s)$	−601.6
sulfur	$S(s) + O_2(g) \longrightarrow SO_2(g)$	−296.8
carbon monoxide	$CO(g) + \frac{1}{2}O_2(g) \longrightarrow CO_2(g)$	−283.0
methane	$CH_4(g) + 2\,O_2(g) \longrightarrow CO_2(g) + 2\,H_2O(l)$	−890.8
acetylene	$C_2H_2(g) + \frac{5}{2}O_2(g) \longrightarrow 2\,CO_2(g) + H_2O(l)$	−1301.1
ethanol	$C_2H_5OH(l) + 3\,O_2(g) \longrightarrow CO_2(g) + 3\,H_2O(l)$	−1366.8
methanol	$CH_3OH(l) + \frac{3}{2}O_2(g) \longrightarrow CO_2(g) + 2\,H_2O(l)$	−726.1
isooctane	$C_8H_{18}(l) + \frac{25}{2}O_2(g) \longrightarrow 8\,CO_2(g) + 9\,H_2O(l)$	−5461

Reference:
https://chem.libretexts.org/Courses/City_College_of_San_Francisco/Chemistry_101A/Topic_D%3A_Thermochemistry/6%3A_Thermochemistry/6.07%3A_Tabulated_Enthalpy_Values

Example of standard heat of combustion calculation:

Consider the combustion reaction below:

$CH_4 + O_2 \longrightarrow CO_2 + 2\ H_2O \qquad \Delta H = -\ 802.3$ kJ/mol

If 1.50 L of CH_4 is used for the combustion, calculate the standard enthalpy of combustion.

The density of methane (gas) is: 0.72 g/L

Molar mass of methane: 16.0 g/mole

$\Delta H^o = [1.50\ CH_4\ L] \times [0.72\ CH_4\ g / L] \times [1\ mole\ CH_4 / 16.0\ g\ CH_4] \times [802.3\ kJ / mole\ CH_4] =$ **- 54.2 kJ**

Standard Enthalpy of Formation:

The standard enthalpy of formation is recognized as a change in enthalpy when one mole of a substance in the standard state (1 atm of pressure and 298.15 K) is formed from its pure elements under the same conditions.

The equation for the standard enthalpy of formation id given below:

$$\Delta H^o reaction = \sum \Delta H^o f(products) - \sum \Delta H^o f(Reactants)$$

Remember that the change in enthalpy is considering the enthalpy as a **State Function**.

Examples:

1. Consider the two molecules $Cl_2(g)$ and $Cl_2(l)$ at 298.15 K, which substance has a nonzero standard enthalpy of formation?

$Cl_2(g)$ is most stable. Therefore $Cl_2(g)$ will have the lower enthalpy and $\Delta H^o_f = 0$.
$Cl_2(l)$ is least stable and therefore will have the highest enthalpy and ΔH^o_f has a nonzero value.

2. Calculate the $\Delta H^o_{(reaction)}$ for the reaction below:

$$2\ SO_2 \quad + \quad O_2 \quad \longrightarrow \quad 2\ SO_3$$

$$\Delta H^o reaction = \sum n_p \Delta H^o f(products) - \sum n_r \Delta H^o f(Reactants)$$

n_p = number of moles of products

n_r = number of moles of the reactants

$\Delta H^o reaction = \{ 2 \times \Delta H^o f[SO_3] - [2 \times \Delta H^o f[SO_2] + \Delta H^o f[O_2]$

Using the table below of the standard enthalpy of the formation:

$\Delta H^o f[SO_3] = - 395.2$ kJ / mole
$\Delta H^o f[SO_2] = -296.1$ kJ / mole
$\Delta H^o f[O_2] = 0$ kJ / mole

$\Delta H^o reaction = \{ 2\ mole \times \Delta H^o f[SO_3] - [2\ mole \times \Delta H^o f[SO_2] + \Delta H^o f[O_2]]$

$\Delta H^o reaction = \{ - 2 \times 395.2\ kJ/mole\} - \{[(- 2 \times 296.1\ kJ/mole) + 0]\} = - 790.4 + 592.2 =$ **- 198.2 kJ**
$\Delta H^o reaction$ has negative value and hence the reaction is exothermic.

3. Calculate the $\Delta H^o_{(reaction)}$ for the reaction below:

$2\ NO + O_2 \longrightarrow 2\ NO_2$

$\Delta H^o reaction = \sum n_p \Delta H^o f(products) - \sum n_r \Delta H^o f(Reactants)$

n_p = number of moles of products

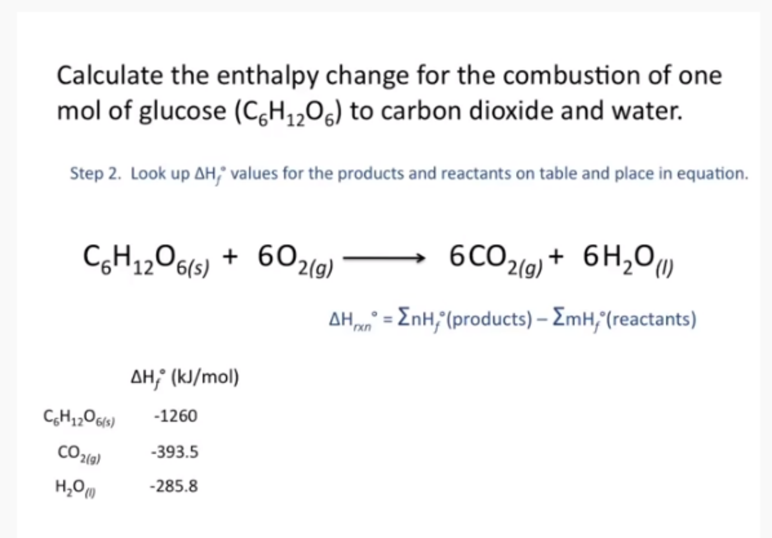
n_r = number of moles of the reactants

Using the table below of the standard enthalpy of the formation:

$\Delta H^o f[NO_2] = 33.18$ kJ / mole
$\Delta H^o f[NO] = 90.25$ kJ / mole
$\Delta H^o f[O_2] = 0$ kJ / mole

$\Delta H^o reaction = \{ 2 \text{ mole} \times \Delta H^o f[NO_2] - [2 \times \Delta H^o f[NO] + \Delta H^o f[O_2]]$
$\Delta H^o reaction = \{2 \text{ mole} \times 33.18 \text{ kJ/mole}\} - \{[(2 \text{ mole} \times 90.25 \text{ kJ/mole}) + 0]\} = 66.36 - 180.50 =$ **-114.14 kJ**
$\Delta H^o reaction$ has negative value and hence the reaction is exothermic.

The videos below illustrate the concept of the standard enthalpy of formation as well as go over some example calculations:



Calculate the enthalpy change for the combustion of one mol of glucose ($C_6H_{12}O_6$) to carbon dioxide and water.

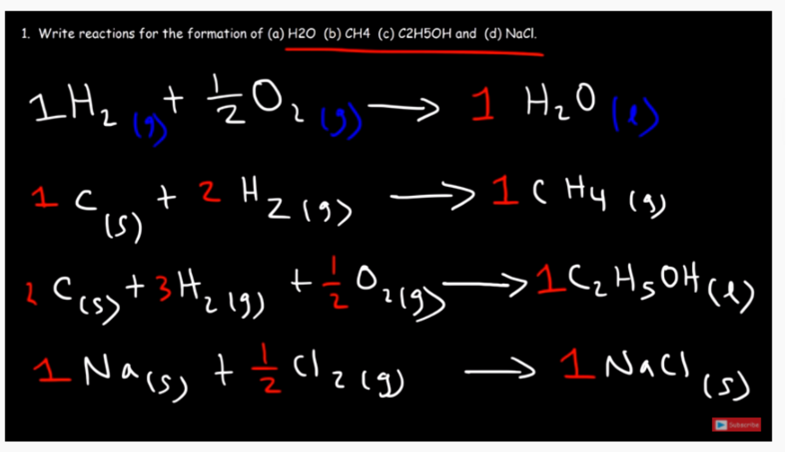
Step 2. Look up ΔH_f° values for the products and reactants on table and place in equation.

$$C_6H_{12}O_{6(s)} + 6O_{2(g)} \longrightarrow 6CO_{2(g)} + 6H_2O_{(l)}$$

$$\Delta H_{rxn}^\circ = \Sigma nH_f^\circ(\text{products}) - \Sigma mH_f^\circ(\text{reactants})$$

	ΔH_f° (kJ/mol)
$C_6H_{12}O_{6(s)}$	-1260
$CO_{2(g)}$	-393.5
$H_2O_{(l)}$	-285.8

https://www.youtube.com/watch?v=PJweE3F_mPY



1. Write reactions for the formation of (a) H2O (b) CH4 (c) C2H5OH and (d) NaCl.

$$1H_{2(g)} + \frac{1}{2}O_{2(g)} \longrightarrow 1\ H_2O_{(l)}$$

$$1\ C_{(s)} + 2\ H_{2(g)} \longrightarrow 1\ CH_{4\ (g)}$$

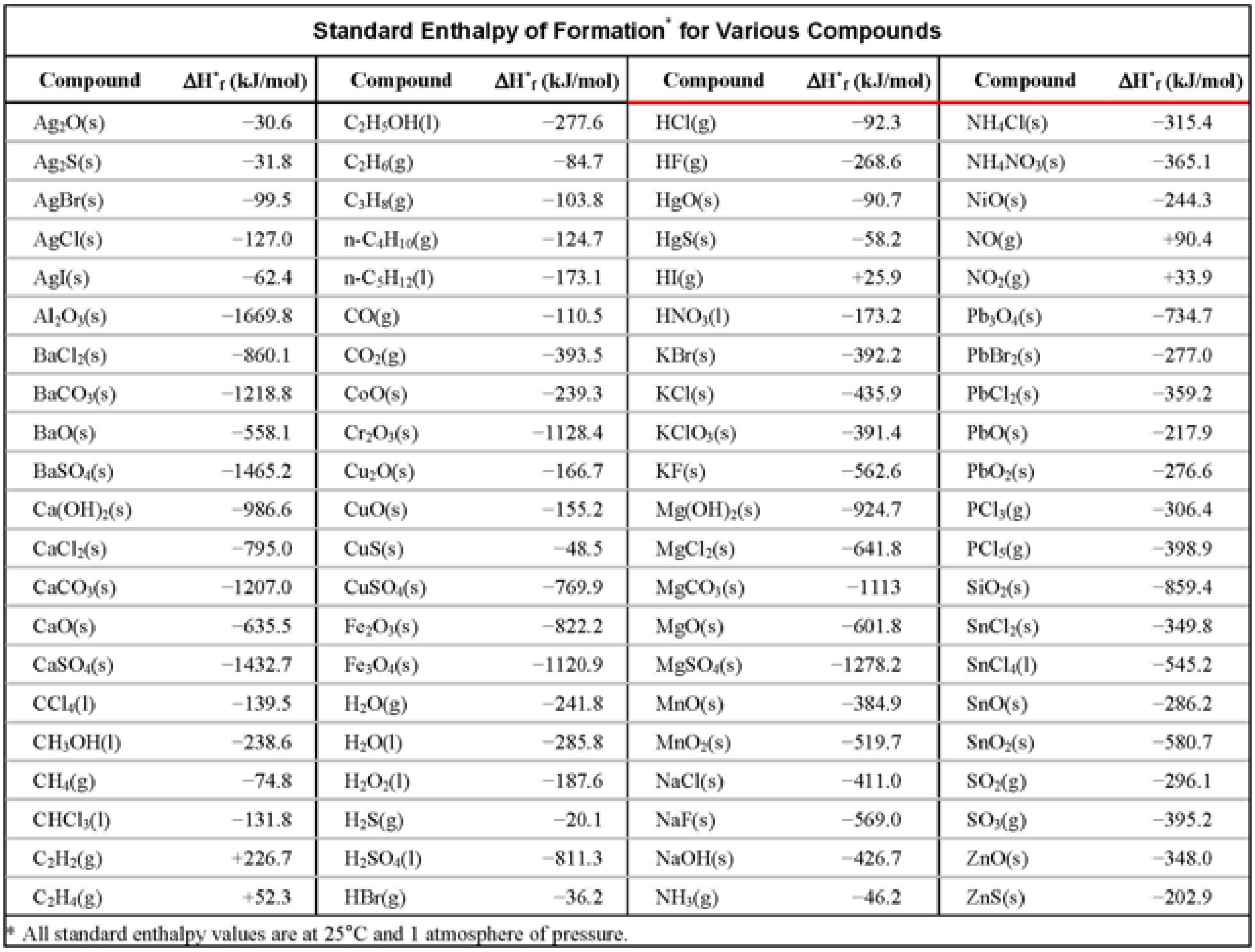
$$2\ C_{(s)} + 3H_{2(g)} + \frac{1}{2}O_{2(g)} \longrightarrow 1C_2H_5OH_{(l)}$$

$$1\ Na_{(s)} + \frac{1}{2}Cl_{2(g)} \longrightarrow 1\ NaCl_{(s)}$$

https://www.youtube.com/watch?v=FP-VYfTYi8Y

Standard Enthalpy of Formation for various Compounds.

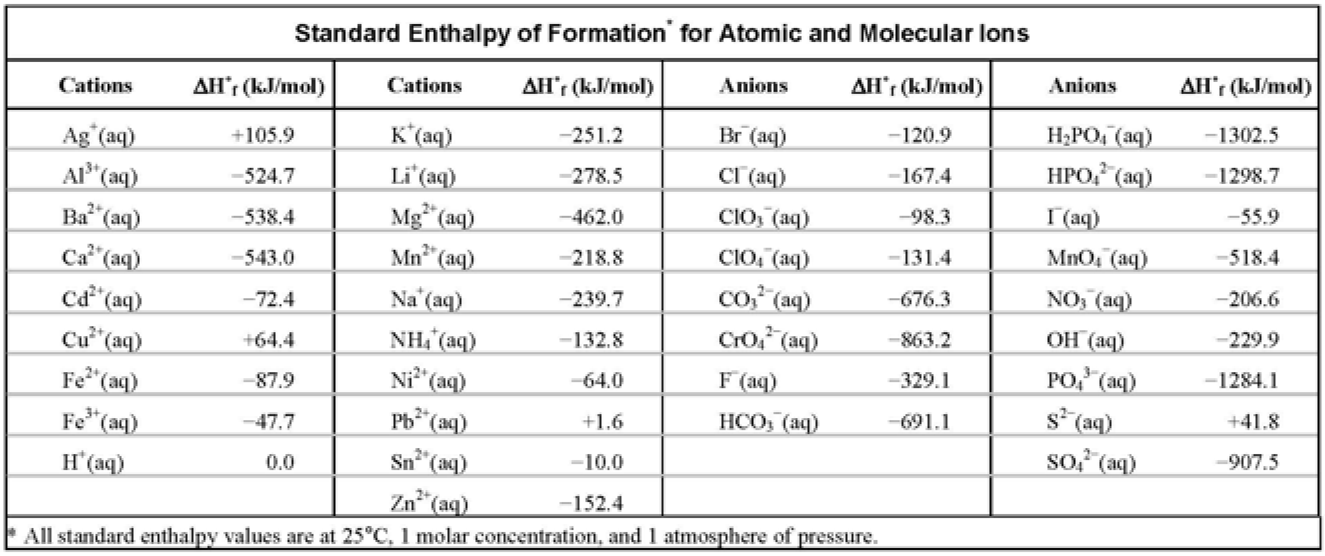
Reference: http://sistemas.eel.usp.br/docentes/arquivos/5817712/TDQ%20I/R-standard_enthalpy_of_formation.pdf



Standard Enthalpy of Formation* for Various Compounds

Compound	ΔH°_f (kJ/mol)	Compound	ΔH°_f (kJ/mol)	Compound	ΔH°_f (kJ/mol)	Compound	ΔH°_f (kJ/mol)
$Ag_2O(s)$	−30.6	$C_2H_5OH(l)$	−277.6	$HCl(g)$	−92.3	$NH_4Cl(s)$	−315.4
$Ag_2S(s)$	−31.8	$C_2H_6(g)$	−84.7	$HF(g)$	−268.6	$NH_4NO_3(s)$	−365.1
$AgBr(s)$	−99.5	$C_3H_8(g)$	−103.8	$HgO(s)$	−90.7	$NiO(s)$	−244.3
$AgCl(s)$	−127.0	n-$C_4H_{10}(g)$	−124.7	$HgS(s)$	−58.2	$NO(g)$	+90.4
$AgI(s)$	−62.4	n-$C_5H_{12}(l)$	−173.1	$HI(g)$	+25.9	$NO_2(g)$	+33.9
$Al_2O_3(s)$	−1669.8	$CO(g)$	−110.5	$HNO_3(l)$	−173.2	$Pb_3O_4(s)$	−734.7
$BaCl_2(s)$	−860.1	$CO_2(g)$	−393.5	$KBr(s)$	−392.2	$PbBr_2(s)$	−277.0
$BaCO_3(s)$	−1218.8	$CoO(s)$	−239.3	$KCl(s)$	−435.9	$PbCl_2(s)$	−359.2
$BaO(s)$	−558.1	$Cr_2O_3(s)$	−1128.4	$KClO_3(s)$	−391.4	$PbO(s)$	−217.9
$BaSO_4(s)$	−1465.2	$Cu_2O(s)$	−166.7	$KF(s)$	−562.6	$PbO_2(s)$	−276.6
$Ca(OH)_2(s)$	−986.6	$CuO(s)$	−155.2	$Mg(OH)_2(s)$	−924.7	$PCl_3(g)$	−306.4
$CaCl_2(s)$	−795.0	$CuS(s)$	−48.5	$MgCl_2(s)$	−641.8	$PCl_5(g)$	−398.9
$CaCO_3(s)$	−1207.0	$CuSO_4(s)$	−769.9	$MgCO_3(s)$	−1113	$SiO_2(s)$	−859.4
$CaO(s)$	−635.5	$Fe_2O_3(s)$	−822.2	$MgO(s)$	−601.8	$SnCl_2(s)$	−349.8
$CaSO_4(s)$	−1432.7	$Fe_3O_4(s)$	−1120.9	$MgSO_4(s)$	−1278.2	$SnCl_4(l)$	−545.2
$CCl_4(l)$	−139.5	$H_2O(g)$	−241.8	$MnO(s)$	−384.9	$SnO(s)$	−286.2
$CH_3OH(l)$	−238.6	$H_2O(l)$	−285.8	$MnO_2(s)$	−519.7	$SnO_2(s)$	−580.7
$CH_4(g)$	−74.8	$H_2O_2(l)$	−187.6	$NaCl(s)$	−411.0	$SO_2(g)$	−296.1
$CHCl_3(l)$	−131.8	$H_2S(g)$	−20.1	$NaF(s)$	−569.0	$SO_3(g)$	−395.2
$C_2H_2(g)$	+226.7	$H_2SO_4(l)$	−811.3	$NaOH(s)$	−426.7	$ZnO(s)$	−348.0
$C_2H_4(g)$	+52.3	$HBr(g)$	−36.2	$NH_3(g)$	−46.2	$ZnS(s)$	−202.9

* All standard enthalpy values are at 25°C and 1 atmosphere of pressure.



Standard Enthalpy of Formation* for Atomic and Molecular Ions

Cations	ΔH°_f (kJ/mol)	Cations	ΔH°_f (kJ/mol)	Anions	ΔH°_f (kJ/mol)	Anions	ΔH°_f (kJ/mol)
Ag^+(aq)	+105.9	K^+(aq)	−251.2	Br^-(aq)	−120.9	$H_2PO_4^-$(aq)	−1302.5
Al^{3+}(aq)	−524.7	Li^+(aq)	−278.5	Cl^-(aq)	−167.4	HPO_4^{2-}(aq)	−1298.7
Ba^{2+}(aq)	−538.4	Mg^{2+}(aq)	−462.0	ClO_3^-(aq)	−98.3	I^-(aq)	−55.9
Ca^{2+}(aq)	−543.0	Mn^{2+}(aq)	−218.8	ClO_4^-(aq)	−131.4	MnO_4^-(aq)	−518.4
Cd^{2+}(aq)	−72.4	Na^+(aq)	−239.7	CO_3^{2-}(aq)	−676.3	NO_3^-(aq)	−206.6
Cu^{2+}(aq)	+64.4	NH_4^+(aq)	−132.8	CrO_4^{2-}(aq)	−863.2	OH^-(aq)	−229.9
Fe^{2+}(aq)	−87.9	Ni^{2+}(aq)	−64.0	F^-(aq)	−329.1	PO_4^{3-}(aq)	−1284.1
Fe^{3+}(aq)	−47.7	Pb^{2+}(aq)	+1.6	HCO_3^-(aq)	−691.1	S^{2-}(aq)	+41.8
H^+(aq)	0.0	Sn^{2+}(aq)	−10.0			SO_4^{2-}(aq)	−907.5
		Zn^{2+}(aq)	−152.4				

* All standard enthalpy values are at 25°C, 1 molar concentration, and 1 atmosphere of pressure.

Writing chemical Equations for ΔH^o_f

Examples:

Write ΔH^o_f for the reactions below:

1. CH3-O-CH_3(l)

2 C(solid, graphite) + ½ O_2(gas) + 3 H_2(g) ⟶ CH3-O-CH_3(l)

2. CH3-CO-CH_3(l)

3 C(solid, graphite) + ½ O_2(gas) + 3 H_2(g) ⟶ CH3-CO-CH_3(l)

Evaluating an Enthalpy of Formation

Hydrogen gas, H_2, reacts explosively with gaseous chlorine, Cl_2, to form hydrogen chloride, HCl(*g*). What is the enthalpy change for the reaction of 1 mole of H_2(*g*) with 1 mole of Cl_2(*g*) if both the reactants and products are at standard state conditions? The standard enthalpy of formation of HCl(*g*) is −92.3 kJ/mol.

$H_2(g) + Cl_2(g) \longrightarrow 2\ HCl(g)$ ΔH°_f = - 92.3 kJ /mole

1 mole of H_2(*g*) will produce 2 moles of HCl(g)
Also 1 mole of Cl_2(*g*) will produce 2 moles of HCl(g)

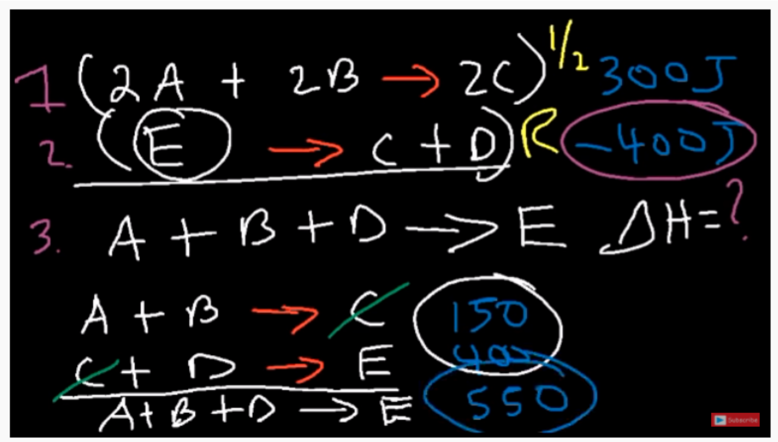
[1 mole H_2(*g*)] x 2 mole HCl(g) / 1 mole H_2(g) = 2 mole HCl(g)

[2 mole HCl(g)] x [- 92.3 kJ / mole H_2(g)] = **- 184.6 kJ**

Hess's Law

Hess was a Russian chemist. This law was named after him in 1840. Hess's law confirms that ΔHº is state function which does not depend on the path of the chemical reaction. **Hess's law states that regardless of the multiple steps that the reaction can take, the total enthalpy change for the reaction is the sum of all changes.**

The videos below illustrate the concept of Hess's Law and some calculations examples:



$1.\ (2A + 2B \rightarrow 2C)^{1/2}\quad 300J$

$2.\ (E \rightarrow C + D)\ R\quad -400J$

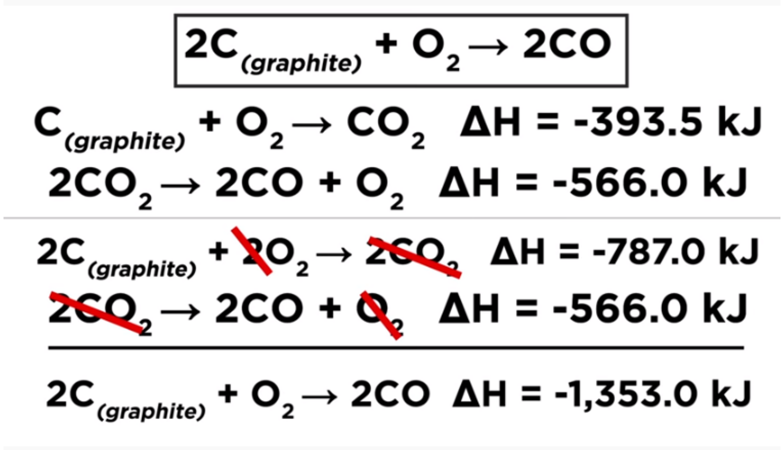
$3.\ A + B + D \rightarrow E\quad \Delta H = ?$

$A + B \rightarrow \cancel{C}\quad 150$

$\cancel{C} + D \rightarrow E\quad 400$

$A + B + D \rightarrow E\quad 550$

https://www.youtube.com/watch?v=Idv2C8HBbug



$$\boxed{2C_{(graphite)} + O_2 \rightarrow 2CO}$$

$$C_{(graphite)} + O_2 \rightarrow CO_2 \quad \Delta H = -393.5\text{ kJ}$$

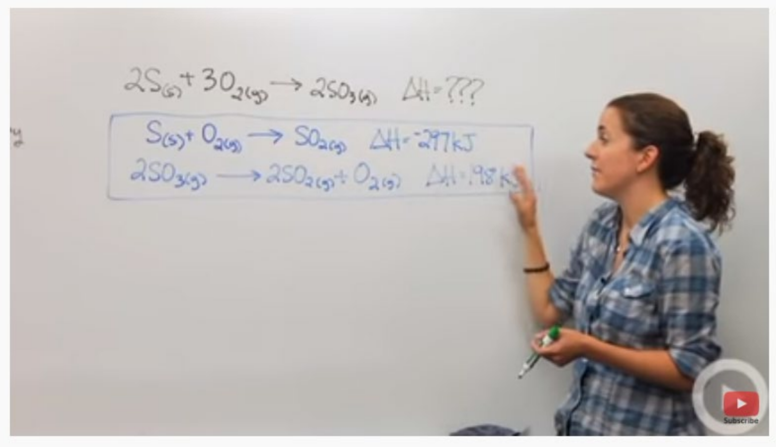
$$2CO_2 \rightarrow 2CO + O_2 \quad \Delta H = -566.0\text{ kJ}$$

$$2C_{(graphite)} + \cancel{2}O_2 \rightarrow \cancel{2CO_2} \quad \Delta H = -787.0\text{ kJ}$$

$$\cancel{2CO_2} \rightarrow 2CO + \cancel{O_2} \quad \Delta H = -566.0\text{ kJ}$$

$$2C_{(graphite)} + O_2 \rightarrow 2CO \quad \Delta H = -1{,}353.0\text{ kJ}$$

https://www.youtube.com/watch?v=2q2u5sj4V00



https://www.youtube.com/watch?v=u7aTBxA7sL8

Examples:

1. Calculate the enthalpy for this reaction ΔH°:

$2\,C(s) + H_2(g) \longrightarrow C_2H_2(g)$ ΔH° = ??? kJ

Given the following thermochemical equations:

$C_2H_2(g) + \frac{5}{2}O_2(g) \longrightarrow 2CO_2(g) + H_2O(l)$ $\Delta H° = -1299.5$ kJ

$C(s) + O_2(g) \longrightarrow CO_2(g)$ $\Delta H° = -393.5$ kJ

$H_2(g) + \frac{1}{2}O_2(g) \longrightarrow H_2O(l)$ $\Delta H° = -285.8$ kJ

Step 1:

Determine what we must do to the three given equations to get our target equation:

a) First equation: flip it so as to put C_2H_2 on the product side
b) Second equation: multiply it by two to get 2C
c) Third equation: do nothing. We need one H_2 on the reactant side and that's what we have.

Step 2:

Rewrite all three equations with changes applied:

$2CO_2(g) + H_2O(l) \longrightarrow C_2H_2(g) + \frac{5}{2}O_2(g)$ $\Delta H° = +1299.5$ kJ

$2C(s) + 2O_2(g) \longrightarrow 2CO_2(g)$ $\Delta H° = -787$ kJ

$H_2(g) + \frac{1}{2}O_2(g) \longrightarrow H_2O(\ell)$ $\Delta H° = -285.8$ kJ

Notice that the ΔH values changed as well.

Step 3:

Checking for what can be canceled:

$2CO_2$ ⟶ first & second equation

H_2O ⟶ first & third equation

$\frac{5}{2}O_2$ ⟶ first & sum of second and third equation

Step 4:

Add up ΔHº values for our answer:

ΔH° = +1299.5 kJ + (−787 kJ) + (−285.8 kJ) = +**226.7 kJ**

2. Calculate the enthalpy of the following chemical reaction:

$CS_2(l) + 3O_2(g) \longrightarrow CO_2(g) + 2SO_2(g)$

Given:

$C(s) + O_2(g) \longrightarrow CO_2(g)$ ΔH = −393.5 kJ/mol
$S(s) + O_2(g) \longrightarrow SO_2(g)$ ΔH = −296.8 kJ/mol
$C(s) + 2S(s) \longrightarrow CS_2(l)$ ΔH = +87.9 kJ/mol

Step 1:

What to do to the data equations:
a) Leave equation 1 untouched (want CO_2 as a product)
b) Multiply second equation by 2 (want to cancel 2S, also want $2SO_2$ on product side)
c) Flip 3rd equation (want CS_2 as a reactant)

Step 2:

The result:
$C(s) + O_2(g) \longrightarrow CO_2(g)$ ΔH = −393.5 kJ/mol
$2S(s) + 2O_2(g) \longrightarrow 2SO_2(g)$ ΔH = −593.6 kJ/mol ← note multiply by 2 on the ΔH
$CS_2(\ell) \longrightarrow C(s) + 2S(s)$ ΔH = −87.9 kJ/mol ← note sign change on the ΔH

Step 3:

Add the three revised equations. C and 2S will cancel.

ΔHº = [-393.5 kJ/mole – 593.6 kJ/mole -87.9 kJ/mole] = **1075.0 kJ/mole**

3. Given the following data:

$SrO(s) + CO_2(g) \longrightarrow SrCO_3(s)$ $\Delta H = -234$ kJ

$2SrO(s) \longrightarrow 2Sr(s) + O_2(g)$ $\Delta H = +1184$ kJ

$2SrCO_3(s) \longrightarrow 2Sr(s) + 2C(s, gr) + 3O_2(g)$ $\Delta H = +2440$ kJ

Find the ΔH of the following reaction:
$C(s, gr) + O_2(g) \longrightarrow CO_2(g)$

Step 1:

Analyze what must happen to each equation:
a) First equation ⟶ flip it (this put the CO_2 on the right-hand side, where we want it)
b) Second equation⟶ do not flip it, divide through by two (no flip because we need to cancel the SrO, divide by two because we only need to cancel one SrO)
c) Third equation ⟶ flip it (to put the $SrCO_3$ on the other side so we can cancel it), divide by two (since we need to cancel only one $SrCO_3$)

Notice that what we did to the third equation also sets up the Sr to be cancelled. Why not also multiply first equation by two (to get 2SrO for canceling)? Because we only want one CO_2 in the final answer, not two. Notice also that I ignored the oxygen. If everything is right, the oxygen will take care of itself.

Step 2:

Apply all the above changes (notice what happens to the ΔH values):

$SrCO_3(s) \longrightarrow SrO(s) + CO_2(g)$ $\Delta H = +234$ kJ

$SrO(s) \longrightarrow Sr(s) + \frac{1}{2}O_2(g)$ $\Delta H = +592$ kJ

$Sr(s) + C(s, gr) + \frac{3}{2}O_2(g) \longrightarrow SrCO_3(s)$ $\Delta H = -1220$ kJ

Step 3:

Here is a list of what gets eliminated when everything is added:

$SrCO_3$, SrO, Sr, $\frac{1}{2}O_2$
The last one comes from $\frac{3}{2}O_2$ on the left in the third equation and $\frac{1}{2}O_2$ on the right in the second equation.

Step 4:

Add the equations and the ΔH values:

$+234 + (+592) + (-1220) = -394$

$C(s, gr) + O2(g) \longrightarrow CO2(g)$

ΔH° = −394 kJ

4. Given the following information:

$2NO(g) + O_2(g) \longrightarrow 2NO_2(g)$ ΔH = −116 kJ

$2N_2(g) + 5O_2(g) + 2H_2O(l) \longrightarrow 4HNO_3(aq)$ ΔH = −256 kJ

$N_2(g) + O_2(g) \longrightarrow 2NO(g)$ ΔH = +183 kJ

Calculate the enthalpy change for the reaction below:

$3NO_2(g) + H_2O(l) \longrightarrow 2HNO_3(aq) + NO(g)$ ΔH = ???

Step 1:

Analyze what must happen to each equation:

a) First equation ⟶ flip; multiply by $\frac{3}{2}$ (this gives $3NO_2$ as well as the 3NO which will be necessary to get one NO in the final answer)
b) Second equation ⟶ divide by 2 (gives two nitric acid in the final answer)
c) Third equation ⟶ flip (cancels 2NO as well as nitrogen)

Step 2:

Notes on the oxygen atoms:
a) step 1a above puts $\frac{3}{2}O_2$ on the right
b) step 1b puts $\frac{5}{2}O_2$ on the left
c) step 1c puts $\frac{2}{2}O_2$ on the right

In addition, a and c give $\frac{5}{2}O_2$ on the right to cancel out the $\frac{5}{2}O_2$ on the left.

Step 3:

Apply all the changes listed above:

$3NO_2(g) \longrightarrow 3NO(g) + \frac{3}{2}O_2(g)$ ΔH = +174 kJ

$N_2(g) + \frac{5}{2}O_2(g) + H_2O(l) \longrightarrow 2HNO_3(aq)$ ΔH = −128 kJ

$2NO(g) \longrightarrow N_2(g) + O_2(g)$ ΔH = −183 kJ

Step 4:

Add the equations and the ΔH values:
+174 + (−128) + (−183) = −137 kJ

$3NO_2(g) + H_2O(\ell)$ ---> $2HNO_3(aq) + NO(g)$ **ΔH° = −137 kJ**

Use of Enthalpy Diagram using Hess's Law:

Comparison and interpretation of enthalpy changes is materially aided by a graphical construction in which the relative enthalpies of various substances are represented by horizontal lines on a vertical energy scale. The zero of the scale can be placed anywhere, since energies are always arbitrary; it is generally most useful to locate the elements at zero energy, which reflects the convention that their standard enthlapies of formation are zero.

This very simple *enthalpy diagram* for carbon and

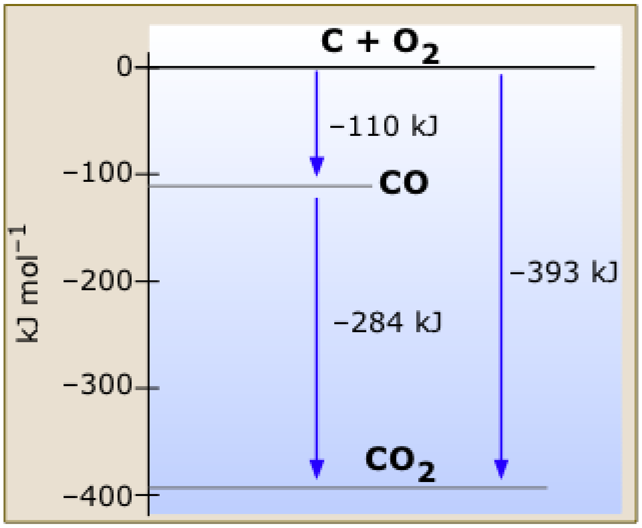


Figure 5.26 Enthalpy Diagram (1)

oxygen and its two stable oxides shows the changes in enthalpy associated with the various reactions this system can undergo. Notice how Hess' law is implicit in this diagram; we can calculate the enthalpy change for the combustion of carbon monoxide to carbon dioxide, for example, by subtraction of the appropriate arrow lengths without writing out the thermochemical equations in a formal way.

The zero-enthalpy reference states refer to graphite, the most stable form of carbon, and gaseous oxygen. All temperatures are 298 K.

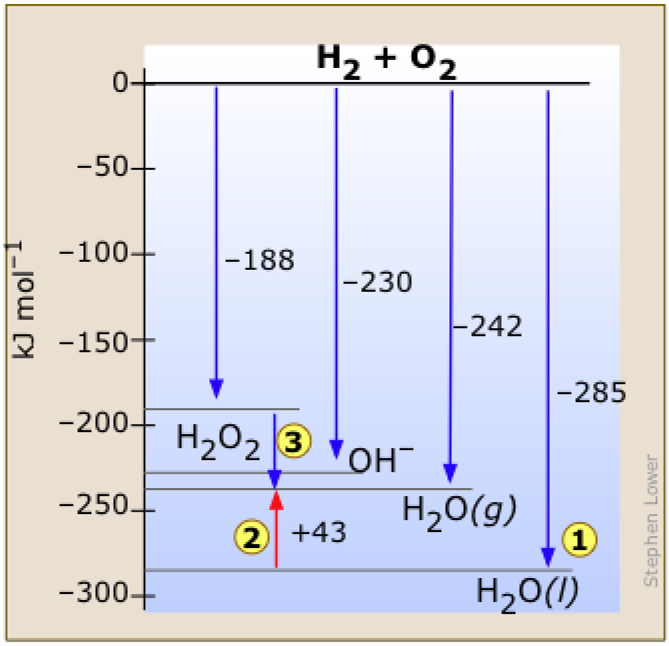


Figure 5.27 Enthalpy Diagram (2)

①

If the H2O is formed in the gaseous state, the energy release will be smaller.

Notice also that...

②

③

has been used to fuel a racing car.

Figure 5.28 Race Cars
Ref: commonswikimedia.org

Why you can't run your car on water ?

You may have heard the venerable urban legend, probably by now over 80 years old, that some obscure inventor discovered a process to do this, but the invention was secretly bought up by the oil companies in order to preserve their monopoly. The enthalpy diagram for the hydrogen-oxygen system shows why this cannot be true — there is simply no known compound of H and O that resides at a lower enthalpy level.

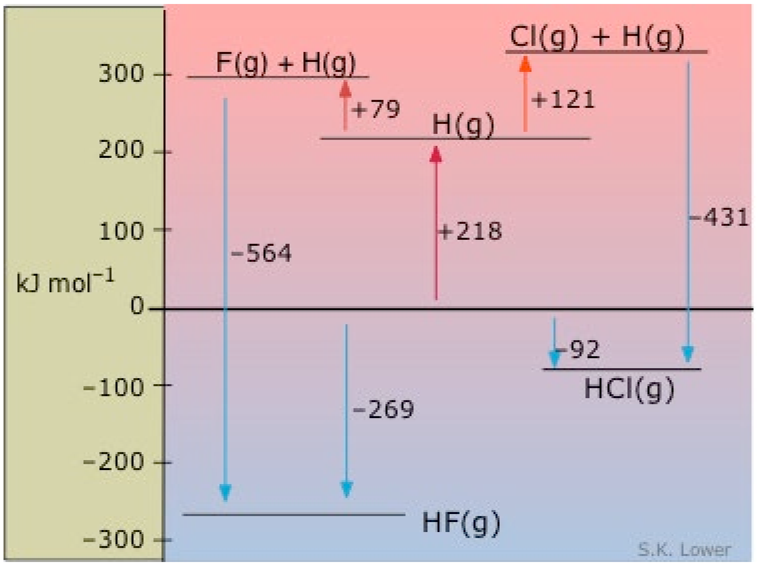


Figure 5.29 Enthalpy Diagram (3)

Enthalpy diagrams are especially useful for comparing groups of substances having some common feature. This one shows the molar enthalpies of species relating to two hydrogen halides, with respect to those of the elements. From this diagram we can see at a glance that the formation of HF from the elements is considerably more exothermic than the corresponding formation of HCl. The upper part of this diagram shows the gaseous atoms at positive enthalpies with respect to the elements. The endothermic processes in which the H2 and the dihalogen are dissociated into atoms can be imagined as taking place in two stages, also shown. From the enthalpy change associated with the dissociation of H_2 (218 kJ mol–1), the dissociation enthalpies of F_2 and Cl_2 can be calculated and placed on the diagram.

How are enthalpy changes determined experimentally?
First, you must understand that the only thermal quantity that can be observed directly is the heat *q* that flows into or out of a reaction vessel, and that *q* is numerically equal to ΔH° only under the special condition of constant pressure. Moreover, *q* is equal to the standard enthalpy change only when the reactants and products are both at the same temperature, normally 25°C.
The measurement of q is generally known as *calorimetry*.

The most common types of calorimeters contain a known quantity of water which absorbs the heat released by the reaction. Because the specific heat capacity of water (4.184 J g–1 K–1) is known to high precision, a measurement of its temperature rise due to the reaction enables one to calculate the quantity of heat released.

The calorimeter constant

In all but the very simplest calorimeters, some of the heat released by the reaction is absorbed by the components of the calorimeter itself. It is therefore necessary to "calibrate" the calorimeter by measuring the temperature change that results from the introduction of a known quantity of heat. The resulting *calorimeter constant*, expressed in J K–1, can be regarded as the “heat capacity of the calorimeter”.

For reactions that can be initiated by combining two solutions, the temperature rise of the solution itself can provide an approximate value of the reaction enthalpy if we assume that the heat capacity of the solution is close to that of the pure water — which will be nearly true if the solutions are dilute.
For example, a very simple calorimetric determination of the standard enthalpy of the reaction H+(aq) + OH–(aq) → H2O(l) could be carried out by combining equal volumes of 0.1M solutions of HCl and of NaOH initially at 25°C. Since this reaction is exothermic, a quantity of heat q will be released into the solution. From the tmperature rise and the specific heat of water, we obtain the number of joules of heat released into each gram of the solution, and q can then be calculated from the mass of the solution. Since the entire process is carried out at constant pressure, we have ΔH° = q. If reactions are carried out in nonstandard conditions then

ΔH= q/mols of limiting reactant

https://www.youtube.com/watch?v=dEfX-nbUMJs

For reactions that cannot be carried out in dilute aqueous solution, the reaction vessel is commonly placed within a larger insulated container of water. During the reaction, heat passes between the inner and outer containers until their temperatures become identical. Again, the temperature change of the water is observed, but in this case we need to know the value of the calorimeter constant described above.

SUPPLEMENTAL

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V. Application

Energy content of fuels

A *fuel* is any substance capable of providing useful amounts of energy through a process that can be carried out in a controlled manner at economical cost. For most practical fuels, the process is combustion in air (in which the oxidizing agent O_2 is available at zero cost.) The *enthalpy of combustion* is obviously an important criterion for a substance's suitability as a fuel, but it is not the only one; a useful fuel must also be easily ignited, and in the case of a fuel intended for self-powered vehicles, its *energy density* in terms of both mass (kJ kg–1) and volume (kJ m–3) must be reasonably large. Thus substances such as methane and propane which are gases at 1 atm must be stored as pressurized liquids for transportation and portable applications.

Energy densities of some common fuels	
Fuel	MJ kg–1
wood (dry)	15
coal (poor)	15
coal (premium)	27
Ethanol	30
petroleum-derived products	45
methane, liquified natural gas	54
hydrogenb	140

Notes on the above table :

a. Ethanol is being strongly promoted as a motor fuel by the U.S. agricultural industry. Note, however, that according to some estimates, it takes 46 MJ of energy to produce 1 kg of ethanol from corn. Some other analyses, which take into account optimal farming practices and the use of by-products arrive at different conclusions; see, for example, this summary with links to several reports.

b. Owing to its low molar mass and high heat of combustion, hydrogen possesses an extraordinarily high energy density, and would be an ideal fuel if its critical temperature (33 K, the temperature above which it cannot exist as a liquid) were not so low. The potential benefits of using hydrogen as a fuel have motivated a great deal of research into other methods of getting a large amount of H2 into a small volume of space. Simply compressing the gas to a very high pressure is not practical because the weight of the heavy-walled steel vessel required to withstand the pressure would increase the effective weight of the fuel to an unacceptably large value. One scheme that has shown some promise exploits the ability of H2 to "dissolve" in certain transition metals. The hydrogen can be recovered from the resulting solid solution (actually a loosely-bound compound) by heating.

Energy content of foods

What, exactly, is meant by the statement that a particular food "contains 1200 calories" per serving? This simply refers to the standard enthalpy of combustion of the foodstuff, as measured in a *bomb calorimeter*. Note, however, that in nutritional usage, the calorie is really a kilocalorie (sometimes called "large calorie"), that is, 4184 J. Although this unit is still employed in the popular literature, the SI unit is now commonly used in the scientific and clinical literature, in which energy contents of foods are usually quoted in kJ per unit of weight.

Although the mechanisms of oxidation of a carbohydrate such as glucose to carbon dioxide and water in a bomb calorimeter and in the body are complex and entirely different, the net reaction involves the same initial and final states, and must be the same for any possible pathway:

$C_6H_{12}O_6 + 6\ O_2 \rightarrow 6\ CO_2 + 6\ H_2O \quad \Delta H° – 20.8\ \text{kJ mol}^{-1}$

Glucose is a *sugar*, a breakdown product of *starch*, and is the most important energy source at the cellular level; fats, proteins, and other sugars are readily converted to glucose. By writing balanced equations for the combustion of sugars, fats, and proteins, a comparison of their relative energy contents can be made. The stoichiometry of each reaction gives the amounts of oxygen taken up and released when a given amount of each kind of food is oxidized; these gas volumes are often taken as indirect measures of energy consumption and metabolic activity; a commonly-accepted value that seems to apply to a variety of food sources is 20.1 J (4.8 kcal) per liter of O2 consumed.

For some components of food, particularly proteins, oxidation may not always be complete in the body, so the energy that is actually available will be smaller than that given by the heat of combustion. Mammals, for example, are unable to break down cellulose (a polymer of sugar) at all; animals that derive a major part of their nutrition from grass and leaves must rely on the action of symbiotic bacteria which colonize their digestive tracts.

The amount of energy available from a food can be found by measuring the heat of combustion of the waste products excreted by an organism that has been restricted to a controlled diet, and subtracting this from the heat of combustion of the food.

Energy content and availability of the major food components			
type of food	food	ΔH°, kJ g–1	percent availability
Protein	meat	22.4	92
	egg	23.4	
Fat	butter	38.2	
	animal fat	39.2	95
Carbohydrate	starch	17.2	
	glucose (sugar)	15.5	99
	ethanol	29.7	100

The amount of energy an animal requires depends on the age, sex, surface area of the body, and of course on the amount of physical activity. The rate at which energy is expended is expressed in watts: 1 W = 1 J sec–1. For humans, this value varies from about 200-800 W. This translates into daily food intakes having energy equivalents of about 10-15 MJ for most working adults. In order to just maintain weight in the absence of any physical activity, about 6 MJ per day is required.

Metabolic rates of some animals		
animal	kJ hr–1	kJ kg–1hr–1
mouse	82	17
cat	34	6.8

dog	78	3.3
sheep	193	2.2
human	300	2.1
horse	1430	1.1
elephant	5380	0.7

https://www.youtube.com/watch?v=FQyFHurneZ4
Calorimetry of Cheeto

The above table is instructive in that although larger animals consume more energy, the energy consumption *per unit of body weight* decreases with size. This reflects the fact the rate of heat loss to the environment depends largely on the surface area of an animal, which increases with mass at a greater rate than does an animal's volume ("size").

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Questions and Answers:

1. Decide whether each of these reactions is exothermic or endothermic:

When two chemicals mix their temperature rises:
a) Exothermic
b) Endothermic
c) None of Above

Answer: A

2. Decide whether each of these reactions is exothermic or endothermic:

A solid burns brightly and releases heat, light and sound:
- a) Exothermic
- b) Endothermic
- c) None of Above

Answer: A

3. Decide whether each of these reactions is exothermic or endothermic:

When two chemicals are mixed their temperature drops:
a) Exothermic
b) Endothermic
c) None of the above

Answer: B

3. Decide whether each of these reactions is exothermic or endothermic:

Two chemicals will only react if you heat them continually:
a) Exothermic
b) Endothermic
c) None of the above

Answer: B

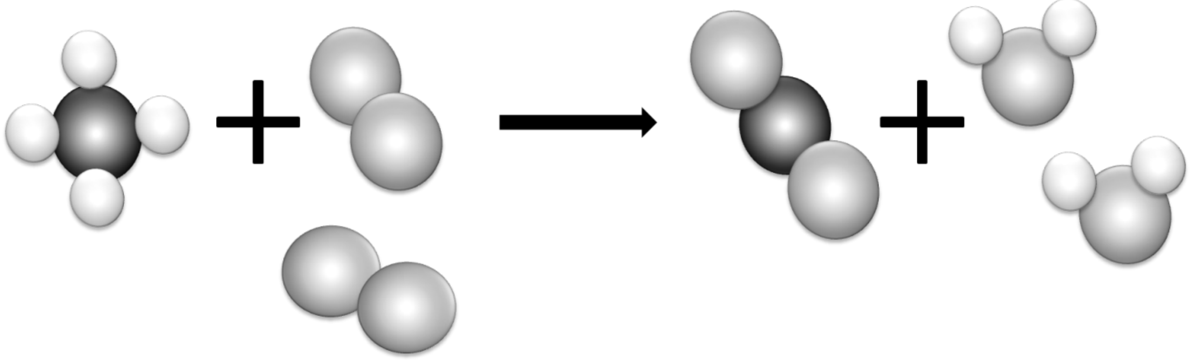
4. Decide whether each of these reactions is exothermic or endothermic:

Plants take in light energy for photosynthesis:
a) Exothermic
b) Endothermic
c) None of the above

Answer: B

5. Most reactions involve bond breaking and bond making. This equation shows what happens when methane (CH_4) burns in oxygen (O_2).

$$CH_4 \quad + \quad 2\ O_2 \quad \longrightarrow \quad CO_2 \quad + \quad 2\ H_2O$$

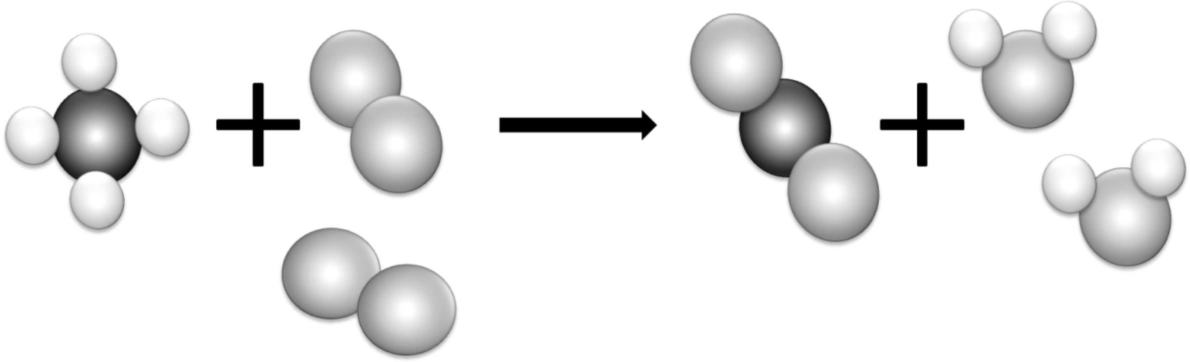


How many bonds are broken between Carbon and Hydrogen atoms?
a) 1
b) 2
c) 3
d) 4
e) None of the above

Answer: D

6. Most reactions involve bond breaking and bond making. This equation shows what happens when methane (CH_4) burns in oxygen (O_2).

$$CH_4 \quad + \quad 2\ O_2 \quad \longrightarrow \quad CO_2 \quad + \quad 2\ H_2O$$



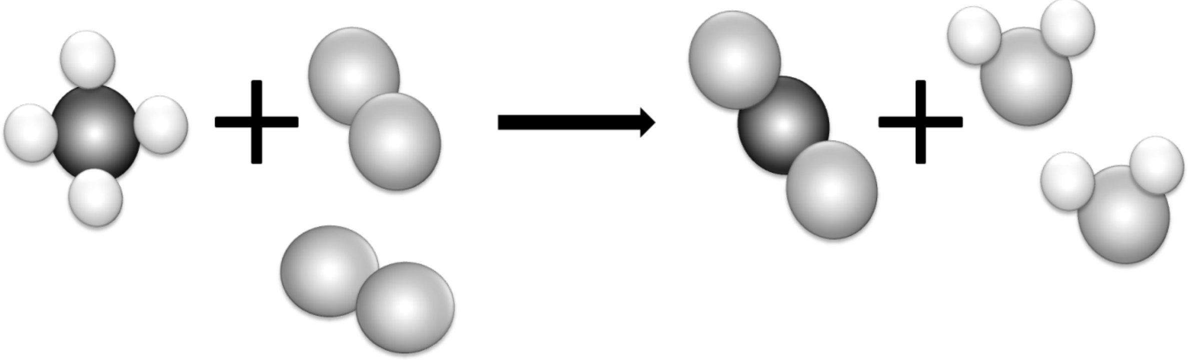
How many bonds are broken between Oxygen atoms?

a) 1
b) 2
c) 3
d) 4
e) None of the above

Answer: B

7. Most reactions involve bond breaking and bond making. This equation shows what happens when methane (CH_4) burns in oxygen (O_2).

$$CH_4 \quad + \quad 2\ O_2 \quad \longrightarrow \quad CO_2 \quad + \quad 2\ H_2O$$



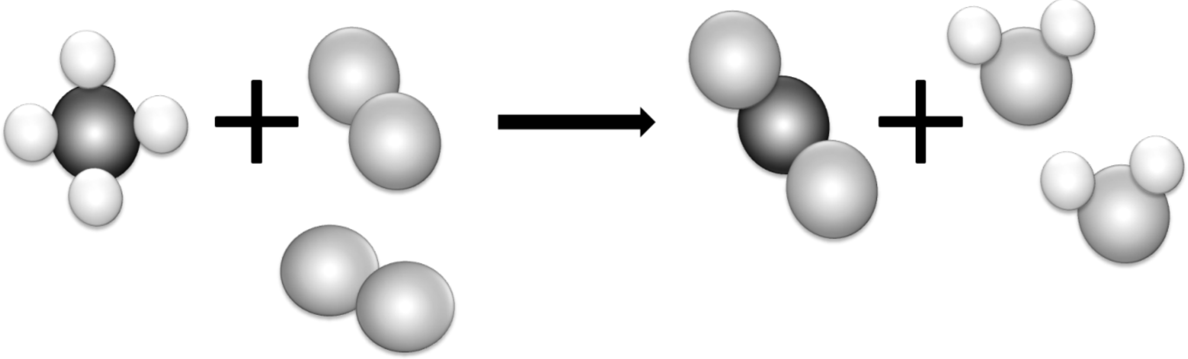
How many bonds are broken between Oxygen atoms?

a) 1
b) 2
c) 3
d) 4
e) None of the above

Answer: B

8. Most reactions involve bond breaking and bond making. This equation shows what happens when methane (CH_4) burns in oxygen (O_2).

$$CH_4 \quad + \quad 2\ O_2 \quad \longrightarrow \quad CO_2 \quad + \quad 2\ H_2O$$



How many bonds are broken between Hydrogen and Oxygen atoms?

a) 1
b) 2
c) 3
d) 4
e) None of the above

Answer: D

9. A chemical reaction has an enthalpy of - 535 kJ /mole
The reaction is:
a) Endothermic
b) Exothermic
c) None of above

Answer: B

10. The complete combustion of methanol proceeds according to the equation:

$$2\ CH_3OH + 3\ O_2 \longrightarrow 2\ CO_2 + 4\ H_2O$$

The reaction enthalpy is −715 kJ/mole. Is the combustion of methanol?
a) Exothermic
b) Endothermic
c) None of the above

Answer: A

11. The temperature of 335 g of water changed from 24.5°C to 26.4°C. How much heat did this sample absorb? Specific heat for water = 4.18 J / g x °C

a) 2.00 kJ
b) 2.66 kJ
c) 3.55 kJ
d) 4.67 kJ
e) 5.13 kJ

Answer: B

12. 12. How much heat in kilojoules has to be removed from 225 g of water to lower its temperature from 25.0 °C to 10.0 °C?

a) - 12.0 kJ
b) - 15.6 kJ
c) - 14.1 kJ
d) - 10.7 kJ
e) -.13.9 kJ

Answer: C

13. To bring 1.0 kg of water from 25 °C to 99 °C takes how much heat input?

a) 309 kJ
b) 505 kJ
c) 983 kJ
d) 256 kJ
e) 794 kJ

Answer: A

14. An insulated cup contains 75.0 g of water at 24.00 °C. A 26.00 g sample of metal at 82.25 °C is added. The final temperature of the water and metal is 28.34 °C. What is the specific heat of the metal?

a) 0.755 J / g x °C
b) 0.823 J / g x °C
c) 0.971 J / g x °C
d) 0.235 J / g x °C
e) 0.765 J / g x °C

Answer: C

15. A calorimeter has a heat capacity of 1265 J / °C. A reaction causes the temperature of the calorimeter to change from 22.34 °C to 25.12 °C. How many joules of heat were released in this process?

a) - 3.09 kJ
b) - 5.05 kJ
c) - 9.83 kJ
d) - 2.56 kJ
e) - 3.25 kJ

Answer: E

16. What is the specific heat of silicon if it takes 192J to raise the temperature of 45.0 g of Si by 6.0 °C?

a) 0.65 J / g x °C
b) 0.79 J / g x °C
c) 0.85 J / g x °C
d) 0.71 J / g x °C
e) 0.54 J / g x °C

Answer: D

17. Aqueous silver ion reacts with aqueous chloride ion to yield a white precipitate of solid silver chloride. When 10.0 mL of 1.00 M $AgNO_3$ solution is added to 10.0 mL of 1.00 M NaCl solution at 25 °C in a calorimeter a white precipitate of AgCl forms and the temperature of the aqueous mixture increases to 32.6 °C. Assuming that the specific heat of the aqueous mixture is 4.18 J / g x °C, that the density of the mixture is 1.00 g / mL, and that the calorimeter itself absorbs a negligible amount of heat, calculate the amount of heat absorbed in kJ / mol of Ag^+.

a) - 64 kJ / mole
b) - 59 kJ / mole
c) - 98 kJ / mole
d) - 25 kJ / mole
e) - 38 kJ / mole

Answer: A

18. Assuming that Coca Cola has the same specific heat as water (4.18 J / g x °C), calculate the amount of heat in kJ transferred when one can (about 350 g) is cooled from 25 °C to 3 °C .

a) 32.2 kJ of heat transferred
b) 92.7 kJ of heat transferred
c) 49.8 kJ of heat transferred
d) 32.6 kJ of heat transferred
e) 20.5 kJ of heat transferred

Answer: A

19. What is the specific heat of lead if it takes 96 J to raise the temperature of a 75 g block by 10 °C?

a) 0.651 J / g x °C
b) 0.792 J / g x °C
c) 0.855 J / g x °C
d) 0.128 J / g x °C
e) 0.545 J / g x °C

Answer: D

20. When 25 mL of 1.0 M H_2SO_4 is added to 50 mL of 1.0 M NaOH at 25 °C in a calorimeter, the temperature of the aqueous solution increases to 33.9 °C. Assuming that the specific heat of the solution is 4.18 J /g x °C, that its density is 1.00 / mL, and that the calorimeter itself absorbs a negligible amount of heat, calculate the amount of heat absorbed for the reaction.

a) 3.09 kJ heat absorbed
b) 5.05 kJ heat absorbed
c) 9.83 kJ heat absorbed
d) 2.56 kJ heat absorbed
e) 2.79 kJ heat absorbed

Answer: E

21. Titanium metal is used as a structural material in many high-tech applications such as jet engines. What is the specific heat of titanium in J / g x °C if it takes 89.7 J to raise the temperature of a 33.0 g block by 5.20 °C? What is the molar heat capacity of titanium in J / mol x °C?

a) 90.0 J / mol x °C
b) 13.0 J / mol x °C
c) 25.0 J / mol x °C
d) 38.0 J / mol x °C
e) 42.0 J / mol x °C

Answer: C

22. Sodium metal is sometimes used as a cooling agent in heat exchange units because of its relatively high molar heat capacity of 28.2 J / mol x °C. What is the specific heat of sodium in J / g x °C?

a) 3.25 J / g x ^{o}C
b) 4.23 J / g x ^{o}C
c) 3.55 J / g x ^{o}C
d) 1.23 J / g x ^{o}C
e) 2.55 J / g x ^{o}C

Answer: D

23. Compound A is burned in a bomb calorimeter that contains 2.50 liters of water. If the combustion of 0.175 moles of this compound causes the temperature of the water to rise 45.0 ^{0}C, what is the molar heat of combustion of compound A?

a) 2.70 kJ / mole
b) 3.85 kJ / mole
c) 4.45 kJ / mole
d) 1.25 kJ /mole
e) 5.23 kJ / mole

Answer: A

24. Compound B is burned in a bomb calorimeter that contains 1.50 L of water. When one had burned 50.0 g of compound B in the calorimeter, the temperature rise of the water in the calorimeter was 35.0 ^{0}C. If the heat of combustion of compound B is 2,150 kJ / mol, what is the molar mass of compound B?

a) 612 g / mole
b) 385 g / mole
c) 250 g / mole
d) 645 g / mole
e) 539 g / mole

Answer: E

25. The molar heat of combustion of compound q is 1,250 kJ / mol. If I were to burn 0.115 moles of this compound in a bomb calorimeter with a reservoir that holds 2.50 L of water, what would the expected temperature increase be?

a) 17.40 ^{o}C
b) 13.80 ^{o}C
c) 15.90 ^{o}C

d) 16.70 °C
e) 19.50 °C

Answer: B

26. Compound A is burned in a bomb calorimeter that contains 2.50 L of water. If the combustion of 0.175 moles of this compound causes the temperature of the water to rise 45.0 ^{0}C, what is the molar heat of combustion of compound A (in kJ/mole)? The heat capacity of water is 4.18 J / g x ^{0}C.

a) -2.69 x 10^3 kJ / mole
b) -3.75 x 10^3 kJ / mole
c) -2.83 x 10^3 kJ / mole
d) -9.86 x 10^3 kJ / mole
e) -5.21 x 10^3 kJ / mole

Answer: A

27. Compound B is burned in a bomb calorimeter that contains 1.50 L of water. When I burned 50.0 g of compound B in the calorimeter, the temperature rise of the water in the calorimeter was 35.0 ^{0}C. If the heat of combustion of compound B is 2150 kJ / mole, what is the molar mass of compound B? The heat capacity of water is 4.18 J / g x ^{0}C.

a) 353. g / mole
b) 545. g / mole
c) 490. g / mole
d) 752. g / mole
e) 609 g / mole

Answer: C

28. A calorimeter was calibrated with an electric heater, which supplied 22.5 kJ of energy to the calorimeter and increased the temperature of the calorimeter and its water from 22.45 ^{0}C to 23.97 ^{0}C. What is the heat capacity of the calorimeter?

a) 26.1 kJ / ^{0}C
b) 35.4 kJ / ^{0}C
c) 14.6 kJ / ^{0}C
d) 34.9 kJ / ^{0}C
e) 14.8 kJ / ^{0}C

Answer: E

29. When 0.113 g of benzene, C_6H_6, burns in excess oxygen in a calibrated constant- pressure calorimeter with a heat capacity of 551 J / ^{0}C, the temperature of the calorimeter rises by 8.60 ^{0}C. Write the thermochemical equation and calculate the reaction enthalpy for the combustion of benzene (which yields carbon dioxide vapor and liquid water).

a) C_6H_6 (l) + 15/2 O_2 ⟶ 6 CO_2(g) + $3H_2O$(l) $\Delta H = -9260$ kJ
b) C_6H_6 (l) + 15/2 O_2 ⟶ 6 CO_2(g) + $3H_2O$(l) $\Delta H = -8250$ kJ
c) C_6H_6 (l) + 15/2 O_2 ⟶ 6 CO_2(g) + $3H_2O$(l) $\Delta H = -5212$ kJ

d) C_6H_6 (l) + 15/2 O_2 ⟶ 6 $CO_2(g)$ + $3H_2O(l)$ $\Delta H = -3270$ kJ
e) C_6H_6 (l) + 15/2 O_2 ⟶ 6 $CO_2(g)$ + $3H_2O(l)$ $\Delta H = -7270$ kJ

Answer: D

30. The value of ΔH^o for the reaction below is +128.1 kJ:
CH_3OH (l) ⟶ CO (g) + $2H_2$ (g)
How many kJ of heat are consumed when 5.10 g of $H_2(g)$ is formed as shown in the equation?

a) 653 kJ
b) 62.0 kJ
c) 324 kJ
d) 162 kJ

Answer: D

31. The value of ΔH^o for the reaction below is +128.1 kJ:
CH_3OH (l) ⟶ CO (g) + $2H_2$ (g)
How many kJ of heat are consumed when 5.10 g of CO(g) is formed as shown in the equation?

a) 533 kJ
b) 32.3 kJ
c) 43.1 kJ
d) 29.5 kJ

Answer: B

32. The value of ΔH^o for the reaction below is -1107 kJ:
2Ba (s) + O_2 (g) ⟶ 2 BaO (s)
How many kJ of heat are released when 5.75 g of BaO (s) is produced?

a) 20.8 kJ
b) 30.3 kJ
c) 40.1 kJ
d) 50.5 kJ

Answer: A

33. A sample of aluminum metal absorbs 9.86 J of heat, calculate the mass sample if it is heated from 23.2 ^oC to 30.5 ^oC. Since the specific heat capacity of aluminum is 0.90 J / g x ^oC.

a) 4.73 g
b) 3.46 g
c) 1.50 g
d) 2.80 g

Answer: C

34. Calculate $\Delta H_{(reaction)}$ for the reaction: C_2H_4 (g) + H_2 (g) $\longrightarrow$ C_2H_6 (g), from the following data.
C_2H_4 (g) + 3 O_2 (g) $\longrightarrow$ 2 CO_2 (g) + 2 H_2O (l) ΔH = -1411. kJ / mole
C_2H_6 (g) + 7/2 O_2 (g) $\longrightarrow$ 2 CO_2 (g) + 3 H_2O (l) ΔH = -1560. kJ / mole
H_2 (g) + 1/2 O_2 (g) $\longrightarrow$ H_2O (l) ΔH = -285.8 kJ / mole

a) -242 kJ
b) -137 kJ
c) -40.1 kJ
d) -150. kJ

Answer: B

35. Calculate $\Delta H_{(reaction)}$ for the reaction: 4 NH_3 (g) + 5 O_2 (g) $\longrightarrow$ 4 NO (g) + 6 H_2O (g), from the following data.
N_2 (g) + O_2 (g) $\longrightarrow$ 2 NO (g) ΔH = -180.5 kJ / mole
N_2 (g) + 3 H_2 (g) $\longrightarrow$ 2 NH_3 (g) ΔH = -91.8 kJ / mole
2 H_2 (g) + O_2 (g) $\longrightarrow$ 2 H_2O (g) ΔH = -483.6 kJ / mole

a) -1425 kJ
b) -1375 kJ
c) -1628. kJ
d) -1983. kJ

Answer: C

36. Find ΔH_f^0 for acetic acid, $HC_2H_3O_2$, using the following thermochemical data.
$HC_2H_3O_2$ (l) + 2 O_2 (g) $\longrightarrow$ 2 CO_2 (g) + 2 H_2O (l) ΔH = -875. kJ / mole
C (s, graphite) + O_2 (g) $\longrightarrow$ CO_2 (g) ΔH = -394.51 kJ / mole
H_2 (g) + 1/2 O_2 (g) $\longrightarrow$ H_2O (l) ΔH = -285.8 kJ / mole

a) -525 kJ
b) -375 kJ
c) -628. kJ
d) -486. kJ

Answer: D

37. Calculate ΔH for the reaction CH_4 (g) + NH_3 (g) $\longrightarrow$ HCN (g) + 3 H_2 (g), from the reactions.
N_2 (g) + 3 H_2 (g) $\longrightarrow$ 2 NH_3 (g) ΔH = -91.8 kJ / mole
C (s, graphite) + 2 H_2 (g) $\longrightarrow$ CH_4 (g) ΔH = -74.9 kJ / mole
H_2 (g) + 2 C (s, graphite) + N_2 (g) $\longrightarrow$ 2 HCN (g) ΔH = +270.3 kJ / mole

a) +256.0 kJ
b) + 1853 kJ
c) + 3421.kJ
d) + 1972 kJ

Answer: A

38. Calculate ΔH for the reaction $2\ Al\ (s) + 3\ Cl_2\ (g) \longrightarrow 2\ AlCl_3\ (s)$ from the following data.

$2\ Al\ (s) + 6\ HCl\ (aq) \longrightarrow 2\ AlCl_3\ (aq) + 3\ H_2\ (g)$	ΔH = -1049. kJ / mole
$HCl\ (g) \longrightarrow HCl\ (aq)$	ΔH = -74.8 kJ /mole
$H_2\ (g) + Cl_2\ (g) \longrightarrow 2\ HCl\ (g)$	ΔH = -1845. kJ / mole
$AlCl_3\ (s) \longrightarrow AlCl_3\ (aq)$	ΔH = -323. kJ /mole

a) +459 kJ
b) -7812 kJ
c) -5348 kJ
d) -6387 kJ

Answer: D

39. If 0.315 moles of hexane (C_6H_{14}) is combusted in a bomb calorimeter containing 5.65 liters of water, calculate the molar heat of combustion of hexane if the water temperature rises 55.4 °C? The specific heat capacity of water is 4.184 J/g °C.

a) 4160 kJ / mole
b) 5893 kJ / mole
c) 6812 kJ / mole
d) 7356 kJ / mole

Answer: A

40. If 22.0 grams of propane (C_3H_8) is combusted in a bomb calorimeter containing 3.25 liters of water, calculate the molar heat of combustion of propane if the water temperature rises 29.5 °C?

a) -160 kJ / mole
b) -587 kJ / mole
c) -872 kJ / mole
d) -802 kJ / mole

Answer: D

41. When 1.38 g of liquid PCl_3 at 25.55 °C is added to 1.00×10^2 g of water at
25.55 °C in a 'coffee-cup' calorimeter, the temperature of the resulting solution increases to 32.00 °C. If the specific heat capacity of the solution is 4.184 J/°Cg, and the heat capacity of the Styrofoam cup is negligible, calculate the molar heat of solution of PCl_3 in water.

a) -170 kJ / mole
b) -271 kJ / mole
c) -398 kJ / mole
d) -802 kJ / mole

Answer: B

42. A 'coffee-cup' calorimeter contains 150g of water at 24.6 °C. A 110 g block of molybdenum metal is heated to 100 °C and then placed in the water in the calorimeter. The contents of the calorimeter come to an average temperature of 28.0 °C. What is the specific heat capacity of the molybdenum metal if the specific heat capacity of water is assumed to be 4.184 J / °C x g**?**

a) 0.34 J / g x °C
b) 0.46 J / g x °C
c) 0.39 J / g x °C
d) 0.18 J / g x °C
e) 0.27 J / g x °C

Answer: E

43. When a 0.235 g sample of benzoic acid, $C_7H_6O_2$, is combusted in a bomb calorimeter, a 3.62 °C rise in temperature occurs. When a 0.305 g sample of citric acid, $C_6H_8O_7$, is burned, a 1.83 °C temperature rise is observed. If the heat of combustion of benzoic acid is 26.38 kJ / g, what is the molar heat of combustion of citric acid?

a) -1476 kJ / mole
b) -2093 kJ / mole
c) -1620 kJ / mole
d) -1780 kJ / mole
e) -1970 kJ / mole

Answer: E

44. The branch of science dealing with the study of the flow of energy is called:

a) kinesiology
b) thermodynamics
c) ergodynamics
d) ergonomics

Answer: B

45. When heat flows into a closed system, its internal energy tends to ………

Answer: increase

46. A process that occurs without heat transfer between a system and its surroundings is called a/an ……..

Answer: adiabatic process.

47. One way of achieving an adiabatic process is by isolating a system from its surroundings.
A system's internal energy is 20 Joules. 30 Joules of work is done on the system in an adiabatic process. What is the system's resultant internal energy?

a) 20 Joules
b) 30 Joules
c) 50 Joules
d) 50 Joules minus dissipated heat

Answer: C

48. Compressing a gas can be considered to be the work done on the gas.

a) True
b) False

Answer: True

49. What is the assumption made by the Zeroth Law of Thermodynamics?

Answer: If two systems are in thermal equilibrium with a third system, they must be in thermal equilibrium with each other.

50. The first law of thermodynamics states that

a) components of a system interact.
b) entropy of a closed system always increases.
c) a closed system always shifts toward disorder or homogeneity.
d) energy is always conserved.

Answer: D

51. The change in the internal energy of a closed system is equal to the amount of heat supplied to the system, minus

a) the amount of heat that is not conserved.
b) the amount of work done by the system on its surroundings.
c) the original internal energy.
d) the volume difference

Answer: B

52. A closed system's internal energy is 30 Joules. Some heat is supplied to it, and it does 20 Joules of work. After this, the closed system's internal energy is 80 Joules. How many Joules of heat were added to the system?

a) 50
b) 60
c) 70
d) 80

Answer: C

53. Which of the following equations is used to represent the First Law of Thermodynamics for a closed system, according to the IUPAC convention?

a) $\Delta U = Q+W$
b) $\Delta U = W-Q$
c) $\Delta U = Q-W$
d) $\Delta U = Q+2W$

Answer: A

54. Which of the following systems does not allow for energy or matter to be exchanged with the surroundings?

a) Open
b) Closed
c) Adiabatic
d) Isolated

Answer: D

55. Which of the following systems only allows for the exchange of energy with the surroundings?

a) Closed
b) Isolated
c) Open
d) None of the above

Answer: A

56. Which system permits energy and matter to be exchanged with the surroundings?

a) Isolated
b) Open
c) Adiabatic
d) Closed

Answer: B

57. In which of the following cases would ΔU
in $\Delta U = Q+W$
be less than zero?

a) Work is done on the system.
b) Work is done by the system.
c) The magnitudes of heat and work are equivalent.
d) The magnitude of heat is greater than that of the work.

Answer: B

58. Which equation is associated with heat in a system that is thermally isolated?

a) $Q < 0$
b) $Q > 0$
c) $Q > W$
d) $Q = 0$

Answer: D

59. Which of the following expressions correctly characterizes an isolated system?

a) $\Delta U < 0$

b) $\Delta U = 0$
c) $\Delta U > 0$
d) None of the above

Answer: B

60. If a process is endothermic, the value of q is less than zero.

a) True
b) False

Answer: B

CHAPTER 6: Electronic Structure and Periodic Properties of Elements

6. Electronic Structure and Periodic Properties of Elements

The study of chemistry must at some point extend to the molecular level, for the physical and chemical properties of a substance that are ultimately explained in terms of the structure and bonding of molecules. This module introduces some basic facts and principles that are needed for a discussion of organic molecules.

Electron configuration or electronic structure of the periodic table elements holds the key to the chemical world in chemistry. Our present-day form of chemical bonding and their properties better understanding by **electronic configuration** formula of elements. A chemical reaction is the change of electron configuration of reactant atoms. Therefore, our inorganic chemistry study of chemicals based on the electronic structure. To find the electron configuration first we find the energy of an electron in s, p, d, and f orbitals or sub-levels, for example, 3s orbital has lower energy than 3p orbitals which again lower energy than 3d level.

6.1 Electromagnetic Energy

Electromagnetic energy is a term used to describe all the different kinds of **energies** released into space by stars such as the Sun. These kinds of **energies** include some that you will recognize and some that will sound strange. They include

- Radio Wave
- Radar waves
- TV wavee
- Heat (infrared radiation)
- Light
- Ultraviolet Light (This is what causes Sunburns)
- X-rays (Just like the kind you get at the doctor's office)
- Short waves
- Microwaves, like in a microwave oven
- Gamma Rays

All these waves do different things (for example, light waves make things visible to the human eye, while heat waves make molecules move and warm up, and x rays can pass through a person and land on film, allowing us to take a picture inside someone's body) but they have some things in common.

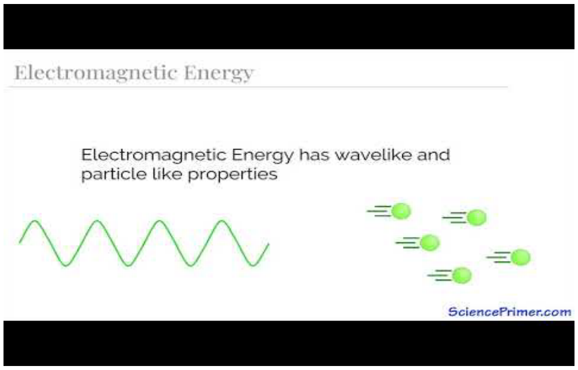
They all travel in waves, like the waves at a beach or like sound waves, and also are made of tiny particles. Scientists are unsure of exactly how the waves and the particles relate to each other. The fact that electromagnetic radiation travels in waves lets us measure the different kind by wavelength or how long the waves are. That is one way we can tell the kinds of radiation apart from each other.

Although all kinds of electromagnetic radiation are released from the Sun, our atmosphere stops some kinds from getting to us. For example, the ozone layer stops a lot of harmful ultraviolet radiation from getting to us, and that's why people are so concerned about the hole in it.

We humans have learned uses for a lot of different kinds of electromagnetic radiation and have learned how to make it using other kinds of energy when we need to. DS1 would not be able to communicate with Earth, for example, if it could not produce radio waves.

The nature of light has been a subject of inquiry since antiquity. In the seventeenth century, Isaac Newton performed experiments with lenses and prisms and was able to demonstrate that white light consists of the individual colors of the rainbow combined together. Newton explained his optics findings in terms of a "corpuscular" view of light, in which light was composed of streams of extremely tiny particles travelling at high speeds according to Newton's laws of motion. Others in the seventeenth century, such as Christiaan Huygens, had shown that optical phenomena such as reflection and refraction could be equally well explained in terms of light as waves travelling at high speed through a medium called "*luminiferous aether*" that was thought to permeate all space. Early in the nineteenth century, Thomas Young demonstrated that light passing through narrow, closely spaced slits produced interference patterns that could not be explained in terms of Newtonian particles but could be easily explained in terms of waves. Later in the nineteenth century, after James

Clerk Maxwell developed his theory of **electromagnetic radiation** and showed that light was the visible part of a vast spectrum of electromagnetic waves, the particle view of light became thoroughly discredited. By the end of the nineteenth century, scientists viewed the physical universe as roughly comprising two separate domains: matter composed of particles moving according to Newton's laws of motion, and electromagnetic radiation consisting of waves governed by Maxwell's equations. Today, these domains are referred to as classical mechanics and classical electrodynamics (or classical electromagnetism). Although there were a few physical phenomena that could not be explained within this framework, scientists at that time were so confident of the overall soundness of this framework that they viewed these aberrations as puzzling paradoxes that would ultimately be resolved somehow within this framework. As we shall see, these paradoxes led to a contemporary framework that intimately connects particles and waves at a fundamental level called wave-particle duality, which has superseded the classical view.



Electromagnetic Energy

Electromagnetic Energy has wavelike and particle like properties

Reference: https://www.youtube.com/watch?v=09vGnzlXlS0

Energy

Energy travels through space or material. This is obvious when you stand near a fire and feel its warmth or when you pick up the handle of a metal pot even though the handle is not sitting directly on the hot stove. Invisible energy waves can travel through air, glass, and even the vacuum of outer space. These waves have electrical and magnetic properties, so they are called **electromagnetic waves**. The transfer of energy from one object to another through electromagnetic waves is known as **radiation**.

Different wavelengths of energy create different types of electromagnetic waves (**Figure** below).

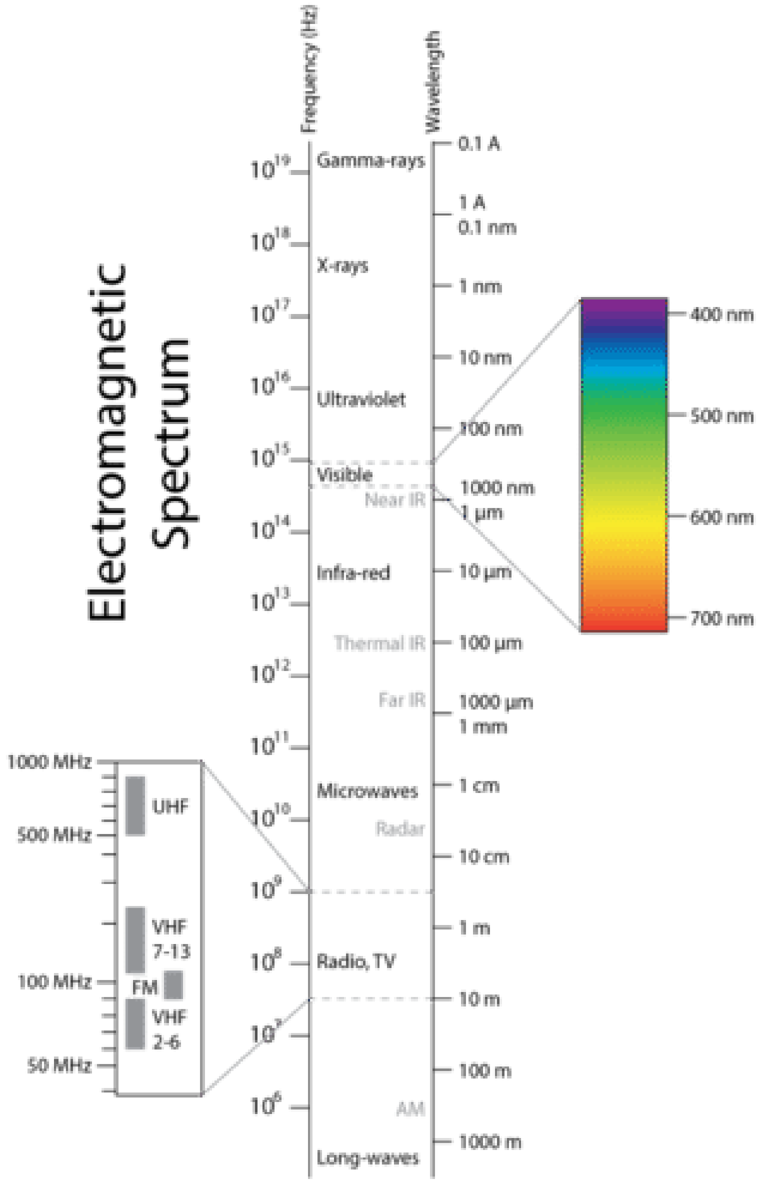


Figure-6.1: The electromagnetic spectrum; short wavelengths are the fastest with the highest energy

Ref: common.wikimedia.org/

Speed of all Electromagnetic Spectrum Waves (c) = 3.0×10^8 m/s = speed of light.

c (m/s) = $\nu \times \lambda$ = speed of light or speed of all electromagnetic spectrum waves

ν (Hz) = c / λ = frequency

λ (m) = c / ν = wavelength

Note that the unit Hz = 1/s (inverse of the seconds)

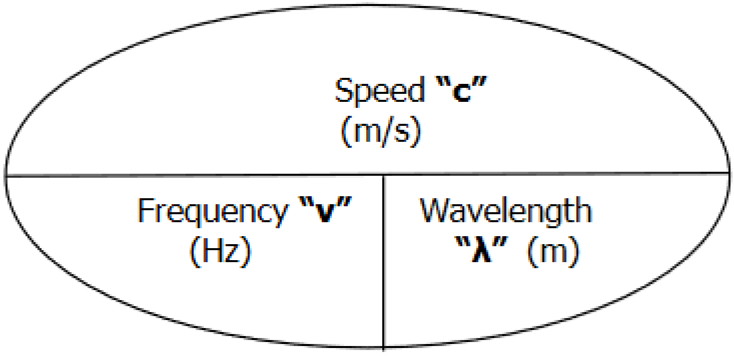


Figure 6.2 Relationship between Frequency, Wavelength & Velocity
Ref: Commons.wikimedia.org/

Examples:

a. Violet light has a wavelength of 4.10 x 10^{-12} m. What is the frequency?

ν (Hz) = c / λ = frequency = [3.0 x 10^{8} m/s] / [4.10 x 10^{-12} m] = 7.31 x 10^{19} Hz

b. Green light has a frequency of 6.01 x 1014Hz. What is the wavelength?

λ (m) = c / ν = wavelength = [3.0 x 10^{8} m/s] / [6.01 x 10^{14} Hz] = 4.99 x 10^{-7} m

The energy of the electromagnetic spectrum can be calculated using the formula below:

Energy (J) = h x ν

h (Planck's Constant) = 6.626 x 10^{-34}J.s

ν (Hz) = c / λ = frequency

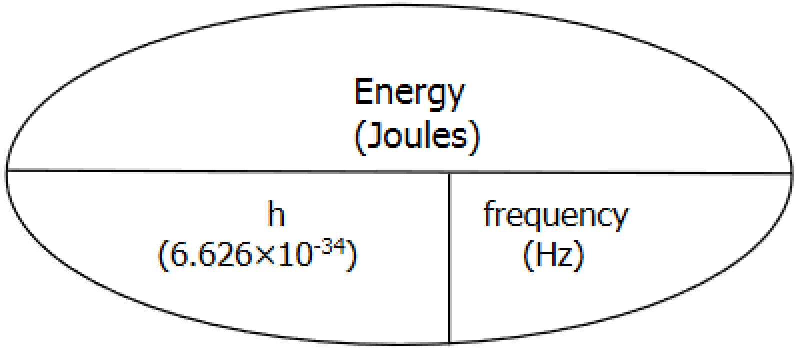


Figure 6.3 Relationship between Frequency, & Energy

Ref: Commons.wikimedia.org/

Examples:

a. Calculate the energy of a photon of radiation with a frequency of 8.5×10^{14}Hz

Energy (J) = $h \times \nu = [\,6.626 \times 10^{-34}\text{J.s}\,] \times [\,8.5 \times 10^{14}\text{Hz}\,] = 5.63 \times 10^{-19}$ J

b. Calculate the energy of a photon of radiation with a wavelength of 6.4×10^{-7}m

Energy (J) = $h \times \nu = h \times [\,c / \lambda\,] = [\,6.626 \times 10^{-34}\text{J.s}\,] \times [\,(3.0 \times 10^{8}\text{ m/s}) / (6.4 \times 10^{-7}\text{m})\,] = 3.1 \times 10^{-19}$ J

c. What is the relationship between frequency and wavelength?
   a) Direct
   b) Inverse

   Answer: Inverse

d. What is the relationship between frequency and energy?
   a) Direct
   b) Inverse

   Answer: Direct

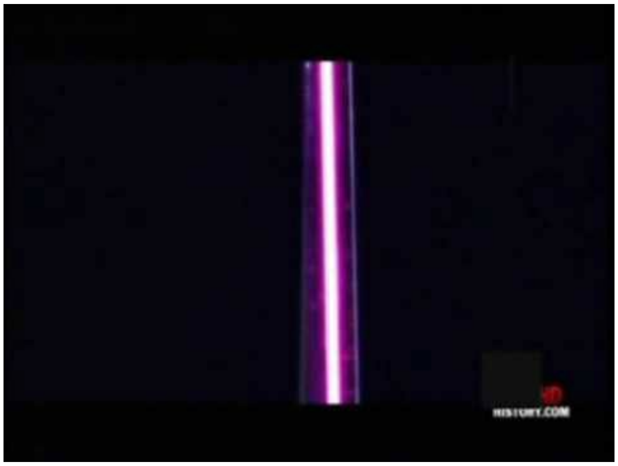
Can you think of some objects that appear to radiate visible light, but actually do not? The Moon and the planets do not emit light of their own; they reflect the light of the Sun. **Reflection** is when light (or another wave) bounces back from a surface. **Albedo** is a measure of how well a surface reflects light. A surface with high albedo reflects a large percentage of light. A snow field has high albedo.

One important fact to remember is that energy cannot be created or destroyed — it can only be changed from one form to another. This is such a fundamental fact of nature that it is a law: the law of conservation of energy.

In photosynthesis, for example, plants convert solar energy into chemical energy that they can use. They do not create new energy. When energy is transformed, some nearly always becomes heat. Heat transfers between materials easily, from warmer objects to cooler ones. If no more heat is added, eventually all of a material will reach the same temperature.

Summary

- Energy travels in waves with electrical and magnetic properties and so is called electromagnetic radiation.
- The wavelengths of visible light vary from long wavelength red to short wavelength violet. Infrared and ultraviolet wavelengths continue outward at longer and shorter wavelengths.
- The law of conservation of energy states that energy cannot be created or destroyed, it can only change forms.



Reference: https://www.youtube.com/watch?v=kfS5Qn0wn2o&feature=youtu.be

Electromagnetic waves

In physics, electromagnetic radiation (EM radiation or EMR) refers to the waves (or their quanta, photons) of the electromagnetic field, propagating (radiating) through space, carrying electromagnetic radiant energy. It includes radio waves, microwaves, infrared, (visible) light, ultraviolet, X-rays, and gamma rays.

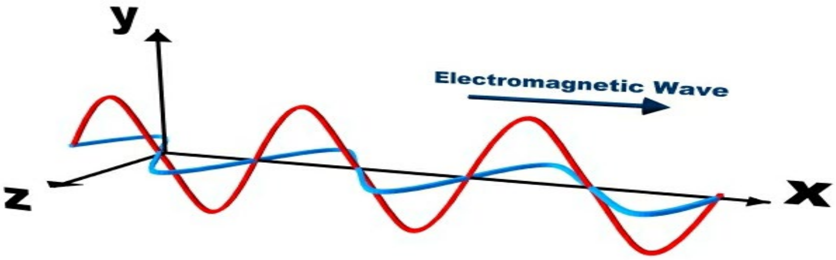


Figure 6.4 Electromagnetic Radiation

Ref: Commons.wikimedia.org/

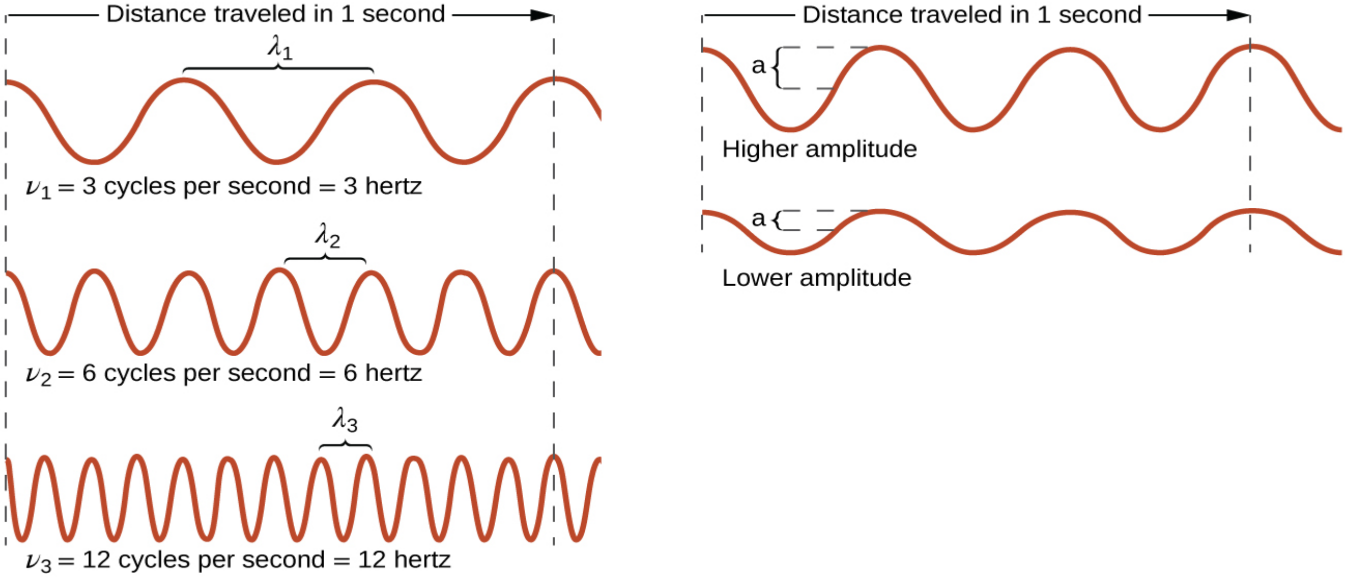


Figure 6.5 Wave Properties

Ref: Commons.wikimedia.org/

Figure: One-dimensional sinusoidal waves show the relationship among wavelength, frequency, and speed. The wave with the shortest wavelength has the highest frequency. Amplitude is one-half the height of the wave from peak to trough.
Reference: ***Chemistry 2e OpenStax.***

Electromagnetic waves are invisible forms of energy that travel though the universe. However, you can "see" some of the results of this energy. The light that our eyes can see is actually part of the electromagnetic spectrum.

This visible part of the electromagnetic spectrum consists of the colors that we see in a rainbow - from reds and oranges, through blues and purples. Each of these colors actually corresponds to a different wavelength of light.

The sound we hear is a result of waves which we cannot see. Sound waves need something to travel through in order for it to move from one place to the next. Sound can travel through air because air is made of molecules.

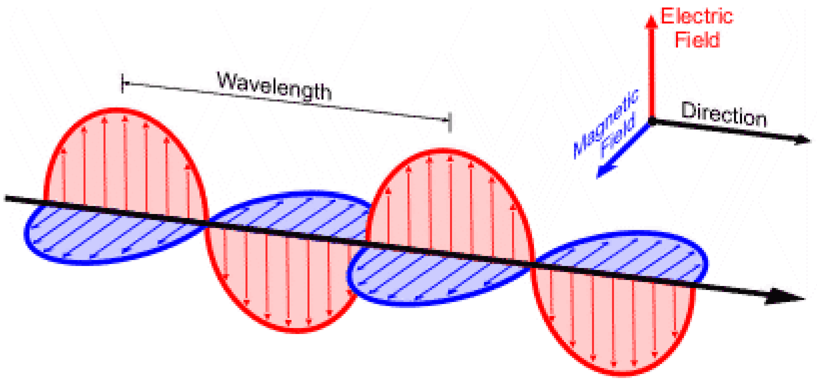


Figure 6.6 Electromagnetic Radiation Properties

Ref: Commons.wikimedia.org/

Electromagnetic Wave

These molecules carry the sound waves by bumping into each other, like dominoes knocking each other over. Sound can travel through anything made of molecules - even water! There is no sound in space because there are no molecules there to transmit the sound waves.

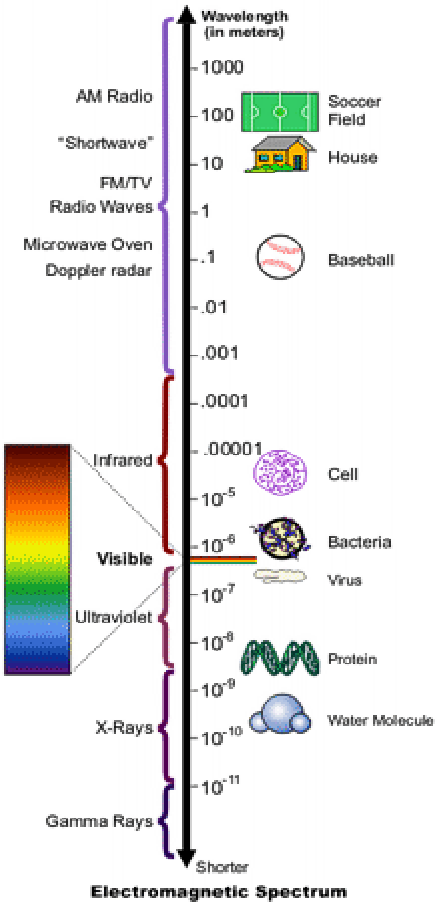


Figure 6.7 Electromagnetic spectrum

Ref: Commons.wikimedia.org/

Electromagnetic waves are not like sound waves because they do not need molecules to travel. This means that electromagnetic waves can travel through air, solid objects and even space. This is how astronauts on spacewalks use radios to communicate. Radio waves are a type of electromagnetic wave.

Electricity can be static, like what holds a balloon to the wall or makes your hair stand on end. Magnetism can also be static like a refrigerator magnet. But when they change or move together, they make waves - electromagnetic waves.

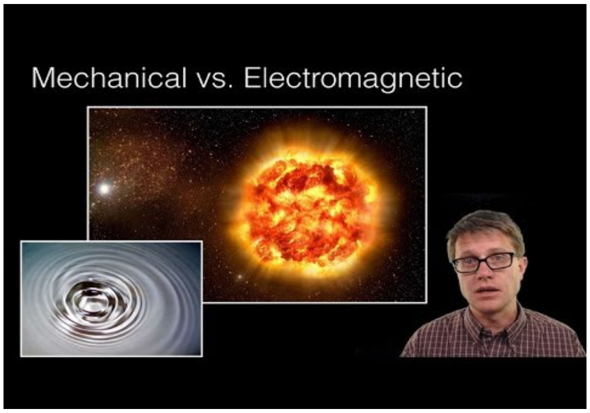
Electromagnetic waves are formed when an electric field (which is shown in red arrows) couples with a magnetic field (which is shown in blue arrows). Magnetic and electric fields of an electromagnetic wave are perpendicular to each other and to the direction of the wave.

When you listen to the radio, watch TV, or cook dinner in a microwave oven, you are using electromagnetic waves. Radio waves, television waves, and microwaves are all types of electromagnetic waves. They only differ from each other in wavelength. Wavelength is the distance between one wave crest to the next.

Waves in the electromagnetic spectrum vary in size from very long radio waves the size of buildings, to very short gamma-rays smaller than the size of the nucleus of an atom. Yet their size can be related to their energy.

The smaller the wavelength the higher the energy. For example, a brick wall blocks visible light wave lengths. Smaller, more energetic, x-rays can pass through brick walls, but themselves are blocked by denser material such as lead.

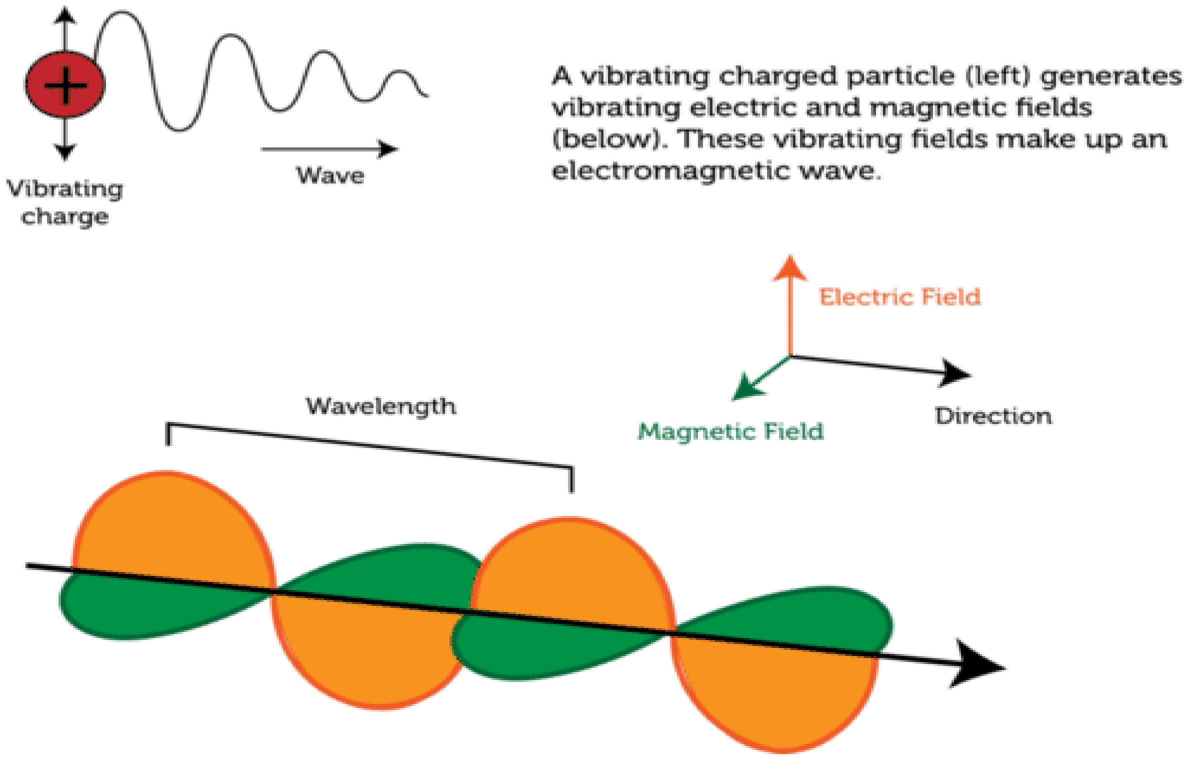
While it can be said waves are "blocked" by certain materials, the correct understanding is that wave lengths of energy are "absorbed" by objects, or not. That is, wave length energy can be *absorbed* by certain material.



Reference: https://www.youtube.com/watch?v=WNkB8IY-k04

Elelectromagnetic wave begins when an electrically charged particle vibrates.
The **Figures** below shows how this happens. A vibrating charged particle causes the electric field surrounding it to vibrate as well. A vibrating electric field, in turn, creates a vibrating magnetic field. The two types of vibrating fields combine to create an electromagnetic wave.

How an



A vibrating charged particle (left) generates vibrating electric and magnetic fields (below). These vibrating fields make up an electromagnetic wave.

Figure 6.8 Electromagnetic Wave Travels

Ref: Commons.wikimedia.org/

As you can see in the **Figure** above, the electric and magnetic fields that make up an electromagnetic wave are perpendicular (at right angles) to each other. Both fields are also perpendicular to the direction that the wave travels. Therefore, an electromagnetic wave is a transverse wave. However, unlike a mechanical transverse wave, which can only travel through matter, an electromagnetic transverse wave can travel through empty space. When waves travel through matter, they lose some energy to the matter as they pass through it. But when waves travel through space, no energy is lost. Therefore, electromagnetic waves don't get weaker as they travel. However, the energy is "diluted" as it travels farther from its source because it spreads out over an ever-larger area.

Electromagnetic Wave Interactions

When electromagnetic waves strike matter, they may interact with it in the same ways that mechanical waves interact with matter. Electromagnetic waves may:

- reflect, or bounce back from a surface;
- refract, or bend when entering a new medium;
- diffract, or spread out around obstacles.

Electromagnetic waves may also be absorbed by matter and converted to other forms of energy. Microwaves are a familiar example. When microwaves strike food in a microwave oven, they are absorbed and converted to thermal energy, which heats the food.

Sources of Electromagnetic Waves

The most important source of electromagnetic waves on Earth is the sun. Electromagnetic waves travel from the sun to Earth across space and provide virtually all the energy that supports life on our planet. Many other sources of electromagnetic waves depend on technology. Radio waves, microwaves, and X rays are examples. We use these electromagnetic waves for communications, cooking, medicine, and many other purposes.

Reference: https://youtu.be/cfXzwh3KadE

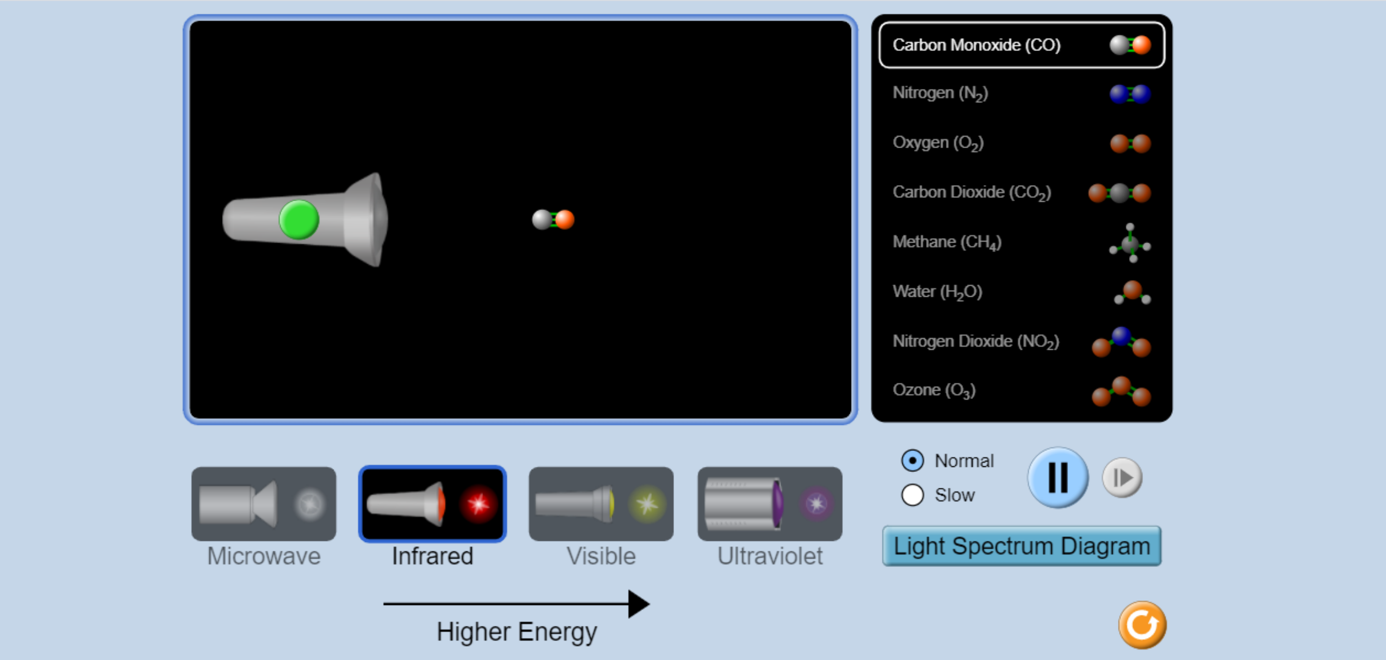
Summary

- Electromagnetic waves are waves that consist of vibrating electric and magnetic fields. They transfer energy through matter or across space. The transfer of energy by electromagnetic waves is called electromagnetic radiation.
- The electric and magnetic fields of an electromagnetic wave are areas of electric or magnetic force. The fields can exert force over objects at a distance.
- An electromagnetic wave begins when an electrically charged particle vibrates. This causes a vibrating electric field, which in turn creates a vibrating magnetic field. The two vibrating fields together form an electromagnetic wave.
- An electromagnetic wave is a transverse wave that can travel across space as well as through matter. When it travels through space, it doesn’t lose energy to a medium as a mechanical wave does.
- When electromagnetic waves strike matter, they may be reflected, refracted, or diffracted. Or they may be absorbed by matter and converted to other forms of energy.
- The most important source of electromagnetic waves on Earth is the sun. Many other sources of electromagnetic waves depend on technology.

Check This Out!

https://phet.colorado.edu/sims/html/molecules-and-light/latest/molecules-and-light_en.html

A nice simulation of electromagnetic radiation reacting with different molecules can be visible and played around it.



● Normal
○ Slow

Black Body Radiation

All objects above the temperature of absolute zero emit electromagnetic radiation consisting of a broad range of wavelengths described by a distribution curve whose peak wavelength λ (lambda) at absolute temperature *T* for a "perfect radiator" known as a black body is given by *Wein's law* which predicts that λ_{max} is inversely proportional to T.

At ordinary temperatures this radiation is entirely in the infrared region of the spectrum, but as the temperature rises above about 1000K, more energy is emitted in the visible wavelength region and the object begins to glow, first with red light, and then shifting toward the blue as the temperature is increased.

This type of radiation has two important characteristics. First, the spectrum is a *continuous* one, meaning that all wavelengths are emitted, although with intensities that vary smoothly with wavelength. The other curious property of black body radiation is that it is independent of the composition of the object; all that is important is the temperature.

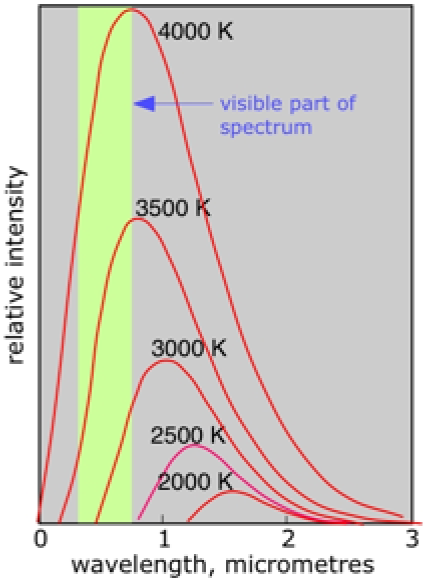


Figure 6.9 Black Body Radiation

Ref: Commons.wikimedia.org/

Planck's Equation

Black body radiation, like all electromagnetic radiation, must originate from oscillations of electric charges which in this case were assumed to be the electrons within the atoms of an object acting somewhat as miniature Hertzian oscillators. It was presumed that since all wavelengths seemed to be present in the continuous spectrum of a glowing body, these tiny oscillators could send or receive any portion of their total energy. However, all attempts to predict the actual shape of the emission spectrum of a glowing object on the basis of classical physical theory proved futile.

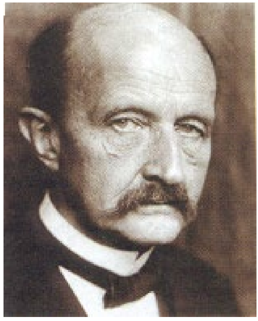


Figure 6.10 Max Planck

In 1900, the great German physicist Max Planck (who earlier in the same year had worked out an empirical formula giving the detailed shape of the black body emission spectrum) showed that the shape of the observed spectrum could be exactly predicted if the energies emitted or absorbed by each oscillator were restricted to integer values of hν, where ν ("nu") is the frequency and *h* is a constant 6.626E–34 J s which we now know as *Planck's Constant*. This means that the allowable energies of each oscillator are *quantized.* (Owing to the minute differences in frequency among the uncountable numbers of oscillators in any visible body, the spectrum appears to be continuous.) This modification of classical theory, the first use of the quantum concept, was as unprecedented as it was simple, and it set the stage for the development of modern quantum physics.

Particle Theory of Light

Photoelectric effect

Shortly after J.J. Thompson's experiments led to the identification of the elementary charged particles we now know as electrons, it was discovered that the illumination of a metallic surface by light can cause electrons to be emitted from the surface. This phenomenon, the photoelectric effect, is studied by illuminating one of two metal plates in an evacuated tube. The kinetic energy of the photoelectrons causes them to move to the opposite electrode, thus completing the circuit and producing a measurable current. However, if an opposing potential (the *retarding potential*) is imposed between the two plates, the kinetic energy can be reduced to zero so that the electron current is stopped. By observing the value of the retarding potential V_r, the kinetic energy of the photoelectrons can be calculated from the electron charge *e*, its mass *m* and the frequency ν of the incident light:

$$V_r e = \frac{m_e V_{\max}}{2}$$

This plot illustrates the photoelectric effect in metallic zinc. No photoelectrons are emitted until the frequency of the incident light reaches 10.4×10^{14} hz = 1.04×10^{15} hz. This frequency corresponds to a wavelength of

(3E8 m s^{-1}) / (1.04E15 s^{-1}) =288E-6 m

which, as the diagram indicates, falls outside the range of visible light, in the ultraviolet region of the spectrum

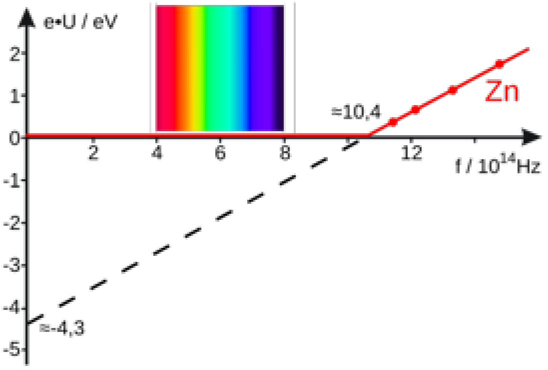


Figure 6.11 Photoelectric Effect on metallic Zinc

Ref: Commons.wikimedia.org/

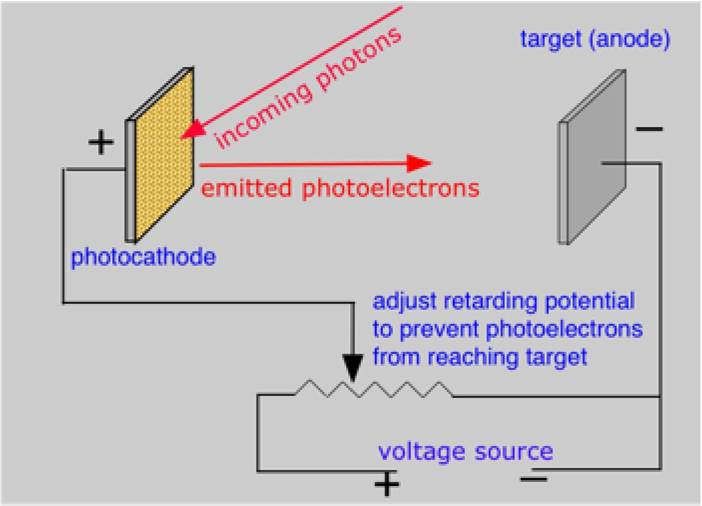


Figure 6.12 Photoelectric Effect

The Idea of Photon

Although the number of electrons ejected from the metal surface per second depends on the intensity of the light, as expected, the kinetic energies of these electrons (as determined by measuring the retarding potential needed to stop them) does not, and this was definitely not expected. Just as a more intense physical disturbance will produce higher energy waves on the surface of the ocean, it was supposed that a more intense light beam would confer greater energy on the photoelectrons. But what was found, to everyone's surprise, is that the photoelectron energy is controlled by the wavelength of the light, and that there is a critical wavelength below which no photoelectrons are emitted at all.

Figure 6.13 Albert Einstein

Ref: Commons.wikimedia.org/

Albert Einstein quickly saw that if the kinetic energy of the photoelectrons depends on the wavelength of the light, then so must its energy. Further, if Planck was correct in supposing that energy must be exchanged in packets restricted to certain values, then light must similarly be organized into energy packets. But a light ray consists of electric and magnetic fields that spread out in a uniform, continuous manner; how can a continuously-varying wave front exchange energy in discrete amounts? Einstein's answer was that the energy contained in each packet of the light must be concentrated into a tiny region of the wave front. This is tantamount to saying that light has the nature of a quantized particle whose energy is given by the product of Planck's constant and the frequency:

$$e = h\nu = \frac{hc}{\lambda}$$

Einstein's publication of this explanation in 1905 led to the rapid acceptance of Planck's idea of energy quantization, which had not previously attracted much support from the physics community of the time. It is interesting to note, however, that this did not make Planck happy at all. Planck, ever the conservative, had been reluctant to accept that his own quantized-energy hypothesis was much more than an artifice to explain black-body radiation; to extend it to light seemed an absurdity that would negate the well-established electromagnetic theory and would set science back to the time before Maxwell.

De Broglie Equation:

Although the photon has no rest mass, it does possess kinetic energy by virtue ot its velocity. The mass-equivalent of this energy is given by Einstein's relation m = e/c^2. Combining this with Planck's relation e = hv, the effctive mass of the photon becomes

$$m = \frac{e}{c^2} = \frac{h\nu}{c^2} = \frac{h}{c\lambda}$$

which corresponds to a momentum *m v* of (*h*/*c*λ) × *c* = *h*/λ .

6.2 The Bohr Model

In atomic physics, the **Rutherford–Bohr** model or Bohr model, presented by Niels Bohr and **Ernest Rutherford** in 1913, is a system consisting of a small, dense nucleus surrounded by orbiting electrons—similar to the structure of the Solar System, but with attraction provided by electrostatic forces in place of gravity.

Development of the Bohr Model

The Bohr model was an improvement on the earlier cubic model (1902), the plum-pudding model (1904), the Saturnian model (1904), and the Rutherford model (1911). Since the Bohr model is a quantum-physics-based modification of the Rutherford model, many sources combine the two: the Rutherford–Bohr model.

Although it challenged the knowledge of classical physics, the model's success lay in explaining the Rydberg formula for the spectral emission lines of atomic hydrogen. While the Rydberg formula had been known experimentally, it did not gain a theoretical underpinning until the Bohr model was introduced. Not only did the Bohr model explain the reason for the structure of the Rydberg formula, it also provided a justification for its empirical results in terms of fundamental physical constants.

Although revolutionary at the time, the Bohr model is a relatively primitive model of the hydrogen atom compared to the valence shell atom. As an initial hypothesis, it was derived as a first-order approximation to describe the hydrogen atom. Due to its simplicity and correct results for selected systems, the Bohr model is still commonly taught to introduce students to quantum mechanics. A related model, proposed by Arthur Erich Haas in 1910, was rejected. The quantum theory from the period between Planck's discovery of the quantum (1900) and the advent of a full-blown quantum mechanics (1925) is often referred to as the old quantum theory.

Early planetary models of the atom suffered from a flaw: they had electrons spinning in orbit around a nucleus—a charged particle in an electric field. There was no accounting for the fact that the electron would spiral into the nucleus. In terms of electron emission, this would represent a continuum of frequencies being emitted since, as the electron moved closer to the nucleus, it would move faster and would emit a different frequency than those experimentally observed. These planetary models ultimately predicted all atoms to be unstable due to the orbital decay. The Bohr theory solved this problem and correctly explained the experimentally obtained Rydberg formula for emission lines.

The **Bohr model** shows that the electrons in atoms are in orbits of differing energy around the nucleus (think of planets orbiting around the sun). **Bohr** used the term energy levels (or shells) to describe these orbits of differing energy. ... The energy level an electron normally occupies is called its ground state.

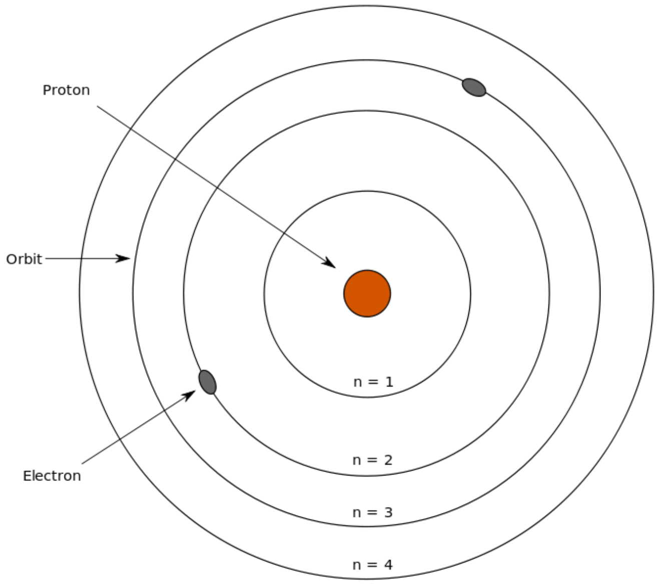
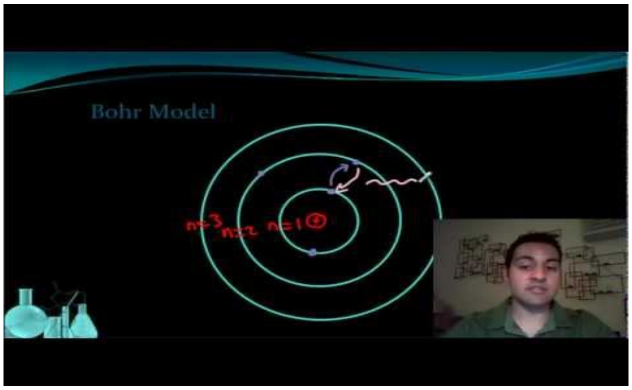


Figure 6.14 Bohr's Orbit

Ref: Commons.wikimedia.org/



Reference: https://www.youtube.com/watch?v=CUk3enr-m0w

The Bohr Model can relate and explain the Rydberg formula for emission spectra lines of several atoms especially of hydrogen atom. The model is based on the fact that electrons orbits around the nucleus in a circular mode at very specific and discrete distances. Each orbit is associated with specific, definite and discrete energy. Such orbit is called energy shell or just energy level.

The orbits are stable and electrons orbiting around the nucleus does not yield a radiation or energy loss as the classical electromagnetic theory assumes.

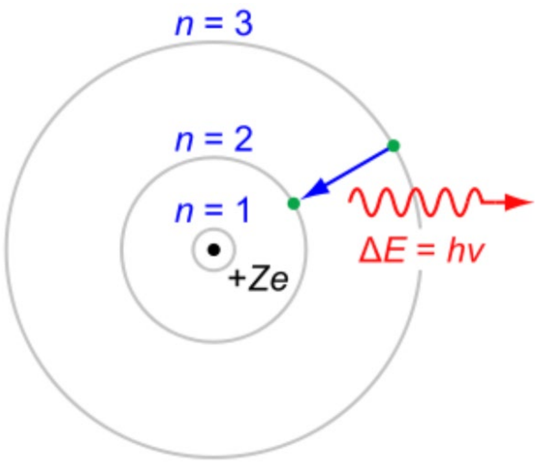


Figure 6.15 Rutherford–Bohr model of the hydrogen atom

Reference: https://courses.lumenlearning.com/introchem/chapter/the-bohr-model/

Properties of Electrons under the Bohr Model

In 1913, Bohr suggested that electrons could only have certain classical motions:

1. Electrons in atoms orbit the nucleus.
2. The electrons can only orbit stably, without radiating, in certain orbits (called by Bohr the "stationary orbits") at a certain discrete set of distances from the nucleus. These orbits are associated with definite energies and are also called energy shells or energy levels. In these orbits, an electron's acceleration does not result in radiation and energy loss as required by classical electromagnetic theory.
3. Electrons can only gain or lose energy by jumping from one allowed orbit to another, absorbing or emitting electromagnetic radiation with a frequency (ν) determined by the energy difference of the levels according to the Planck relation.

Behavior of Electrons: Part 3, The Bohr Model of the Atom – YouTube We combine our new found knowledge of the nature of light with Bohr's atomic theory.

https://youtu.be/66WsP1NCVIY

Bohr's model is significant because the laws of classical mechanics apply to the motion of the electron about the nucleus only when restricted by a quantum rule. Although Rule 3 is not completely well defined for small orbits, Bohr could determine the energy spacing between levels using Rule 3 and come to an exactly correct quantum rule—the angular momentum *L* is restricted to be an integer multiple of a fixed unit:

$\Delta E = E_2 - E_1 = h.\nu$, h= Planck's constant, $6.626 * 10^{-34}$ J.s

E_2 and E_1 are the corresponding energy levels of the orbits. Orbits are denoted by n. n = 1, 2, 3, … is called the principal quantum number. The lowest value of n is 1; this gives a smallest possible orbital radius of 0.0529 nm, known as the Bohr radius. Once an electron is in this lowest orbit, it can get no closer to the proton. Starting from the angular momentum quantum rule, Bohr was able to calculate the energies of the allowed orbits of the hydrogen atom and other hydrogen-like atoms and ions.

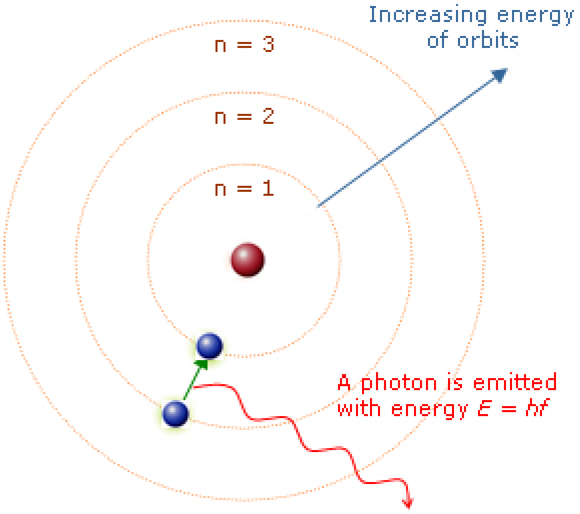


Figure 6.16 Energy Transition in Bohr's Orbit

Ref: Commons.wikimedia.org/

The Correspondence Principle

Bohr atom model postulate had corrected the Rutherford's atom's model. Bohr postulated that the electrons can orbit around the nucleus without radiating any energy and each orbit has its own definite energy. The stable orbit has discrete distance from the nucleus.

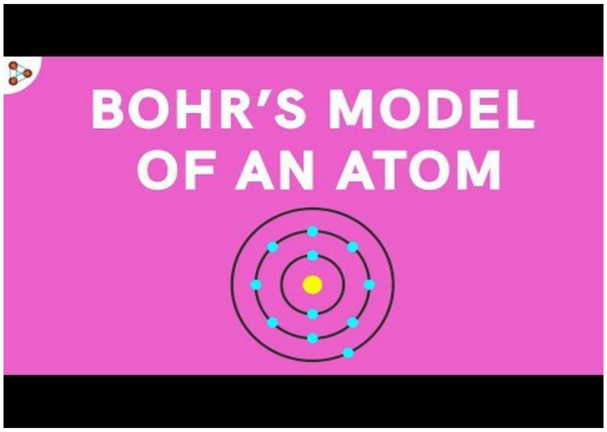
Furthermore, each orbit will have very distinct angular momentum which is an integer multiple of the reduced Planck constant with the principle quantum number n = 1, 2, 3, 4 etc.

In addition, Bohr was dependent on the old classical electromagnetic theory of Maxwell theory and one of weakest point of Bohr's model was that the Bohr himself did not believe in the concept of photons as explained by Einstein.

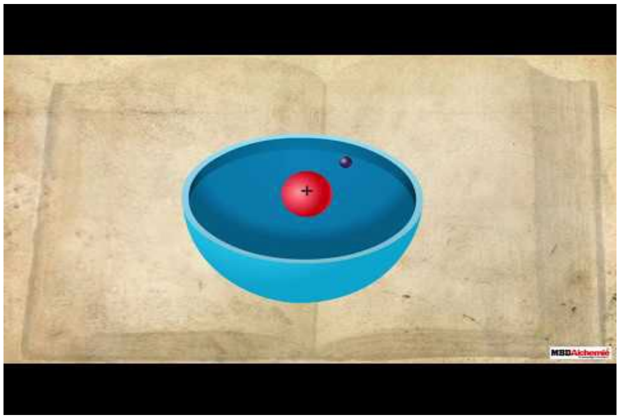
Maxwell theory states that the frequency *ν* of old classical radiation is equal to the rotation frequency of the electron in its orbit, with harmonics at integer multiples of this frequency. Bohr model predicted that the transfer of the electron from one level to another will acquire specific energy levels E_n and E_{n-k} where k is much smaller than n. F

In case of larger values of n (Rydberg states), the two orbits involved in the emission process have nearly the same rotation frequency, so that the classical orbital frequency is clear. But for small n (or large k), the radiation frequency has clear explanation.

Reference: ***https://en.wikipedia.org/wiki/Bohr_model***



Reference: https://www.youtube.com/watch?v=S1LDJUu4nko



Reference: https://www.youtube.com/watch?v=uXUqWlcZrss

6.2.1 Rydberg Equation

Planck's and Rydberg's Principles

Freshman students are taking a general chemistry class at Georgia State University. One day during the semester, their professor decided to take them to Las Vegas for field trip and to visit the University of Nevada, Las Vegas department of chemistry and look at their labs and undergraduate research.

They took the plane and arrived Las Vegas in the morning. They took the whole morning a calm rest at one of the Las Vegas Hotels.

At night they walked through Las Vegas Down Town. Las Vegas was looking very impressive with lots of fancy lights with different colors.

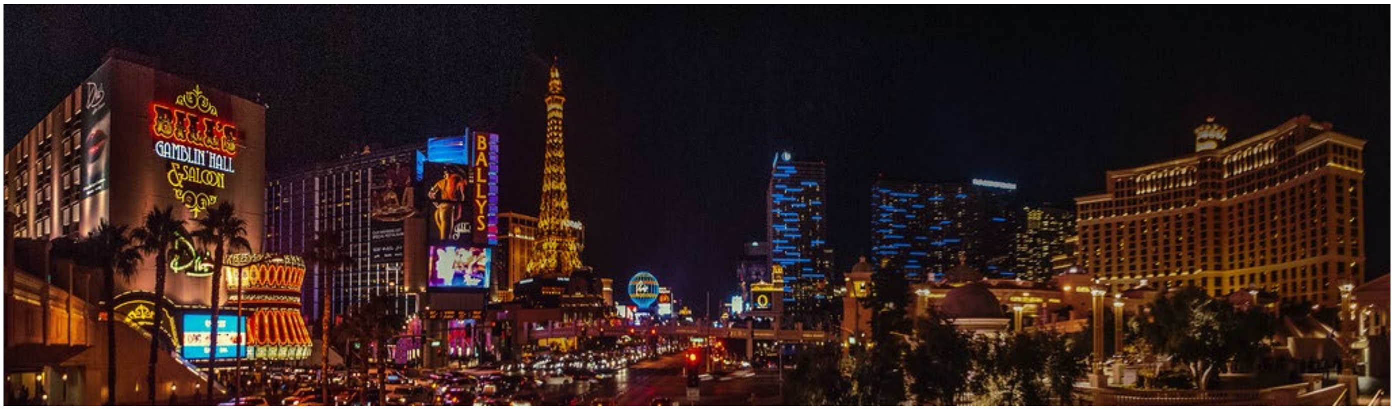


Figure 6.17 Night Sky of Las Vegas

Ref: Commons.wikimedia.org/

Las Vegas at night

Reference: https://www.flickr.com/photos/whsieh78/8222313719

The students were very excited and impressed with all the colors of light they saw.

One student asked his professor about the origins of these different colors of lights they saw.

The professor replied to his class: “Let us enjoy the night tonight and tomorrow after the breakfast and before visiting the chemistry department at the University of Nevada, I will gather everyone and will go over the origin of these beautiful lights”.

Next day, the professor and his class gathered around the professor’s laptop after the breakfast.

He started explaining the emission and absorption concept to his students. Luckily, they covered some of the materials covering the aspects of emission and absorption.

The professor explained them the concept of the emission and absorption.

Absorption: When an atom is absorbing energy from outside source and the valence electrons get excited to higher levels. This excitation is not stable and the valence electrons can give away the absorbed energy and the valence electrons go back to their original levels. This process is called emission because the valence electrons emit photons (releasing the absorbed energy). Each element has specific transitions of absorption and emission.

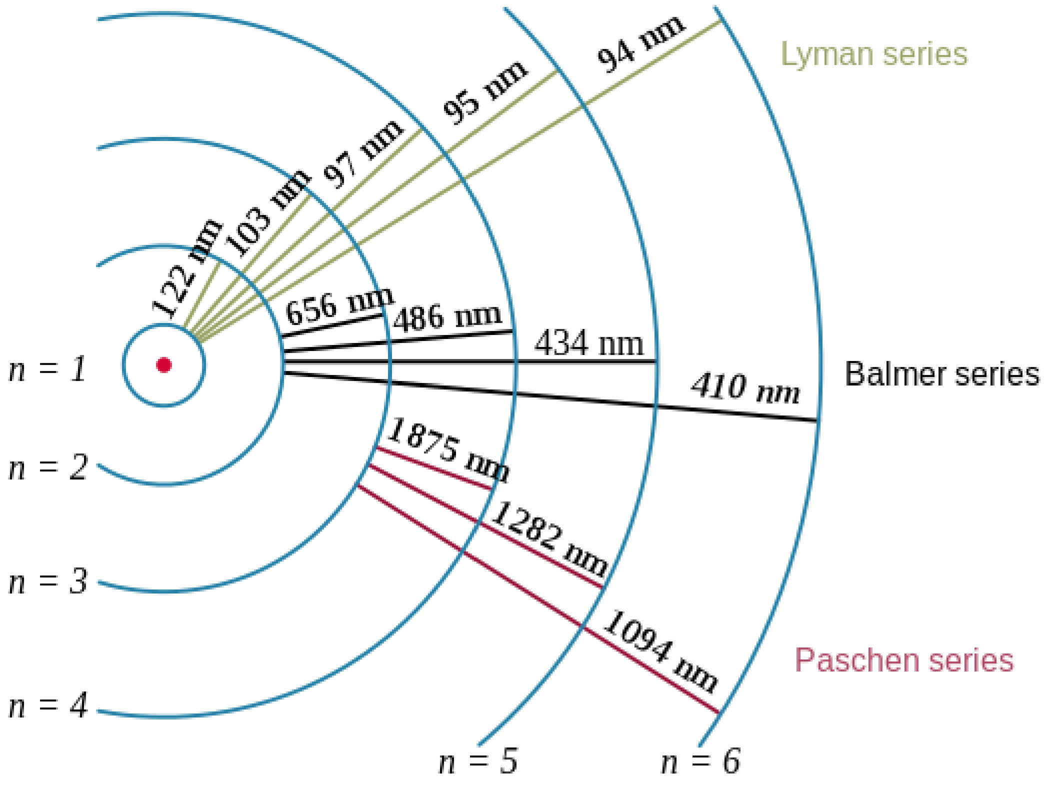


Figure 6.18 H-Atom Emission Spectrum

Ref: Commons.wikimedia.org/

Reference: https://intl.siyavula.com/read/science/grade-12/optical-phenomena-and-properties-of-matter/12-optical-phenomena-and-properties-of-matter-03

In the figure above, electron energy levels for the hydrogen atom. The arrows indicate the electron transitions from higher energy levels to lower energy levels. The energies of the emitted photons are the same as the energy difference between two energy levels.

The absorption process (arrows up) can be considered as the opposite process of the emission process (arrows down)..

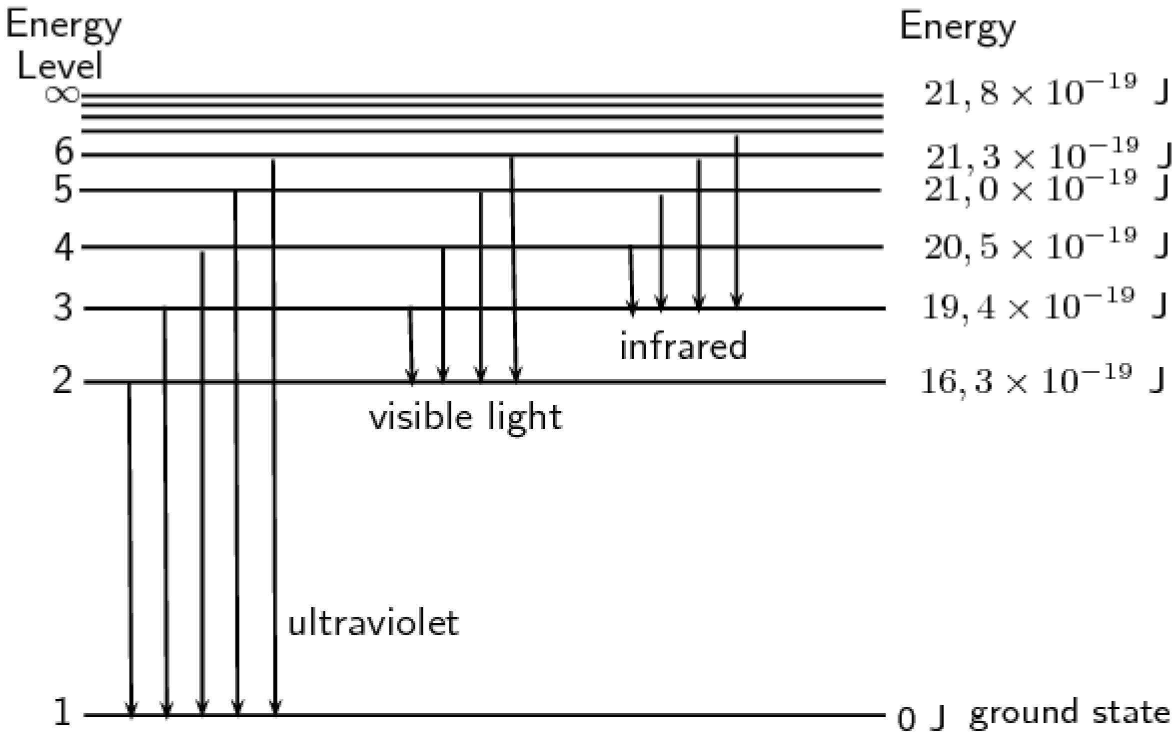


Figure 6.19 Different Wavelengths of Absorption and Emission Energy

Ref: Commons.wikimedia.org/

Reference: https://intl.siyavula.com/read/science/grade-12/optical-phenomena-and-properties-of-matter/12-optical-phenomena-and-properties-of-matter-03

$$\Delta E_{(\text{electron})} = \textbf{E(final)} - \textbf{E(initial)} = \textbf{h x } \vartheta = [\textbf{h x c / } \lambda]$$

The above formula is called Planck's formula or Principle

$\Delta E_{(\text{electron})}$ = Photon's energy is equal to the energy difference between the two energy levels (final – initial).

h = Planck's constant

ϑ = frequency

c = speed of light

λ = wavelength

Each specific photon frequency (or wavelength) for each transition will give very specific color. An example of this is the hydrogen spectra photon transitions in the visible range. The figure below illustrates these unique spectra. Each element in the periodic table will have its own unique line spectra.

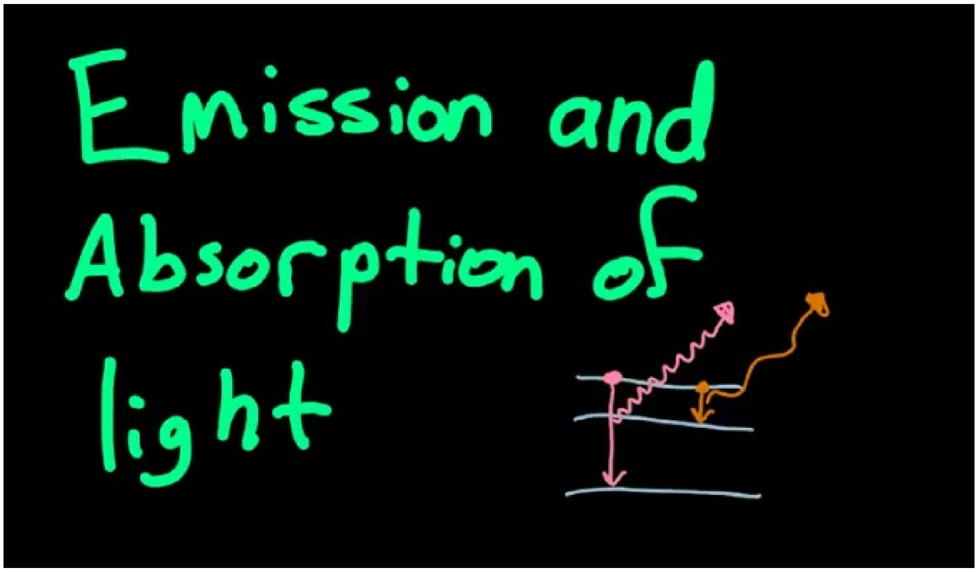
Figure 6.20 Discrete Emission Spectrum Lines

Ref: Commons.wikimedia.org/

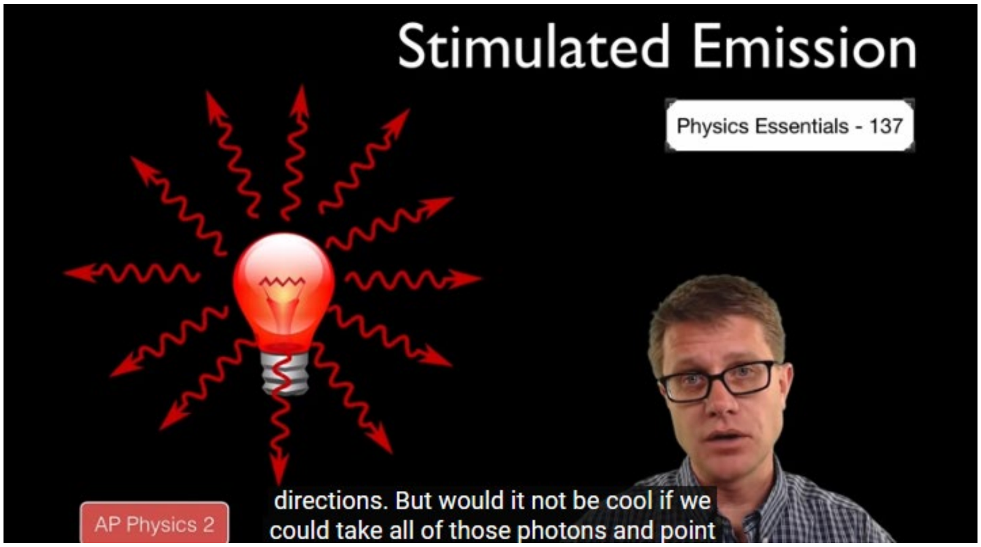
Reference: https://intl.siyavula.com/read/science/grade-12/optical-phenomena-and-properties-of-matter/12-optical-phenomena-and-properties-of-matter-03

The professor went further and recommended his students the following YouTube videos:

.



https://www.youtube.com/watch?v=XQj0VwM-Hfs



directions. But would it not be cool if we could take all of those photons and point

https://www.youtube.com/watch?v=YHmGNDMV1cY

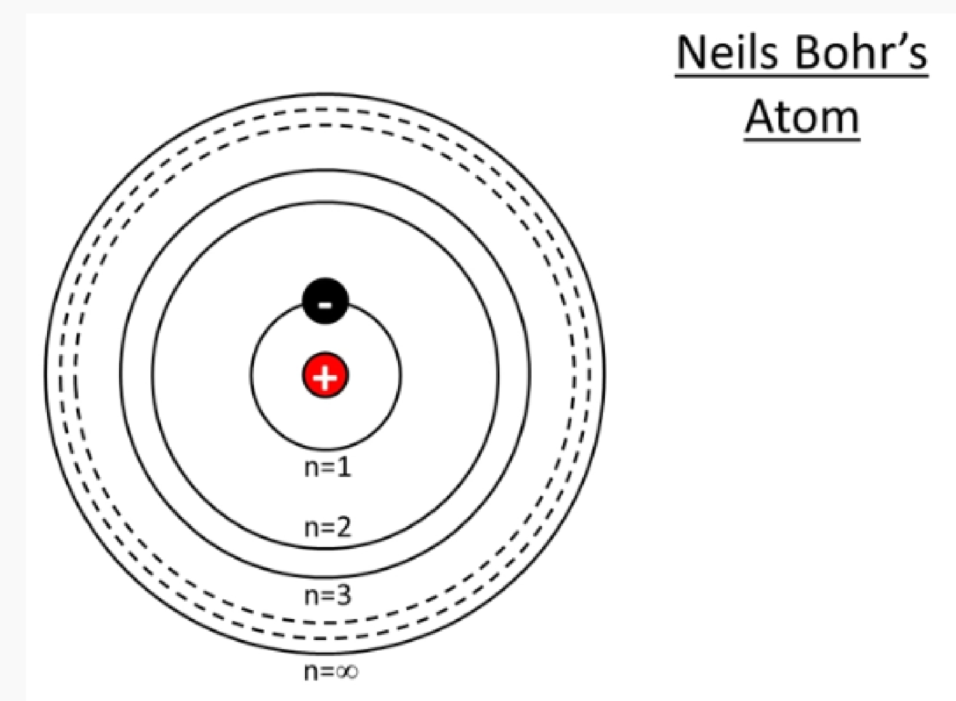
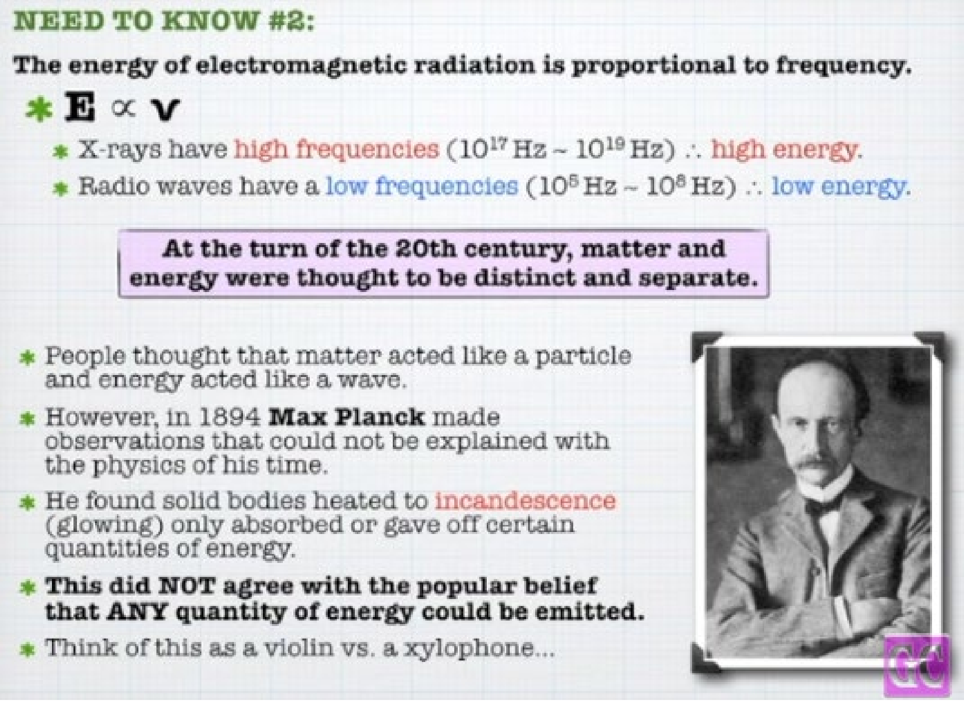


Figure 6.21 Bohr's Orbit based on Rydberg Equation

Ref: Commons.wikimedia.org/

https://www.youtube.com/watch?v=h3E9jNDnrDo



NEED TO KNOW #2:

The energy of electromagnetic radiation is proportional to frequency.

- $E \propto \nu$
  - X-rays have high frequencies (10^{17} Hz ~ 10^{19} Hz) ∴ high energy.
  - Radio waves have a low frequencies (10^{5} Hz ~ 10^{8} Hz) ∴ low energy.

At the turn of the 20th century, matter and energy were thought to be distinct and separate.

- People thought that matter acted like a particle and energy acted like a wave.
- However, in 1894 **Max Planck** made observations that could not be explained with the physics of his time.
- He found solid bodies heated to incandescence (glowing) only absorbed or gave off certain quantities of energy.
- **This did NOT agree with the popular belief that ANY quantity of energy could be emitted.**
- Think of this as a violin vs. a xylophone...

https://www.youtube.com/watch?v=vhxjQ3-gYko

https://www.youtube.com/watch?v=uMUi3o78qgQ

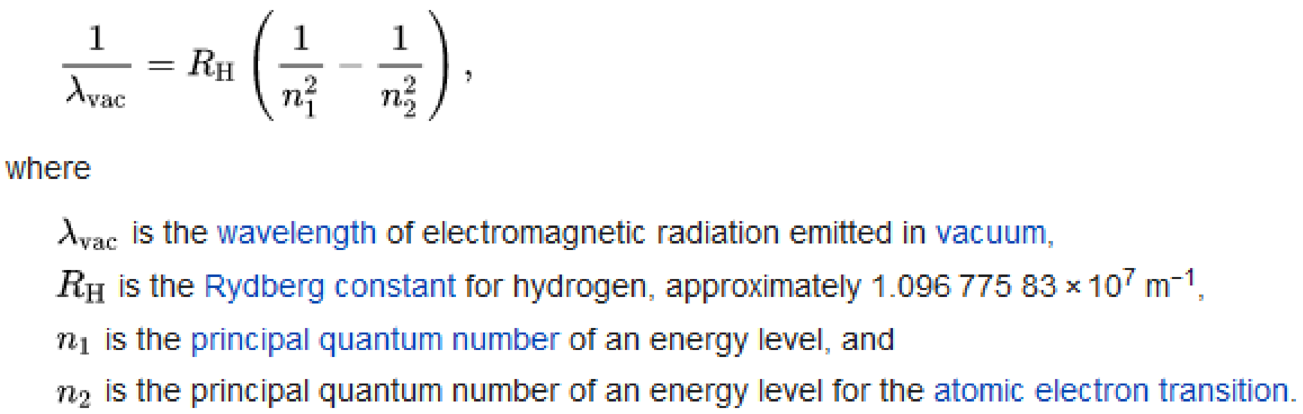
The professor went on his talk and recommended his students to wait till they will hear the concept of **Rydberg's Principle.**

Rydberg's Principle

The Rydberg's Principle concept explains spectral lines of each element related to their frequencies which can be either the sum or the difference of the frequencies of two other lines. Lines of the spectra of elements could be predicted from existing lines.

Rydberg's Formula

The formula for hydrogen is given in the figure below:



$$\frac{1}{\lambda_{\mathrm{vac}}} = R_{\mathrm{H}} \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right),$$

where

λ_{vac} is the wavelength of electromagnetic radiation emitted in vacuum,

R_{H} is the Rydberg constant for hydrogen, approximately $1.096\,775\,83 \times 10^{7}\ \mathrm{m}^{-1}$,

n_1 is the principal quantum number of an energy level, and

n_2 is the principal quantum number of an energy level for the atomic electron transition.

n_2 is greater than n_1

Reference: https://en.wikipedia.org/wiki/Rydberg_formula

The figure below illustrates the origin of the line spectra of hydrogen:

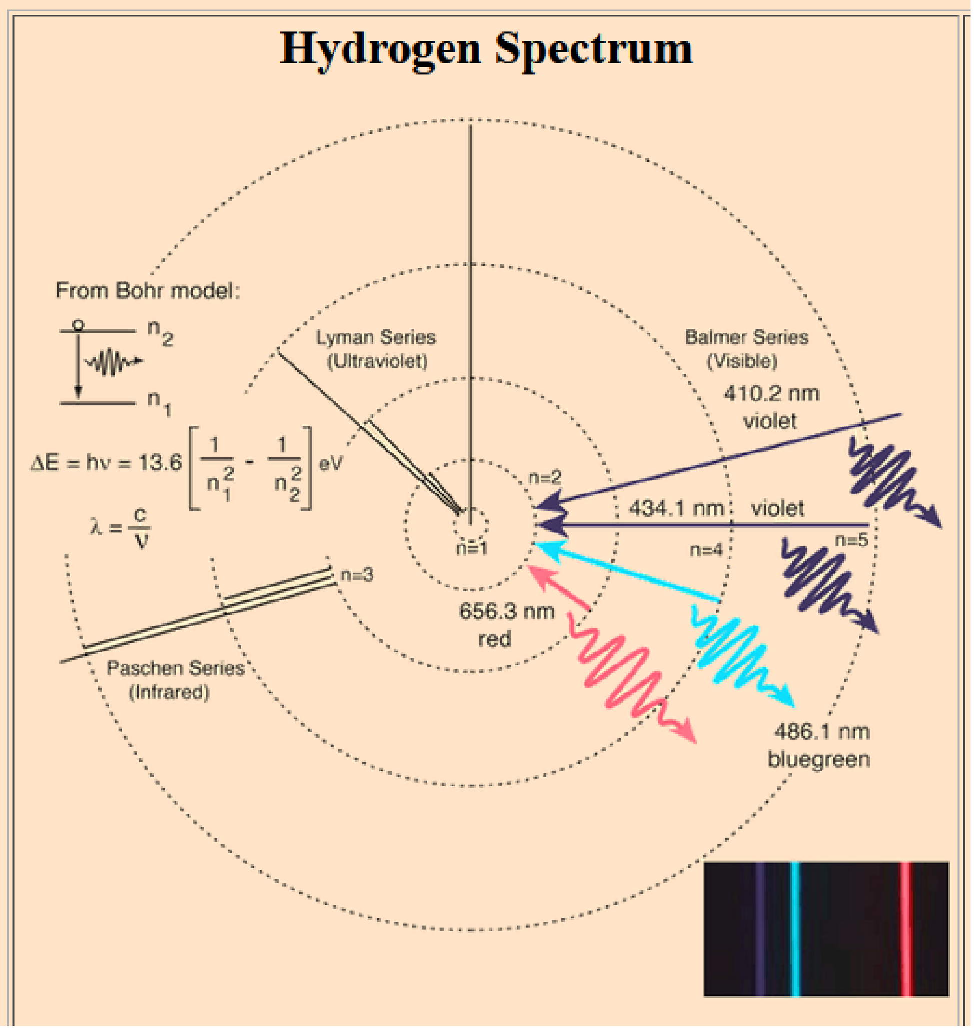


Figure 6.22 Spectral Lines of Bohr's Orbit

Ref: Commons.wikimedia.org

http://hyperphysics.phy-astr.gsu.edu/hbase/hyde.html

There is another form of Rydberg Equation which is popularly used:

$$\Delta E = -2.18 * 10\text{-}18 \left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right)$$

Above equation is frequently used for energy difference and followed by Planck's equation to determine wavelength.

For example, suppose, that an electron in a hydrogen atom relaxes from an orbital in the n=3 level to an orbital in the n=2 level. We determine ΔE, the energy difference corresponding to the transition from n=3 to n=2 as follows,

$\Delta E_{atom} = E_2 - E_3$

$= -2.18 * 10^{-18}(1/2^2) - -2.18 * 10\text{-}18(1/3^2) = = -2.18 * 10^{-18}(1/2^2 - 1/3^2) = -3.03 * 10^{-19}$ J

Since energy must be conserved, the exact amount of energy emitted by atom is carried by the photon.

$-\Delta E_{atom}=\Delta E_{photon}$

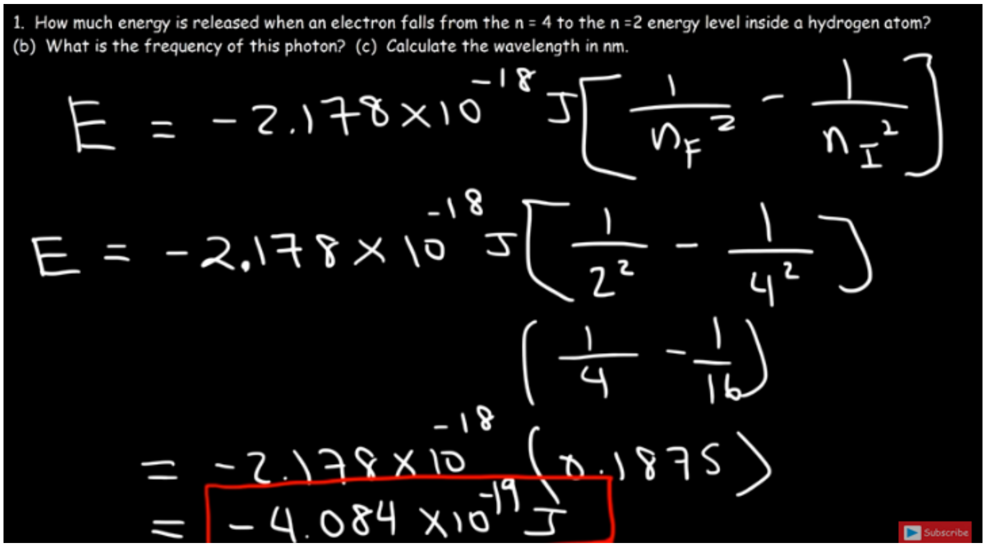
Since wavelength of a photon is related to its energy, E= hc/λ, we calculate wavelength of the photon as:

$\Lambda = hc/E = (6.626 * 10^{-34} * 3.00 * 10^{8})/3.03 * 10^{-19}$

$= 6.56 * 10^{-7}$ m or 656 nm

With the help of Rydberg formula, one can calculate the wavelength of each transition and the hence the colors of the line spectra will be determined as shown in the hydrogen spectrum.

At the end of his long talk (almost a lecture), the professor recommended his students the videos below which cover the Rydberg Principle and Formula and Calculations:



1. How much energy is released when an electron falls from the n = 4 to the n =2 energy level inside a hydrogen atom? (b) What is the frequency of this photon? (c) Calculate the wavelength in nm.

$$E = -2.178\times10^{-18}\,J\left[\frac{1}{n_F{}^2} - \frac{1}{n_I{}^2}\right]$$

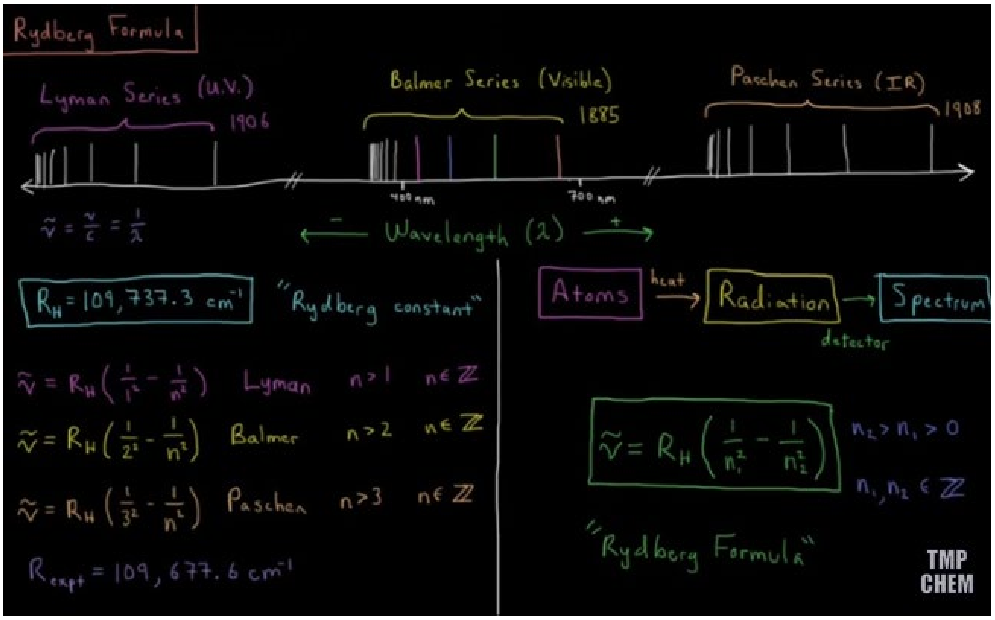
$$E = -2.178\times10^{-18}\,J\left[\frac{1}{2^2} - \frac{1}{4^2}\right]$$

$$\left(\frac{1}{4} - \frac{1}{16}\right)$$

$$= -2.178\times10^{-18}\,(0.1875)$$

$$= \boxed{-4.084\times10^{-19}\,J}$$

https://www.youtube.com/watch?v=mXxsT1ut35Q



https://www.youtube.com/watch?v=DLmnh74MfSA

https://www.youtube.com/watch?v=au2HCVn9IJI

Rydberg Formula

$$\frac{1}{\lambda} = RZ^2(\frac{1}{n_1^2} - \frac{1}{n_2^2})$$

Where

λ	The wavelength of the photon.
R	Rydberg's constant $(1.0973731568539(55) \times 10^7 m^{-1})$
Z	The atomic number of the atom
$n_1 and n_2$	Integers where $n_2 > n_1$.

Figure 6.23 Rydberg Equation

Ref: Commons.wikimedia.org

It was later found that n_2 and n_1 were related to the principal quantum number or energy quantum number. This formula works very well for transitions between energy levels of the hydrogen atom. It is because H is with only one electron.

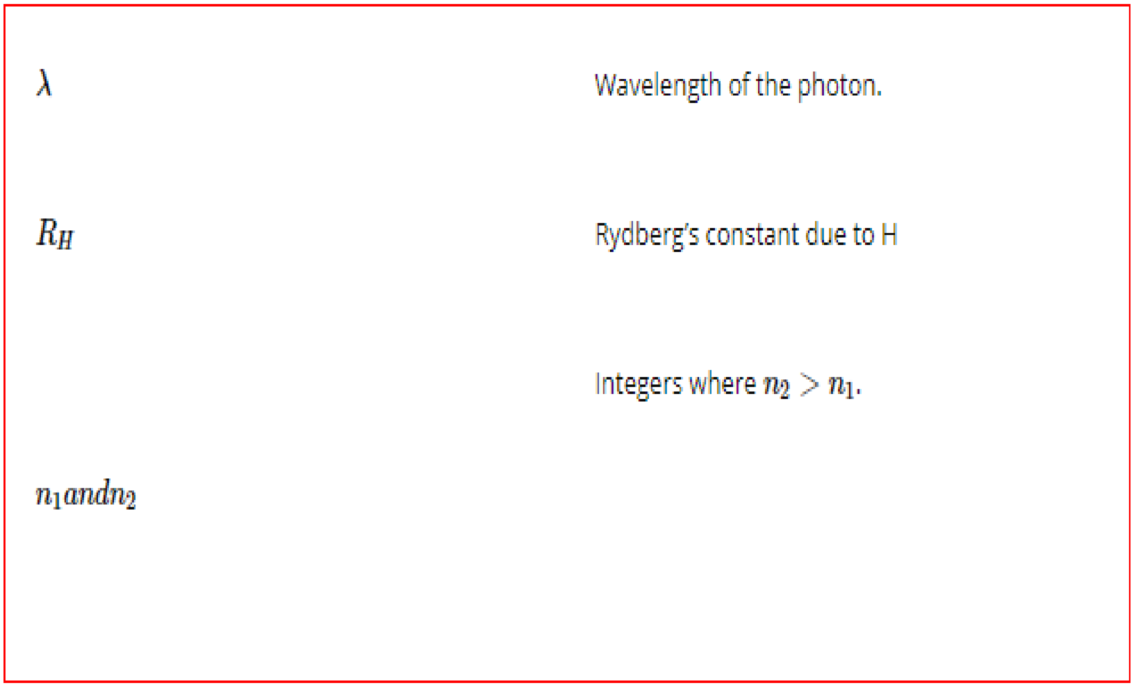
For atoms with more than one electron, this formula begins to break down and give incorrect results. This was due to the inaccuracy that the amount of screening for inner electrons for outer electron transitions varies.

We can use the Rydberg formula for hydrogen to obtain its spectral lines. Setting n_1 to 1 and running n_2 from 2 to infinity yields to get the Lyman series.

For most problems, we will deal with hydrogen so we can use the formula:

$$\frac{1}{\lambda} = R_H\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right)$$

where



λ	Wavelength of the photon.
R_H	Rydberg's constant due to H
$n_1 and n_2$	Integers where $n_2 > n_1$.

Figure 6.24 Numerical Problems on Rydberg Equation

Ref: Commons.wikimedia.org

Solution: We have the Rydberg equation:

This formula gives a wavelength in meters using this value for Rydberg's constant.

$$\frac{1}{\lambda} = R_H(\frac{1}{n_1^2} - \frac{1}{n_2^2})$$

Now put the known vakues,

$n_1 = 1$

and $n_2 = 3$.

Use $R_H = 1.9074 \times 10^7 m^{-1}$.

$$\frac{1}{\lambda} = R_H(\frac{1}{n_1^2} - \frac{1}{n_2^2})$$

$$= 1.0947 \times 10^7(\frac{1}{1^2} - \frac{1}{3^2})$$

$$= 1.0947 \times 10^7 \times \frac{8}{9}$$

$$= 0.973 \times 10^7$$

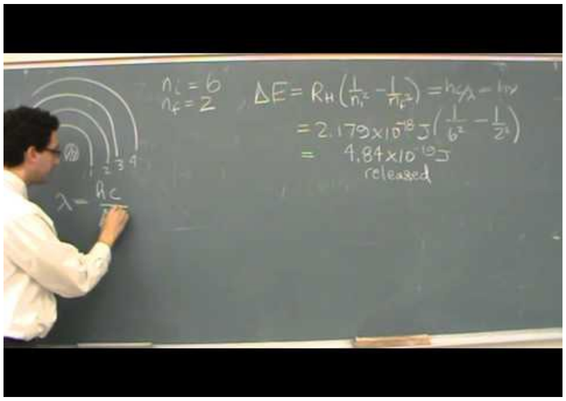
$$\lambda = 1.025 \times 10^{-7}\ meter$$

More Practice problems:

1) Determine the wavelength of the light absorbed when an electron in a hydrogen atom makes a transition from the orbital in the n=2 level to an orbital in the n=7 level.
2) An electron in the n=6 level of the hydrogen atom relaxes to a lower energy level, emitting light of λ= 93.8 nm. Find the principal level to which the electron relaxed.

The Rydberg equation works only for hydrogen because it is an empirical formula that is based on the Bohr model of the hydrogen atom and can only apply to it and other hydrogenic species. The Bohr model assumes that hydrogen and all subsequent elements have quantized shells with each taking discrete principle energy levels. However, the Bohr model breaks apart past hydrogen due to the presence of two or more electrons in higher atomic numbered elements, which introduces electron-electron interactions that complicate things significantly and can only be explained by more in-depth and rigorous quantum mechanics.

The video below illustrates Rydberg equation and calculations.



https://www.youtube.com/watch?v=4kOdbqoycmY

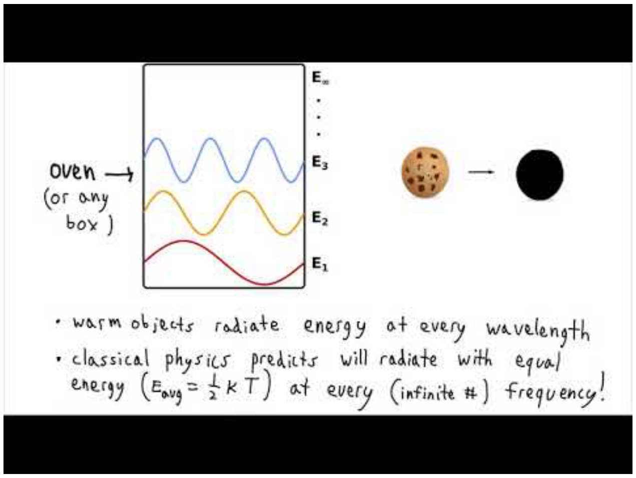
6.3 Development of Quantum Theory

- In 1900, Planck made the assumption that energy was made of individual units, or quanta.
- In 1905, Albert Einstein theorized that not just the energy, but the radiation itself was *quantized* in the same manner.
- In 1924, Louis de Broglie proposed that there is no fundamental difference in the makeup and behavior of energy and matter; on the atomic and subatomic level either may behave as if made of either particles or waves. This theory became known as the *principle of wave-particle duality*: elementary particles of both energy and matter behave, depending on the conditions, like either particles or waves.

In 1927, Werner Heisenberg proposed that precise, simultaneous measurement of two complementary values - such as the position and momentum of a subatomic particle - is impossible. Contrary to the principles of classical physics, their simultaneous measurement is inescapably flawed; the more precisely one value is measured, the more flawed will be the measurement of the other value. This theory became known as the uncertainty principle, which prompted Albert Einstein's famous comment, "God does not play dice."

In 1900, physicist Max Planck presented his quantum theory to the German Physical Society. Planck had sought to discover the reason that radiation from a glowing body changes in color from red, to orange, and, finally, to blue as its temperature rises. He found that by making the assumption that energy existed in individual units in the same way that matter does, rather than just as a constant electromagnetic wave - as had been formerly assumed - and was therefore *quantifiable*, he could find the answer to his question. The existence of these units became the first assumption of quantum theory.

Planck wrote a mathematical equation involving a figure to represent these individual units of energy, which he called *quanta*. The equation explained the phenomenon very well; Planck found that at certain discrete temperature levels (exact multiples of a basic minimum value), energy from a glowing body will occupy different areas of the color spectrum. Planck assumed there was a theory yet to emerge from the discovery of quanta, but, in fact, their very existence implied a completely new and fundamental understanding of the laws of nature. Planck won the Nobel Prize in Physics for his theory in 1918, but developments by various scientists over a thirty-year period all contributed to the modern understanding of quantum theory.



Reference: https://www.youtube.com/watch?v=CejaM4NeSLE

Evolution of Quantum Theory

Early Developments

While the theory of relativity was largely the work of one man, Albert Einstein, the quantum theory was developed principally over a period of thirty years through the efforts of many scientists. The first contribution was the explanation of blackbody radiation in 1900 by Max Planck, who proposed that the energies of any harmonic oscillator (see harmonic motion), such as the atoms of a blackbody radiator, are restricted to certain values, each of which is an integral (whole number) multiple of a basic, minimum value. The energy E of this basic quantum is directly proportional to the frequency ν of the oscillator, or $E = h\nu$, where h is a constant, now called Planck's constant, having the value 6.62607×10^{-34} joule-second. In 1905, Einstein proposed that the radiation itself is also quantized according to this same formula, and he used the new theory to explain the photoelectric effect. Following the discovery of the nuclear atom by Rutherford (1911), Bohr used the quantum theory in 1913 to explain both atomic structure and atomic spectra, showing the connection between the electrons' energy levels and the frequencies of light given off and absorbed.

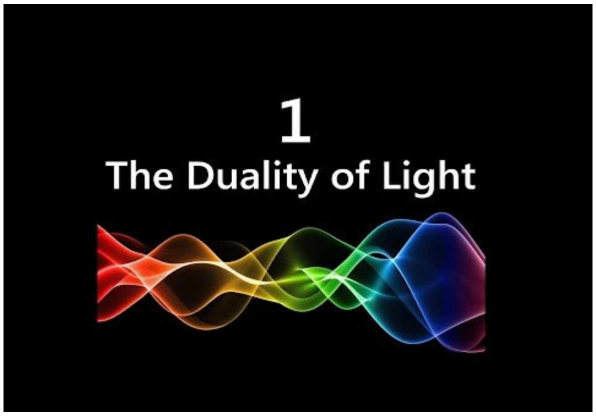
Quantum Mechanics and Later Developments

Quantum mechanics is the foundation of **chemistry**, because it deals with subatomic particles, as well as atoms, molecules, elements, compounds, and much larger systems. The **quantum theory** does much more than explaining the structure of the simplest atom, it rationalizes the existence of the **chemical** elements.

The quantum theory has many mathematical approaches, but the philosophy is essentially the same. Quantum mechanics is the foundation of chemistry, because it deals with subatomic particles, as well as atoms, molecules, elements, compounds, and much larger systems.

At the sub-atomic scale, there is no boundary between particles and waves. In fact, both **particles and wave properties must be considered simultaneously** for a system. The study of quantum mechanics lead us to understand the material and the universe beyond the general perception of matter by our ordinary senses of tasting, seeing, hearing, feeling, and sensing.

Furthermore, when coupled with the theory of relativity developed by Einstein, **there is no boundary between material and energy**. Energy and mass are equivalent, and they can convert into each other.



Reference: https://www.youtube.com/watch?v=e5_V78SWGF0

Quantum mechanics is an essential development of modern physics progress. The quantum mechanics started with different inventions and discoveries. Cathode rays were discovered by Michael Faraday.

Gustav Kirchhoff in about 1860 had development the concept of black – body radiation. About ten years later about 1877, Ludwig Boltzmann suggested that any physical system can be discrete. This had led to the development of the photoelectric effect by Heinrich Hertz in 1887. Later in 1900, Max Planck postulated a hypothesis that stated that the atomic system when radiating energy into a number of discrete energy elements ε (epsilon) which direct proportional to the frequency ν:

$$\varepsilon = h\,\nu$$

h is a numerical value called Planck's constant.

P. Dirac in 1928 had combined both the relativity theory with the quantum mechanics. This approach had led to the prediction of the antiparticle’s existence. In 1927, Heisenberg used the quantum mechanics to discover the uncertainty principle which had put theoretical limitation of the accuracy of specific measurements. In the past, it was thought that the measurements have to yield absolute values and data.

Einstein and Bose had developed the Bose – Einstein Statistics which put the limitation on the absolute’s values of the measurements. This development had similar approach in the Fermi – Dirac – Statistics.

So What Is Quantum Mechanics?

Quantum Mechanics is one of the branches of physics dealing small scale of the atoms and electrons. The classical mechanics deals with the matter and its studies at specific time and place.

Classical mechanics deals also with everyday size and not small subatomic sizes.

Three revolutionary principles

1. **Quantized properties**:

A **quantized property:** is definite size and the property which may be found in a multiple of that definite size.

2. **Particles of light:** It was demonstrated experimentally that the light has a dual character: wave and particle.

3. **Waves of matter**: Electron was also demonstrated experimentally that the light has a dual character.

Quantized properties?

Specific physical properties, such as position, speed and color, can sometimes only occur in specific, set of similar amounts.

Particles of light?

Light particles are called photons by Einstein which means that the light is made of flow of photons. Energy of these photons has specific oscillation frequency. The intensity of the light is the quantity of its photons

Waves of matter?

Matter waves are essential section of the quantum mechanics theory. All matter show wave – particle duality behavior. The dual character of the matter is referred to as the de Broglie hypothesis. Matter waves are known as de Broglie waves.

The uncertainty principle

The uncertainty principle is known as Heisenberg's uncertainty principle which states that there fundamental limitations occur for the accuracy values of physical quantities of particles such as momentum and position. The position and the momentum are known complementary variables The uncertainty principles will limit to what extent other properties will main their relative and approximate values.

In 1927, Werner Heisenberg

δ δ

$$(\delta x)\times(\delta p)\geq\frac{h}{2\pi}$$

As with the de Broglie particle wavelength, this has practical consequences only for electrons and other particles of very small mass. It is very important to understand that these "uncertainties" are not merely limitations related to experimental error or observational technique, but instead they express an underlying fact that Nature does not allow a particle to possess definite values of position and momentum at the same time. This principle (which would be better described by the term "indeterminacy" than "uncertainty") has been thoroughly verified and has far-reaching practical consequences which extend to chemical bonding and molecular structure.

SUPPLEMENTAL

****

Is the Uncertainty Principle consistent with Particle Waves?

Yes; either one really implies the other. Consider the following two limiting cases: · A particle whose velocity is known to within a very small uncertainty will have a sharply-defined energy (because its kinetic energy is known) which can be represented by a probability wave having a single, sharply-defined frequency. A"monochromatic" wave of this kind must extend infinitely in space:

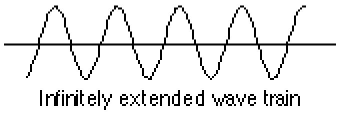


Figure 6.25 Standing Wave

But if the peaks of the wave represent locations at which the particle is most likely to manifest itself, we are forced to the conclusion that it can "be" virtually anywhere, since the number of such peaks is infinite! Now think of the opposite extreme: a particle whose location is closely known. Such a particle would be described by a short wavetrain having only a single peak, the smaller the uncertainty in position, the more narrow the peak.

To help you see how waveforms of different wavelength combine, two such combinations are shown below:

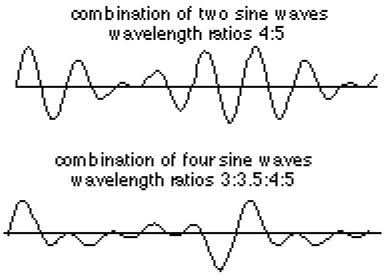


Figure 6.26 Combination of Standing Wave

It is apparent that as more waves of different frequency are mixed, the regions in which they add constructively diminish in extent. The extreme case would be a wavetrain in which destructive interference occurs at all locations except one, resulting in a single pulse:

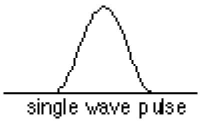
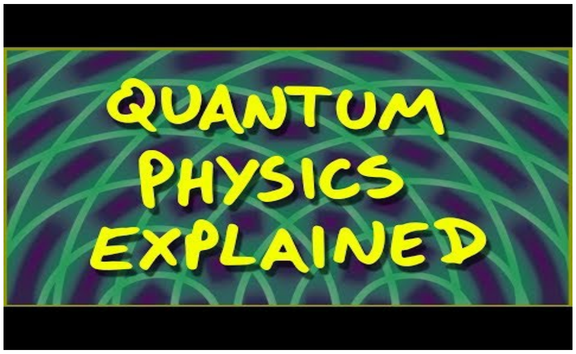
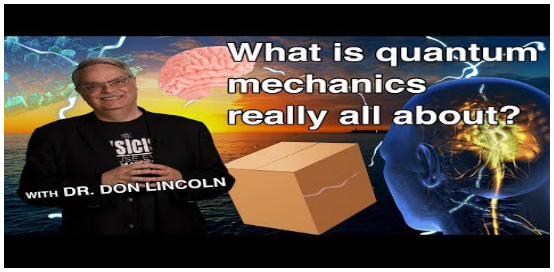


Figure 6.27 Single Wave Pulse

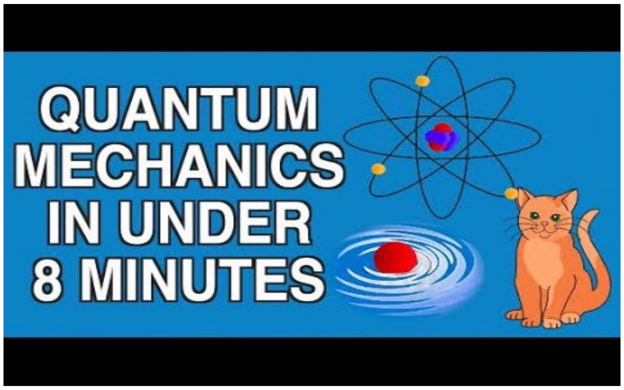
Is such a wave possible, and if so, what is its wavelength? Such a wave is possible, but only as the sum (interference) of other waves whose wavelengths are all slightly different. Each component wave possesses its own energy (momentum), and adds that value to the range of momenta carried by the particle, thus increasing the uncertainty δp. In the extreme case of a quantum particle whose location is known exactly, the probability wavelet would have zero width which could be achieved only by combining waves of all wavelengths-- an infinite number of wavelengths, and thus an infinite range of momentum δp and thus kinetic energy.



Reference: https://youtu.be/Usu9xZfabPM



Reference: https://www.youtube.com/watch?v=K0VY9_hB_WU



Reference: https://www.youtube.com/watch?v=8HkPAE_9Q1Y

Should we call them Particle or Wave?

only conclusion possible is that quantum particles have no well defined paths; each photon (or electron) seems to have an infinity of paths which thread their way through space, seeking out and collecting information about all possible routes, and then adjusting its behavior so that its final trajectory, when combined with that of others, produces the same overall effect that we would see from a train of waves of wavelength $\lambda = h/mv$.

From orbits to Orbitals

About ten years after Bohr had developed his theory, de Broglie showed that the electron should have wavelike properties of its own, thus making the analogy with the mechanical theory of standing waves somewhat less artificial. One serious difficulty with the Bohr model still remained, however: it was unable to explain the spectrum of any atom more complicated than hydrogen. A refinement suggested by Sommerfeld assumed that some of the orbits are elliptical instead of circular, and invoked a second quantum number,
ℓ, that indicated the degree of ellipticity. This concept proved useful, and it also began to offer some correlation with the placement of the elements in the periodic table.

The Schrödinger equation

By 1926, de Broglie's theory of the wave nature of the electron had been experimentally confirmed, and the stage was set for its extension to all matter. At about the same time, three apparently very different theories that attempted to treat matter in general terms were developed. These were Schrödinger's wave mechanics, Heisenberg's matrix mechanics, and a more abstract theory of P.A.M. Dirac. These eventually were seen to be mathematically equivalent, and all continue to be useful.

Of these alternative treatments, the one developed by Schrödinger is the most easily visualized. Schrödinger started with the simple requirement that the total energy of the electron is the sum of its kinetic and potential energies:

$$E = \frac{mv^2}{2} + \frac{-e^2}{r}$$

The second term represents the potential energy of an electron (whose charge is denoted by *e*) at a distance *r* from a proton (the nucleus of the hydrogen atom). In quantum mechanics it is generally easier to deal with equations that use momentum ($p = mv$) rather than velocity, so the next step is to make this substitution:

$$E = \frac{p^2}{2m} - \frac{e^2}{r}$$

Figure 6.28 Ernest Schrödinger

This is still an entirely classical relation, as valid for the waves on a guitar string as for those of the electron in a hydrogen atom. The third step is the big one: in order to take into account the wavelike character of the hydrogen atom, a mathematical expression that describes the position and momentum of the electron at all points in space is applied to both sides of the equation. The function, denoted by Ψ (*psi*), "modulates" the equation of motion of the electron so as to reflect the fact that the electron manifests itself with greater probability in some locations that at others. This yields the celebrated ***Schrödinger equation***:

If this equation looks a bit weird to you, don't be too concerned; we show it here only because one hears so much about it — quite justifiably, as it "drives" every atom in the universe.

$$\left(\frac{mv^2}{2} - \frac{e^2}{r}\right)\Psi = E\Psi$$

Physical significance of the wave function Ψ

How can such a simple-looking expression contain within it the quantum-mechanical description of an electron in an atom— and thus, by extension, of all matter? The catch, as you may well suspect, lies in discovering the correct form of Ψ , which is known as the ***wave function***. As this name suggests, the value of Ψ is a function of location in space relative to that of the proton which is the source of the binding force acting on the electron. As in any system composed of standing waves, certain boundary conditions must be applied, and these are also contained in Ψ; the major ones are that the value of Ψ must approach zero as the distance from the nucleus approaches infinity, and that the function be continuous.

When the functional form of Ψ has been worked out, the Schrödinger equation is said to have been *solved* for a particular atomic system. The details of how this is done are beyond the scope of this course, but the consequences of doing so are extremely important to us. Once the form of is known, the allowed energies E of an atom can be predicted from the above equation. Soon after Schrödinger's proposal, his equation was solved for several atoms, and in each case the predicted energy levels agreed exactly with the observed spectra.

There is another very useful kind of information contained in Ψ. Recalling that its value depends on the location in space with respect to the nucleus of the atom, the square of this function Ψ^2, evaluated at any given point in space, represents the probability of finding the electron at that particular location. The significance of this cannot be overemphasized; although the electron remains a particle having a definite charge and mass, the question of "where" it is located is no longer meaningful.

Any single experimental observation will reveal a definite location for the electron, but this will in itself have little significance; only a large number of such observations (similar to a series of multiple exposures of a photographic film) will yield meaningful results which will show that the electron can "be" anywhere with at least some degree of probability. This does not mean that the electron is "moving around" to all of these places, but that (in accord with the uncertainty principle) the concept of location has limited meaning for a particle as small as the electron. If we count only those locations in space at which the probability of the electron manifesting itself exceeds some arbitrary value, we find that the Ψ function defines a definite three-dimensional region which we call an ***orbital***.

Why doesn't the electron fall into the nucleus?

We can now return to the question which Bohr was unable to answer in 1912. Even the subsequent discovery of the wavelike nature of the electron and the analogy with standing waves in mechanical systems did not really answer the question; the electron is still a particle having a negative charge and is attracted to the nucleus.

The answer comes from the Heisenberg uncertainty principle, which says that a quantum particle such as the electron cannot simultaneously have sharply-defined values of location and of momentum (and thus kinetic energy). To understand the implications of this restriction, suppose that we place the electron in a small box. The walls of the box define the precision δ*x* to which the location is known; the smaller the box, the more exactly will we know the location of the electron. But as the box gets smaller, the uncertainty in the electron's kinetic energy will increase. As a consequence of this uncertainty, the electron will at times possess so much kinetic energy (the "confinement energy") that it may be able to penetrate the wall and escape the confines of the box.

This process is known as ***quantum tunneling***. It is exploited in various kinds of semiconductor devices, and it is the mechanism whereby electrons jump between dissolved ions and the electrode in batteries and other electrochemical devices.

(For more, see this Wikipedia article on quantum tunneling)

The region near the nucleus can be thought of as an extremely small funnel-shaped box, the walls of which correspond to the electrostatic attraction that must be overcome if an electron confined within this region is to escape. As an electron is drawn toward the nucleus by electrostatic attraction, the volume to which it is confined diminishes rapidly. Because its location is now more precisely known, its kinetic energy must become more uncertain; the electron's kinetic energy rises more rapidly than its potential energy falls, so that it gets ejected back into one of its allowed values of *n*.

The electron well of the atom

The red circles show the average distance of the electron from the nucleus for the allowed quantum levels (standing wave patterns) of

n=1 through n=3. As *n* decreases, the potential energy of the system becomes more negative and the electron becomes more confined in space. According to the uncertainty principle, this increases the momentum of the electron, and hence its kinetic energy. The latter acts as a kind of "confinement energy" that restores the electron to one of the allowed levels.

The values of *n* in the above diagram correspond to the *principal quantum number* of the hydrogen atom. When the H atom is in its normal "ground state", $n = 1$ and the radius of this circle corresponds exactly to the radius predicted by Bohr's model. The big difference between Bohr's model and the quantum model is that in the latter, the n=1 circle defines the radius at which the electron is *most likely* to be

found, rather than the radius *to which it is confine*d as Bohr's theory predicts.

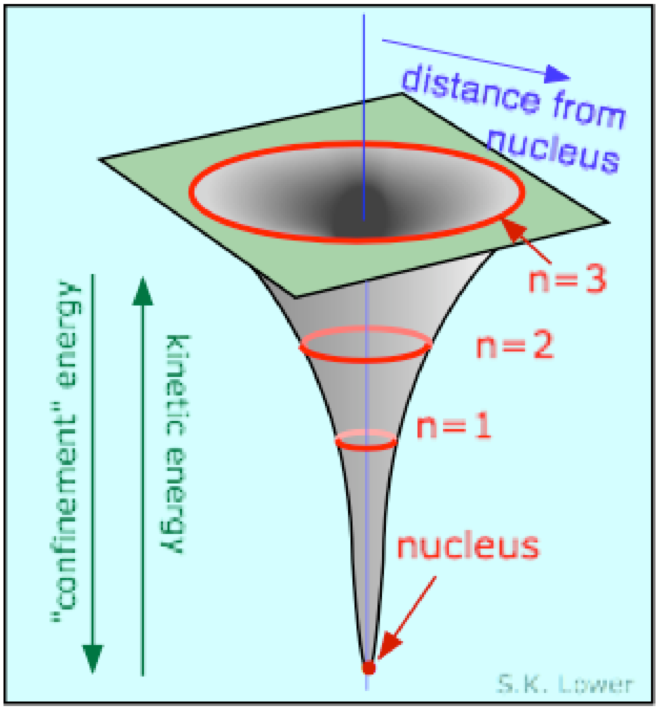


Figure 6.29 Electron tunneling of Atom

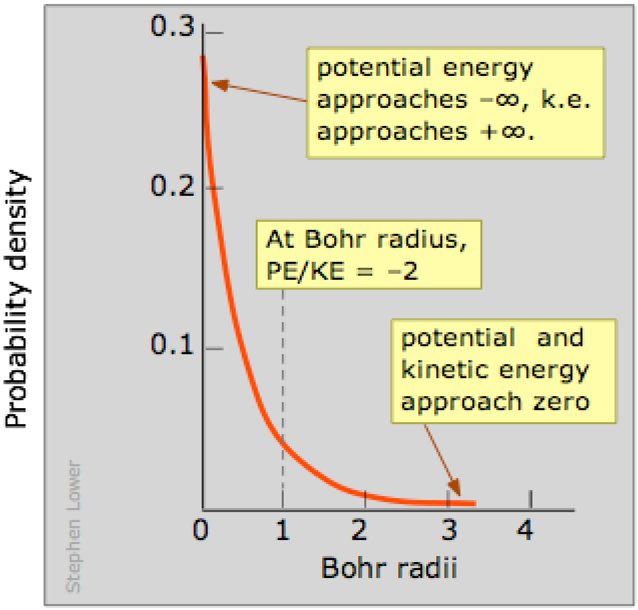


Figure 6.30 Probability Density vs. Bohr Radii

The nature of the n=1 *orbital* of the H atom is more clearly visualized by this 2-dimensional plot which shows the quantity of electron charge *per unit volume of space* at various distances from the nucleus. This is known as a *probability density plot*. The "*per unit volume of space"* part is very important here; as we consider radii closer to the nucleus, these volumes become very small, so the number of electrons per unit volume increases very rapidly. In this view, it appears as if the electron *does* fall into the nucleus!

But it doesn't quite make it; as the electron approaches the tiny volume of space occupied by the nucleus, its potential energy dives down toward minus-infinity, and its kinetic energy (momentum and velocity) shoots up toward positive-infinity. This "battle of the infinities" cannot be won by either side, so a compromise is reached in which theory tells us that *the fall in potential energy is just twice the kinetic energy*, and the electron dances at an average distance that corresponds to the Bohr radius.

Orbits give way to orbitals and electron clouds

The modern view of atomic structure dismisses entirely the old but comfortable planetary view of electrons circling around the nucleus in fixed orbits.

We can also dispose of the question of why the orbiting electron does not radiate its kinetic energy away as it revolves around the nucleus. The Schrödinger equation completely discards any concept of a definite path or trajectory of a particle; what was formerly known as an "orbit" is now an "orbital", defined as the locations in space at which the probability of finding electrons exceeds some arbitrary value. It should be noted that this wavelike character of the electron coexists with its possession of a momentum, and thus of an effective velocity, even though its motion does not imply the existence of a definite path or trajectory that we associate with a more massive particle.

The term "electron cloud" is commonly used to denote the region of space in which an electron has a significant (90-95 percent) probability of manifesting itself. It is important to understand that this does not mean that the electron is itself "smeared out" in space. If you had a magical camera that could take pictures of the electron at random instants, it would always record it as being at some definite location with a probability that corresponds to the curve labeled "radial probability" in this representation of the n=1 orbital of the hydrogen atom.

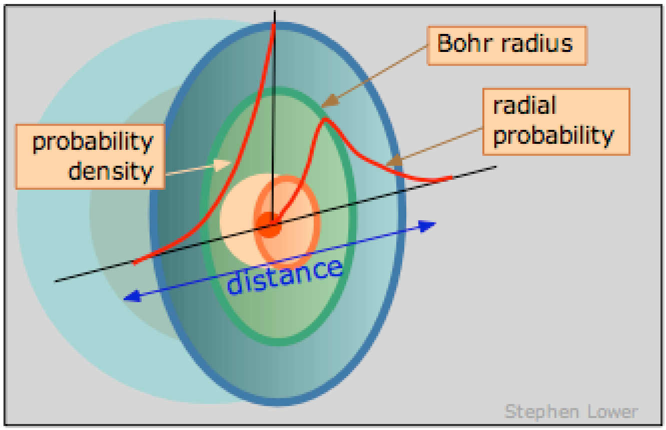


Figure 6.31 Top view of Probability Density vs. Bohr Radius

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The Quantum Numbers

Modern quantum theory tells us that the various allowed states of existence of the electron in the hydrogen atom correspond to different standing wave patterns. In the preceding lesson we showed examples of standing waves that occur on a vibrating guitar string. The wave patterns of electrons in an atom are different in two important ways:

1. Instead of indicating displacement of a point on a vibrating string, the electron waves represent the *probability* that an electron will manifest itself (appear to be located) at any particular point in space. (Note carefully that this is *not* the same as saying that "the electron is smeared out in space"; at any given instant in time, it is either at a given point or it is not.)
2. The electron waves occupy all three dimensions of space, whereas guitar strings vibrate in only two dimensions.

This one (8 min) is especially helpful in showing how the three quantum numbers *n*, *l*, and *m* arise from the wave function of the atom.

https://youtu.be/luB5a39kGkA

Other videos

Orbital energies and the principal quantum number (4 min)

https://youtu.be/Aoi4j8es4gQ

s Orbitals of the hydrogen atom
(3½ min)

https://youtu.be/Nr40fnfHccQ

Multi-electron atoms and shielding
(4½ min)

https://youtu.be/phkcJo-94pQ

Radial nodes of orbitals (quiz)

https://youtu.be/Rk6g0lfSVZI

Restrictions on quantum numbers

https://youtu.be/wnLcJH-Heyo

Electron spin, magnetism (7 min)

https://youtu.be/Bl-zUmeYj74

Aside from this, the similarities are striking. Each wave pattern is identified by an integer number *n*, which in the case of the atom is known as the ***principal quantum number***. The value of *n* tells how many peaks of amplitude (antinodes) exist in that particular standing wave pattern; the more peaks there are, the higher the energy of the state.

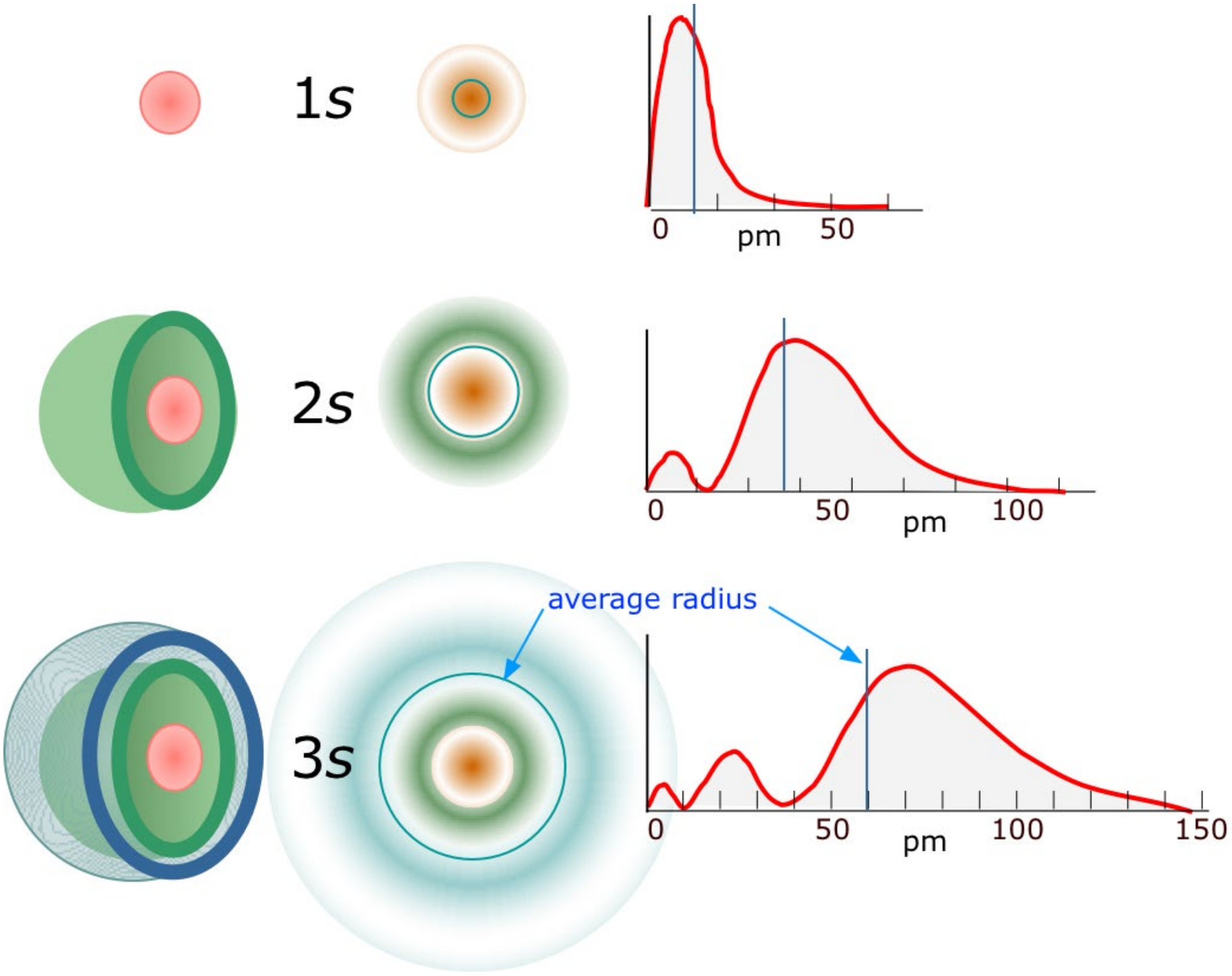

Figure 6.32 Electron Density vs. Distance from Nucleus

The three simplest orbitals of the hydrogen atom are depicted above in pseudo-3D, in cross-section, and as plots of probability (of finding the electron) as a function of distance from the nucleus. The average radius of the electron probability is shown by the blue circles or plots in the two columns on the right. These radii correspond exactly to those predicted by the Bohr model.

SUPPLEMENTAL

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Physical significance of *n*

The potential energy of the electron is given by the formula

$$E = \frac{-4\pi^2 e^4 m}{h^2 n^2}$$

in which *e* is the charge of the electron, *m* is its mass, *h* is Planck's constant, and *n* is the principal quantum number. The negative sign ensures that the potential energy is always negative. Notice that this energy in inversely proportional to the *square* of *n*, so that the energy rises toward zero as *n* becomes very large, but it can never exceed zero.

This formula was actually part of Bohr's original theory, and is still applicable to the hydrogen atom, although not to atoms containing two or more electrons. In the Bohr model, each value of *n* corresponded to an orbit of a different radius. The larger the orbital radius, the higher the potential energy of the electron; the inverse square relationship between electrostatic potential energy and distance is reflected in the inverse square relation between the energy and *n* in the above formula.

Although the concept of a definite trajectory or "orbit" of the electron is no longer tenable, the same orbital radii that relate to the different values of *n* in Bohr's theory now have a new significance: they give the average distance of the electron from the nucleus. As you can see from the figure, the averaging process must encompass several probability peaks in the case of higher values of *n*. The spatial distribution of these probability maxima defines the particular orbital.

This physical interpretation of the principal quantum number as an index of the average distance of the electron from the nucleus turns out to be extremely useful from a chemical standpoint, because it relates directly to the tendency of an atom to lose or gain electrons in chemical reactions.

The angular momentum quantum number

The electron wave functions that are derived from Schrödinger's theory are characterized by several quantum numbers. The first one, *n*, describes the nodal behavior of the probability distribution of the electron, and correlates with its potential energy and average distance from the nucleus as we have just described.

The angular momentum quantum number is conventionally represented by lower-case L: l. In order to avoid confusion with the numeral 1, it is ordinarily italized:
l. Additional clarity, which we employ here, is provided by using the scripted form: ℓ.

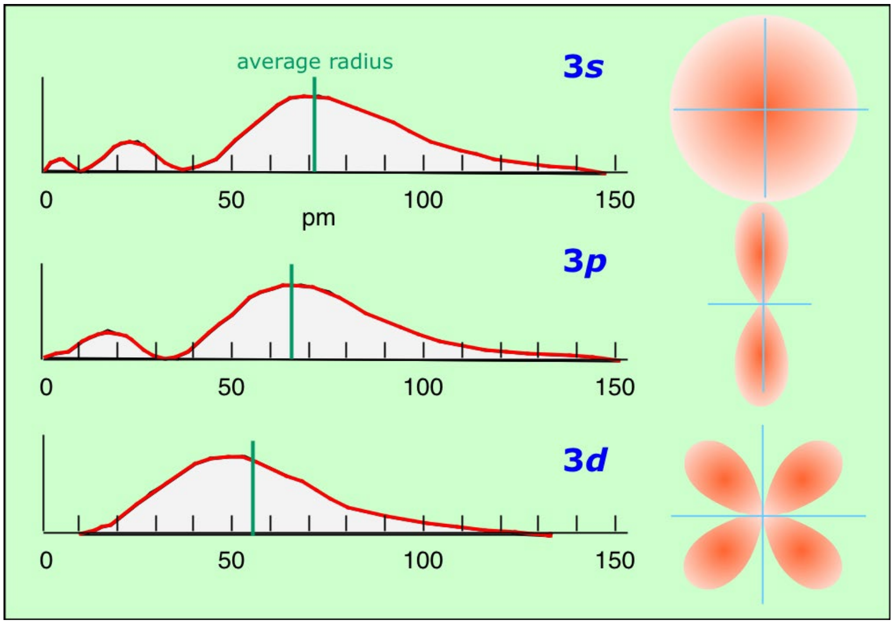

Figure 6.33 Probability Density vs. shapes of Orbitals

The theory also predicts that orbitals having the same value of *n* can differ in shape and in their orientation in space. The quantum number ℓ, known as the *angular momentum quantum number*, determines the shape of the orbital. (More precisely, ℓ determines the number of angular nodes, that is, the number of regions of zero probability encountered in a 360° rotation around the center.)

When $\ell = 0$, the orbital is spherical in shape.

If $\ell = 1$, the orbital is elongated into something resembling a figure-8 shape, and higher values of ℓ correspond to still more complicated shapes— but note that the number of peaks in the radial probability distributions (below) decreases with increasing ℓ. The possible values that ℓ can take are strictly limited by the value of the principal quantum number; ℓ can be no greater than $n - 1$. This means that for
$n = 1$, ℓ can only have the single value zero which corresponds to a spherical orbital. For historical reasons, the orbitals corresponding to different values of ℓ are designated by letters, starting with *s* for $\ell = 0$, *p* for $\ell = 1$, *d* for $\ell = 2$, and *f* for $\ell = 3$.

The shapes and radial distributions of the orbitals corresponding to the three allowed values of ℓ for the $n = 3$ level of hydrogen are shown above. Notice that the average orbital radius *r* decreases somewhat at higher values of ℓ. The function relationship is given by

$$\bar{r} = (5.29\,pm)\frac{n^2}{z}\left[\frac{3}{2} - \frac{l(l-1)}{2n^2}\right]$$

in which *z* is the nuclear charge of the atom, which of course is unity for hydrogen.

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The magnetic quantum number

An *s*-orbital, corresponding to $\ell = 0$, is spherical in shape and therefore has no special directional properties. The probability cloud of a *p* orbital is aligned principally along an axis extending along any of the three directions of space. The additional quantum number *m* is required to specify the particular direction along which the orbital is aligned.

"Direction in space" has no meaning in the absence of a force field that serves to establish a reference direction. For an isolated atom there is no such external field, and for this reason there is no distinction between the orbitals having different values of *m*. If the atom is placed in an external magnetic or electrostatic field, a coordinate system is established, and the orbitals having different values of *m* will split into slightly different energy levels. This effect was first seen in the case of a magnetic field, and this is the origin of the term *magnetic quantum number*.

In chemistry, however, electrostatic fields are much more important for defining directions at the atomic level because it is through such fields that nearby atoms in a molecule interact with each other. The electrostatic field created when other atoms or ions come close to an atom can cause the energies of orbitals having different direction properties to split up into different energy levels; this is the origin of the colors seen in many inorganic salts of transition elements, such as the blue color of copper sulfate.

The quantum number m can assume $2\ell + 1$ values for each value of ℓ, from $-\ell$ through 0 to $+\ell$. When $\ell = 0$ the only possible value of *m* will also be zero, and for the *p* orbital ($\ell = 1$), *m* can be –1, 0, and +1. Higher values of ℓ introduce more complicated orbital shapes which give rise to more possible orientations in space, and thus to more values of *m*.

Electron spin and the Exclusion Principle

Certain fundamental particles have associated with them a *magnetic moment* that can align itself in either of two directions with respect to an external magnetic field. The electron is one such particle, and the direction of its magnetic moment is called its *spin*.

The mechanical analogy implied by the term *spin* is easy to visualize, but should not be taken literally. Physical rotation of an electron is meaningless. However, the *coordinates* of the electron's wave function can be rotated mathematically; when this is done, it is found that a rotation of 720° is required to restore the function to its initial value— rather weird, considering that a 360° rotation will leave any extended body unchanged! Electron spin is basically a relativistic effect in which the electron's momentum distorts local space and time. It has no classical counterpart and thus cannot be visualized other than through mathematics.

Exclusion principle and Hund's rule
UC-Berkeley, 6 min)

https://youtu.be/Z08pNaGQPv8

How the Schrödinger equation predicts the exclusion principle
(TinaHuang, 4 min)

https://youtu.be/I93gZ_zfOpg

A basic principle of modern physics states that for particles such as electrons that possess half-integral values of spin, no two of them can be in identical quantum states within the same system. The quantum state of a particle is defined by the values of its quantum numbers, so what this means is that **no two electrons in the same atom can have the same set of quantum numbers.** This is known as the ***Pauli exclusion principle***, named after the German physicist Wolfgang Pauli (1900-1958, Nobel Prize 1945).

The best non-mathematical explanation of the exclusion principle that I have come across is Phil Fraundorf's Candle Dances and Atoms page at U. Missouri-St. Louis.

The exclusion principle was discovered empirically and was placed on a firm theoretical foundation by Pauli in 1925. A complete explanation requires some familiarity with quantum mechanics, so all we will say here is that if two electrons possess the same quantum numbers n, l, m and s (defined below), the wave function that describes the state of existence of the two electrons together becomes zero, which means that this is an "impossible" situation.

A given *orbital* is characterized by a fixed set of the quantum numbers n, ℓ, and m. The electron spin itself constitutes a fourth quantum number s, which can take the two values +1 and –1. Thus **a given orbital can contain two electrons having opposite spins**, which "cancel out" to produce zero magnetic moment. Two such electrons in a single orbital are often referred to as an ***electron pair***.

More on the Pauli exclusion principle from answers.com

If it were not for the exclusion principle, the atoms of all elements would behave in the same way, and there would be no need for a science of Chemistry!

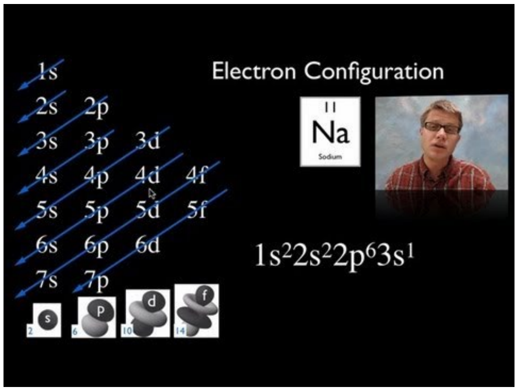
As we have seen, the lowest-energy standing wave pattern the electron can assume in an atom corresponds to n=1, which describes the state of the single electron in hydrogen, and of the two electrons in helium. Since the quantum numbers m and ℓ are zero for n=1, the pair of electrons in the helium orbital have the values $(n, l, m, s) = (1,0,0,+1)$ and $(1,0,0,-1)$— that is, they differ only in spin. These two sets of quantum numbers are the only ones that are possible for a n=1 orbital. The additional electrons in atoms beyond helium must go into higher-energy (n>1) orbitals.

Electron wave patterns corresponding to these greater values of n are concentrated farther from the nucleus, with the result that these electrons are less tightly bound to the atom and are more accessible to interaction with the electrons of neighboring atoms, thus influencing their *chemical behavior*. If it were not for the Pauli principle, all the electrons of every element would be in the lowest-energy n=1 state, and the differences in the chemical behavior the different elements would be minimal. Chemistry would certainly be a simpler subject, but it would not be very interesting!

6.4 Electronic Structure of Atoms (Electron Configurations)

In atomic physics and quantum chemistry, the electron configuration is the distribution of electrons of an atom or molecule (or other physical structure) in atomic or molecular orbitals.

Electrons in an atom are grouped around the nucleus into shells. Shell (electron): A grouping of electrons in an atom according to energy. The farther a shell is from the nucleus, the larger it is, the more electrons it can hold, and the higher the energies of those electrons.



Reference: https://www.youtube.com/watch?v=2AFPfg0Como

Introduction: What are Electron Configurations?

The **electron configuration** of an element describes how electrons are distributed in its atomic orbitals. **Electron configurations** of atoms follow a standard notation in which all **electron**-containing atomic subshells (with the number of electrons they hold written in superscript) are placed in a sequence. For example, the electron configuration of sodium is $1s^22s^22p^63s^1$.

However, the standard notation often yields lengthy electron configurations (especially for elements having a relatively large atomic number). In such cases, an abbreviated or condensed notation may be used instead of the standard notation. In the abbreviated notation, the sequence of completely filled subshells that correspond to the electronic configuration of a noble gas is replaced with the symbol of that noble gas in square brackets. Therefore, the abbreviated electron configuration of sodium is $[Ne]3s^1$ (the electron configuration of neon is $1s^22s^22p^6$, which can be abbreviated to $[He]2s^22p^6$). This is called spectroscopic notation of electron configurations.

Electron Configurations are useful for:

- Determining the valency of an element.
- Predicting the properties of a group of elements (elements with similar electron configurations tend to exhibit similar properties).
- Interpreting atomic spectra.

This notation for the distribution of electrons in the atomic orbitals of atoms came into practice shortly after the Bohr model of the atom was presented by Ernest Rutherford and Niels Bohr in the year 1913.

Writing Electron Configurations

Shells

The maximum number of electrons that can be accommodated in a shell is based on the principal quantum number (n). It is represented by the formula $2n^2$, where 'n' is the shell number. The shells, values of n, and the total number of electrons that can be accommodated are tabulated below.

Shell and 'n' value	**Max. Electrons in the Electron Configuration**
K shell, n=1	$2*1^2 = 2$
L shell, n=2	$2*2^2 = 8$
M shell, n=3	$2*3^2 = 18$
N shell, n=4	$2*4^2 = 32$

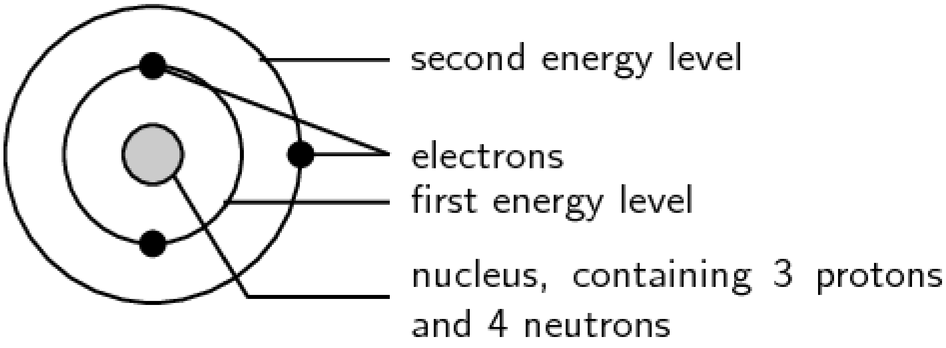


Figure 6.34 Multi-electron System

Subshells

- The subshells into which electrons are distributed are based on the azimuthal quantum number (denoted by 'l').
- This quantum number is dependent on the value of the principal quantum number, n. Therefore, when n has a value of 4, four different subshells are possible.
- When n=4. the subshells correspond to l=0, l=1, l=2, and l=3 and are named the s, p, d, and f subshells respectively.
- The maximum number of electrons that can be accommodated by a subshell is given by the formula $2*(2l + 1)$.

- Therefore, the s, p, d, and f subshells can accommodate a maximum of 2, 6, 10, and 14 electrons respectively.

All the possible subshells for values of n up to 4 are tabulated below.

Principle Quantum Number Value	**Value of Azimuthal Quantum Number**	**Resulting Subshell in the Electron Configuration**
n=1	l=0	1s
n=2	l=0	2s
	l=1	2p
n=3	l=0	3s
	l=1	3p
	l=2	3d
n=4	l=0	4s
	l=1	4p
	l=2	4d
	l=3	4f

Thus, it can be understood that the 1p, 2d, and 3f orbitals do not exist because the value of the azimuthal quantum number is always less than that of the principal quantum number.

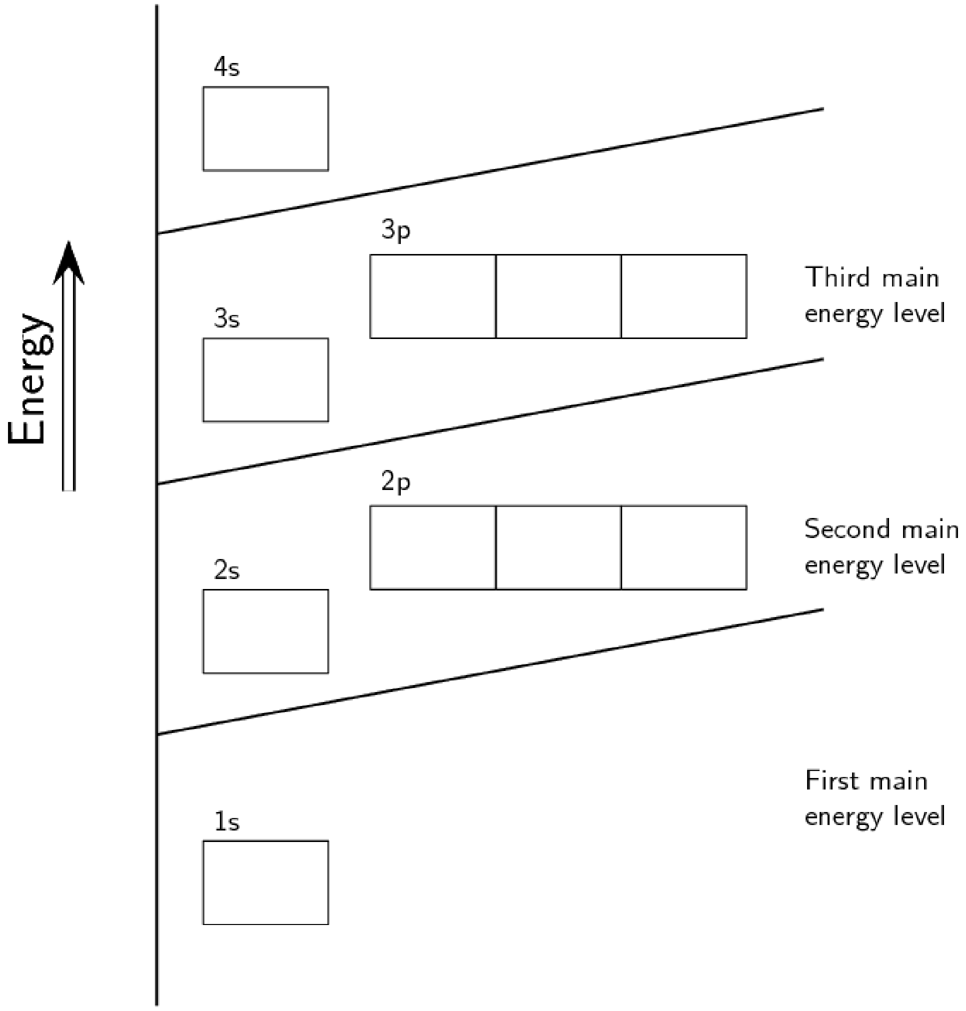


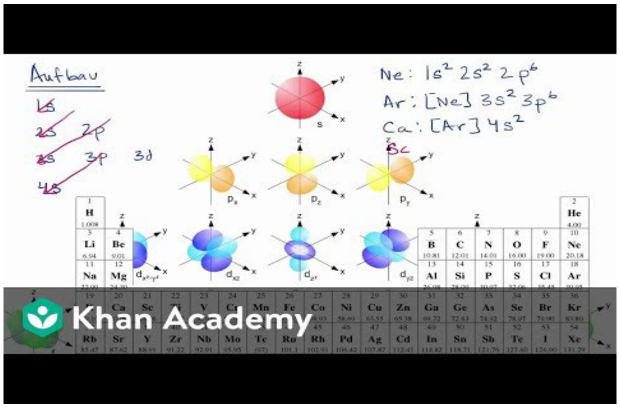
Figure 6.35 Energy level of Orbitals

Notation

- The electron configuration of an atom is written with the help of subshell labels.
- These labels contain the shell number (given by the principal quantum number), the subshell name (given by the azimuthal quantum number), and the total number of electrons in the subshell in superscript.
- If two electrons are filled in the ‘s’ subshell of the first shell, the resulting notation is ‘$1s^2$’.
- With the help of these subshell labels, the electron configuration of magnesium (atomic number 12) can be written as $1s^2\ 2s^2\ 2p^6\ 3s^2$.

Filling of Atomic Orbitals

The Aufbau principle, from the German Aufbau prinzip, also called the aufbau rule, states that in the ground state of an atom or ion, electrons fill atomic orbitals of the lowest available energy levels before occupying higher levels. For example, the 1s subshell is filled before the 2s subshell is occupied.



Reference: https://www.youtube.com/watch?v=Zersl0Ji3P0

- It states that in ground state of atom, the orbitals are filled in increasing order of their energies.
- So electrons first occupy the lowest energy orbital available to them and enter into higher energy orbitals only after the lower energy orbitals are filled as per Pauli Exclusion principle & Hund Rule
- Now we know that energy of a given orbital depends upon effective nuclear charge and different type of orbitals are affected to different extent. So there is no single ordering of energies of orbitals which will be universally correct for all atoms
- But Following ordering can be used to predict the configuration of electrons in atom
  1s, 2s ,2p, 3s ,3p ,4s ,3d ,4p, 5s,4d,5p,4f,5d,6p

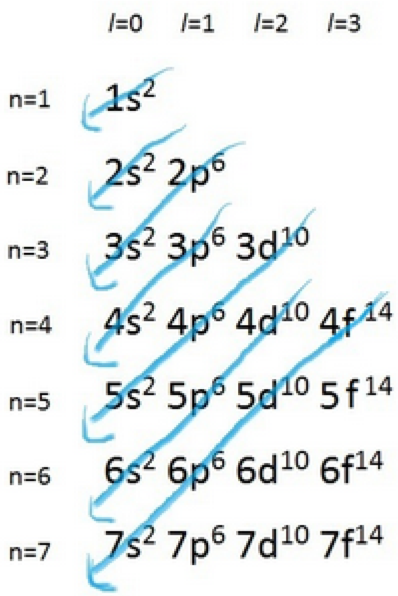


Figure 6.36 Aufbau Principle

Summary:

Type of orbital

Each shell in an atom has a different type of orbital.
For example:

1. *The innermost shell (n=1) only has an s orbital.*
2. *The second shell (n=2) has an s orbital and a p orbital.*
3. *The third shell (n=3) has s, p, d orbitals.*
4. *From the fourth shell (n>=4) there are s, p, d, f orbitals.*

Each orbital has a fixed number of electrons.

1. *s Orbital can contain 2 electrons.*
2. *p Orbital can contain 6 electrons.*
3. *d Orbital can contain 10 electrons.*
4. *f Orbital can contain 14 electrons.*

Each orbital has a slightly different electrical potential energy.

$$s < p < d < f$$

The s orbital has the lowest energy so that the electrons can be the most stable.
If both the s orbital and the p orbital of the same shell are empty, the electrons first try to fill the s orbital first.

Rules for electrons to be filled

In a stable atom, electrons are filled from the innermost shell.
In the same shell, electrons are filled in the order of s, p, d, f orbitals.
In other words, as the energy increases in the order of s → p → d → f, the energy level increases.

When the number of shells exceeds 3, the energy boundary begins to become unclear.
For example, a 4s orbital has a lower energy value compared to a 3d orbital. So, before the 3d orbital is filled with electrons, the 4s orbital is filled with electrons first.
Similarly, before the 4d orbital is filled with electrons, it is first filled in the 5s orbital.

Besides, electrons have the property of being in pairs (even) as can as possible.
Also, there are cases where electrons become stable as they fill the upper orbital first. In this case, an exception occurs.

Reference:
https://chem.libretexts.org/Bookshelves/Physical_and_Theoretical_Chemistry_Textbook_Maps/Supplemental_Modules_(Physical_and_Theoretical_Chemistry)/Quantum_Mechanics/10%3A_Multi-electron_Atoms/Electron_Configuration

The above order is based on Madelung's Rule which states that

a) The sum of the values of the principal quantum numbers (n) and azimuthal quantum number (l) i.e (n+l) determined the energy level of an orbital. Subshell having lower n+l value will be filled first.

b) The lower value of the sum of (n+l) implies that the energy of the orbital is low. If the value of n+l for two orbitals is equal then the orbital with a lower value of n will have a lower energy level.

The table below shows the electron configuration for each element in the periodic table:

Reference:
https://chem.libretexts.org/Bookshelves/General_Chemistry/Book%3A_ChemPRIME_(Moore_et_al.)/05%3A_The_Electronic_Structure_of_Atoms/5.17%3A_Electron_Configurations_and_the_Periodic_Table

Table: Atomic Electron Configurations

Z (atomic number)	Element	Configuration
1	H	$1s^1$
2	He	$1s^2$
3	Li	[He] $2s^1$
4	Be	[He] $2s^2$
5	B	[He] $2s^2$ $2p^1$
6	C	[He] $2s^2$ $2p^2$

Z	Element	Configuration
7	N	[He] $2s^{2} 2p^{3}$
8	0	[He] $2s^{2} 2p^{4}$
9	F	[He] $2s^{2} 2p^{5}$
10	Ne	[He] $2s^{2} 2p^{6}$
11	Na	[Ne] $3s^{1}$
12	Mg	[Ne] $3s^{2}$
13	Al	[Ne] $3s^{2} 3p^{1}$
14	Si	[Ne]$3s^{2} 3p^{2}$
15	P	[Ne] $3s^{2} 3p^{3}$
16	S	[Ne] $3s^{2} 3p^{4}$
17	Cl	[Ne] $3s^{2} 3p^{5}$
18	Ar	[Ne] $3s^{2} 3p^{6}$
19	K	[Ar] $4s^{1}$
20	Ca	[Ar] $4s^{2}$
21	Sc	[Ar] $3d^{1} 4s^{2}$
22	Ti	[Ar] $3d^{2} 4s^{2}$
23	V	[Ar] $3d^{3} 4s^{2}$
24	Cr	[Ar] $3d^{5} 4s^{1}$
25	Mn	[Ar] $3d^{5} 4s^{2}$
26	Fe	[Ar] $3d^{6} 4s^{2}$
27	Co	[Ar] $3d^{7} 4s^{2}$
28	Ni	[Ar] $3d^{8} 4s^{2}$
29	Cu	[Ar] $3d^{10} 4s^{1}$
30	Zn	[Ar] $3d^{10} 4s^{2}$
31	Ga	[Ar] $3d^{10} 4s^{2} 4p^{1}$
32	Ge	[Ar] $3d^{10} 4s^{2} 4p^{2}$
33	As	[Ar] $3d^{10} 4s^{2} 4p^{3}$
34	Se	[Ar] $3d^{10} 4s^{2} 4p^{4}$
35	Br	[Ar] $3d^{10} 4s^{2} 4p^{5}$
36	Kr	[Ar] $3d^{10} 4s^{2} 4p^{6}$
37	Rb	[Kr] $5s^{1}$

38	Sr	[Kr] $5s^{2}$
39	Y	[Kr] $4d^{1}\ 5s^{2}$
40	Zr	[Kr] $4d^{2}\ 5s^{2}$
41	Nb	[Kr] $4d^{4}\ 5s^{1}$
42	Mo	[Kr] $4d^{5}\ 5s^{1}$
43	Tc	[Kr] $4d^{5}\ 5s^{2}$
44	Ru	[Kr] $4d^{7}\ 5s^{1}$
45	Rh	[Kr] $4d^{8}\ 5s^{1}$
46	Pd	[Kr] $4d^{10}$
47	Ag	[Kr] $4d^{10}\ 5s^{1}$

Z	Element	Configuration
48	Cd	$[\mathrm{Kr}]\ 4d^{10}\ 5s^{2}$
49	In	$[\mathrm{Kr}]\ 4d^{10}\ 5s^{2}\ 5p^{1}$
50	Sn	$[\mathrm{Kr}]\ 4d^{10}\ 5s^{2}\ 5p^{2}$
51	Sb	$[\mathrm{Kr}]\ 4d^{10}\ 5s^{2}\ 5p^{3}$
52	Te	$[\mathrm{Kr}]\ 4d^{10}\ 5s^{2}\ 5p^{4}$
53	I	$[\mathrm{Kr}]\ 4d^{10}\ 5s^{2}\ 5p^{5}$
54	Xe	$[\mathrm{Kr}]\ 4d^{10}\ 5s^{2}\ 5p^{6}$
55	Cs	$[\mathrm{Xe}]\ 6s^{1}$
56	Ba	$[\mathrm{Xe}]\ 6s^{2}$
57	La	$[\mathrm{Xe}]\ 5d^{1}\ 6s^{2}$
58	Ce	$[\mathrm{Xe}]\ 4f^{1}\ 5d^{1}\ 6s^{2}$
59	Pr	$[\mathrm{Xe}]\ 4f^{3}\ 6s^{2}$
60	Nd	$[\mathrm{Xe}]\ 4f^{4}\ 6s^{2}$
61	Pm	$[\mathrm{Xe}]\ 4f^{5}\ 6s^{2}$
62	Sm	$[\mathrm{Xe}]\ 4f^{6}\ 6s^{2}$
63	Eu	$[\mathrm{Xe}]\ 4f^{7}\ 6s^{2}$
64	Gd	$[\mathrm{Xe}]\ 4f^{7}\ 5d^{1}\ 6s^{2}$
65	Tb	$[\mathrm{Xe}]\ 4f^{9}\ 6s^{2}$
66	Dy	$[\mathrm{Xe}]\ 4f^{10}\ 6s^{2}$
67	Ho	$[\mathrm{Xe}]\ 4f^{11}\ 6s^{2}$
68	Er	$[\mathrm{Xe}]\ 4f^{12}\ 6s^{2}$
69	Tm	$[\mathrm{Xe}]\ 4f^{13}\ 6s^{2}$
70	Yb	$[\mathrm{Xe}]\ 4f^{14}\ 6s^{2}$
71	Lu	$[\mathrm{Xe}]\ 4f^{14}\ 5d^{1}\ 6s^{2}$
72	Hf	$[\mathrm{Xe}]\ 4f^{14}\ 5d^{2}\ 6s^{2}$
73	Ta	$[\mathrm{Xe}]\ 4f^{14}\ 5d^{3}\ 6s^{2}$
74	W	$[\mathrm{Xe}]\ 4f^{14}\ 5d^{4}\ 6s^{2}$
75	Re	$[\mathrm{Xe}]\ 4f^{14}\ 5d^{5}\ 6s^{2}$
76	0s	$[\mathrm{Xe}]\ 4f^{14}\ 5d^{6}\ 6s$

		^{2}
77	Ir	[Xe] $4f^{14}\ 5d^{7}\ 6s^{2}$
78	Pt	[Xe] $4f^{14}\ 5d^{9}\ 6s^{1}$
79	Au	[Xe] $4f^{14}\ 5d^{10}\ 6s^{1}$
80	Hg	[Xe] $4f^{14}\ 5d^{10}\ 6s^{2}$
81	Tl	[Xe] $4f^{14}\ 5d^{10}\ 6s^{2}\ 6p^{1}$
82	Pb	[Xe] $4f^{14}\ 5d^{10}\ 6s^{2}\ 6p^{2}$
83	Bi	[Xe] $4f^{14}\ 5d^{10}\ 6s^{2}\ 6p^{3}$
84	Po	[Xe] $4f^{14}\ 5d^{10}\ 6s^{2}\ 6p^{4}$
85	At	[Xe] $4f^{14}\ 5d^{10}\ 6s^{2}\ 6p^{5}$
86	Rn	[Xe] $4f^{14}\ 5d^{10}\ 6s^{2}\ 6p^{6}$
87	Fr	[Rn] $7s^{1}$
88	Ra	[Rn] $7s^{2}$

Z	Element	Configuration
89	Ac	[Rn] $6d^{1}\,7s^{2}$
90	Th	[Rn] $6d^{2}\,7s^{2}$
91	Pa	[Rn] $5f^{2}\,6d^{1}\,7s^{2}$
92	U	[Rn] $5f^{3}\,6d^{1}\,7s^{2}$
93	Np	[Rn] $5f^{4}\,6d^{1}\,7s^{2}$
94	Pu	[Rn] $5f^{6}\,7s^{2}$
95	Am	[Rn] $5f^{7}\,7s^{2}$
96	Cm	[Rn] $5f^{7}\,6d^{1}\,s^{2}$
97	Bk	[Rn] $5f^{9}\,s^{2}$
98	Cf	[Rn] $5f^{10}\,s^{2}$
99	Es	[Rn] $5f^{11}\,s^{2}$
100	Fm	[Rn] $5f^{12}\,s^{2}$
101	Md	[Rn] $5f^{13}\,s^{2}$
102	No	[Rn] $5f^{14}\,s^{2}$
103	Lr	[Rn] $5f^{14}\,6d^{1}\,s^{2}$
104	Rf	[Rn] $5f^{14}\,6d^{2}\,s^{2}$

The first period of the periodic table has the elements of H (Hydrogen) and He (Helium). Both are distinguished with the electron configuration of $1\,s^{1}$ and $1\,s^{2}$ respectively.

The group 1 A and 2 A will have the general valence electrons subshell of $1\,s^{x}$ and $2\,s^{y}$ where x and y are number of valence electrons which equals number of the group. The most general formula is $n\,s^{1}$ and $n\,s^{2}$ for group the S block of the periodic table of the elements where n is number of the period.

The second period of the periodic table starts with the element Li (Lithium) that has the electron configuration $1\,s^{2}\,2\,s^{1}$ followed by Be (Beryllium) with electron configuration $1\,s^{2}\,2\,s^{2}$. After these two elements, element Boron (B) which starts filling the p orbital. The electrum configuration of Boron (B) is $1\,s^{2}\,2\,s^{2}\,2\,p^{1}$ or [He] $2\,s^{2}\,2\,p^{1}$ with the 3 valence electrons hosted in $2\,s^{2}\,2\,p^{1}$. The 2-p subshell will be filled starting from B (Boron) till Ne (Neon).

The groups 2 A through 8 A will have the general valence electrons subshell of $2\,s^{x}\,2\,p^{y}$ where x + y equals the number of valence electrons which equals number of the group.

The third period of the periodic table then starts with Na (Sodium) and Mg (Magnesium) where the 3 s orbital starts to be filled. The electron configuration of Na (sodium) is [Ne] $3\,s^{1}$. Mg (Magnesium) will have the electron configuration of [Ne] $3\,s^{2}$. Starting with the Al (Aluminum) the 3 p orbitals will start to be filled till Ar (Argon).

The groups 3 A through 8 A will have the general valence electrons subshell of $3\,s^{x}\,3\,p^{y}$ where x + y equals the number of valence electrons which equals number of the group. More generally the valence electron subshells have the general formula $ns^x np^y$ where n is number of the period and x + y is number of the valence electrons. This formula can be used for All elements of the P block

The transition metals are hosted in group B and called the D block elements. In these elements the d orbitals will be utilized and filled. The general formula for the electron valence subshell is

$(n-1)d^x ns^y$ where n number of the period and x + y is number of the valence electrons which equals number of the group.

The Lanthanides and the Actinides are utilizing the f subshells. The general formula for the electron subshell is $(n-2)f^x (n-1)d^y ns^z$ where x + y + z equals the valence electrons and equals number of the main groups. The Lanthanides and Actinides (inner transition elements) occupy periods 6 and 7 respectively.

The Lanthanides and Actinides occupy the groups extending from the D and the P blocks as can be seen below:

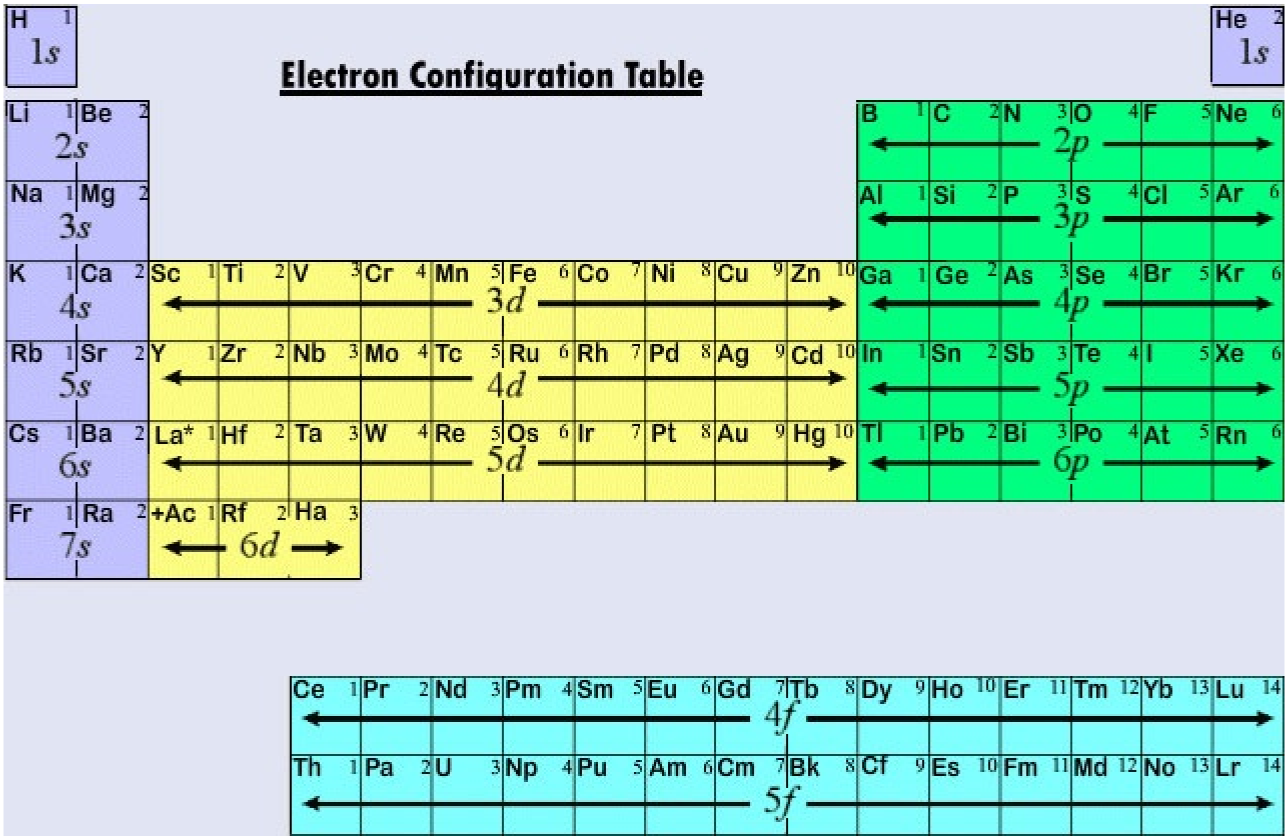


Figure 6.37 Periodic Classification of Electron Configuration

Reference:
https://chem.libretexts.org/Bookshelves/General_Chemistry/Book%3A_ChemPRIME_(Moore_et_al.)/05%3A_The_Electronic_Structure_of_Atoms/5.17%3A_Electron_Configurations_and_the_Periodic_TablePau

Pauli Exclusion Principle

A basic principle of modern physics states that for particles such as electrons that possess half-integral values of spin, no two of them can be in identical quantum states within the same system. The quantum state of a particle is defined by the values of its quantum numbers, so what this means is that **no two electrons in the same atom can have the same set of quantum numbers.** This is known as the *Pauli exclusion principle*, named after the German physicist Wolfgang Pauli (1900-1958, Nobel Prize 1945).

Hund's Rule

When the two electrons are entering an orbital, they should enter this orbital singly and parallel to each other (with the same spin).

An example of Hund's Rule is given below:

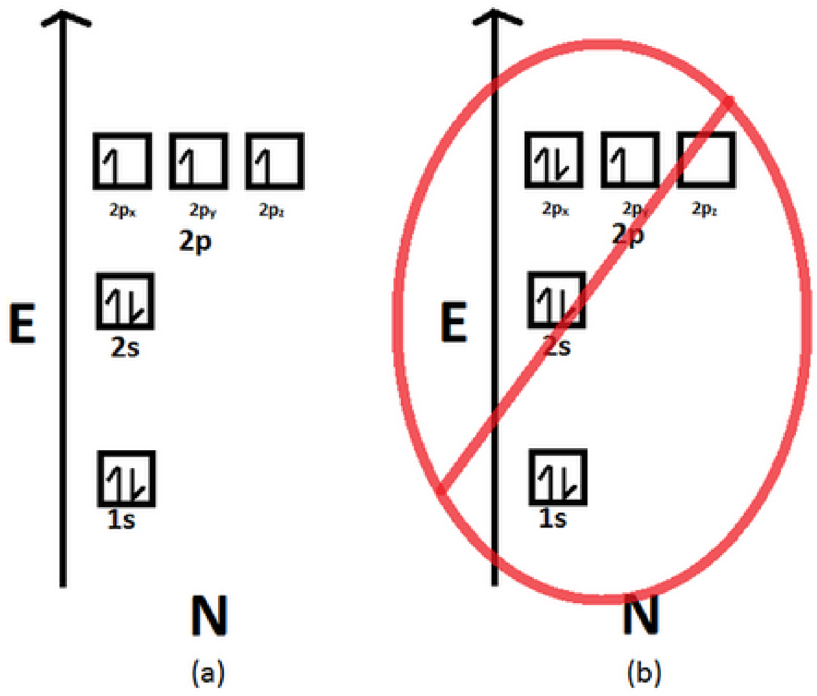


Figure 6.38 Hund's Rule

Below is some electronic arrangements of atoms for period I and II elements.

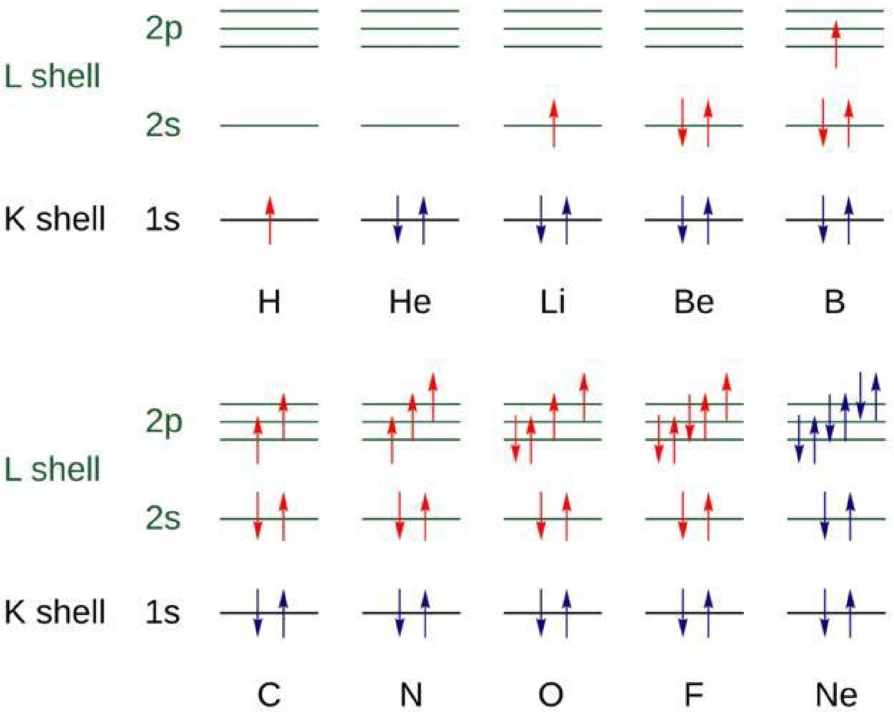


Figure 6.39 location of electrons in different shells and subshells

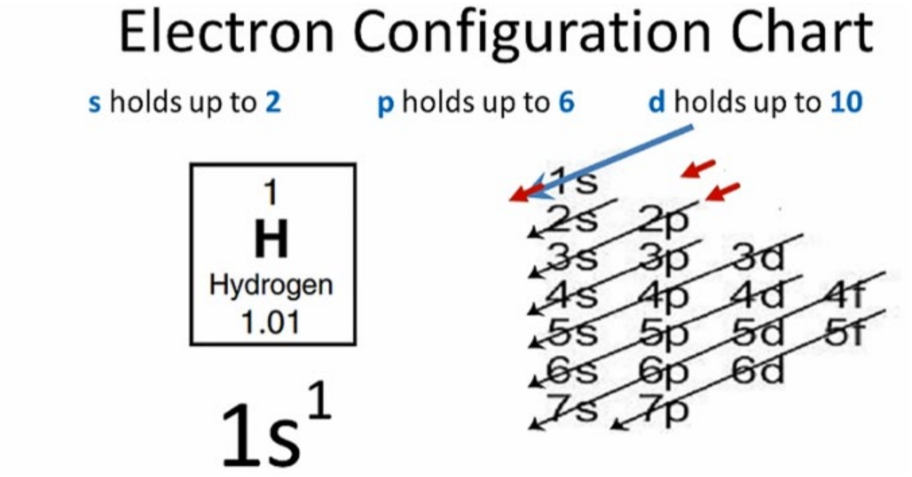
Reference:
https://chem.libretexts.org/Bookshelves/Physical_and_Theoretical_Chemistry_Textbook_Maps/Supplemental_Modules_(Physical_and_Theoretical_Chemistry)/Quantum_Mechanics/10%3A_Multi-electron_Atoms/Electron_Configuration

Examples

The electron configurations of a few elements are provided with illustrations in this subsection.

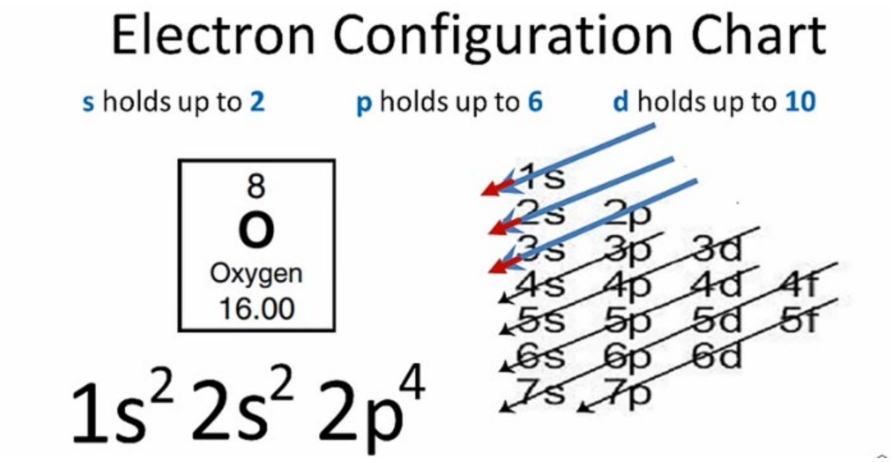
Worked Example 1: Electron Configuration of Hydrogen

The atomic number of hydrogen is 1. Therefore, a hydrogen atom contains 1 electron, which will be placed in the s subshell as shown below:



Reference: https://www.youtube.com/watch?v=Wwb8fSXr6oo

Worked Example 2: Electron Configuration of Oxygen



Reference: https://www.youtube.com/watch?v=Wwb8fSXr6oo

$1s^2$ is the electron configuration of Helium [He}

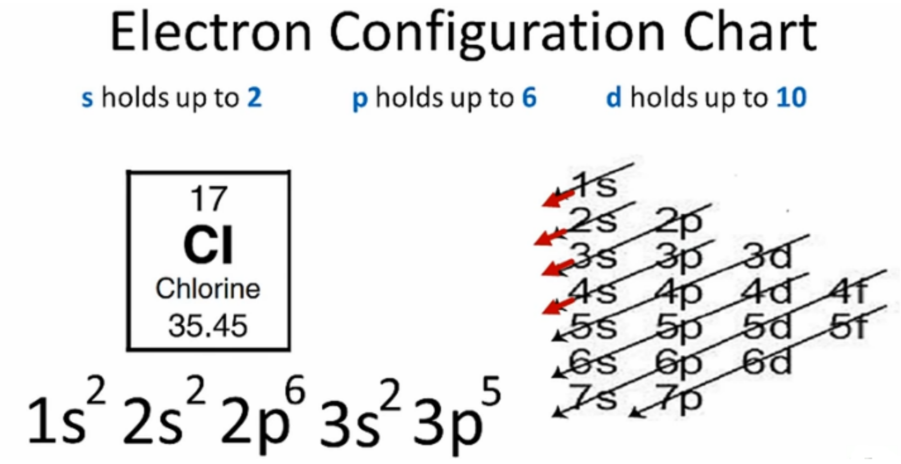
Electron Configuration of Oxygen based on inert gas core:

[He] $2s^2$ $2p^4$

The valence electron is equal the number of the group. Oxygen is found in the 6th group and hence the valence electrons are 6.

The orbitals that are hosting the valence electrons are $2s^2$ $2p^4$

Worked Example 3: Electron Configuration of Chlorine



Reference: https://www.youtube.com/watch?v=5cfC28KFHRQ

$1s^2$ $2s^2$ $2p^6$ is the electron configuration of Neon [Ne]

Electron Configuration of chlorine based on inert gas core:

[Ne] $3s^2$ $3p^5$

The valence electron is equal the number of the group. Chlorine is found in the 7th group and hence the valence electrons are 7.

The orbitals that are hosting the valence electrons are $3s^2$ $3p^5$

Worked Example 4: AUFBAU DIAGRAMS AND SPECTROSCOPIC ELECTRON CONFIGURATION

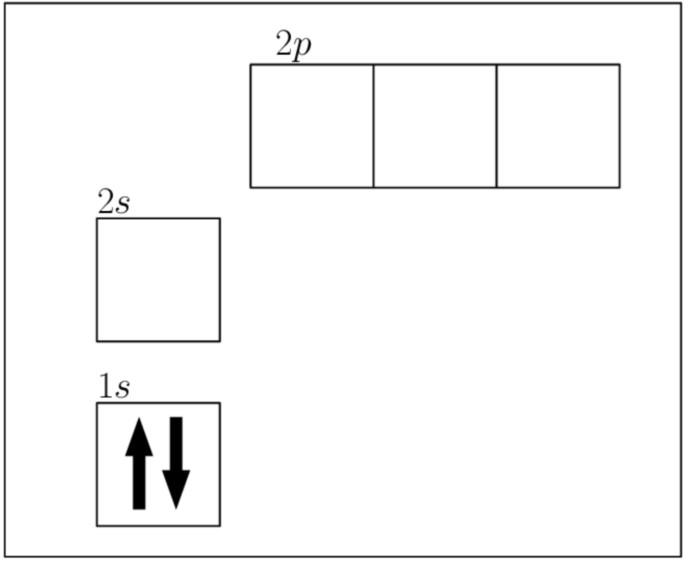
Give the electron configuration for nitrogen (N) and draw an Aufbau diagram.

Give the number of electrons

Nitrogen has seven electrons.

Place two electrons in the 1s orbital

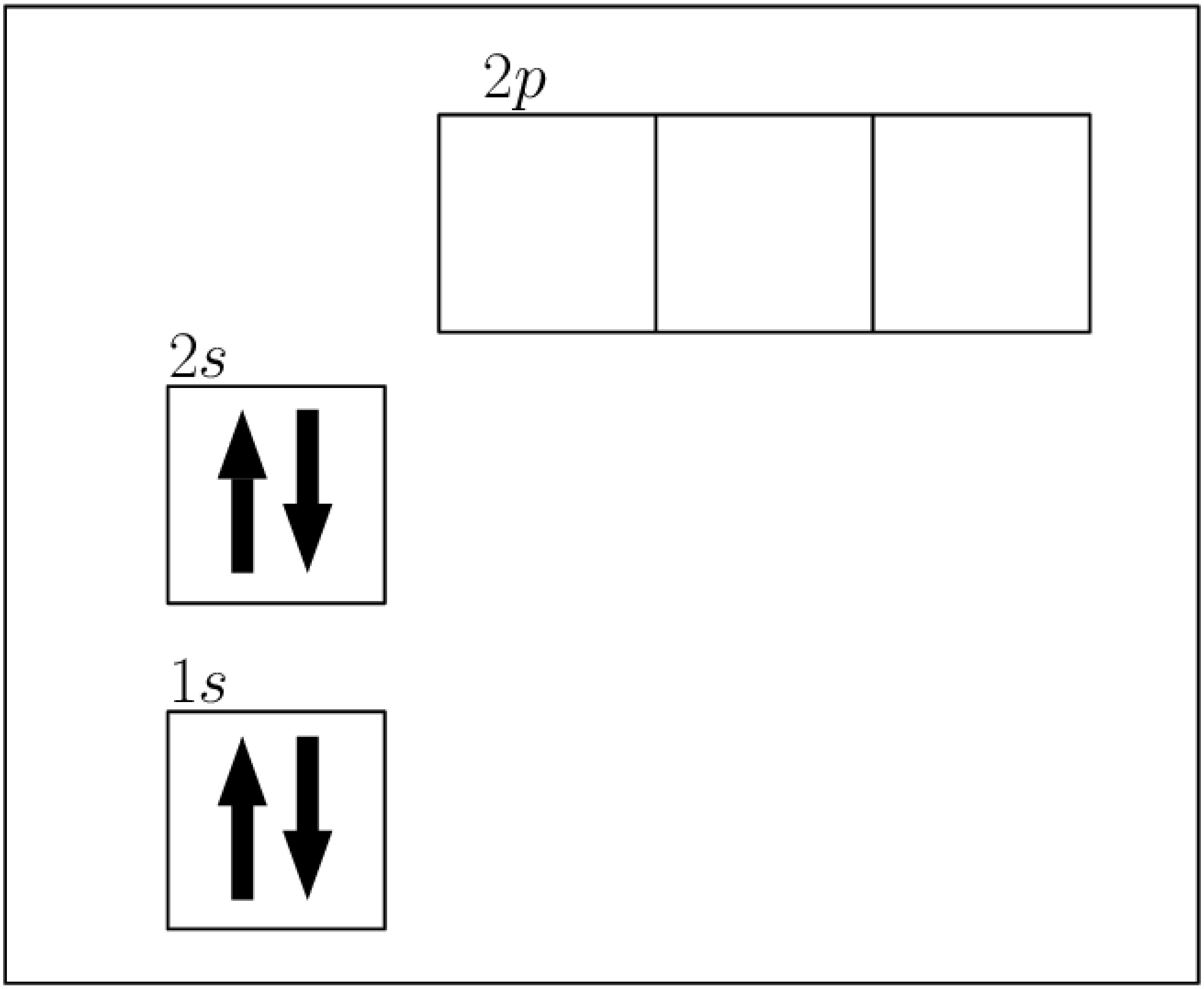
We start by placing two electrons in the 1s orbital: $1s^2 1s^2$.



Now we have five electrons left to place in orbitals.

Place two electrons in the 2s orbital

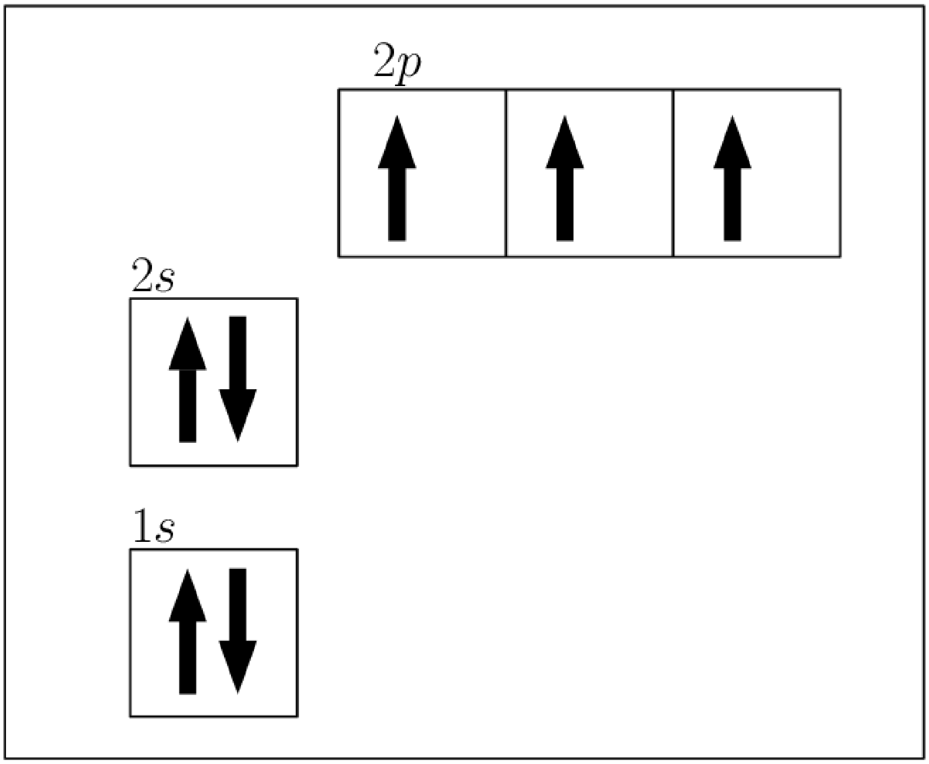
We put two electrons in the 2s orbital: $2s^2 2s^2$.



There are now three electrons to place in orbitals.

Place three electrons in the 2p orbital

We place three electrons in the 2p orbital: $2p^3 2p^3$.



Write the final answer

The electron configuration is: $1s^{2}2s^{2}2p^{3}1s^{2}2s^{2}2p3$. The Aufbau diagram is given in the step above.

Electron Configuration of Ions:

WORKED EXAMPLE 5: AUFBAU DIAGRAM FOR AN ION

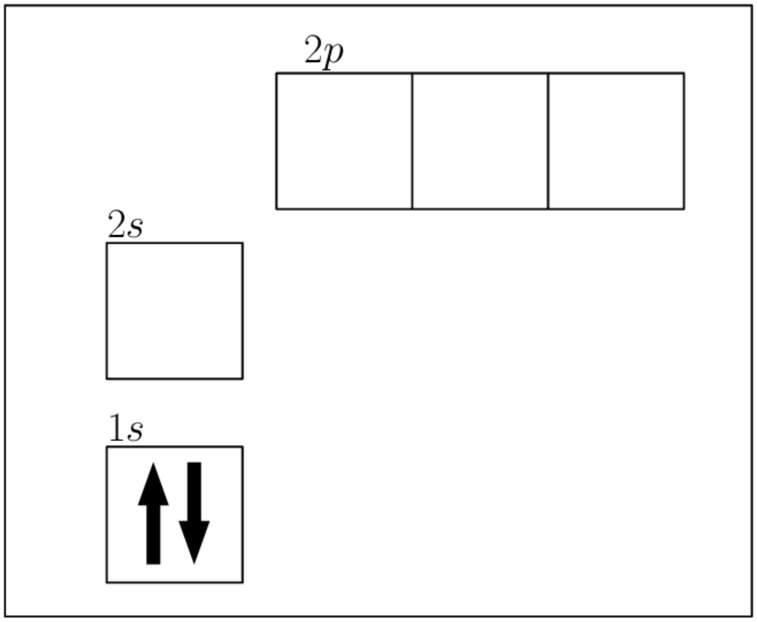
Give the electron configuration for (O^{2-}) and draw an Aufbau diagram.

Give the number of electrons

Oxygen has eight electrons. The oxygen anion has gained two electrons and so the total number of electrons is ten.

Place two electrons in the 1s orbital

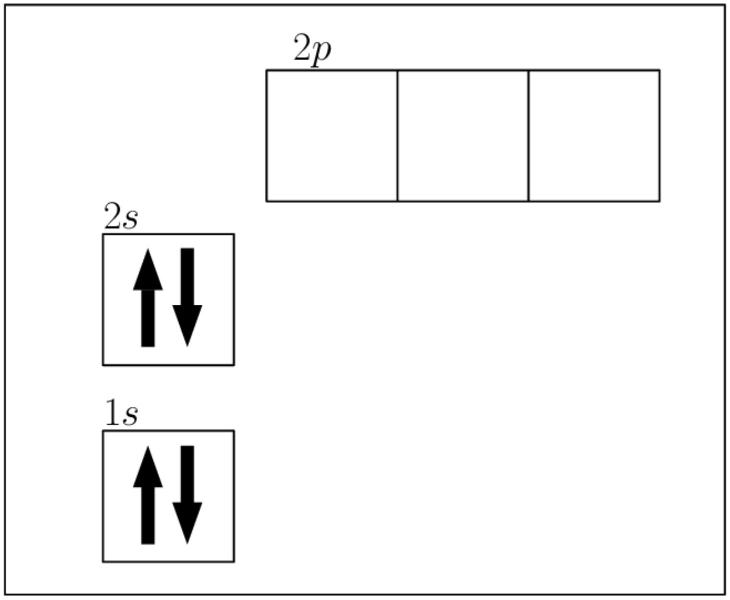
We start by placing two electrons in the 1s orbital: $1s^{2}$.



Now we have eight electrons left to place in orbitals.

Place two electrons in the 2s orbital

We put two electrons in the 2s orbital: 2s2.



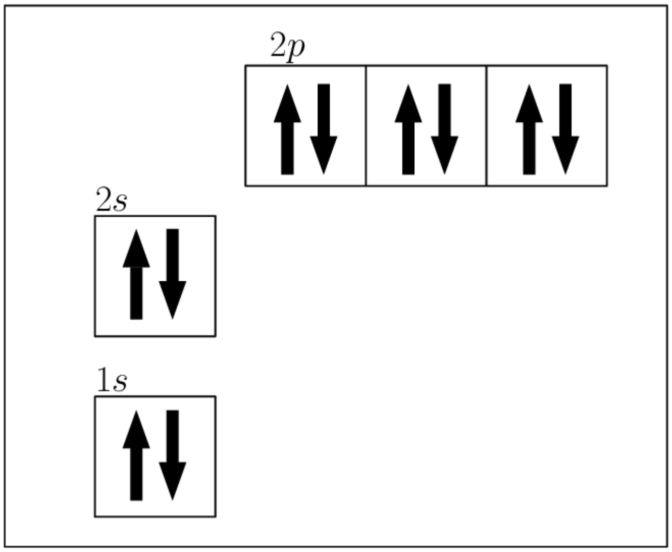
There are now six electrons to place in orbitals.

Place six electrons in the 2p orbital

We place six electrons in the 2p orbital: $2p^6$.

Write the final answer

The electron configuration is: $1s^22s^22p^6$. The Aufbau diagram is:

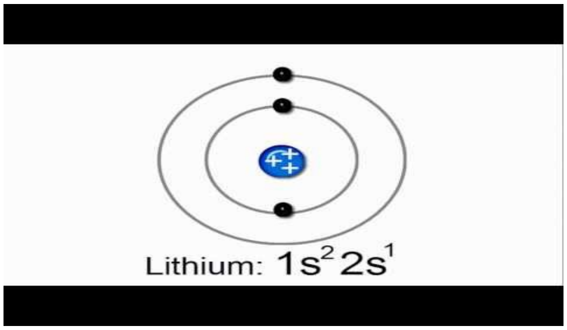


Reference: https://intl.siyavula.com/read/science/grade-10/the-atom/04-the-atom-06

How to Write Electron Configuration

The following videos illustrate the electron configuration concepts in details:

How to write electron configuration?



Reference: https://youtu.be/J-v9_ieCqJI

There are two ways to write the electronic configuration of electrons in atoms. The first is more conceptually cohesive and involves using the Periodic Table to write the notation. The second way is use the configuration chart ((Aufbau Principle).)

[redacted]

Practice Exercise:

Element or Ion	Electron configuration	Core electrons	Valence electrons
Potassium (K)			
Helium (He)			
Oxygen ion (O^{2-})			
Magnesium ion (Mg^{2+})			
Copper(Cu)			
Mercury(Hg)			
Arsenic ion (As^{3-})			
Lead ion (Pb^{4+})			
Uranium (U)			

Contact your instructor for solutions

Orbital shapes

Each orbital type has a unique shape based on the energy of its electrons. The s orbital is a spherical shape. The p orbital is a dumbbell shape. There are three **p orbitals** that differ in orientation along a three-dimensional axis.

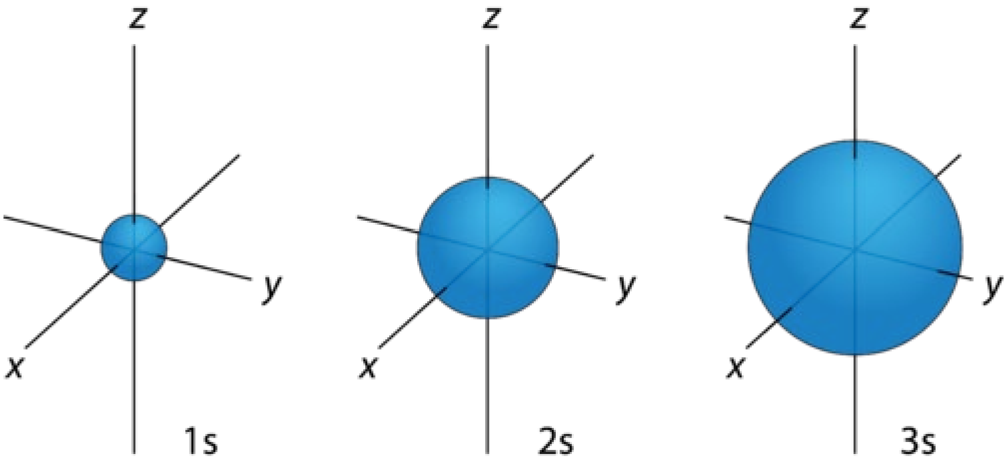
Figure 6.40 Shapes of s, p, d orbitals

Ref: commons.wikimedia.org/

s Orbitals (l=0)

Three things happen to **s** orbitals as **n** increases

1. They become larger, extending farther from the nucleus.
2. They contain more nodes. This is similar to a standing wave that has regions of significant amplitude separated by nodes, points with zero amplitude.
3. For a given atom, the **s** orbitals also become higher in energy as **n** increases because of theirr increased distance from the nucleus.



S orbitals

Figure 6.41 s-orbitals

Ref: commons.wikimedia.org/

p Orbitals (l=1)

Only **s** orbitals are spherically symmetrical. As the value of **l** increases, the numberr of orbitals in a given subshell increases, and the shapes of the orbitals become more complex. Because the 2**p** subshell has **l** = 1, with three values of $\mathbf{m}_l$ (−1, 0, and +1), there are three 2**p** orbitals.

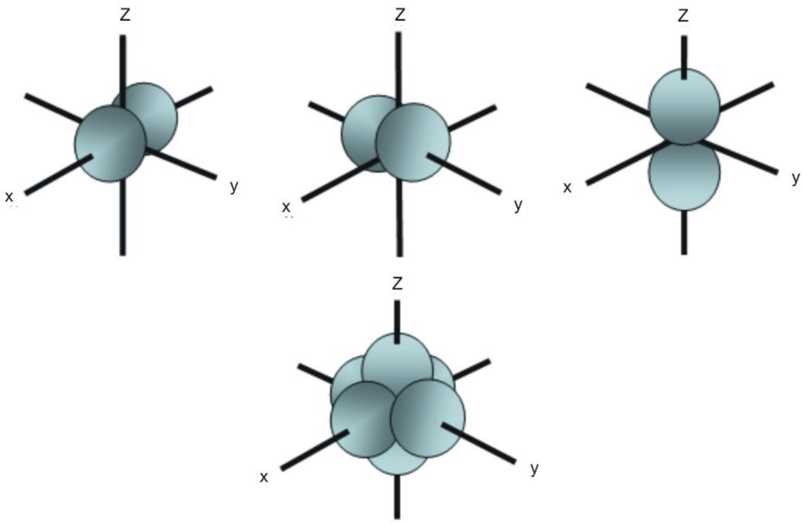


Figure 6.42 p-orbitals

Ref: commons.wikimedia.org/

d Orbitals (l=2)

Subshells with **l** = 2 have five **d** orbitals; the first principal shell to have a **d** subshell corresponds to **n** = 3. The five **d** orbitals have $\mathbf{m}_l$ values of −2, −1, 0, +1, and +2.

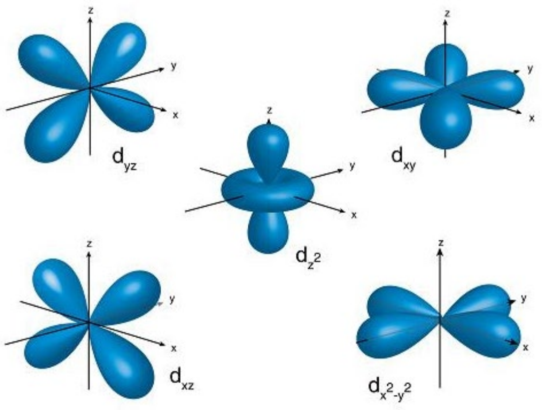


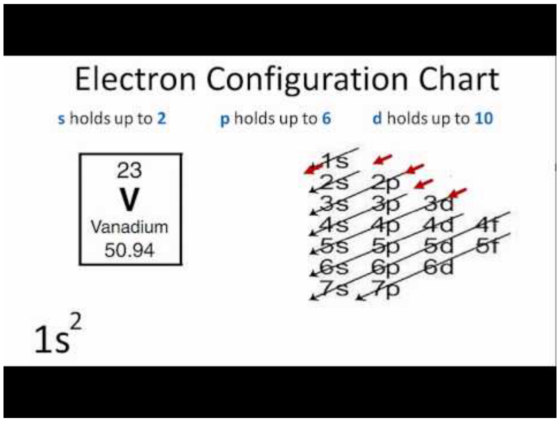
Figure 6.43 d-orbitals

Ref: commons.wikimedia.org/

Reference:
https://chem.libretexts.org/Bookshelves/General_Chemistry/Map%3A_A_Molecular_Approach_(Tro)/07%3A_The_Quantum-Mechanical_Model_of_the_Atom/7.06%3A_The_Shape_of_Atomic_Orbitals

Core and valence electrons

Electrons in the outermost energy level of an atom are called **valence electrons**. The electrons that are in the energy shells closer to the nucleus are called **core electrons**. Core electrons are all the electrons in an atom, excluding the valence electrons. An element that has its valence energy level full is *more stable* and *less likely to react* than other elements with a valence energy level that is not full



Reference: https://youtu.be/TjVrcw2sZLs

The importance of understanding electron configuration

By this stage, you may well be wondering why it is important for you to understand how electrons are arranged around the nucleus of an atom. Remember that during chemical reactions, when atoms come into contact with one another, it is the *electrons* of these atoms that will interact first. More specifically, it is the **valence electrons** of the atoms that will determine how they react with one another.

To take this a step further, an atom is at its most stable (and therefore *unreactive*) when all its orbitals are full. On the other hand, an atom is least stable (and therefore most *reactive*) when its valence electron orbitals are not full. This will make more sense when we go on to look at chemical bonding in a later chapter. To put it simply, the valence electrons are largely responsible for an element's chemical behaviour and elements that have the same number of valence electrons often have similar chemical properties.

The most stable configurations are the ones that have full energy levels. These configurations occur in the noble gases. The noble gases are very stable elements that do not react easily (if at all) with any other elements. This is due to the full energy levels. All elements would like to reach the most stable electron configurations, i.e. all elements want to be noble gases.

Electron Configurations and the Periodic Table

Main group elements (also known as **representative elements**:

These elements occupy s and/or p orbitals in their outermost shells. These elements are called S and P blocks elements.

Transition elements or transition metals.

These elements are metals that occupy the d orbitals in their outermost shells. These elements are called transition metals.

Inner transition elements are metals called Lanthanides and Actinides and occupy the f and d orbitals in their outermost shells. The lanthanide series: Lanthanide (La) through lutetium (Lu). The actinide series: Actinide (Ac) through lawrencium (Lr).

Lanthanides and actinides exhibit similar chemical and physical properties and therefore they are grouped within the same series. Also Lanthanides and Actinides exhibit similar chemical and physical properties similar to the transition elements with the similar corresponding groups although these transition elements have no f orbitals in their outermost shells.

Electron Configurations of Ions

The electron configurations of ions follow the same electron configurations of the neutral elements except adding extra valence electrons in case the ion is negative (anion) or subtracting extra valence electrons in case of the ion is positive (cation).

Key Concepts and Summary

The relative energies of the subshells dictate the order of the atomic orbitals to be filled (1*s*, 2*s*, 2p, 3*s*, 3*p*, 4*s*, 3*d*, 4*p* etc). Electron configurations and orbital diagrams can be determined by applying the Pauli exclusion principle which states that no two electrons can have the same set of four quantum numbers and Hund’s rule what states that electrons keep the unpaired spins status in degenerate orbitals.

Electrons in the outermost orbitals, called valence electrons, are responsible for most of the chemical and physical properties and reactions. The number of the valence electrons equals the number of the group that element is found in. It means that all elements within the same groups will exhibit similar physical and chemical properties.

In the periodic table, elements with similar valence electron configurations are grouped in the same group. There are some exceptions to the predicted filling order, particularly when half-filled or completely filled orbitals can be formed. The periodic table can be divided into four blocks based on the orbital in which the last electron to be added is placed: main group elements (s *and* p orbitals), transition elements (d orbitals), and inner transition elements (f orbitals).

6.5 Periodic Variations in Element Properties

Our goal in this lesson is to help you understand how the shape and organization of the modern periodic table are direct consequences of the atomic electronic structure of the elements.

We begin with the image you saw in the preceding lesson, showing the long form of the table with the "block" structure emphasized. You will recall that the two *f* blocks are written at the bottom merely to keep the table from becoming inconveniently wide; these two blocks actually go in between La-Hf and Ac-Db, respectively, in the *d* block.

Periods, groups and blocks

To construct the table, we place each sequence (denoted by the vertical red bar above) in a separate row, which we call a *period*. The rows are aligned in such a way that the elements in each vertical column possess certain similarities. Thus the first short-period elements H and He are chemically similar to the elements Li and Ne at the beginning and end of the second period. Notice that the first period is split in order to reflect these chemical similarities.

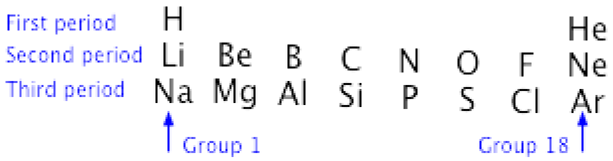


Figure 6.44 Periods, Groups, Blocks

Take a moment to see how the above image relates to the complete periodic table, which we reproduce below. Each row that begins with H down through Fr corresponds to a period; in this table, there are seven periods.

Each column, labeled with small blue numbers 1-18 along the top of the table corresponds to a *group*.

In the past, two different systems of Roman numerals and letters were used to denote the various groups. North Americans added the letter *B* to denote the *d*-block groups and *A* for the others; this is the system shown in the table above. But the rest of the world used *A* for the *d*-block elements and *B* for the others.

In 1985, a new international system was adopted in which the columns were simply labeled 1-18.

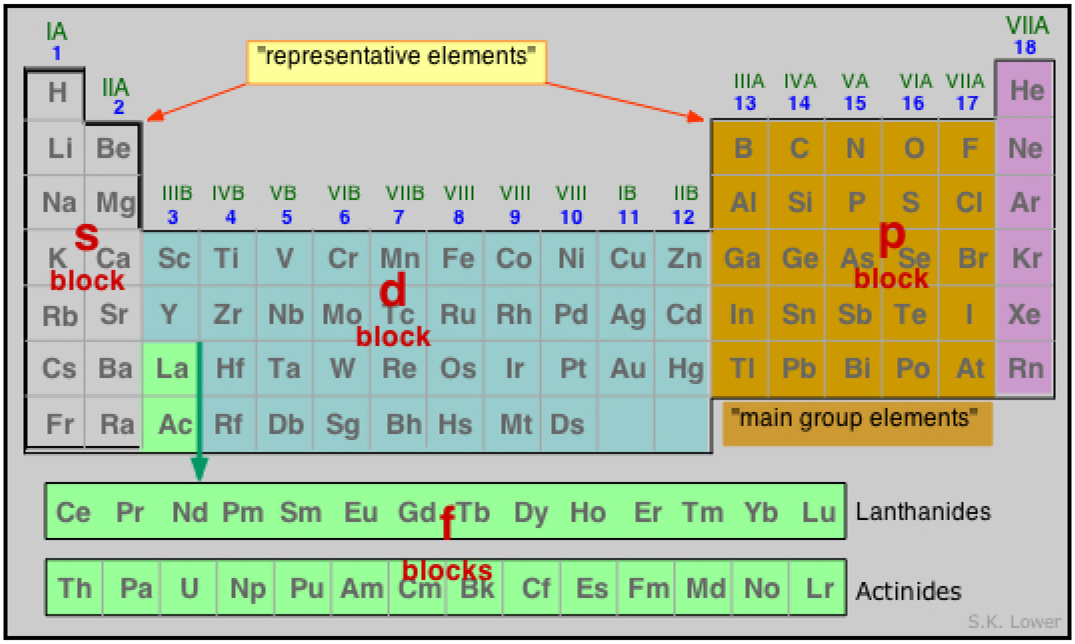


Figure 6.45 Periodic blocks of Elements

Now look at the section of the table containing groups 3 through 12, labeled **d-block**. At the bottom of Group 3 in this block, notice the elements Lanthanum and Actinium, which are shaded in light green. You will see a downward-pointing arrow that points to rwo more rows, also shaded in green.

These two **f-blocks**, as they are called, are not considered separate periods in this "short form" of the table, but have been squeezed in, beginning at the third period, where Scandium Sc is the first element at which the 3*d* shell begins to fill.

The "block" nomenclature of the periodic table refers to the sub-orbital type (quantum number ℓ, or *s-p-d-f* classification) of the highest-energy orbitals that are occupied in a given element. Notice that:

- For n=1 there is no *p* block, and the *s* block is split so that helium is placed in the same group as the other inert gases, which it resembles chemically.
- For the second period (n=2) there is a *p* block but no *d* block; in the usual "long form" of the periodic table it is customary to leave a gap between these two blocks in order to accommodate the *d* blocks that occur at n=3 and above.
- At n=6 we introduce an *f* block, but in order to hold the table to reasonable dimensions the *f* blocks are placed below the main body of the table.

Periodic table families

Chemists have long found it convenient to refer to certain categories of elements by the by special names, commonly known as families. The labels superimposed on the periodic table below are widely used, and worth knowing.

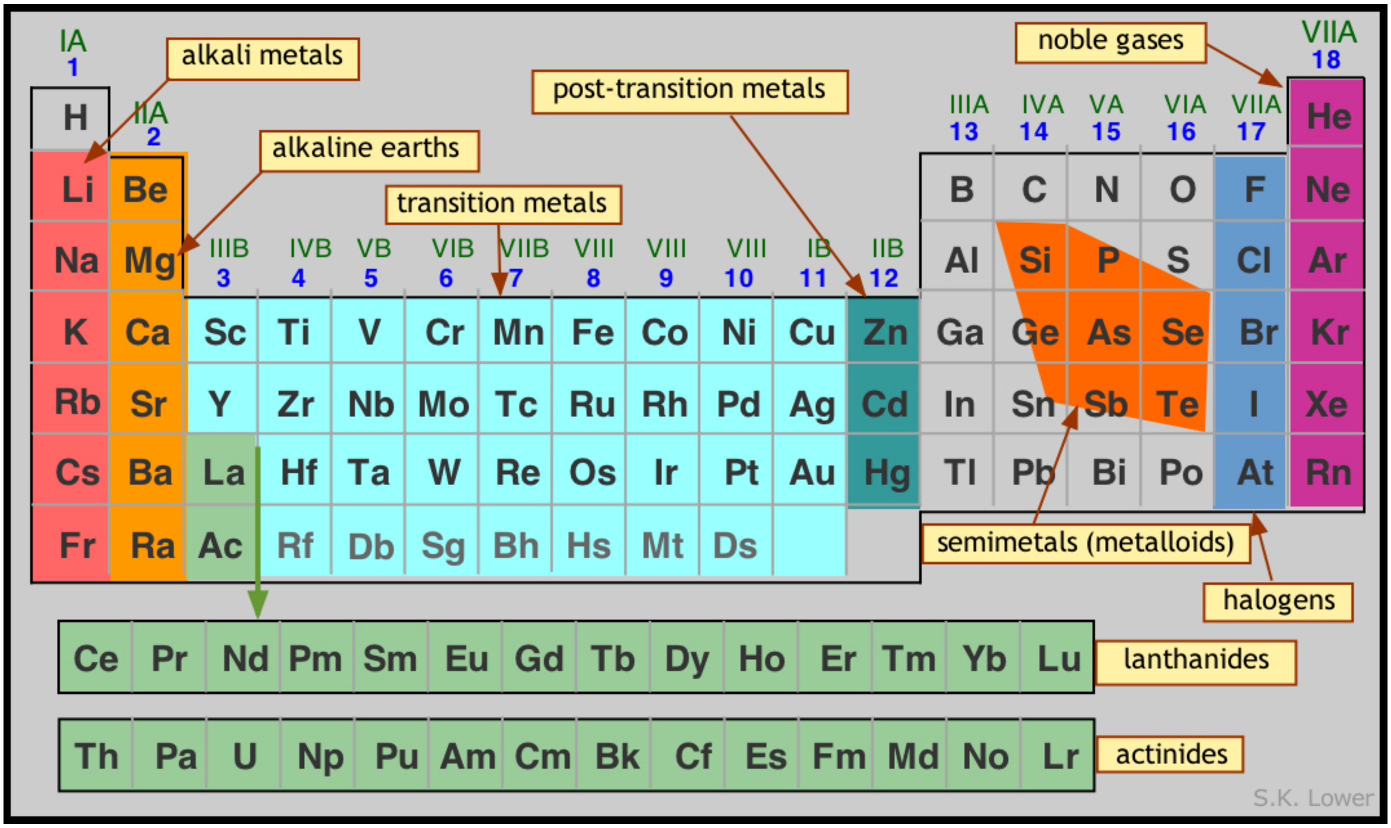


Figure 6.46 Group names of Periodic Table

Of the families shown in the image, it is particularly important that you be able to recognize the *alkali metals* which begin each row, *transition metals* (all elements in the d-block Groups 3-12) and the *noble gases* of Group 18; these families relate directly to the electron configurations of the elements.

Other element families can be entirely arbitrary, such as the elements present in living organisms, the *precious* or *coinage* metals, the *structural metals* such as iron, aluminum and titanium, the elements that are commercially mined in a given country, etc.

2 How electron structures shape the periodic table

The properties of an atom depend ultimately on the number of electrons in the various orbitals, and on the nuclear charge which determines the compactness of the orbitals.

The shell model of the atom

In order to relate the properties of the elements to their locations in the periodic table, it is often convenient to make use of a simplified view of the atom in which the nucleus is surrounded by one or more concentric spherical "shells", each of which consists of the highest-principal quantum number orbitals (always *s*- and *p*-orbitals) that contain at least one electron.

As with any scientific model, the shell model offers a simplified view that helps us to understand and correlate diverse phenomena. The principal simplification here is that it deals only with the *main group* *elements* of the *s*- and *p*-blocks, omitting the *d*- and *f*-block elements whose properties tend to be less closely tied to their group numbers.

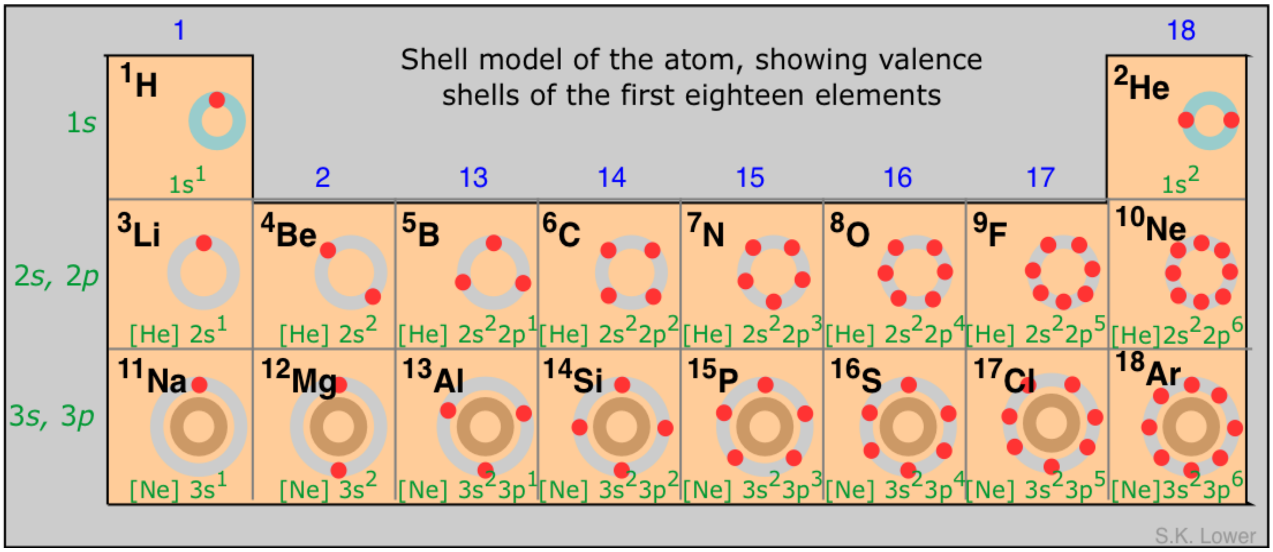


Figure 6.47 Valence electrons

This diagram shows the first three rows of what are known as the *representative elements*—that is, the *s*- and *p*-block elements only. As we move farther down (into the fourth row and below), the presence of *d*-electrons exerts a complicating influence which allows elements to exhibit multiple valances. This effect is especially noticeable in the transition-metal elements, and is the reason for not including the d-block with the representative elements.

The electrons (denoted by the red dots) in the outer-most shell of an atom are the ones that interact most readily with other atoms, and thus play a major role in governing the chemistry of an element. Notice the use of noble-gas symbols to simplify the electron-configuration notation.

[Valence electrons and the periodic table](https://youtu.be/yADrWdNTWEc)

https://youtu.be/yADrWdNTWEc

In particular, the number of outer-shell electrons (which is given by the rightmost digit in the *group number*) is a major determinant of an element's "combining power", or *valence*. The general trend is for an atom to gain or lose electrons, either directly (leading to formation of *ions*) or by sharing electrons with other atoms so as to achieve an outer-shell configuration of s^2p^6. This configuration, known as an *octet*, corresponds to that of one of the noble-gas elements of Group 18.

- the elements in Groups 1, 2 and 13 tend to give up their valence electrons to form positive ions such as Na^+, Mg^{2+} and Al^{3+}, as well as compounds NaH, MgH_2 and AlH_3. The outer-shell configurations of the metal atoms in these species correspond to that of neon.
- elements in Groups 15-17 tend to acquire electrons, forming ions such as P^{3-}, S^{2-} and Cl^- or compounds such as PH_3, H_2S and HCl. The outer-shell configurations of these elements correspond to that of argon.
- the Group 14 elements do not normally form ions at all, but share electrons with other elements in tetravalent compounds such as CH_4.

Effective nuclear charge

Those electrons in the outmost or valence shell are especially important because they are the ones that can engage in the sharing and exchange that is responsible for chemical reactions; how tightly they are bound to the atom determines much of the chemistry of the element. The degree of binding is the result of two opposing forces: the attraction between the electron and the nucleus, and the repulsions between the electron in question and all the other electrons in the atom. All that matters is the net force, the difference between the nuclear attraction and the totality of the electron-electron repulsions.

We can simplify the shell model even further by imagining that the valence shell electrons are the *only* electrons in the atom, and that the nuclear charge has whatever value would be required to bind these electrons as tightly as is observed experimentally. Because the number of electrons in this model is less than the atomic number *Z*, the required nuclear charge will also be smaller, and is known as the *effective nuclear charge*. Effective nuclear charge is essentially the positive charge that a valence electron "sees".

Part of the difference between *Z* and $Z_{effective}$ is due to other electrons in the valence shell, but this is usually only a minor contributor because these electrons tend to act as if they are spread out in a diffuse spherical shell of larger radius. The main actors here are the electrons in the much more compact inner shells which surround the nucleus and exert what is often called a shielding or "*screening*" effect on the valence electrons.

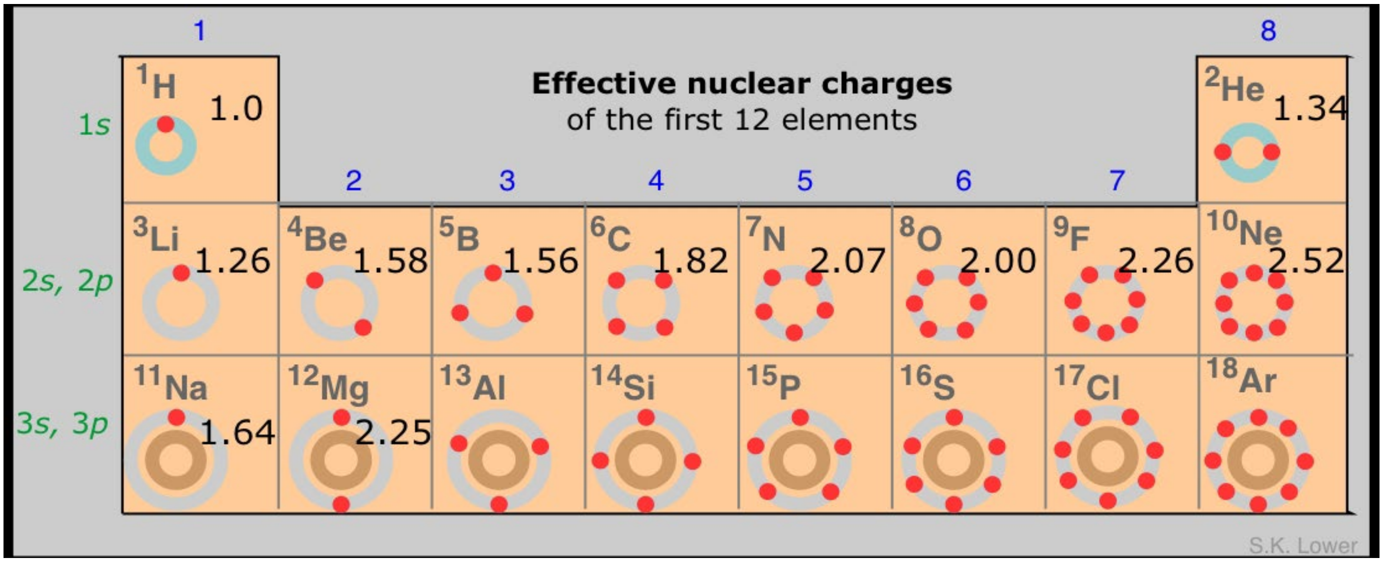


Figure 6.47 Effective Nuclear Charge

The formula for calculating effective nuclear charge is not very complicated, but we will skip a discussion of it here. An even simpler although rather crude procedure is to just subtract the number of inner-shell electrons from the nuclear charge; the result is a form of effective nuclear charge which is called the *core charge* of the atom.

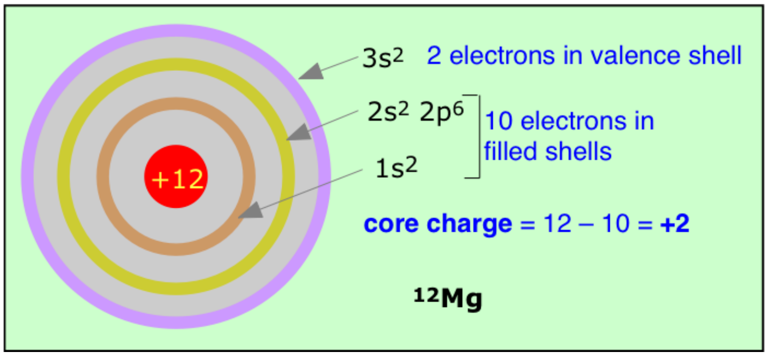


Figure 6.48 Shielding effect

https://youtu.be/ZPfDBu8Mhk8

Periodic trends in atomic and ionic radii

The original purpose of the periodic table was to organize the chemical elements in a manner that would make sense of the ways in which the observed physical and chemical properties of the elements vary with the atomic number.

In this section, we look at some of these trends and try to understand the reasons for them based on the electron structures of the elements.

Periodic trends in the sizes of atoms

What do we mean by the "size" of an atom?

The concept of "size" is somewhat ambiguous when applied to the scale of atoms and molecules. The reason for this is apparent when you recall that an atom has no definite boundary; there is a finite (but very small) probability of finding the electron of a hydrogen atom, for example, 1 cm, or even 1 km from the nucleus. It is not possible to specify a definite value for the radius of an isolated atom; the best we can do is to define a spherical shell within whose radius some arbitrary percentage of the electron density can be found.

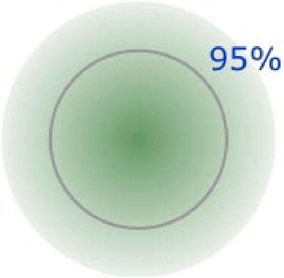


Figure 6.49 Size of an Atom

When an atom is combined with other atoms in a solid element or compound, an effective radius can be determined by observing the distances between adjacent rows of atoms in these solids. This is most commonly carried out by X-ray scattering experiments. Because of the different ways in which atoms can aggregate together, several different kinds of atomic radii can be defined.

Distances on the atomic scale have traditionally been expressed in Ångstrom units (1Å = 10^{-8} cm = 10^{-10} m), but nowadays the picometer is preferred;
1 pm = 10^{-12} m = 10^{-10} cm = 10^{-2} Å, or 1Å = 100 pm. The radii of atoms and ions are typically in the range 70-400 pm.

Periodic trends 1 - radii

https://youtu.be/s85Esq12DPk

Atomic and ionic radii

https://youtu.be/62pf6YOG6Ag

Atomic radius

https://youtu.be/u2xEJdSJZOs

A rough idea of the size of a metallic atom can be obtained simply by measuring the *density* of a sample of the metal. This tells us the number of atoms per unit volume of the solid. The atoms are assumed to be spheres of radius *r* in contact with each other, each of which sits in a cubic box of edge length 2*r*. The volume of each box is just the total volume of the solid divided by the number of atoms in that mass of the solid; the atomic radius is the cube root of *r*.

Although the radius of an atom or ion cannot be measured directly, in most cases it can be inferred from measurements of the distance between adjacent nuclei in a crystalline solid.

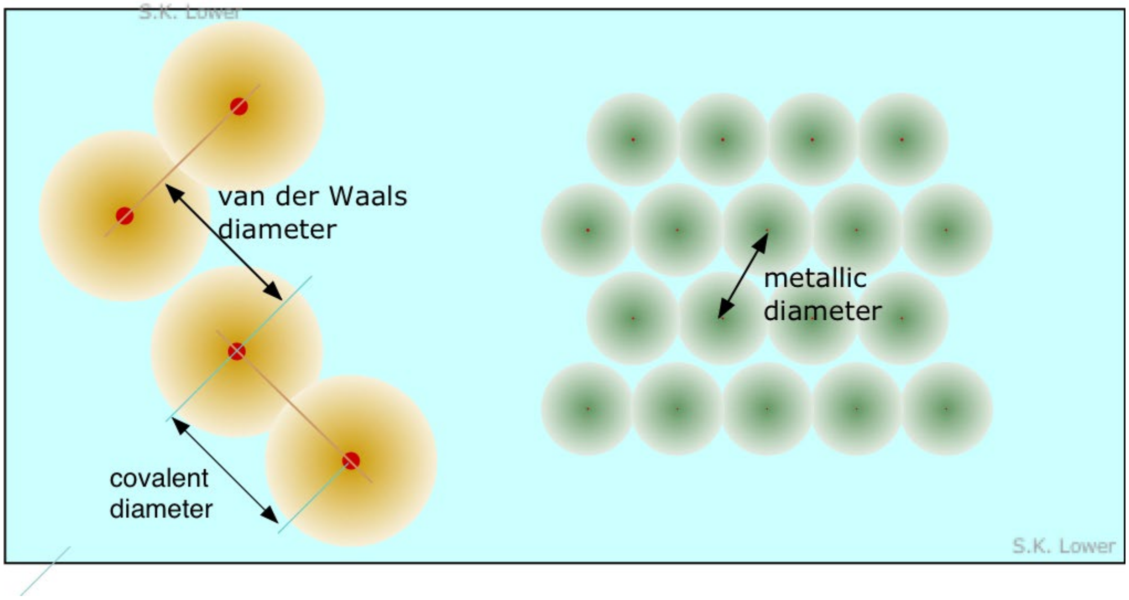


Figure 6.50 Diameter of an Atom

Because solids fall into several different classes, several kinds of atomic radius are defined. Many atoms have several different radii; for example, sodium forms a metallic solid and thus has a metallic radius, it forms a gaseous molecule Na_2 in the vapor phase (covalent radius), and of course it forms ionic solids such as NaCl.

- *Metallic radius* is half the distance between nuclei in a metallic crystal.
- *Covalent radius* is half the distance between like atoms that are bonded together in a molecule.
- *van der Waals radius* is the effective radius of adjacent atoms which are not chemically bonded in a solid, but are presumably in "contact". An example would be the distance between the iodine atoms of adjacent I_2 molecules in crystalline iodine.

Many atoms have several different radii; for example, sodium forms a metallic solid and thus has a metallic radius, it forms a gaseous molecule Na_2 in the vapor phase (covalent radius), and of course it forms ionic solids as mentioned above.

Periodic trends in atomic radius

We would expect the size of an atom to depend mainly on the principal quantum number of the highest occupied orbital; in other words, on the "number of occupied electron shells". Since each row in the periodic table corresponds to an increment in n, atomic radius increases as we move down a column. The other important factor is the nuclear charge; the higher the atomic number, the more strongly will the electrons be drawn toward the nucleus, and the smaller the atom. This effect is responsible for the contraction we observe as we move across the periodic table from left to right.

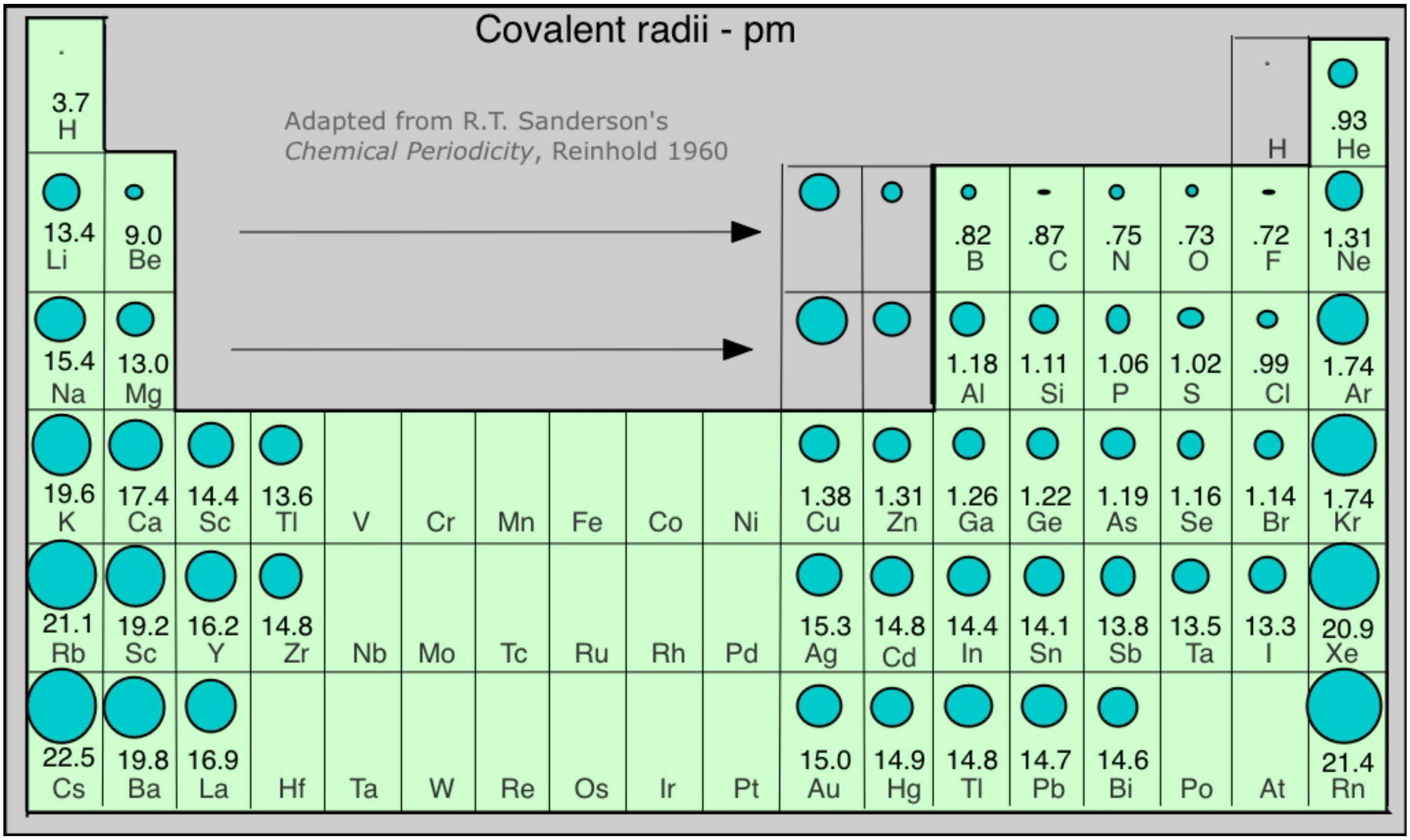


Figure 6.51 Covalent Radii Trend

The figure shows a periodic table in which the sizes of the atoms are represented graphically. The apparent discontinuities in this diagram reflect the difficulty of comparing the radii of atoms of metallic and nonmetallic bonding types. Radii of the noble gas elements are estimates from those of nearby elements.

How ionic radii are estimated

The size of an *ion* can be defined only for those present in *ionic solids*. When an ion dissolves in water, it acquires a *hydration shell* of loosely-attached H_2O molecules that increase its effective radius in ways that are difficult to define in a systematic way.

By observing the diffraction of X-rays by an ionic crystal, it is an easy task to measure the distance between adjacent rows of Na^+ and Cl^- ions, but there is no unambiguous way to decide what portions of this distance are attributable to each ion. The best one can do is make estimates based on studies of several different ionic solids (LiI, KI, NaI, for example) that contain one ion in common. Many such estimates have been made, and they turn out to be remarkably consistent.

For example, the lithium ion is sufficiently small that in LiI, the iodide ions are in contact, so I-I distances are twice the ionic radius of I^-. This is not true for KI, but in this solid, adjacent potassium and iodide ions are in contact, allowing estimation of the K^+ ionic radius.

Comparing the radii of atoms and their ions

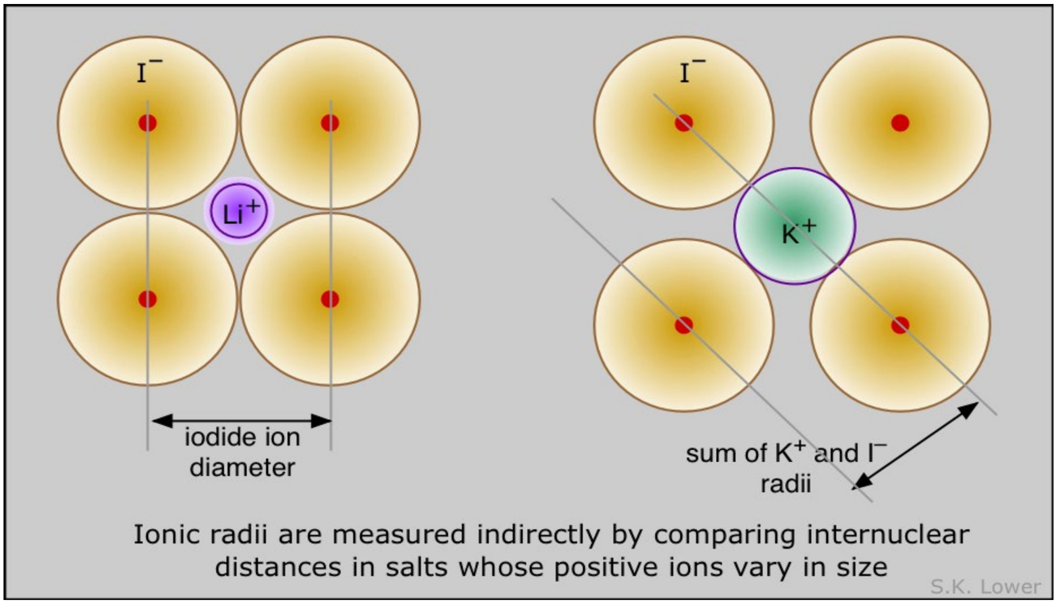


Figure 6.52 Comparison of atomic vs. Ionic Radii

A positive ion is always smaller than the neutral atom, owing to the diminished electron-electron repulsion. If a second electron is lost, the ion gets even smaller; for example, the ionic radius of Fe^{2+} is 76 pm, while that of Fe^{3+} is 65 pm. If formation of the ion involves complete emptying of the outer shell, then the decrease in radius is especially great.

The hydrogen ion H^+ is in a class by itself; having no electron cloud at all, its radius is that of the bare proton, or about 0.1 pm— a contraction of 99.999%! Because the unit positive charge is concentrated into such a small volume of space, the *charge density* of the hydrogen ion is extremely high; it interacts very strongly with other matter, including water molecules, and in aqueous solution it exists only as the *hydronium ion* H_3O^+.

Negative ions are always larger than the parent ion; the addition of one or more electrons to an existing shell increases *electron-electron repulsion* which results in a general expansion of the atom.

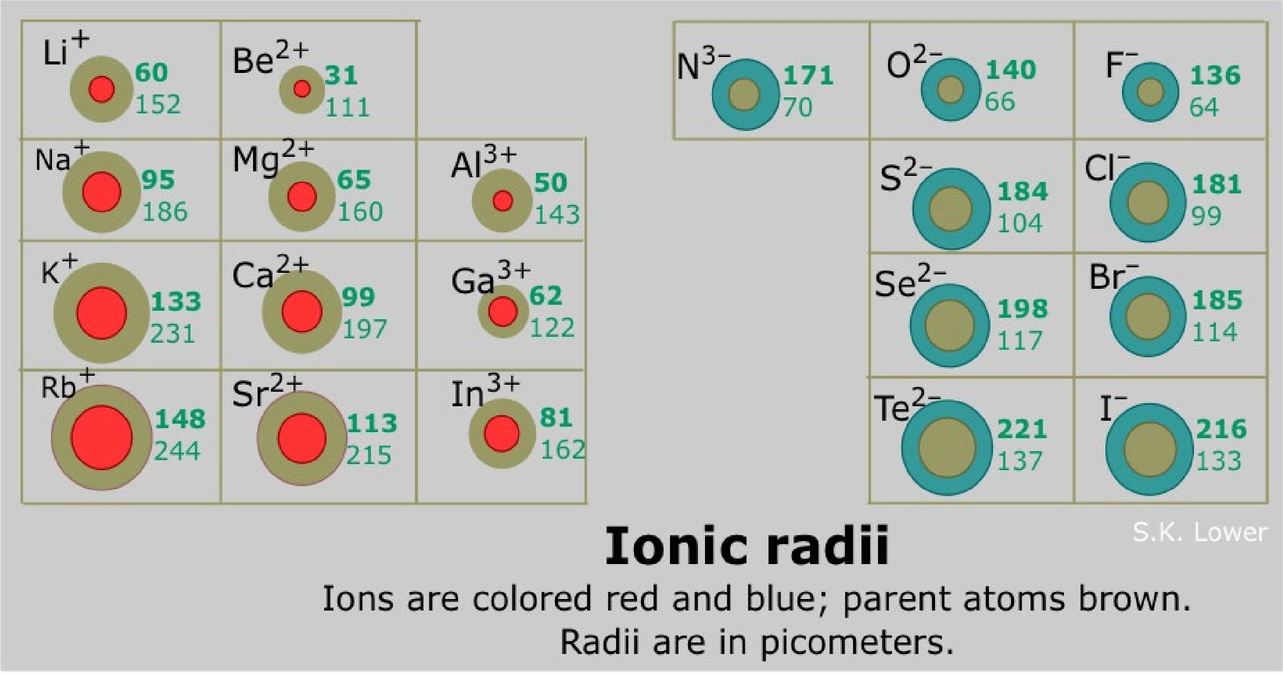


Figure 6.53 Ionic Radii

Periodic trends in ionic radii

The best way of visualizing these trends is to compare the radii of an *isoelectronic series* — a sequence of species all having the same number of electrons (and thus the same amount of electron-electron repulsion) but differing in nuclear charge. Of course, only one member of such a sequence can be a neutral atom (neon in the series shown below.) The effect of increasing nuclear charge on the radius is clearly seen.

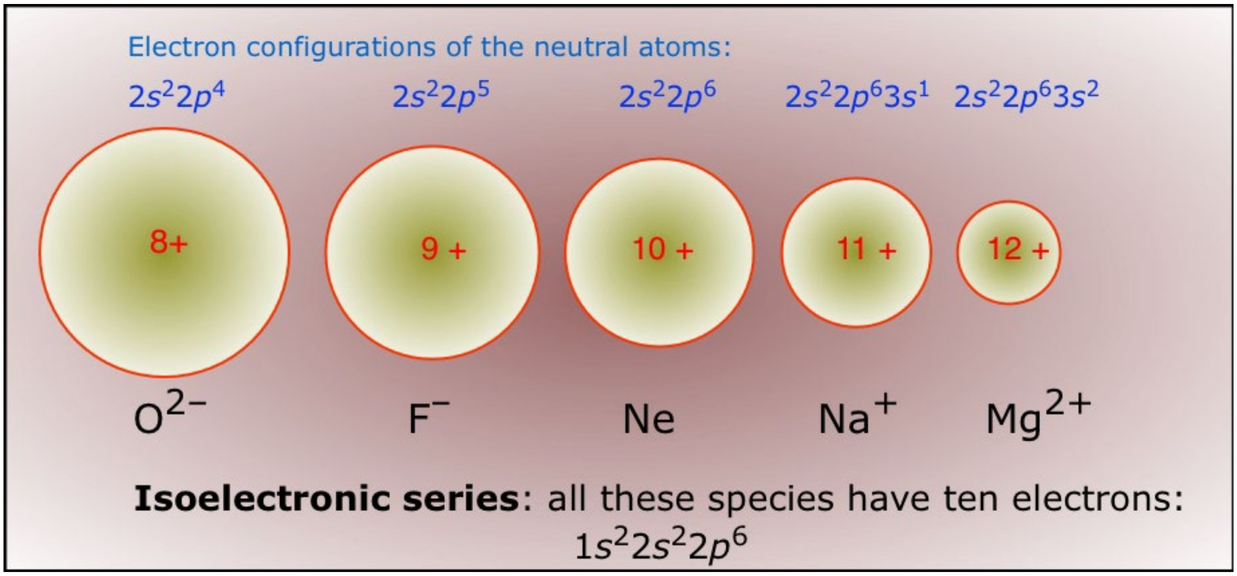


Figure 6.53 Periodic Trend in Ionic Radii

Periodic trends in the energetics of ion formation

Chemical reactions are based largely on the interactions between the most loosely bound electrons in atoms, so it is not surprising that the tendency of an atom to gain, lose or share electrons should play an important role in determining its chemical properties.

Periodic trends in ionization energy

The term "ionization energy" always refers to removal of electrons of an atom, leading to the formation of *positive* ions. In order to remove an electron from an atom, work must be done to overcome the electrostatic attraction between the electron and the nucleus; this work is called the *ionization energy* of the atom and corresponds to the exothermic process

$$M(g) \rightarrow M^{+}(g) + e^{-}$$

in which M(*g*) stands for any isolated (gaseous) atom.

An excellent series of YouTube videos on ionization energy and electron affinity from UC-Berkeley:

Ionization energy, electron affinity (6 min)

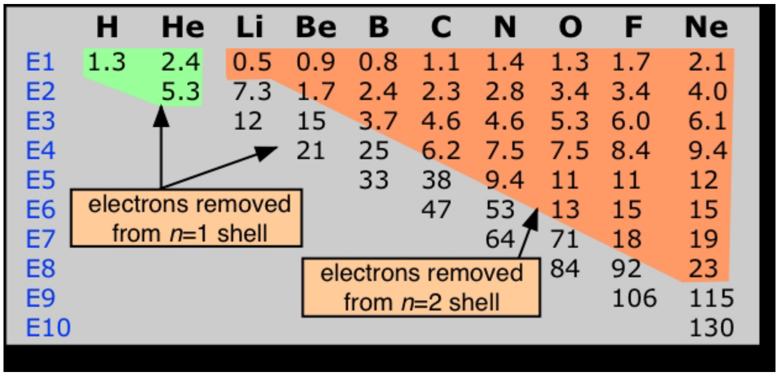
https://youtu.be/jGRhNqkYK18

Quiz on ionization energy

https://youtu.be/fJcz5SBq3Ik

An atom has as many ionization energies as it has electrons. Electrons are always removed from the highest-energy occupied orbital. An examination of the successive ionization energies of the first ten elements (below) provides experimental confirmation that the binding of the two innermost electrons (1*s* orbital) is significantly different from that of the *n*=2 electrons. Successive ionization energies of an atom increase rapidly as reduced electron-electron repulsion causes the electron shells to contract, thus binding the electrons even more tightly to the nucleus.

The table lists the energies, in electron volts, required to remove each successive electron from the first ten elements.



	H	He	Li	Be	B	C	N	O	F	Ne
E1	1.3	2.4	0.5	0.9	0.8	1.1	1.4	1.3	1.7	2.1
E2		5.3	7.3	1.7	2.4	2.3	2.8	3.4	3.4	4.0
E3			12	15	3.7	4.6	4.6	5.3	6.0	6.1
E4				21	25	6.2	7.5	7.5	8.4	9.4
E5					33	38	9.4	11	11	12
E6						47	53	13	15	15
E7							64	71	18	19
E8								84	92	23
E9									106	115
E10										130

Figure 6.54 Ionization energy Trend

It's worth taking some time to examine the rather abrupt jumps in the sequence E1 through E10 as the atomic number increases. Note the very large jumps in the energies required to remove electrons from the 1s orbitals of atoms of the second-row elements Li-Ne.

Ionization energies increase with the nuclear charge *Z* as we move *across* the periodic table. They decrease as we move *down* the table because in each period the electron is being removed from a shell one step farther from the nucleus than in the atom immediately above it. This results in the familiar zig-zag lines when the first ionization energies are plotted as a function of Z.

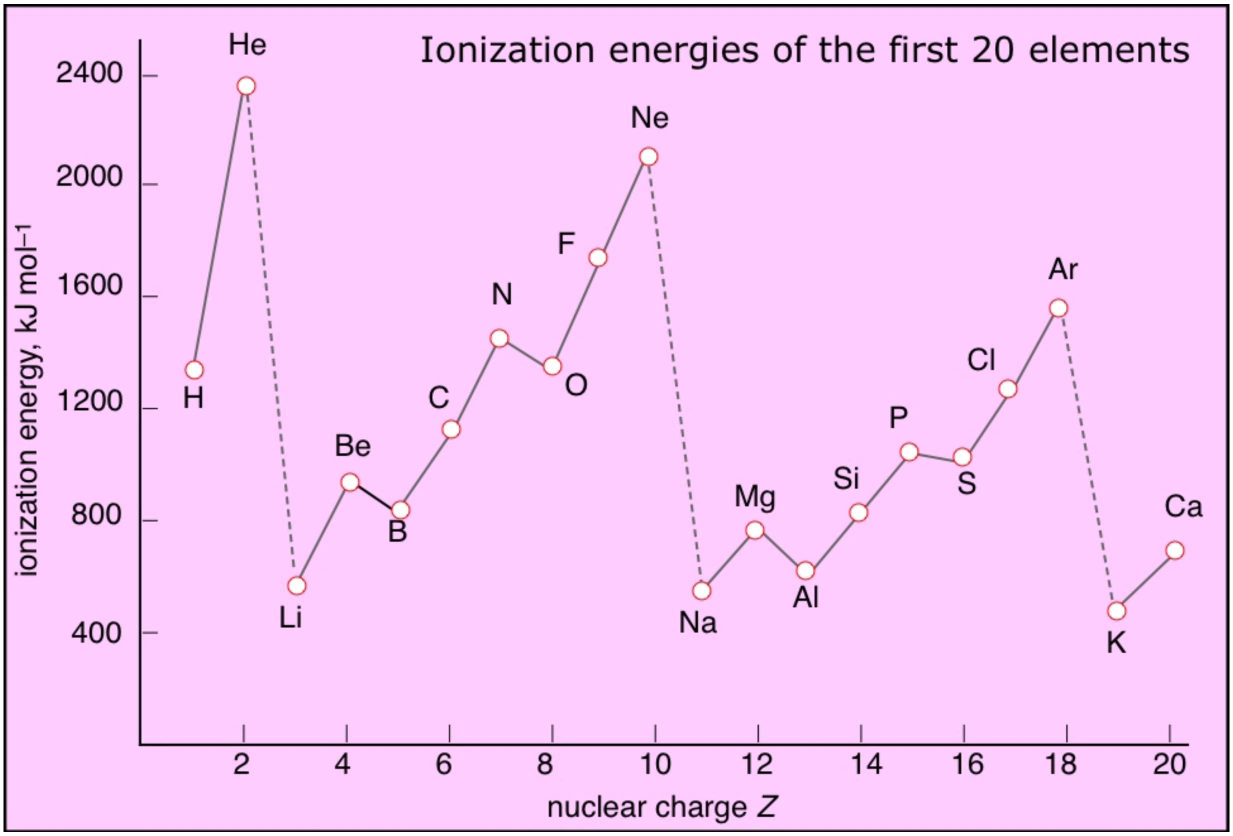


Figure 6.55 Periodic Trend in first Ionization energy

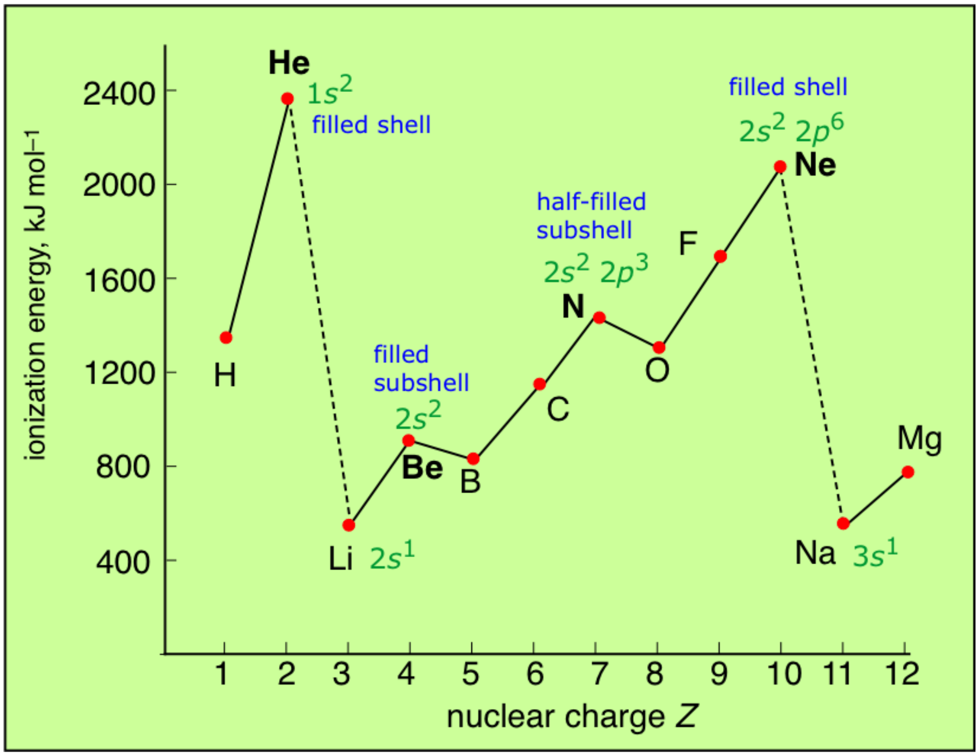


Figure 6.56 Periodic Trend in Period 2 Ionization energy

This more detailed plot of the ionization energies of the atoms of the first ten elements reveals some interesting irregularities that can be related to the slightly lower energies (greater stabilities) of electrons in half-filled (spin-unpaired) relative to completely-filled subshells.

Depicting the ionization energies of the main group elements in the context of the periodic table offers a more comprehensive view of these trends.

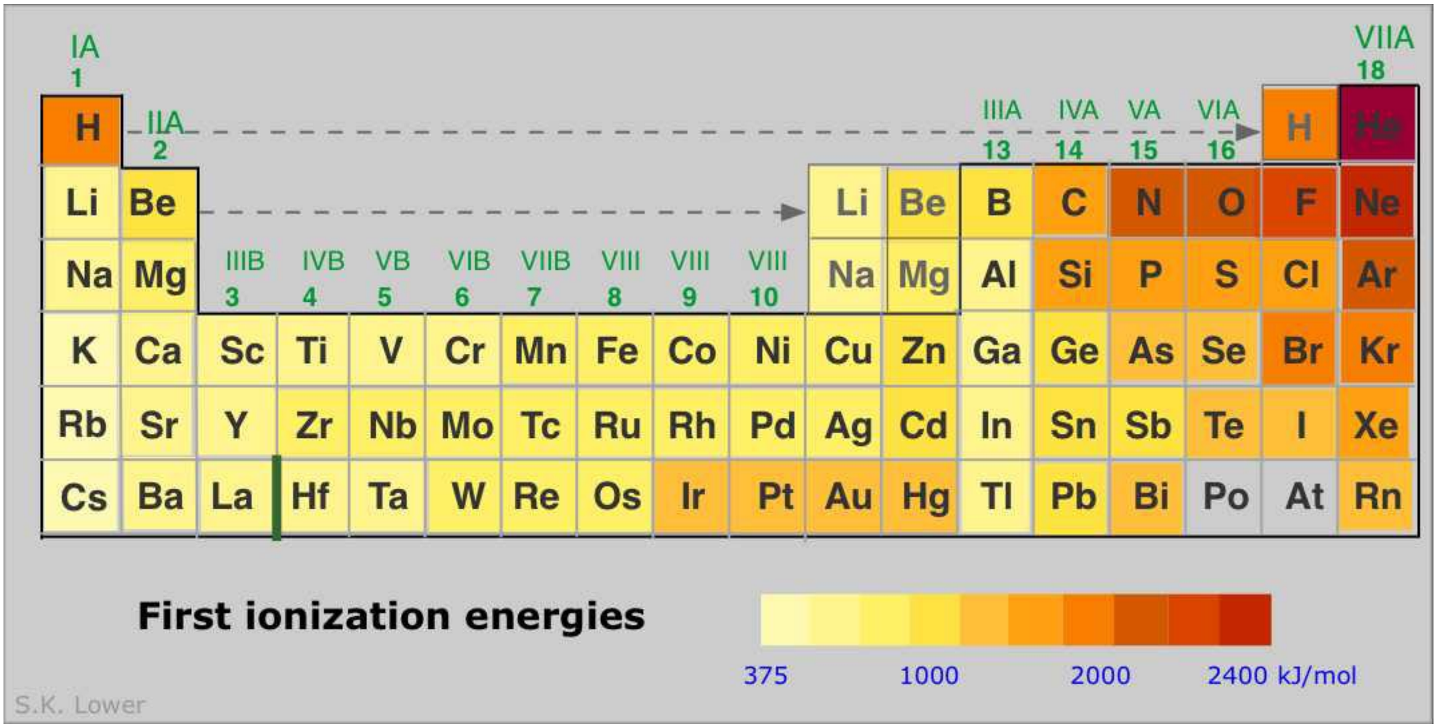


Figure 6.57 Periodic Trend in Ionization energy

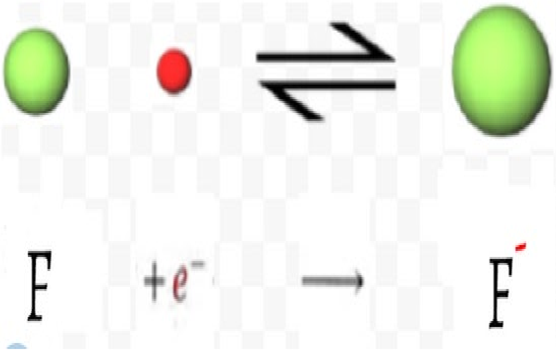
Some points to note:

- The noble gases have the highest IE's of any element in the period. This has nothing to do with any mysterious "special stability" of the s^2p^6 electron configuration; it is simply a matter of the high nuclear charge acting on more contracted orbitals.
- IE's (as well as many other properties) tend not to vary greatly amongst the *d*-block elements. This reflects the fact that as the more-compact *d* orbitals are being filled, they exert a screening effect that partly offsets that increasing nuclear charge on the outermost *s* orbitals of higher principal quantum number.
- Each of the Group 13 elements has a lower first-IE than that of the element preceding it. The reversal of the IE trend in this group is often attributed to the more easy removal of the single outer-shell p electron compared to that of electrons contained in filled (and thus spin-paired) *s*- and *d*-orbitals in the preceding elements.

Periodic trends in electron affinity

Formation of a negative ion occurs when an electron from some external source enters the atom and become incorporated into the lowest energy orbital that possesses a vacancy. Because the entering electron is attracted to the positive nucleus, the formation of negative ions is usually exothermic. The energy given off is the *electron affinity* of the atom. For some atoms, the electron affinity appears to be slightly negative, suggesting that electron-electron repulsion is the dominant factor in these instances.

In general, electron affinities tend to be much smaller than ionization energies, suggesting that they are controlled by opposing factors having similar magnitudes. These two factors are, as before, the nuclear charge and electron-electron repulsion. But the latter, only a minor actor in positive ion formation, is now much more significant. One reason for this is that the electrons contained in the inner shells of the atom exert a collective negative charge that partially cancels the charge of the nucleus, thus exerting a so-called shielding effect which diminishes the tendency for negative ions to form.



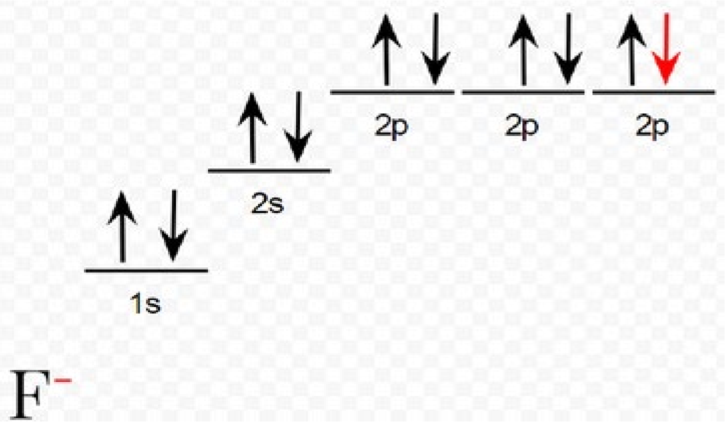
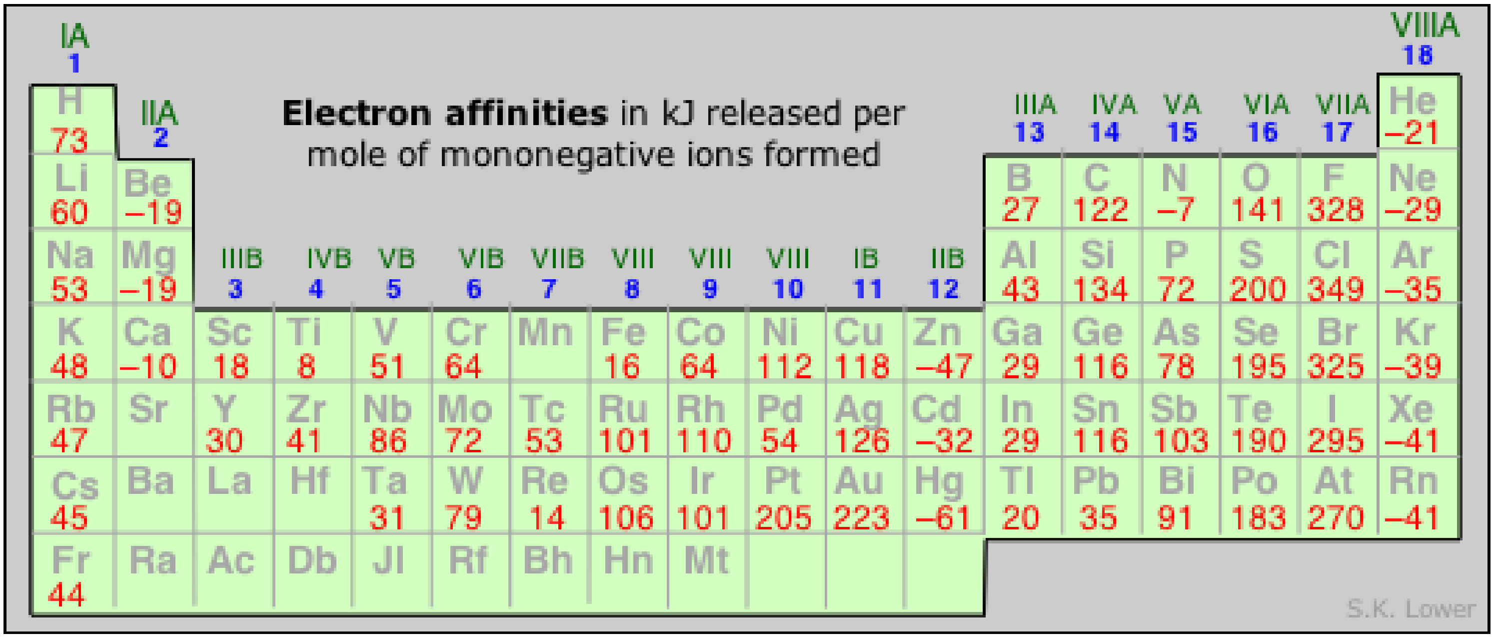


Figure 6.58(a) Electron Affinity

Figure 6.58(b) Anion formation

Because of these opposing effects, the periodic trends in electron affinities are not as clear as are those of ionization energies. This is particularly evident in the first few rows of the periodic table, in which small effects tend to be magnified anyway because an added electron produces a large percentage increase in the number of electrons in the atom.



Electron affinities in kJ released per mole of mononegative ions formed

IA 1	IIA 2	IIIB 3	IVB 4	VB 5	VIB 6	VIIB 7	VIII 8	VIII 9	VIII 10	IB 11	IIB 12	IIIA 13	IVA 14	VA 15	VIA 16	VIIA 17	VIIIA 18
H 73																	He −21
Li 60	Be −19											B 27	C 122	N −7	O 141	F 328	Ne −29
Na 53	Mg −19											Al 43	Si 134	P 72	S 200	Cl 349	Ar −35
K 48	Ca −10	Sc 18	Ti 8	V 51	Cr 64	Mn	Fe 16	Co 64	Ni 112	Cu 118	Zn −47	Ga 29	Ge 116	As 78	Se 195	Br 325	Kr −39
Rb 47	Sr	Y 30	Zr 41	Nb 86	Mo 72	Tc 53	Ru 101	Rh 110	Pd 54	Ag 126	Cd −32	In 29	Sn 116	Sb 103	Te 190	I 295	Xe −41
Cs 45	Ba	La	Hf	Ta 31	W 79	Re 14	Os 106	Ir 101	Pt 205	Au 223	Hg −61	Tl 20	Pb 35	Bi 91	Po 183	At 270	Rn −41
Fr 44	Ra	Ac	Db	Jl	Rf	Bh	Hn	Mt									

S.K. Lower

Figure 6.59 Periodic Trend in Electron Affinity

In general, we can say that electron affinities become more exothermic as we move from left to right across a period (owing to increased nuclear charge and smaller atom size). There are some interesting irregularities, however:

- In the Group 2 elements, the filled 2*s* orbital apparently shields the nucleus so effectively that the electron affinities are slightly endothermic.
- The Group 15 elements have rather low values, due possibly to the need to place the added electron in a half-filled *p* orbital; why the electron affinity of nitrogen should be endothermic is not clear. The vertical trend is for electron affinity to become less exothermic in successive periods owing to better shielding of the nucleus by more inner shells and the greater size of the atom, but here also there are some apparent anomalies.

Electronegativity

When two elements are joined in a chemical bond, the element that attracts the shared electrons more strongly is more *electronegative*. Elements with low electronegativities (the metallic elements) are said to be *electropositive*.

It is important to understand that electronegativities are properties of atoms that are chemically bound to each other; there is no way of measuring the electronegativity of an isolated atom.

[Electron affinity periodic trends](https://youtu.be/YGz4YgTTs8Q)

https://youtu.be/YGz4YgTTs8Q

[How electron affinity, ionization energy and electronegativity relate to each other](https://youtu.be/mvu73OQkLsw)

https://youtu.be/mvu73OQkLsw

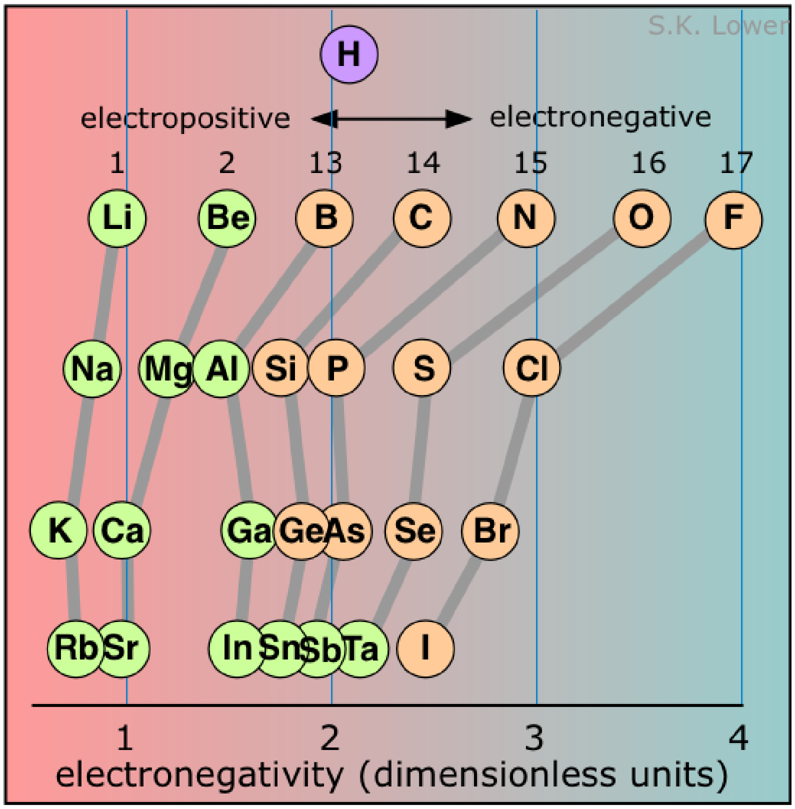


Figure 6.60 Periodic Trend in Electronegativity

Moreover, the same atom can exhibit different electronegativities in different chemical environments, so the "electronegativity of an element" is only a general guide to its chemical behavior rather than an exact specification of its behavior in a particular compound. Nevertheless, electronegativity is eminently useful in summarizing the chemical behavior of an element. You will make considerable use of electronegativity when you study chemical bonding and the chemistry of the individual elements.

Because there is no single definition of electronegativity, any numerical scale for measuring it must of necessity be somewhat arbitrary. Most such scales are themselves based on atomic properties that are directly measurable and which relate in one way or the other to electron-attracting propensity.

The most widely used of these scales was devised by Linus Pauling and is related to ionization energy and electron affinity.

The Pauling scale runs from 0 to 4; the highest electron affinity, 4.0, is assigned to fluorine, while cesium has the lowest value of 0.7. Values less than about 2.2 are usually associated with electropositive, or metallic character. In the representation of the scale shown in figure, the elements are arranged in rows corresponding to their locations in the periodic table. The correlation is obvious; electronegativity is associated with the higher rows and the rightmost columns.

The location of **hydrogen** on this scale reflects some of the significant chemical properties of this element. Although it acts like a metallic element in many respects (forming a positive ion, for example), it can also form hydride-ion (H^-) solids with the more electropositive elements, and of course its ability to share electrons with carbon and other *p*-block elements gives rise to a very rich chemistry, including, of course, the millions of organic compounds.

a) Metallic character

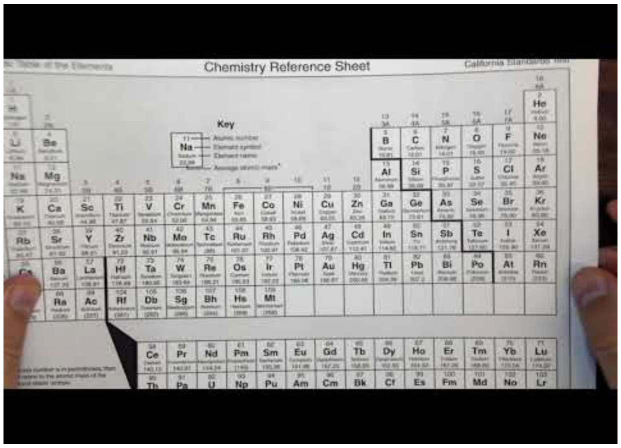
The metallic trend follows the trend of the atomic radius. It increases within a group of the periodic table from the top to the bottom and it decreases within a period of the periodic table from left to right.

What you should be able to do

Make sure you thoroughly understand the following essential concepts that have been presented above.

- You should be able to sketch out the general form of the periodic table and identify the various *blocks* and identify the *groups* corresponding to the *alkali metals*, the *transition elements*, the *halogens*, and the *noble gases*.
- For the first eighteen elements, you should be able to predict the formulas of typical binary compounds they can be expected to form with hydrogen and with oxygen.
- Comment on the concept of the "size" of an atom, and give examples of how radii are defined in at least two classes of of substances.
- Define *ionization energy* and *electron affinity*, and explain the periodic general trends.
- State the meaning and significance of *electronegativity*.

The video below illustrates the concepts of the atomic radius.



Reference: https://www.youtube.com/watch?v=3tFOr1Jh_bs

a) Ionization Energy: It is defined as the amount of energy needed to remove the valence electrons from an atom in the gas phase.
The Ionization Energy trend is the opposite of the atomic radii of the atoms within the groups and the periods of the periodic table.
Ionization energy increases within the period from the left to the left to the right and decreases within a group from top to bottom.
Ionization energies can be measured experimentally.

Example: Aluminum atom ionization energies:

$Al(g) \rightarrow Al^{+}(g) + 1\,e^{-}$ [First Ionization Energy I_1]
$Al^{+}(g) \rightarrow Al^{2+}(g) + 1\,e^{-}$ [Second Ionization Energy I_2]
$Al^{2+}(g) \rightarrow Al^{3+}(g) + 1\,e^{-}$ [Third Ionization Energy I_3]

The third ionization is the largest since it will require more energy to remove the last third valence electron because it is very close to the nucleus compared with the other two valence electrons.

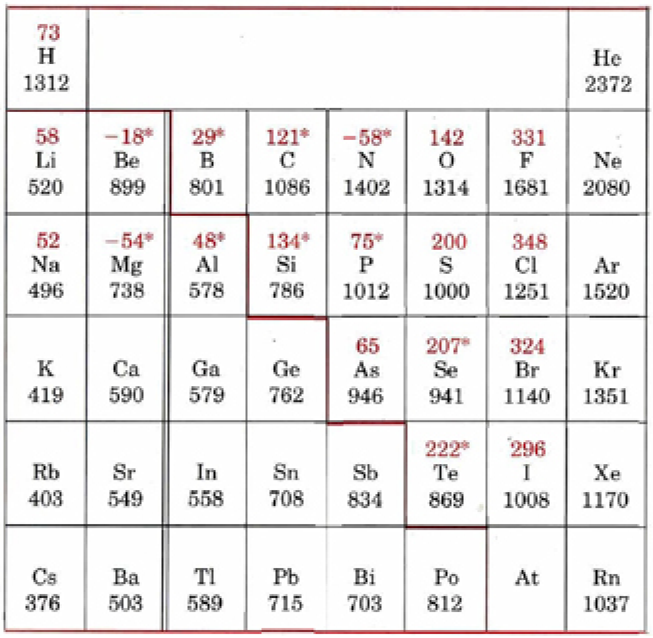
The video below illustrates the concepts of the ionization energy.

Reference: https://www.youtube.com/watch?v=LNVEBURpTcQ

b) Electron affinities: The ability to attract valence electrons to an atom to form an ion in the gas phase.
Example: Fluorine ion

Reference:
https://chem.libretexts.org/Bookshelves/General_Chemistry/Book%3A_ChemPRIME_(Moore_et_al.)/06%3A_Chemical_Bonding_-_Electron_Pairs_and_Octets/6.08%3A_Electron_Affinities

Electron affinities are difficult to be measured experimentally compared with the ionization energies' measurements.
The figure below shows the ionization energies calculated (values are given in black) and the electron affinities estimated (values are given in red)



73 H 1312							He 2372
58 Li 520	−18* Be 899	29* B 801	121* C 1086	−58* N 1402	142 O 1314	331 F 1681	Ne 2080
52 Na 496	−54* Mg 738	48* Al 578	134* Si 786	75* P 1012	200 S 1000	348 Cl 1251	Ar 1520
K 419	Ca 590	Ga 579	Ge 762	65 As 946	207* Se 941	324 Br 1140	Kr 1351
Rb 403	Sr 549	In 558	Sn 708	Sb 834	222* Te 869	296 I 1008	Xe 1170
Cs 376	Ba 503	Tl 589	Pb 715	Bi 703	Po 812	At	Rn 1037

Reference:
https://chem.libretexts.org/Bookshelves/General_Chemistry/Book%3A_ChemPRIME_(Moore_et_al.)/06%3A_Chemical_Bonding_-_Electron_Pairs_and_Octets/6.08%3A_Electron_Affinities

The videos below illustrate the concepts of the electron affinities in some details:

Reference: https://www.youtube.com/watch?v=KhLijA77WQE

Reference: https://www.youtube.com/watch?v=OcPvtr1EuTc

c) Metallic Trend
The metallic trend follows the trend of the atomic radius. It increases within a group of the periodic table from the top to the bottom and it decreases within a period of the periodic table from left to right.

The summary of variation of the electron properties in periodic table is given in the figure and the videos below:

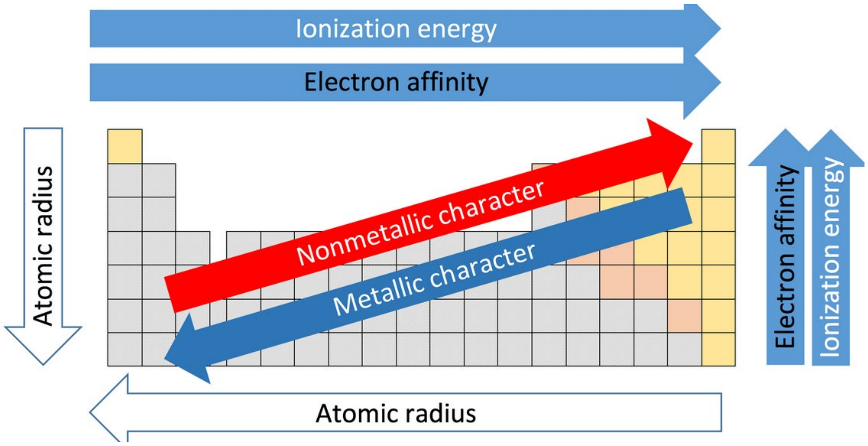
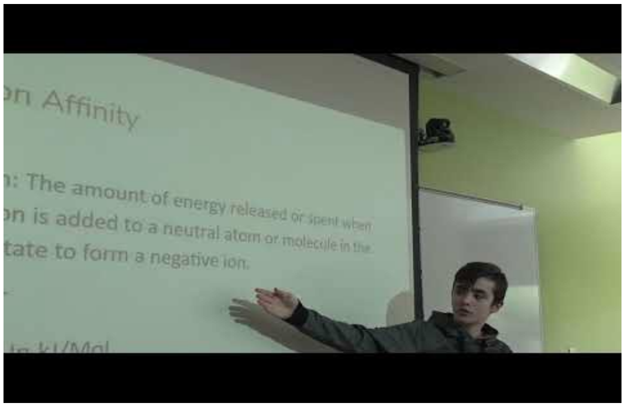


Figure 6.61Summary of all Periodic Trend

Reference: https://chem.libretexts.org/Courses/Oregon_Tech_PortlandMetro_Campus/OT_-_PDX_-_Metro%3A_General_Chemistry_II/02%3A_Periodic_Patterns/2.04%3A_Trends_in_Electron_Affinity_and_Metallic_Character

Reference: https://www.youtube.com/watch?v=A3dTn2at0Hw



Reference: https://www.youtube.com/watch?v=K0YokTyEAMg

WORKSHEET WITH ANSWERS

Q 1: All electromagnetic waves have the same...

A- frequency
B- speed
C- wavelength
D- energy

Answer: B

Q 2: electromagnetic waves with the longest wavelengths are:

A- gamma rays
B- x-rays
C- infrared waves
D- radio waves

Answer: D

Q 3: Which waves are used to show heat loss with heat sensitive cameras?

A- Infrared radiation
B- ultraviolet radiation
C- microwaves
D- gamma rays

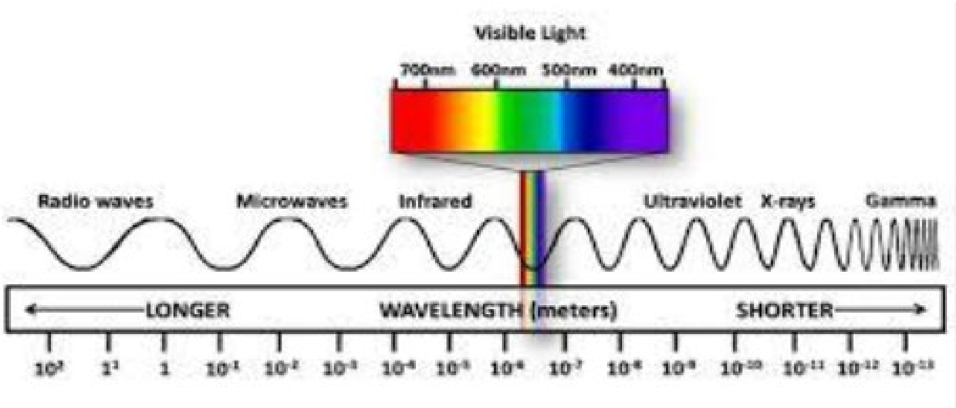
Answer: A

Q 4: Which rays can be felt as heat?

A- X-Rays
B- Infrared Radiation
C- Ultraviolet Radiation
D- Microwaves

Answer: B

Q 5: The acronym (letters) used to remember visible light is____________



A- KTPERRY
B- ROYGBIV
C- DOGPOUND
D- ROMERO

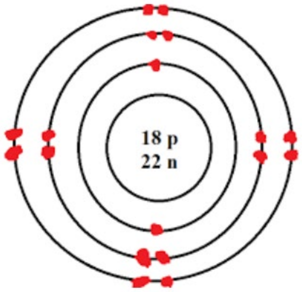
Answer: B

Q 6: A horizontal row of elements in the periodic table.

A- column
B- group
C- period

Answer: C

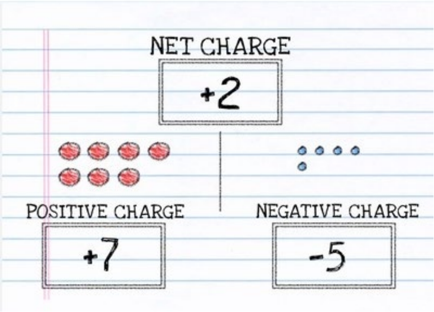
Q 7: What element is this?



A- Helium
B- Hydrogen
C- Argon
D- Silver

Answer: C

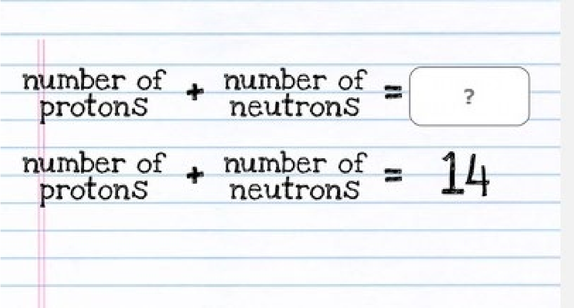
Q 8: For an atom to be electrically neutral, it must contain the same number of _____



A- protons and neutrons
B- neutrons and electrons
C- protons and electrons
D- nucleons and electrons

Answer: C

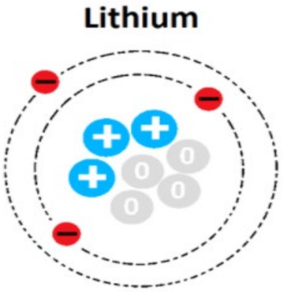
Q 9: The sum of the number of protons and the number of neutrons is called the _____



A- atomic number
B- mass number
C- isotope number
D- average weigh

Answer: B

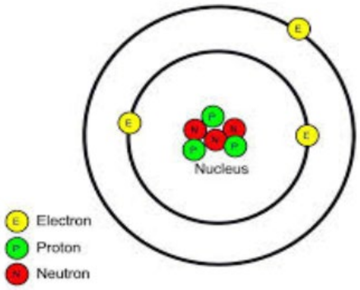
Q 10: What is the mass number of this atom?



A- 1
B- 3
C- 4
D- 7

Answer: D

Q 11: What element is represented in this Bohr Model?



A- Carbon
B- Hydrogen
C- Aluminum
D- Lithium

Answer: D

Q 12: When electron changes its orbit from outer to inner energy is:

A- absorbed
B- released
C- no change
D- remains constant

Answer: B

Q 13: Which subatomic particle is negatively charged?

A- proton
B- neutron
C- electron
D- quark

Answer: C

Q 14: What do electrons constantly do?

A- They pop in and out of appearing.
B- They pop in and out of existence.

C- They pop in and out of consciousness.
D- They pop in and out of disappearing.

Answer: B

Q 15: What's the name of the infamous experiment in Quantum Physics?

A- Double-Split Experiment
B- One-Slit Experiment
C- Double-Decker Experiment
D- Double-Slit Experiment

Answer: D

Q 16: When the top of one wave meets the bottom of another wave, they...

A- all each other out.
B- cancel each other out.
C- cancel each other off.
D- don't cancel each other out.

Answer: B

Q 17: What is inside the nucleus of the atom?

A- electrons and protons
B- protons and quarks
C- protons and neutrons
D- neutrons and electrons
Answer: C

Q 18: The observer creates the material world simply by...

A- experimenting.
B- studying.
C- observing.
D- doing nothing.

Answer: C

Q 19: Who proposed that electrons are only found in specific, discrete circular orbits around the nucleus?

A- Albert Einstein
B- Erwin Schrodinger
C- Ernest Rutherford
D- Niels Bohr

Answer: D

Q 20: Particles whose motions are better described by quantum mechanics can only gain or lose energy in discrete units called…

A- monsters
B- Quanta
C- Protons
D- Electrons

Answer: B

Q 21: What atom matches this electron configuration?
$1s^2 2s^2 2p^6 3s^2$

A- Neon
B- Magnesium
C- Aluminum
D- Potassium

Answer: B

Q 22: What electron configuration matches an oxygen atom?

A- $1s^2 2s^2 2p^6 3s2, 3p^6 4s^2 3d^{10} 4p^5$
B- $1s^2 2s^2 2p^4$
C- $1s^2 2s^2 2p^6$
D- $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^1$

Answer: B

Q 23: Which of the following is the smallest in size?

A- N
B- S
C- I
D- Fr

Answer: A

Q 24: How many valence electrons does Si contain?

A- 14
B- 28
C- 2
D- 4

Answer: D

Q 25: An orbital can at most hold how many electrons?

A- 1 electron
B- 2 electrons
C- 3 electrons
D- 4 electrons

Answer: B

Q 26: Which of the following will have a higher electronegativity than arsenic (As)?

A- Carbon (C)
B- Neon (Ne)
C- Antimony (Sb)
D- Germanium (Ge)

Answer: A

Q 27: As atoms of elements in group 16 are considered in order from top to bottom, the electronegativity of each successive element....

A- decreases
B- increases
C- remains the same
D- none of the above

Answer: A

Q 28: As you move down the periodic table atoms get bigger.This is because _____________.

A- The atoms have more mass.
B- The atoms have more protons.
C- The atoms have more energy levels
D- The atoms have more neutrons

Answer: C

Q 29: Electronegativity is...

A- the ability of an atom to attract/ accept electrons
B- the ability of an atom to lose electrons
C- the energy required to remove an electron from a specific atom
D- how easy it is to make friends.

Answer: A

Q 30: Ionization energy is...

A- the energy required to add an electron to a specific atom
B- how much energy it takes to remove an electron from an atom
C- the energy required to shield the outer electrons from the nucleus
D- a measure of the ability of an atom to attract electrons

Answer: B

Q 31: Radiowaves are about 1m long. Calculate their frequency.

$$\frac{c}{\lambda} = \frac{\nu\lambda}{\lambda} \Rightarrow \frac{c}{\lambda} = \nu = \frac{3.0\times10^{8}\,{}^{m}/_{s}}{1\,m} = 3.0\times10^{8}\,Hz$$

Q 32: A hypothetical wave has 6.6 J of energy. What is its hypothetical, approximate frequency?

$$E = h\nu \qquad \nu = \frac{E}{h} \qquad \nu = \frac{6.6J}{6.626\times10^{-34}\,J{\cdot}s} = 0.9\times10^{34}\,Hz$$

Q 33: A photon with enough energy, 5.1 electron volts (eV) of energy -to be precise, will eject an electron from a piece of gold! What frequency and wavelength does light with this energy have?
Note: 1eV = 1.60 ×10^{-19} Joules

$$\nu = \frac{E}{h} = \frac{(5.1eV)\left(1.60\times10^{-19}\,{}^{J}/_{eV}\right)}{(6.626\times10^{-34}J\cdot s)} = 1.2\times\times10^{15}\,Hz$$

$$\lambda = \frac{c}{\nu} = \frac{(3.0\times10^{8}\,{}^{m}/_{s})}{\left(1.2\times10^{15}\,{}^{1}/_{s}\right)} = 2.5\times10^{-7}\,m$$

Q 34: A red laser pointer emits light with a wavelength of 700nm. A fancy green laser pointer emits light with a wavelength of 500nm. Which emits more energy per photon? (You might also compare the two tools' operating frequencies.)

$$green = \frac{hc}{\lambda} = \frac{(6.626\times10^{-34} J\cdot s)(3.0\times10^{8}\, {}^{m}/_{s})}{(500\times10^{-9}m)} = 4.0\times10^{-19}\, J\ for\ green$$

$$red = E = h\nu = \frac{hc}{\lambda} = \frac{(6.626\times10^{-34} J\cdot s)(3.0\times10^{8}\, {}^{m}/_{s})}{(700\times10^{-9}m)} = 0.028\times10^{-17} J = 2.8\times10^{-19}\, J\ for\ red$$

note: $E_{green} > E_{red}$

CHAPTER 7: Chemical Bonding and Molecular Geometry

INTRODUCTION

I. What *is* a chemical bond?

You probably learned some time ago that chemical bonds are what hold atoms together to form the more complicated aggregates that we know as molecules and extended solids. Chemists talk about bonds all the time, and draw pictures of them as lines joining atom symbols. Teachers often identify them as the little sticks that connect the spheres that represent atoms in a plastic molecular model. So it's not surprising that we sometimes tend to think of chemical bonds as “things”. But no one has ever *seen* a chemical bond, and there is no reason to believe that they really even exist as physical objects.

"SOMETIMES IT SEEMS to me that a bond between two atoms has become so real, so tangible, so friendly, that I can almost see it. Then I awake with a little shock, for a chemical bond is not a real thing. It does not exist. No one has ever seen one. No one ever can. It is a figment of our own imagination."

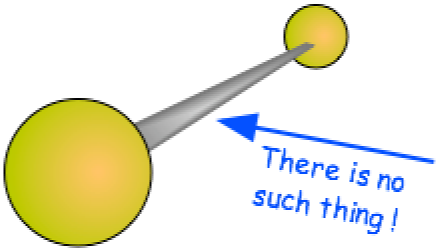


Figure 7.1 Chemical Bond

C.A. Coulson (1910-1974) was an English theoretical chemist who played a central role in the development of quantum theories of chemical bonding.

It is probably more useful to regard a chemical bond as an *effect* that causes certain atoms to join together to form enduring structures that have unique physical and chemical properties.

So although the "chemical bond" (as a physical object) may be no more than a convenient fiction, *chemical bonding*, which leads to the near-infinity of substances (31 million in mid-2007), lies at the very core of chemistry.

The forces that hold bonded atoms together are basically just the same kinds of electrostatic attractions that bind the electrons of an atom to its positively-charged nucleus;

chemical bonding occurs when one or more electrons are simultaneously attracted to *two* nuclei.

This is the most important fact about chemical bonding that you should know, but it is not of itself a workable ***theory*** of bonding because it does not describe the conditions under which bonding occurs, nor does it make useful predictions about the properties of the bonded atoms.

Our views of what constitutes chemical bonding are still evolving, according to a 2007 article in *Chemical and Engineering News*(**85** 37-40). This "buckyball-and-mitt" synthesized in 2007 by Andrzej Sygula is a case in point. The buckyball C_{60} resides in the $C_{60}H_{28}$"buckybowl". There are no traditional "chemical bonds" between the ball and the tube.

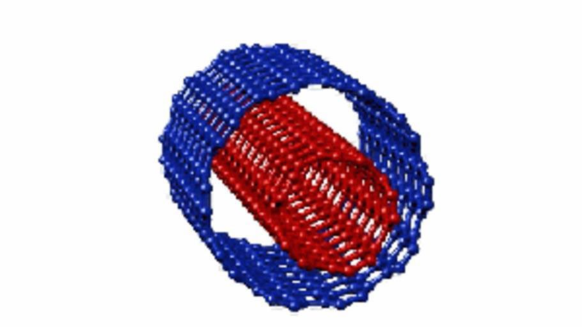


Figure 7.2 Carbon nanotube

Ref: www.snappygoat.com

What is a *molecule*?

Even at the end of the 19th century, when compounds and their formulas had long been in use, some prominent chemists doubted that molecules (or atoms) were any more than convenient models. Molecules suddenly became real in 1905, when Albert Einstein showed that Brownian motion, the irregular microscopic movements of tiny pollen grains floating in water, could be directly attributed to collisions with molecule-sized particles.

Most people think of molecules as the particles that result when atoms become joined together in some way. This conveys the general picture, but a somewhat better definition that we will use in these lessons is

A molecule is an aggregate of atoms that possesses distinctive observable properties

A more restrictive definition distinguishes between a "true" molecule that exists as an independent particle, and an ***extended solid*** that can only be represented by its simplest formula. Methane, CH_4, is an example of the former, while sodium chloride, which does not contain any discrete NaCl units, is the most widely-known extended solid. But because we want to look at chemical bonding in the most general way, we will avoid making this distinction here except in a few special cases. In order to emphasize this "aggregate of atoms" definition, we will often use terms such as "chemical species" and "structures" in place of "molecules" in this lesson.

The definition written above is an *operational* one; that is, it depends on our ability to observe and measure the molecule's properties. Clearly, this means that the molecule must retain its identity for a period of time long enough to carry out these observations. For most of the molecules of chemical interest, this presents no difficulty. But it does happen that some structures that we can write formulas for, such as He_2, have such brief lives that no significant properties have been observed. So to some extent, what we consider to be a molecule depends on the technology we use to observe them, and this will necessarily change with time.

Structure, structure, structure!

And what are those properties that characterize a particular kind of molecule and distinguish it from others? Just as real estate is valued by "location, location, location", the identity of a chemical species is defined by its ***structure***. In its most fundamental sense, the structure of a molecule is specified by the identity of its constituent atoms and the sequence in which they are joined together, that is, by the ***bonding connectivity***. This, in turn, defines the ***bonding geometry***— the spatial relationship between the bonded atoms.

The importance of bonding connectivity is nicely illustrated by the structures of the two compounds *ethanol* and *dimethyl ether*, both of which have the *simplest formula* C_2H_6O. The *structural formulas* reveal the very different connectivity of these two molecules whose physical and chemical properties are quite different:

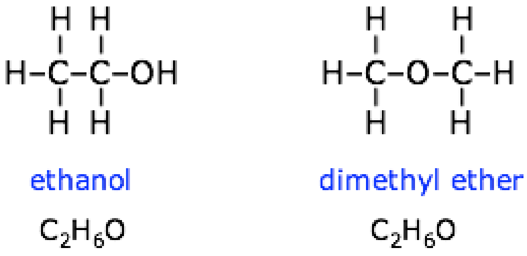


Figure 7.3 Ethanol and Ditheyl ether structure

Ref: commons.wikimedia.org/

Structures without molecules: stability and reactivity

The precise definition of bonding energy is described in another lesson and is not important here. For the moment you only need to know that in any stable structure, the potential energy of its atoms is lower than that of the individual isolated atoms. Thus the formation of methane from its gaseous atoms (a reaction that cannot be observed under ordinary conditions but for which the energetics are known from indirect evidence)

$$4\ H(g) + C(g) \rightarrow CH_4$$

is accompanied by the release of heat, and is thus an *exothermic* process. The quantity of heat released is related to the stability of the molecule. The smaller the amount of energy released, the more easily can the molecule absorb thermal energy from the environment, driving the above reaction in reverse and leading to the molecule's decomposition. A highly stable molecule such as methane must be subjected to temperatures of more than 1000°C for significant decomposition to occur. But the noble-gas molecule KrF_2 is so weakly bound that it decomposes even at 0°C, and the structure He_2 has never been observed. If a particular arrangement of atoms is too unstable to reveal its properties at any achievable temperature, then it does not qualify to be called a molecule.

There are many molecules that are energetically stable enough to meet the above criterion, but are so ***reactive*** that their lifetimes are too brief to make their observation possible. The molecule CH_3, *methyl*, is a good example: it can be formed by electrical discharge in gaseous CH_4, but it is so reactive that it combines with almost any molecule it strikes (even another CH_3) within a few collisions. It was not until the development of spectroscopic methods (in which a molecule is characterized by the wavelengths of light that it absorbs or emits) that methyl was recognized as a stable albeit shamelessly promiscuous molecule that is an important intermediate in many chemical processes ranging from flames to atmospheric chemistry.

SUPPLEMENTAL

****

How we depict molecular structures

Chemical species are traditionally represented by ***structural formulas*** such as the ones for phosphoric acid, H_3PO_4, which we show here. The lines, of course, represent the "chemical bonds" of the molecule.
More importantly, the structural formula of a molecule defines its ***connectivity***, as was illustrated in the comparison of ethanol and dimethyl ether shown in the previous section.

One limitation of such formulas is that they are drawn on a two-dimensional surface, whereas most molecules have a three-dimensional shape.

The wedge-shaped lines in the structural formula on the right are one way of indicating which bonds extend above or below the viewing plane, providing a kind of pseudo-3D view. You will probably be spared having to learn this convention until you get into Organic Chemistry.

Three-dimensional models (either real plastic ones or images that incorporate perspective and shading) reveal much more about a molecule's structure. The ball-and-stick and space-filling renditions are widely employed, but each has its limitations, as seen in the following examples that compare different ways of depicting the structures of the same two molecules:

Simple structural formulas in two dimensions show the molecule's connectivity, but nothing more.

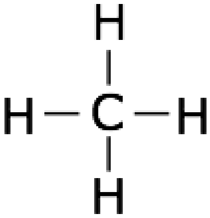


Figure 7.4 Structural Formula of methane

Ref: commons.wikimedia.org/

↑ This simple structural formula of methane, CH_4, projects its 3-dimentional structure onto a 2D surface.

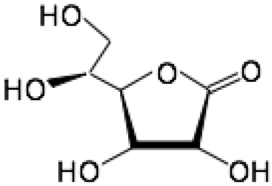


Figure 7.5 Structure formula of vitamin C

Ref: commons.wikimedia.org/

↑ The structural formula of ascorbic acid (vitamin C) is commonly enhanced with wedge-shaped bonds to show that they extend above the plane of the paper or screen.

Ball-and-stick models show 3-dimensional views of the "chemical bonds" and their geometry. although with the individual atoms unrealisticly separated.

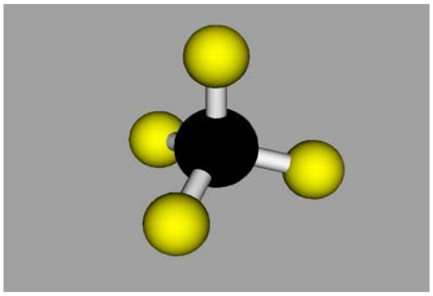


Figure 7.6 3D Shape of methane

Ref: commons.wikimedia.org/

This image correctly expresses the tetrahedral coordination of the four C—H bonds.

[U. Rochester]

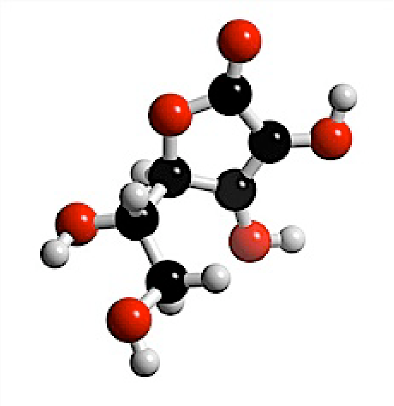
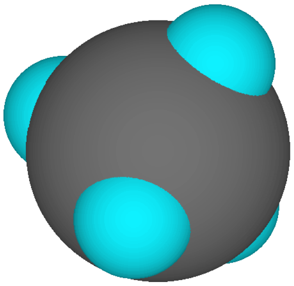


Figure 7.7 3D Shape of Vitamic C

Ref: commons.wikimedia.org/

Ascorbic acid

Space-filling models don't attempt to depict the bonds, but show the relative sizes of the atoms and general shape of the molecule, at the expense of hiding some of the atoms.



Note how this shows CH_4 to be roughly spherical.

[U. Alberta]

Figure 7.8 3D Space filling model of methane

Ref: commons.wikimedia.org/

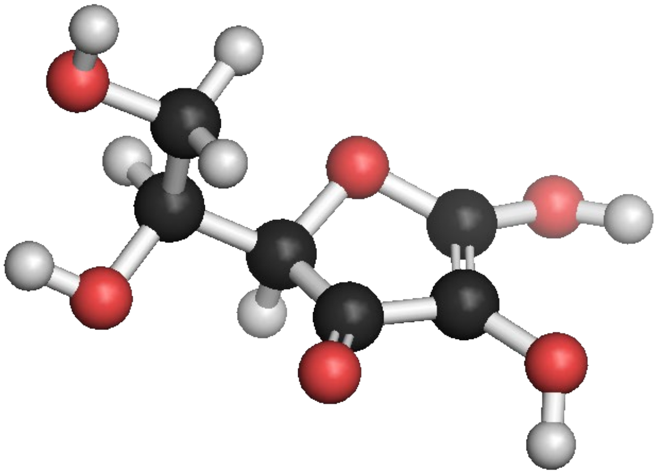


Figure 7.9 Ball and stick model of Ascorbic Acid

Ref: commons.wikimedia.org/

But what would a molecule "really" look like if you could view it through a magical microscope of some kind? A possible answer would be this computer-generated view of nicotine. At first you might think it looks more like a piece of abstract sculpture than a molecule, but it does reveal the shape of the negative charge-cloud that envelops the collection of atom cores (i.e., nuclei) hidden within. This can be very important for understanding how the molecule interacts with the similar charge-clouds that clothe solvent and bioreceptor molecules.

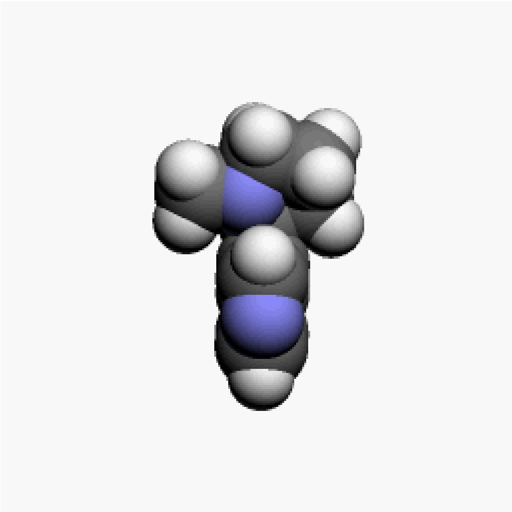


Figure 7.10 Space filling model of Nicotine

Ref: commons.wikimedia.org/

Molecular modeling and visualization

The purpose of rendering a molecular structure in a particular way is not to achieve "realism" (whatever that might be), but rather to convey useful information of some kind. Modern computer rendering software takes its basic data from various kinds of standard structural databases which are compiled either from experimental X-ray scattering data, or are calculated from theory.

Figure 7.11 Cup of coffee

Ref: commons.wikimedia.org/

Example: Caffeine

Caffeine's *molecular formula*, $C_8H_{10}N_4O_2$, tells us its composition, but conveys no information about how its 24 atoms are connected, and thus how it differs from any number of other compounds having the same formula. In order to reveal its connectivity, we use its ***structural formula***.

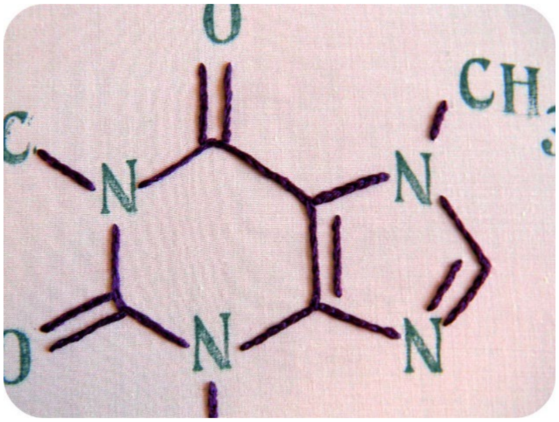


Figure 7.12 Structural Formula of Nicotine

Ref: www.flickr.com

Although the structure at the right does not look like the one on the cup, their connectivity is identical, so the two structures are equivalent. As an exercise, see if you are able to confirm this.

For most "ordinary" chemistry, the structural formula is all we need. Suppose, however, that you wish to understand more about how caffeine exerts its stimulating effect on the body. Like many drugs, caffeine binds to specific sites on proteins; the efficacy of this binding is usually highly dependent on the both the shape of the drug and the manner in which electric charge is distributed over this shape.

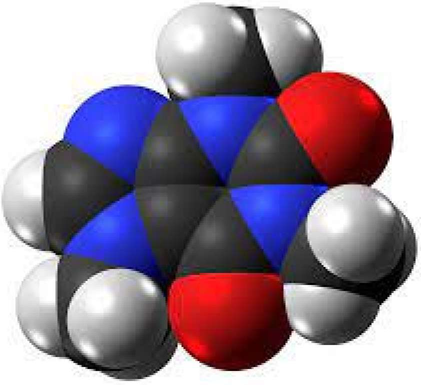


Figure 7.13 Space filling model of Cafeine

Ref: commons.wikimedia.org/

In this context, it is important to understand that the outer "surface" of a molecule is defined by the veil of negative charge that originates in the valence electrons of the atoms but which tends to be spread over the entire molecule to a distance that can significantly affect ***van der Waals interactions*** with neighboring molecules.

For this purpose, one employs a mixture of chemical intuition and *molecular modeling* computer software to generate an image such as the one shown here.

In this depiction of Caffeine, the atoms are coded by color: white=H, red=O, light blue=C, dark blue=N.

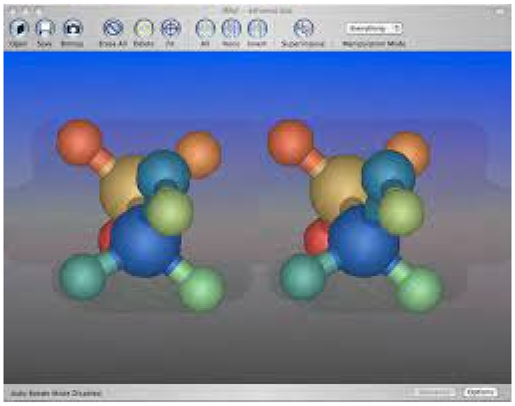


Figure 7.14 Space filling model of ethanol

Another example is C_2H_5OH Ethanol molecule (Ref: www.flickr.com)

Example: Sucrose

Figure 7.15 3D structure of Sucrose

Ref: commons.wikimedia.org/

Sucrose — ordinary "sugar" — occurs naturally in fruits and vegetables, as well as in everyone's kitchen and in all too many foods and beverages. Its structural formula shows that it is really a "double sugar" (a *disaccharide*) in which two *monosaccharides*, *glucose* and *fructose*, are joined together.

The overall shape and distribution of electric charge at the surface enable it to bind to the sweetness receptors on the tongue, and — more importantly to the enzyme that catalyzes the hydrolysis reaction that breaks the sucrose into its two monosaccharide components, releasing the glucose which fuels our body's cells.

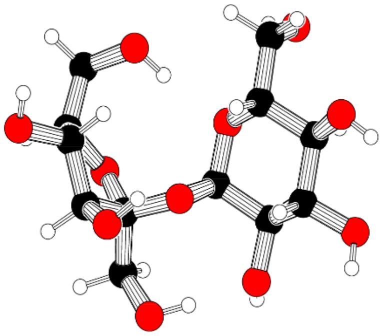
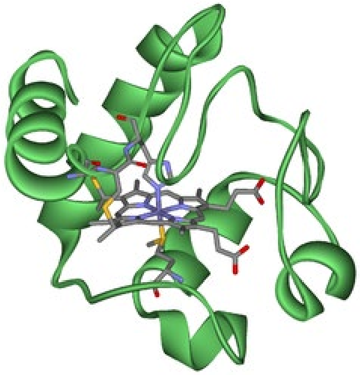


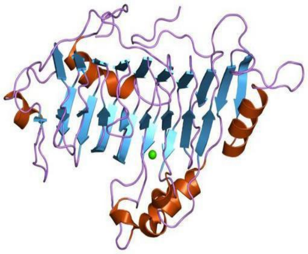
Figure 7.16 ball and stick model of Sucrose

Ref: commons.wikimedia.org/

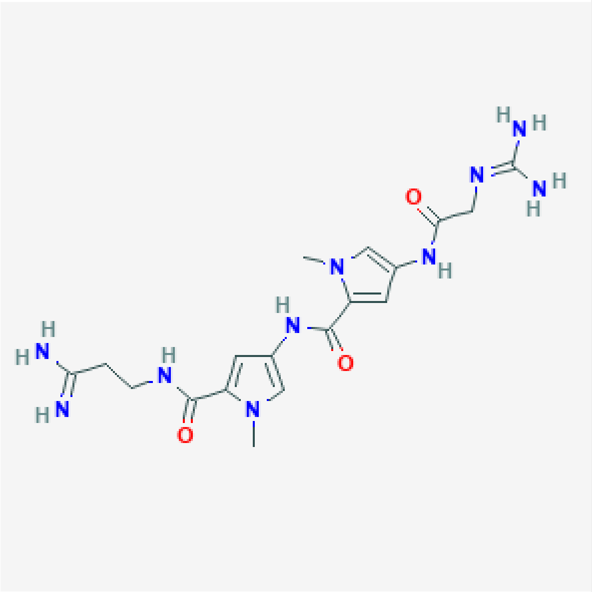
Visualizing **very large molecules** such as carbohydrates and proteins that may contain tens of thousands of atoms presents obvious problems. The usual technique is to simplify parts of the molecule, representing major kinds of extended structural units by shapes such as ribbons or tubes which are twisted or bent to approximate their conformations. These are then gathered to reveal the geometrical relations of the various units within the overall structure. Individual atoms, if shown at all, are restricted to those of special interest.



A cytochrome heme-binding protein composed of five peptide helices (gold and blue). A heme molecule lodged in its binding site is shown in green, with the central Fe(II) ion in white. Cytochromes are essential elements of respiratory electron transfer.



This worm-like creature is as evil as it looks; it is a highly nuanced rendering of the enzyme *pectate lyase* that is involved in the rotting of plant tissue.



Netropsin is a naturally-occurring antibiotic that binds to specific sites on DNA. The netropsin itself is rendered as a ball-and-stick model with an extended molecular surface.

Figure 7.17 Molecular modelling view of Bio-molecules: Cytochrome(left), pectane lyase(middle) & Netropsin(right)

Ref: www.snappygoat.com

Ref: https://pubchem.ncbi.nlm.nih.gov/compound/Netropsin

Study of the surface properties of large molecules is crucial for understanding how proteins, carbohydrates, and DNA interact with smaller molcules, especially those involved in transport of ions and small molecule across cell membranes, immune-system behavior, and signal transduction processes such as the "turning on" of genes.

See here for links to a wide variety of sources relating to visualization and molecular modeling.

Observable properties of chemical bonds

When we talk about the properties of a particular chemical bond, we are really discussing the relationship between two adjacent atoms that are part of the molecule. *Diatomic* molecules are of course the easiest to study, and the information we derive from them helps us interpret various kinds of experiments we carry out on more complicated molecules.

It is important to bear in mind that the exact properties of a specific kind of bond will be determined in part by the nature of the other bonds in the molecule; thus the energy and length of the C–H bond will be somewhat dependent on what other atoms are connected to the carbon atom. Similarly, the C-H bond length can vary by as much a 4 percent between different molecules. For this reason, the values listed in tables of bond energy and bond length are usually averages taken over a variety of compounds that contain a specific atom pair..

In some cases, such as C—O and C—C, the variations can be much greater, approaching 20 percent. In these cases, the values fall into groups which we interpret as representative of single- and *multiple* bonds: double, and triple.

Potential energies of bonded atoms

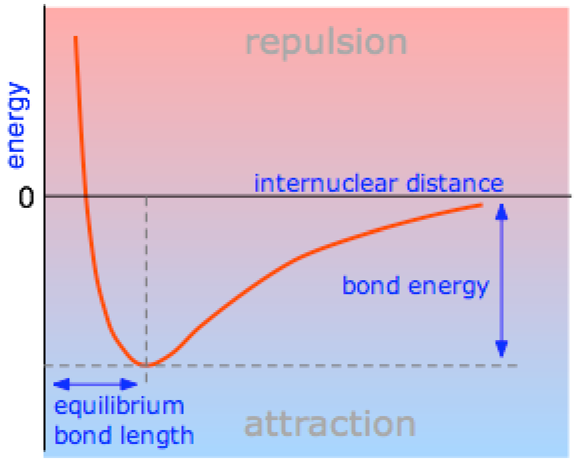


Figure 7.18 Potential energy Curve

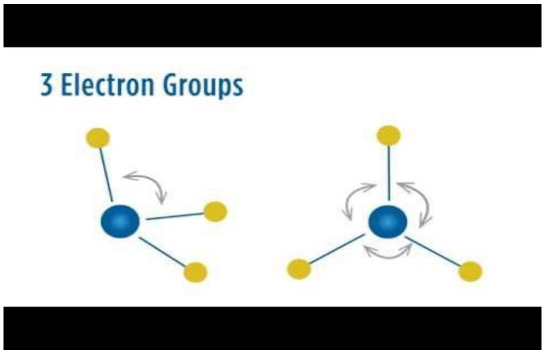
The energy of a system of two atoms depends on the distance between them. At large distances the energy is zero, meaning “no interaction”. At distances of several atomic diameters attractive forces dominate, whereas at very close approaches the force is repulsive, causing the energy to rise. The attractive and repulsive effects are balanced at the minimum point in the curve. Plots that illustrate this relationship are known as ***Morse curves***, and they are quite useful in defining certain properties of a chemical bond.

The internuclear distance at which the potential energy minimum occurs defines the **bond length**. This is more correctly known as the *equilibrium* bond length, because thermal motion causes the two atoms to vibrate about this distance. In general, the stronger the bond, the smaller will be the bond length.

Attractive forces operate between all atoms, but unless the potential energy minimum is at least of the order of RT, the two atoms will not be able to withstand the disruptive influence of thermal energy long enough to result in an identifiable molecule. Thus we can say that a chemical bond exists between the two atoms in H_2. The weak attraction between argon atoms does not allow Ar_2 to exist as a molecule, but it does give rise to the ***van Der Waals force*** that holds argon atoms together in its liquid and solid forms.

Potential energy and kinetic energy Quantum theory tells us that an electron in an atom possesses ***kinetic energy*** K as well as ***potential energy*** P, so the total energy E is always the sum of the two: $E = P + K$. The relation between them is surprisingly simple: $K = –0.5\ P$. This means that when a chemical bond forms (an exothermic process with $\Delta E < 0$), the decrease in potential energy is accompanied by an increase in the kinetic energy (embodied in the momentum of the bonding electrons), but the magnitude of the latter change is only half as much, so the change in potential energy always dominates. The ***bond energy*** $–\Delta E$ has half the magnitude of the fall in potential energy.

In summary, a chemical bond is an attraction between atoms that allows the formation of chemical substances that contain two or more atoms. The bond is caused by the electrostatic force of attraction between opposite charges, either between electrons and nuclei, or as the result of a dipole attraction. All bonds can be explained by quantum theory, but, in practice, simplification rules allow chemists to predict the strength, directionality, and polarity of bonds. The octet rule and VSEPR theory are two examples. More sophisticated theories are valence bond theory which includes orbital hybridization and resonance, and the linear combination of atomic orbitals molecular orbital method. Electrostatics are used to describe bond polarities and the effects they have on chemical substances.



Reference: https://www.youtube.com/watch?v=YB09OjAIh8k

Intramolecular interactions, such as covalent bonding and ionic bonding, and intermolecular interactions, such as London dispersion forces and hydrogen bonding, affect the chemical bonding and molecular geometry of substances. These interactions result from attractive and repulsive electrostatic interactions between electric charges. The physical and chemical properties of materials depend on these forces. In intramolecular and ionic interactions, the electronegativity of the involved atoms plays an important role. Two atoms with identical electronegativities can share electrons equally and form nonpolar covalent bonds, two atoms with different electronegativities can share electrons unequally and form polar covalent bonds, and two atoms with greatly differing electronegativities can transfer electrons, forming ionic bonds. Lewis structures allow for modeling covalent bonds and can predict how molecules form. Intermolecular forces are attractions between atoms, ions, or molecules that form matter. Intermolecular forces can occur between molecules with permanent dipole moments, two polar molecules, or an ion and a polar molecule (ion-dipole). Intermolecular forces can also occur between nonpolar molecules.

At A Glance

Chemical bonds form because of electrostatic interactions between protons and electrons. A chemical bond is stable if the total energy of the bonded atoms is less than the total energy of free atoms.

Ionic bonds form between atoms with large differences in electrostatic forces of oppositely charged ions.

Covalent bonds form between atoms with similar electronegativity values. Electrons are shared between atoms in a covalent bond.

When covalent bonds form between atoms with different electronegativities, the bonding electrons are shared unequally, forming a polar bond.

Lewis structures model covalent bonds by using element symbols and dots around the symbol to represent valence electrons. Lines represent covalent bonds between atoms.

Molecules can have more than one valid Lewis structure. Formal charge can be used to determine which representation is likely to be lower in energy. Resonance occurs when two or more Lewis structures have equivalent formal charges.

Dipoles carry an unequal charge distribution and can interact with other dipoles or ions. Hydrogen bonding is a special case of dipole-dipole interaction.

Nonpolar molecules have intermolecular interactions called London dispersion forces. London dispersion forces increase with molecule size.

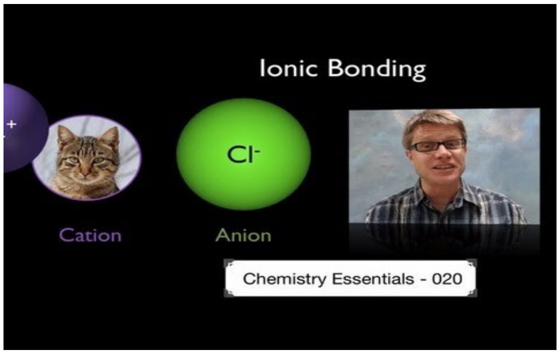
****

II. Ionic Bonding

When a metal loses its valence electrons, it becomes positive charged ion called cation, while the none metal accepts these valence electrons and it becomes negative charged called an anion.

There are electrostatic forces causing the cation and anion attracted to each other.

Reference https://youtu.be/zpaHPXVR8WU



Reference: https://youtu.be/hiyTfhjeF_U

Forming an Ion

An example for an ion formation is sodium cation. Neutral sodium Na has 11 protons and 11 electrons. When Na loses an electron, number of the protons does not change but number of electrons will be less by one electron. The number of electrons will be 10 electrons and therefore, Na will have one positive charge. Na^+

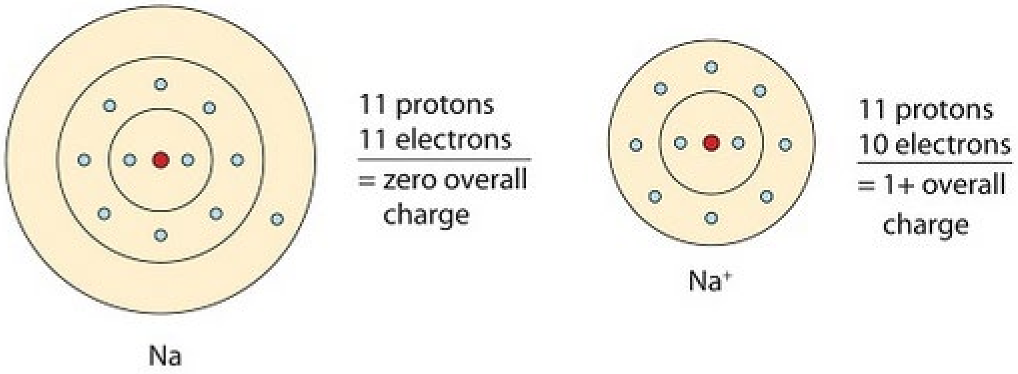


Figure 7.19 Formation of Na^+ Ion

Ref: commons.wikimedia.org/

The none metal chlorine Cl has 17 protons and 17 electrons. When the chlorine atom gains an extra electron, the number of the protons does not change but number of electrons will be increased by one electron. A negative ion of chlorine called anion is formed as shown below:

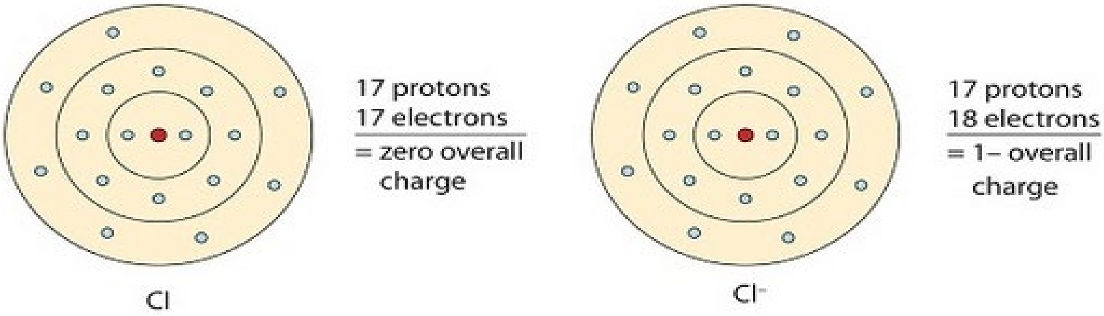
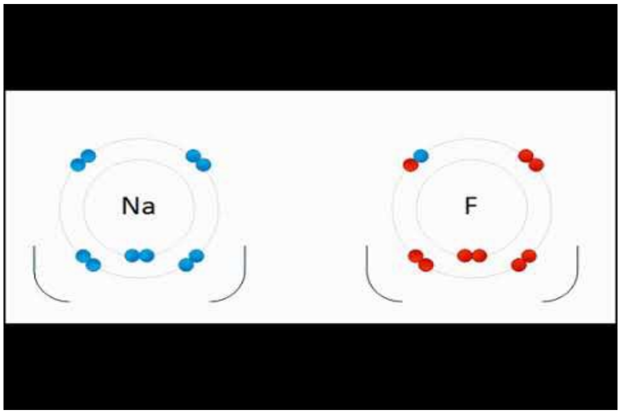


Figure 7.20 Formation of Cl^- Ion

Ref: commons.wikimedia.org/

Forming an Ionic Bond

The video below illustrates the formation of an ionic bond. Once the oppositely charged ions form Na^+ and F^-, they are attracted by their positive and negative charges and form an ionic compound. Ionic bonds are also formed when there is a large electronegativity difference between two atoms. This difference causes an unequal sharing of electrons such that one atom completely loses one or more electrons and the other atom gains one or more electrons, such as in the creation of an ionic bond between a metal atom (sodium) and a nonmetal (fluorine).



Reference: https://www.youtube.com/watch?v=r23klS9fzdc&feature=youtu.be

Naming an Ionic Compound from a Formula

1. Start naming the metal cation for example Ba $^{2+}$ (barium cation)
2. Then follow the name of the metal cation with the name of the none metal anion.
3. Discard the **ine** ending of the none metal chlor**ine** and replace it with the **ide** ending
   The name of the ionic compound ion $BaCl_2$ is called **barium chloride**.

Determining the Formula of Ionic Compound with Metal has one positive charge from a Name

Example:

Barium chloride
1.Barium is found in second group 2A. According the periodic table barium has +2 positive charges Ba $^{2+}$. See figure below:
2.Chlorine anion called chloride has one negative charge Cl^{-}.
3. Now, one has to swap the values of the charges of the ions only not the signs of ion:
Ba cation will take the value 1 as subscript and the chloride will take the value of 2 as subscript:
$Ba_1 Cl_2$ which is written as $BaCl_2$. The value of 1 is understood but it is not written.

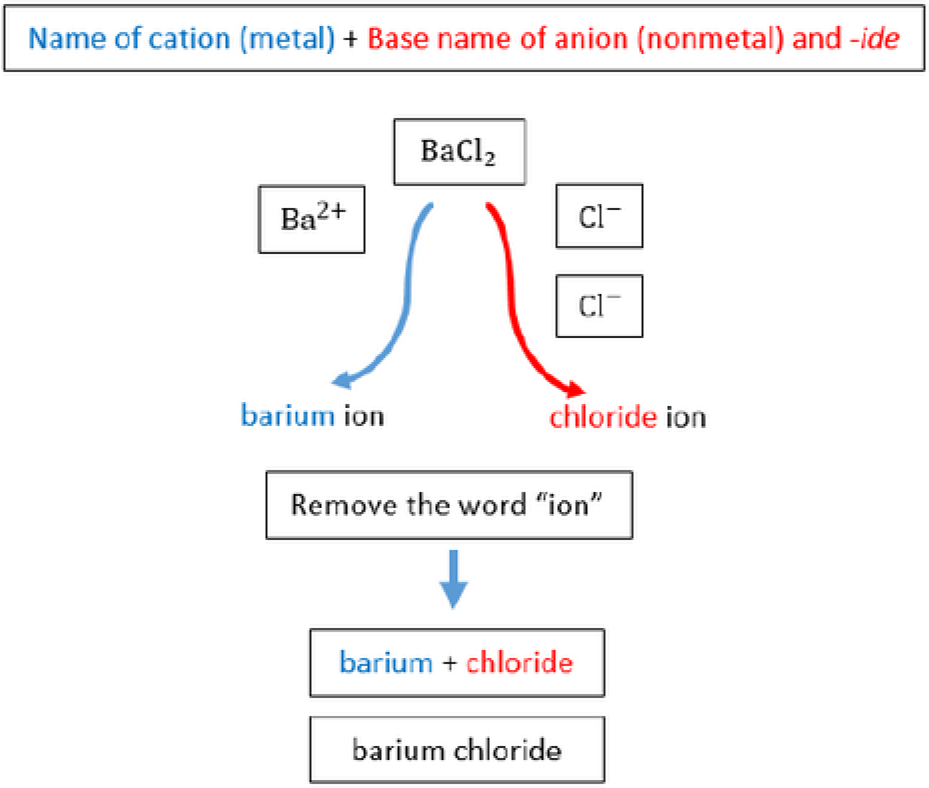
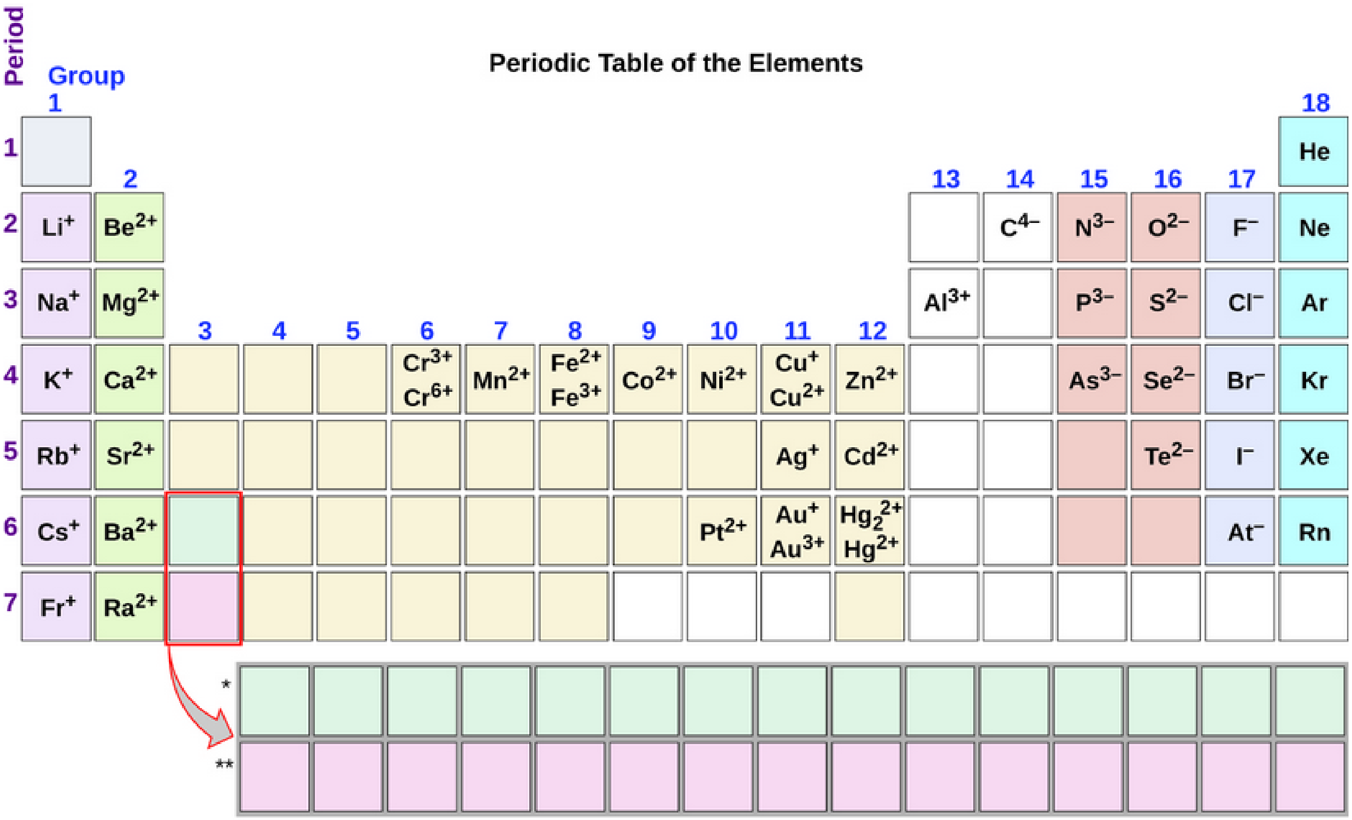


Figure 7.21 Nomenclature of Ionic compound

Ref: commons.wikimedia.org/

Reference:

https://chem.libretexts.org/Courses/College_of_Marin/CHEM_114%3A_Introductory_Chemistry/05%3A_Molecules_and_Compounds/5.07%3A_Naming_Ionic_Compounds



Periodic Table of the Elements

Period	Group 1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1																		He
2	Li^+	Be^{2+}												C^{4-}	N^{3-}	O^{2-}	F^-	Ne
3	Na^+	Mg^{2+}											Al^{3+}		P^{3-}	S^{2-}	Cl^-	Ar
4	K^+	Ca^{2+}				Cr^{3+} Cr^{6+}	Mn^{2+}	Fe^{2+} Fe^{3+}	Co^{2+}	Ni^{2+}	Cu^+ Cu^{2+}	Zn^{2+}			As^{3-}	Se^{2-}	Br^-	Kr
5	Rb^+	Sr^{2+}									Ag^+	Cd^{2+}				Te^{2-}	I^-	Xe
6	Cs^+	Ba^{2+}								Pt^{2+}	Au^+ Au^{3+}	Hg_2^{2+} Hg^{2+}					At^-	Rn
7	Fr^+	Ra^{2+}																

Figure 7.21 Charge of Ions from Periodic Table

Reference: https://chem.libretexts.org/Courses/Oregon_Tech_PortlandMetro_Campus/OT_-_PDX_-_Metro%3A_General_Chemistry_I/03%3A_Nuclei_Ions_and_the_Periodic_Table/3.03%3A_Predicting_Charges_of_Ions

Determining the Formula of Ionic Compound with Metal has Multiple positive charges from a Name and Determining Its name from the Formula

Name of cation (metal) + (Roman Numeral in parenthesis) + Base name of anion (nonmetal) and *-ide*

Figure 7.22 Nomenclature of Ionic compound(Transition metal)

Reference:
https://chem.libretexts.org/Courses/College_of_Marin/CHEM_114%3A_Introductory_Chemistry/05%3A_Molecules_and_Compounds/5.07%3A_Naming_Ionic_Compounds

Some metal ions have multiple charges. The periodic table shows some metals with their multiple charges.

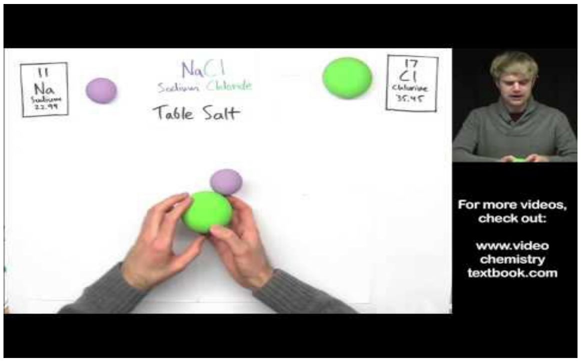
To name the ionic compound or to write the correct ionic formula, one has to use the Roman Numbers to distinguish the different charges of the metal cation

For example:

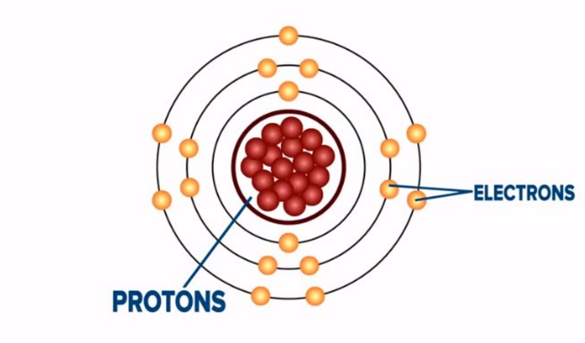
Iron-III-chloride is written as a formula as:
Fe^{3+} and Cl^{-}. Swap the values of the charges only not the sign, then one obtains $Fe_1 Cl_3$.
The ionic compound will be $FeCl_3$. The value of 1 is understood but it is not written.

$FeCl_3$ is named as Iron -III-Chloride. Note that the subscript of 3 means came from Fe and hence Fe has to have 3 positive charges.

The same approach on can name and obtain the formula of Iron-II-chloride as shown in the figure above.



Reference: https://www.youtube.com/watch?v=Qf07-8Jhhpc



Reference: https://www.youtube.com/watch?v=IQ4JOBZRAKQ

III. Covalent Bonding

Covalent bonding is made from the combination of two or more nonmetals. Nonmetals in the covalent bonding do not transfer electron (valence electrons) instead they share them to form single, double or even triple bonds.

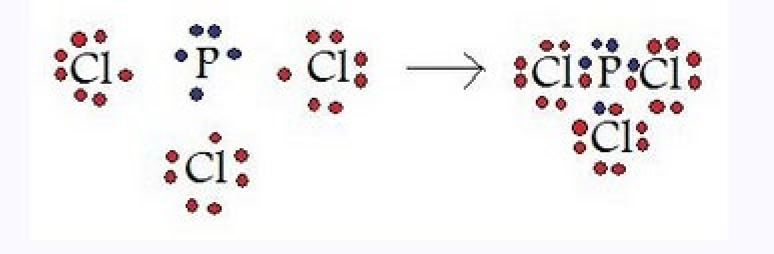


Figure 7.23 Covalent Bond Formation

Or:

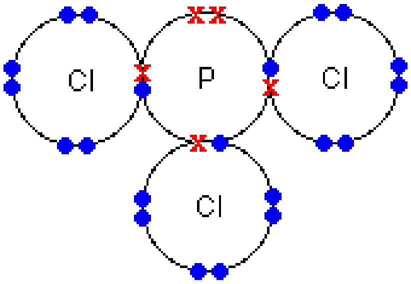


Figure 7.24 Sharing of Electrons in Covalent Bond Formation

There are three single bonds and one set of lone pair in PCl_3.

Reference:
https://chem.libretexts.org/Bookshelves/Physical_and_Theoretical_Chemistry_Textbook_Maps/Supplemental_Modules_(Physical_and_Theoretical_Chemistry)/Chemical_Bonding/Fundamentals_of_Chemical_Bonding/Covalent_Bonding

Another example: Methane CH_4. Hydrogen is ingroup 1 A, and it has one valence electron and carbon is in group 4 A, and therefore it has four valence electrons. Methane has four single covalent bonds.

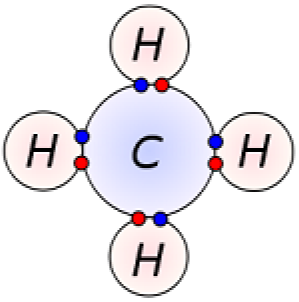


Figure 7.25 Sharing of Electrons in methane

Reference:
https://chem.libretexts.org/Bookshelves/Physical_and_Theoretical_Chemistry_Textbook_Maps/Supplemental_Modules_(Physical_and_Theoretical_Chemistry)/Chemical_Bonding

Octet Rule

The first really successful theory of chemical bonding was formulated by G.N.Lewis, whose 1902 lab notes eventually led to his classic article *The Atom and the Molecule* in 1916.

G.N. Lewis (1875-1946) created the College of Chemistry at the University of California, Berkeley, and made it into one of the world's most productive centers of chemistry research. His other notable work included acid-base theory, the thermodynamics of solutions, the first isolation of heavy water (D_2O), and the phosphorescence and magnetic properties of molecules.

Although Lewis originated the idea of the electron-pair bond, much of the credit for its early acceptance must go to **Irving Langmuir**, who extended it somewhat and enthusiastically popularized it to the extent that it began to be known as the Lewis-Langmuir theory, and even (to Lewis' annoyance) as the "Langmuir theory".

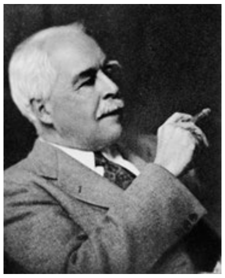


Figure 7.26 C.N. Lewis

Irving Langmuir (1881-1967, Nobel Prize 1932) was an industrial scientist employed by the General Electric Co. His most notable work was on the chemistry of surfaces and monomolecular layers. He originated the concept of "seeding" clouds to induce precipitation— a field of sufficient public interest at the time to get him on the cover of *Time Magazine* in 1950.

Figure 7.27 Irving Langmuir

Lewis and Langmuir were probably the two greatest American chemists of the first half of the twentieth century. Two interesting articles about them can be found at the Chemical Heritage Foundation site and at this Chemical Achievers site. Both scientists had earlier been involved in developing the cubical atom model which Lewis formulated in 1902 and which eventually led to the octet rule.

At the time Lewis began developing his ideas in 1902, it was widely believed that chemical bonding involved electrostatic attraction between ion-like entities. This seemed satisfactory for compounds such as NaCl that were known to dissociate into ions when dissolved in water, but it failed to explain the bonding in non-electrolytes such as CH_4. Atomic orbitals had not yet been thought of, but the concept of "valence" electrons was known, and the location of the noble gases in the periodic table suggested that all except helium possess eight valence electrons. It was also realized that elements known to form simple ions such as Ca^{2+} or Cl^- do so by losing or gaining whatever number of electrons is needed to leave eight in the valence shell of each. Lewis sought a way of achieving this octet in a way that did not involve ion formation, and he found it in his shared electron-pair theory published in 1916.

Present-day shared electron-pair theory is based on the premise that the s^2p^6 octet in the outermost shells of the noble gas elements above helium represents a particularly favorable configuration. This is not because of any mysterious properties of octets (or of noble gas atoms); it simply reflects the fact that filling an existing *s*-*p* valence shell is energetically more favorable than placing electrons in orbitals of higher principal quantum number. The sharing of electrons in this way between atoms means that more electrons are effectively "seeing" more nuclei, which you should remember is always the fundamental energetic basis of bond formation.

"Noble gas" valence electron configurations

The idea that the noble-gas configuration is a particularly favorable one which can be achieved through formation of electron-pair bonds with other atoms is known as the ***octet rule***.

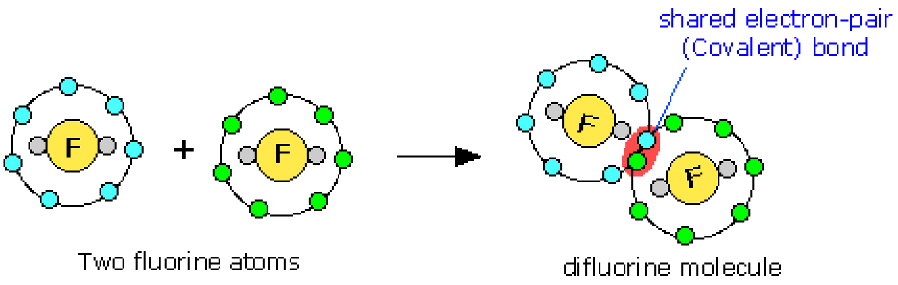


Figure 7.28 Formation of F_2 molecule

Noble gas configuration (in this case, that of neon, s^2p^6) is achieved when two fluorine atoms (s^2p^5) are able to share an electron pair, which becomes the covalent bond. Notice that only the outer (valence shell) electrons are involved.

Lewis' idea that the electrons are shared in pairs stemmed from his observation that most molecules possess an even number of electrons. This paired sharing also allows the formulas of a large number of compounds to be rationalized and predicted— a fact that led to the widespread acceptance of the Lewis model by the early 1920s.

Scope of the octet rule

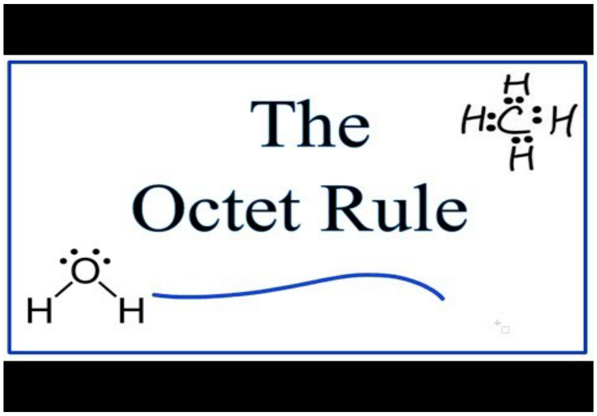
For the lightest atoms the octet rule must be modified, since the noble-gas configuration will be that of helium, which is simply s^2 rather than s^2p^6. Thus we write LiH as Li**:**H, where the electrons represented by the two dots come from the 2*s* orbital of lithium and the 1*s* orbital of hydrogen.

The octet rule applies quite well to the first full row of the periodic table (Li through F), but beyond this it is generally applicable only to the non-transition elements, and even in many of these it cannot explain many of the bonding patterns that are observed. The principal difficulty is that a central atom that is bonded to more than four peripheral atoms must have more than eight electrons around it if each bond is assumed to consist of an electron pair. In these cases, we hedge the rule a bit, and euphemistically refer to the larger number of electrons as an "expanded octet".

These situations tend to occur in atoms whose *d* orbitals are energetically close enough to the most highly-occupied s^2p^6 orbitals that they can become involved in electron-sharing with other atoms.

In spite of the octet rule's many exceptions and limitations, the shared electron-pair model is the one that chemists most frequently employ in their day-to-day thinking about molecules. It continues to serve as a very useful guiding principle and can be a good starting point for more sophisticated theories.

The video below illustrates the Octet rule:



Reference: https://www.youtube.com/watch?v=6Ecr7m-0E0E

Covalent compounds

The ***shared-electron pair model*** introduced by G.N. Lewis showed how chemical bonds could form in the absence of electrostatic attraction between oppositely-charged ions. As such, it has become the most popular and generally useful model of bonding in all substances other than metals. A chemical bond occurs when electrons are simultaneously attracted to two nuclei, thus acting to bind them together in an energetically-stable arrangement. The ***covalent bond*** is formed when two atoms are able to share a pair of electrons:

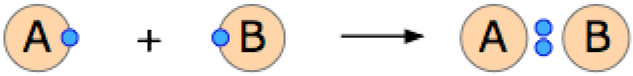


Figure 7.29 Formation of covalent Bond

In general, however, different kinds of atoms exert different degrees of attraction on their electrons, so in most cases the sharing will not be equal. One can even imagine an extreme case in which the sharing is so unequal that the resulting "molecule" is simply a pair of ions:

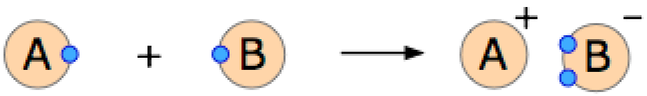


Figure 7.30 Formation of Ion Pair

The resulting substance is sometimes said to contain an ***ionic bond***. Indeed, the properties of a number of compounds can be adequately explained using the ionic model. But does this mean that there are really two kinds of chemical bonds, ionic and covalent?

Comparison Study: Bonding in ionic solids

According to the ionic electrostatic model, solids such as NaCl consist of positive and negative ions arranged in a crystal lattice. Each ion is attracted to neighboring ions of opposite charge, and is repelled by ions of like charge; this combination of attractions and repulsions, acting in all directions, causes the ion to be tightly fixed in its own location in the crystal lattice.

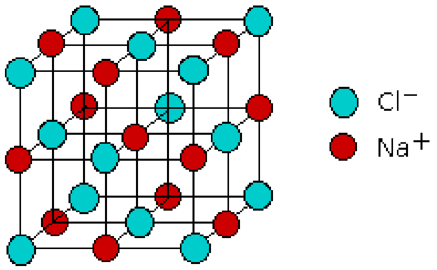


Figure 7.31 Formation of Ionic Crystal

Since electrostatic forces are non-directional, the structure of an ionic solid is determined purely by geometry: two kinds of ions, each with its own radius, will fall into whatever repeating pattern will achieve the lowest possible potential energy. Surprisingly, there are only a small number of possible structures; one of the most common of these, the ***simple cubic*** lattice of NaCl, is shown here.

Is there really such a thing as an ionic bond?

When two elements form an ionic compound, is an electron really lost by one atom and transferred to the other one? In order to deal with this question, consider the data on the ionic solid LiF. The average radius of the neutral Li atom is about 2.52Å. Now if this Li atom reacts with an atom of F to form LiF, what is the average distance between the Li nucleus and the electron it has "lost" to the fluorine atom? The answer is 1.56Å; the electron is now closer to the lithium nucleus than it was in neutral lithium!

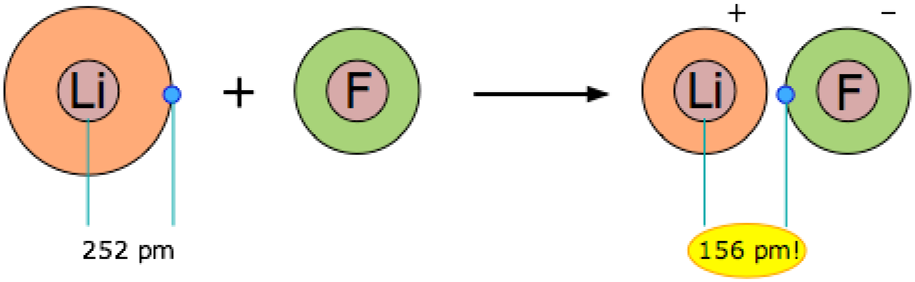


Figure 7.32 Formation of Ionic bond

So the answer to the above question is both yes and no: yes, the electron that was now in the 2*s* orbital of Li is now within the grasp of a fluorine 2*p* orbital, but no, the electron is now even closer to the Li nucleus than before, so how can it be "lost"? The one thing that is inarguably true about LiF is that there are more electrons closer to positive nuclei than there are in the separated Li and F atoms. But this is just the rule we stated at the beginning of this unit: **chemical bonds form when electrons can be simultaneously near two or more nuclei.**

It is obvious that the electron-pair bond brings about this situation, and this is the reason for the stability of the covalent bond. What is not so obvious (until you look at the numbers such as are quoted for LiF above) is that the "ionic" bond results in the same condition; even in the most highly ionic compounds, both electrons are close to both nuclei, and the resulting mutual attractions bind the nuclei together. This being the case, is there really any fundamental difference between the ionic and covalent bond?

The answer, according to modern chemical thinking is probably "no"; in fact, there is some question as to whether it is realistic to consider that these solids consist of "ions" in the usual sense. The preferred picture that seems to be emerging is one in which the electron orbitals of adjacent atom pairs are simply skewed so as to place more electron density around the "negative" element than around the "positive" one.

This being said, it must be reiterated that the ionic model of bonding is a useful one for many purposes, and there is nothing wrong with using the term "ionic bond" to describe the interactions between the atoms in the very small class of "ionic solids" such as LiF and NaCl.

More on polar covalence

"Covalent, ionic or metallic" is an oversimplification!

If there is no such thing as a "completely ionic" bond, can we have one that is completely covalent? The answer is yes, if the two nuclei have equal electron attracting powers. This situation is guaranteed to be the case with homonuclear diatomic molecules-- molecules consisting of two identical atoms. Thus in Cl_2, O_2, and H_2, electron sharing between the two identical atoms must be exactly even; in such molecules, the center of positive charge corresponds exactly to the center of negative charge: halfway between the two nuclei.

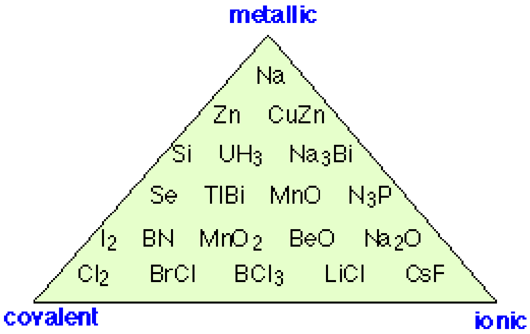


Figure 7.33 Metallic, covalent and ionic Compounds of different elements

Categorizing all chemical bonds as either ionic, covalent, or metallic is a gross oversimplification; as this diagram shows, there are examples of substances that exhibit varying degrees of all three bonding characteristics.

- A bond's percent ionic character (discussed more in detail later under "Electronegativity section) is the amount of electron sharing between two atoms; limited electron sharing corresponds with a high percent ionic character.
- To determine a bond's percent ionic character, the atoms' electronegativities are used to predict the electron sharing between the atoms.

Electron donor-acceptor bonds

In most covalent bonds, we think of the electron pair as having a dual parentage, one electron being contributed by each atom. There are, however, many cases in which both electrons come from only one atom. This can happen if the donor atom has a non-bonding pair of electrons and the acceptor atom has a completely empty orbital that can accommodate them.

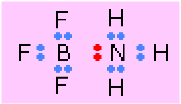


Figure 7.34 Electronic arrangement in donor-acceptor bond

This is the case, for example, with boron trifluoride and ammonia. In BF_3, one the 2p orbitals is unoccupied and can accommodate the lone pair on the nitrogen atom of ammonia. The electron acceptor, BF_3, acts as a ***Lewis acid*** here, and NH_3 is the ***Lewis base***.

Bonds of this type (sometimes known as ***coordinate covalent*** or ***dative*** bonds) tend to be rather weak (usually 50-200kJ/mol); in many cases the two joined units retain sufficient individuality to justify writing the formula as a molecular ***complex*** or ***adduct***.

Single, Double and Triple Covalent Bonding

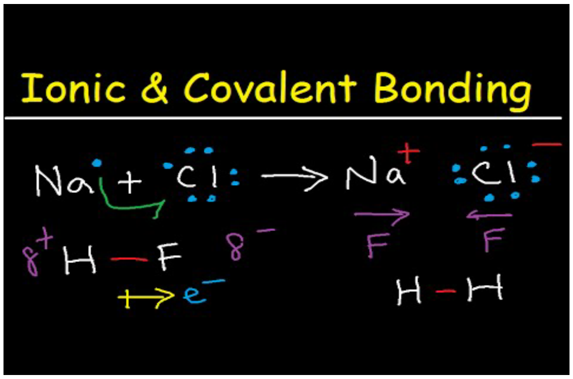
Covalent bonding requires a very discrete and specific orientation to establish the overlap between the bonding orbitals. The overlap can form sigma (single) bonds or pi (double and triple) bonds. the sigma bonds have very strong interaction due to the fact shared electrons are moving freely along the axis and the overlapping orbital are lying exactly on the orbital axis, while the pi bonds have weak interaction because the overlapping orbitals are laying above or below the orbital axis.

Single bonds are made when two electrons are shared, they form one sigma bond between the two atoms. Double bonds are made when four electrons are shared between the two atoms. As a result, sigma bond and one pi bond is formed. Triple bonds occur when six electrons are shared between the two atoms and as result one sigma bond and two pi bonds are formed.

More information on this type of bonding is discussed in next module.(Module 8) Advance Theories of Bonding.

The videos below illustrate the concept of the covalent bonds.

Reference: https://www.youtube.com/watch?v=ZxWmyZmwXtA



Reference: https://www.youtube.com/watch?v=S_k0kr2eZSQ

Polar and Nonpolar Covalent Bonds

Two important types of covalent bonds are nonpolar or pure covalent bonds and polar covalent bonds. Nonpolar bonds occur when atoms equally share electron pairs. Since only identical atoms (having the same electronegativity) truly engage in equal sharing, the definition is expanded to include covalent bonding between any atoms with an electronegativity difference less than 0.4. Examples of molecules with nonpolar bonds are H_2, N_2, and CH_4.

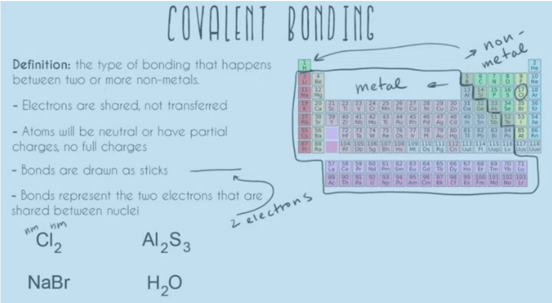
As the electronegativity difference increases, the electron pair in a bond is more closely associated with one nucleus than the other. If the electronegativity difference is between 0.4 and 1.7, the bond is polar. If the electronegativity difference is greater than 1.7, the bond is ionic.

Covalent Bond Examples

There is a covalent bond between the oxygen and each hydrogen in a water molecule (H_2O). Each of the covalent bonds contains two electrons, one from a hydrogen atom and one from the oxygen atom. Both atoms share the electrons.

A hydrogen molecule, H_2, consists of two hydrogen atoms joined by a covalent bond. Each hydrogen atom needs two electrons to achieve a stable outer electron shell. The pair of electrons is attracted to the positive charge of both atomic nuclei, holding the molecule together.

Phosphorus can form either PCl_3 or PCl_5. In both cases, the phosphorus and chlorine atoms are connected by covalent bonds. PCl_3 assumes the expected noble gas structure, in which the atoms achieve complete outer electron shells. Yet PCl_5 is also stable, so it's important to remember covalent bonds in chemistry don't always abide by the octet rule.



COVALENT BONDING

Definition: the type of bonding that happens between two or more non-metals.

- Electrons are shared, not transferred
- Atoms will be neutral or have partial charges, no full charges
- Bonds are drawn as sticks
- Bonds represent the two electrons that are shared between nuclei

Cl_2 Al_2S_3

NaBr H_2O

Reference: https://www.youtube.com/watch?v=RK07Bwwxkjg

Electronegativity

Electronegativity is a measure of the tendency of an atom to attract electrons (or electron density) towards itself. It determines how the shared electrons are distributed between the two atoms in a bond. The more strongly an atom attracts the electrons in its bonds, the larger its electronegativity.

In general, the electronegativity describes the degree to which an atom attracts electrons in a chemical bond. The difference in the electronegativity of two atoms determines their bond type. If the electronegativity difference is more than 1.7, the bond will have an ionic character. If the electronegativity difference is between 0.4 and 1.7, the bond will have a polar covalent character. Lastly, if the electronegativity difference is less than 0.4, the bond will have a nonpolar covalent character.

Unlike many other periodic trends, electronegativity does not have actual units. Instead, it is a way of combining two other periodic trends: ionization energy and electron affinity. Ionization energy is the amount of energy required to remove an electron from a neutral atom. Electron affinity is the amount of energy given off or required when a neutral atom gains an electron. Electronegativity does not have any units. However, the Pauling scale for electronegativity lists cesium as the least electronegative element, with a value of 0.79. In this scale, fluorine is the most electronegative element, with a value of 4.0.

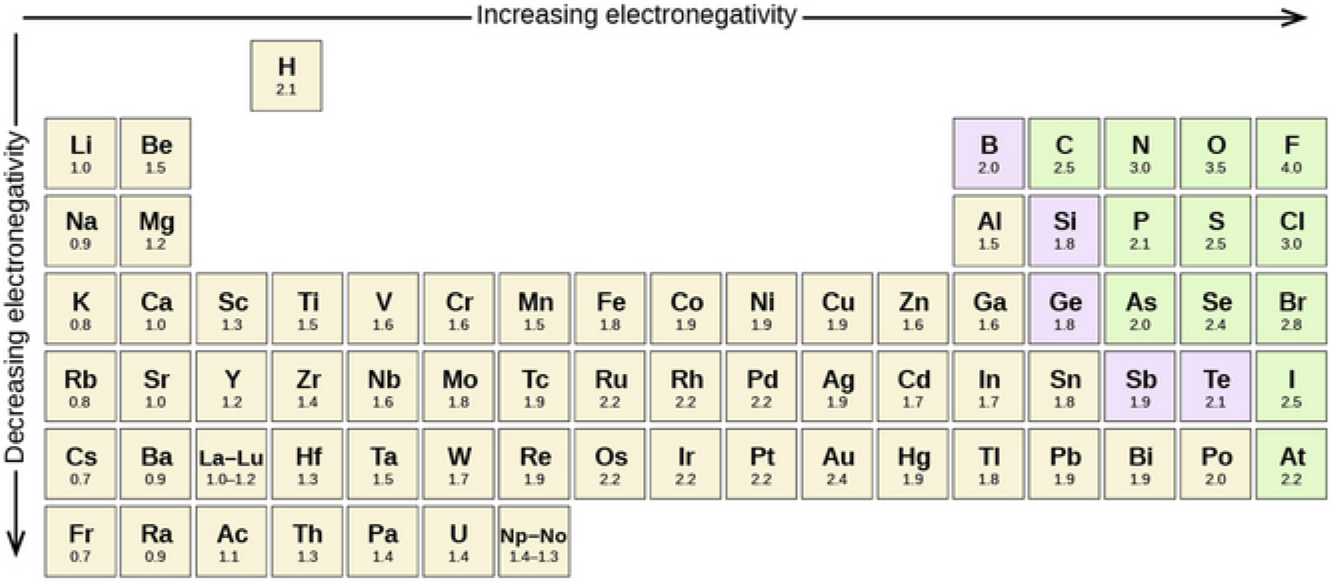


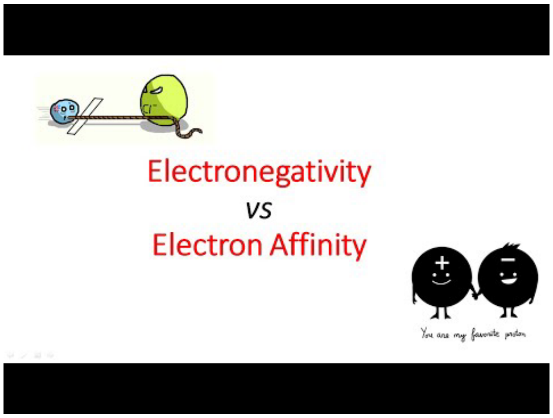
Figure 7.35 Electronegativity trend on Periodic table

Reference: https://iu.pressbooks.pub/openstaxchemistry/chapter/7-2-covalent-bonding/

Above is the electronegativity values derived by Pauling follow predictable periodic trends, with the higher electronegativities toward the upper right of the periodic table.

Electronegativity versus Electron Affinity

Electronegativity and electron affinity are the two chemical properties associated with elements. The major difference between electronegativity and electron affinity is that electronegativity is the property associated with the attracting ability of electron towards an atom. As against, electron affinity is associated with the release of energy when an electron is added to an atom.



Reference: https://www.youtube.com/watch?v=m12wZMbOGFQ

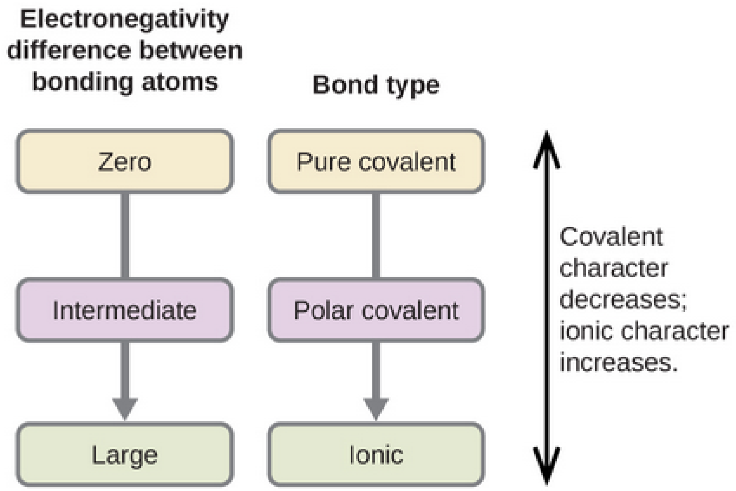
Ionic Compounds vs. Molecular Compounds

A covalent bond that is formed from the same none metal atoms will result a none polar covalent bond. The electronegativity is zero. A covalent bond that is formed from different none metal atoms with different electronegativity will yield a polar covalent bond.

Ionic bond are polar and the electronegativity difference is higher than that found in the polar covalent bond.

Ionic solids are generally characterized by high melting and boiling points along with brittle, crystalline structures. Covalent compounds, have lower melting and boiling points. They tend to be not soluble in water and do not conduct electricity when they dissolved in water.

With the help of the electronegativity difference chart is given below, one can determine if the bond none polar covalent or it is polar covalent, or polar ionic:

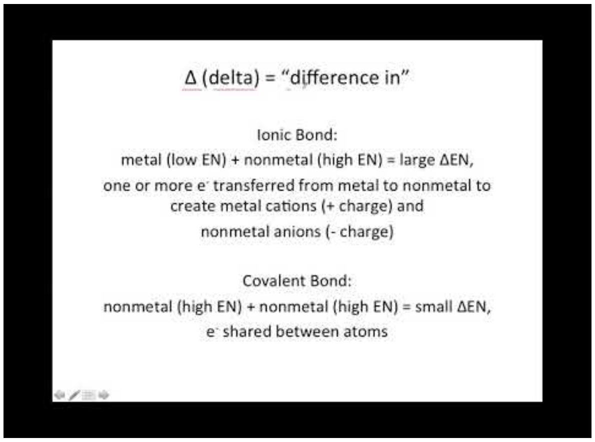


Bond Type	Electronegativity Difference
pure covalent	< 0.4
polar covalent	between 0.4 and 1.8
ionic	> 1.8

Figure 7.36 Electronegativity and nature of Bonds

Reference: https://iu.pressbooks.pub/openstaxchemistry/chapter/7-2-covalent-bonding/

The video below illustrates the electronegativity difference in some details:



Δ (delta) = "difference in"

Ionic Bond:
metal (low EN) + nonmetal (high EN) = large ΔEN,
one or more e$^-$ transferred from metal to nonmetal to create metal cations (+ charge) and nonmetal anions (- charge)

Covalent Bond:
nonmetal (high EN) + nonmetal (high EN) = small ΔEN,
e$^-$ shared between atoms

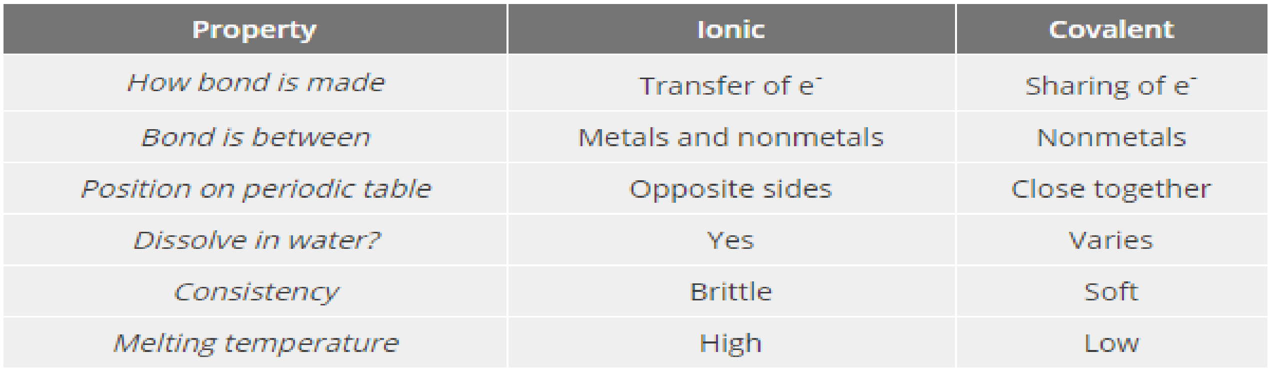
Reference: https://www.youtube.com/watch?v=SwTrBcTAznI

Comparison of Ionic and Covalent Bonds

A molecule or compound is made when two or more atoms form a chemical bond that links them together. As we have seen, there are two types of bonds: ionic bonds and covalent bonds. In an ionic bond, the atoms are bound together by the electrostatic forces in the attraction between ions of opposite charge. Ionic bonds usually occur between metal and nonmetal ions. For example, sodium (Na), a metal, and chloride (Cl), a nonmetal, form an ionic bond to make NaCl. In a covalent bond, the atoms bond by sharing electrons. Covalent bonds usually occur between nonmetals. For example, in water (H_2O) each hydrogen (H) and oxygen (O) share a pair of electrons to make a molecule of two hydrogen atoms single bonded to a single oxygen atom.

In general, ionic bonds occur between elements that are far apart on the periodic table. Covalent bonds occur between elements that are close together on the periodic table. Ionic compounds tend to be brittle in their solid form and have very high melting temperatures. Covalent compounds tend to be soft, and have relatively low melting and boiling points. Water, a liquid composed of covalently bonded molecules, can also be used as a test substance for other ionic and covalently compounds. Ionic compounds tend to dissolve in water (e.g., sodium chloride, NaCl); covalent compounds sometimes dissolve well in water (e.g., hydrogen chloride, HCl), and sometimes do not (e.g., butane, C_4H_{10}). Properties of ionic and covalent compounds are listed in the following Table.

Table: Properties of ionic and covalent compounds.



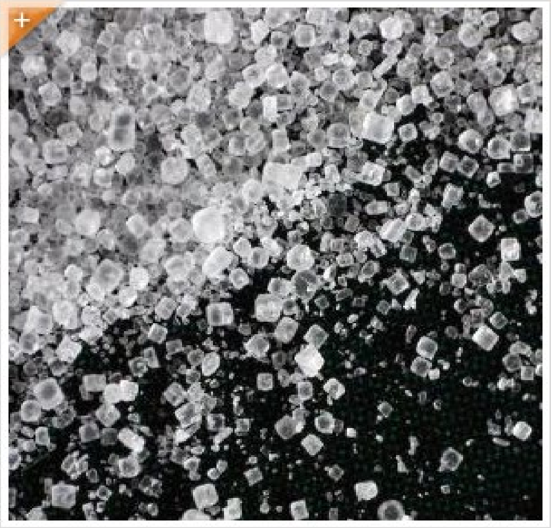
Property	Ionic	Covalent
How bond is made	Transfer of e^-	Sharing of e^-
Bond is between	Metals and nonmetals	Nonmetals
Position on periodic table	Opposite sides	Close together
Dissolve in water?	Yes	Varies
Consistency	Brittle	Soft
Melting temperature	High	Low

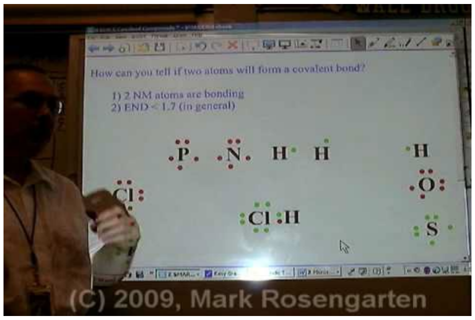
The properties listed in the above Table are exemplified by sodium chloride (NaCl) and chlorine gas (Cl_2). Like other ionic compounds, sodium chloride (See the following Fig A) contains a metal ion (sodium) and a nonmetal ion (chloride), is brittle, and has a high melting temperature. Chlorine gas (Fig.B) is similar to other covalent compounds in that it is a nonmetal and has a very low melting temperature.

Fig7.37 (**A**) sodium chloride (NaCl), an ionic compound

Fig. (**B**) chlorine gas (Cl_2), a covalent compound

Reference*:* Image courtesy of Edal Anton Lefterov from Wikipedia





How can you tell if two atoms will form a covalent bond?

1) 2 NM atoms are bonding
2) END < 1.7 (in general)

Reference: https://youtu.be/-Eh_0Dseg3E

It all depends on electronegativity differences

The electronegativity of an atom denotes its relative electron-attracting power in a chemical bond.

See here for more on ionization energy, electron affinity, electronegativity, and their periodic trends.

It is important to understand that electronegativity is not a measurable property of an atom in the sense that ionization energies and electron affinities are, although it can be correlated with both of these properties. The actual electron-attracting power of an atom depends in part on its chemical environment (that is, on what other atoms are bonded to it), so tabulated electronegativities should be regarded as no more than predictors of the behavior of electrons, especially in more complicated molecules.

There are several ways of computing electronegativities, which are expressed on an arbitrary scale. The concept of electronegativity was introduced by LINUS PAULING, and his 0-4 scale continues to be the one most widely used.

TRENDS IN ELECTRONEGATIVITY:

Electronegativities of the main-group elements

The 0-4 electronegativity scale of Pauling is the best known of several arbitrary scales of this kind. Electronegativity values are not directly observable, but are derived from measurable atomic properties such as ionization energy and electron affinity. The place of any atom on this scale provides a good indication of its ability to compete with another atom in attracting a shared electron pair to it, but the presence of bonds to other atoms, and of multiple- or nonbonding electron pairs may make predictions about the nature a given bond less reliable.

An atom that has a small electronegativity is said to be ***electropositive***. As the diagram shows, the metallic elements are generally electropositive. The position of hydrogen in this regard is worth noting; although physically a nonmetal, much of its chemistry is metal-like.

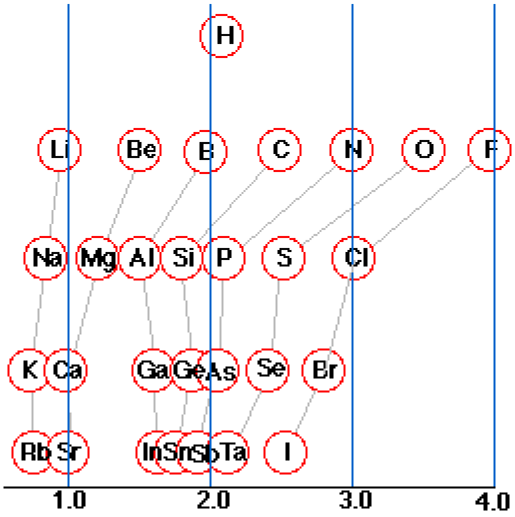


Figure 7.38 Electronegativity in main group elements

Molecular dipole moments

When non-identical atoms are joined in a covalent bond, the electron pair will be attracted more strongly to the atom that has the higher electronegativity. As a consequence, the electrons will not be shared equally; the center of the negative charges in the molecule will be displaced from the center of positive charge. Such bonds are said to be ***polar*** and to possess ***partial ionic character***, and they may confer a polar nature on the molecule as a whole.

A polar molecule acts as an ***electric dipole*** which can interact with electric fields that are created artificially or that arise from nearby ions or polar molecules. Dipoles are conventionally represented as arrows pointing in the direction of the negative end. The magnitude of interaction with the electric field is given by the ***permanent electric dipole moment*** of the molecule. The dipole moment corresponding to an individual bond (or to a diatomic molecule) is given by the product of the quantity of charge displaced q and the bond length r:

$$\mu = q \times r$$

In SI units, q is expressed in coulombs and r in meters, so μ has the dimensions of C-m. If one entire electron charge is displaced by 100 pm (a typical bond length), then

$$\mu = (1.6022 \times 10^{-19}\ \text{C}) \times (10^{-10}\ \text{m}) = 1.6 \times 10^{-29}\ \text{C-m} = \mathbf{4.8\ D}$$

The quantity denoted by D, the ***Debye*** unit, is still commonly used to express dipole moments. It was named after PETER DEBYE (1884-1966), the Dutch-American physicist who pioneered the study of dipole moments and of electrical interactions between particles; he won the Nobel Prize for Chemistry in 1936.

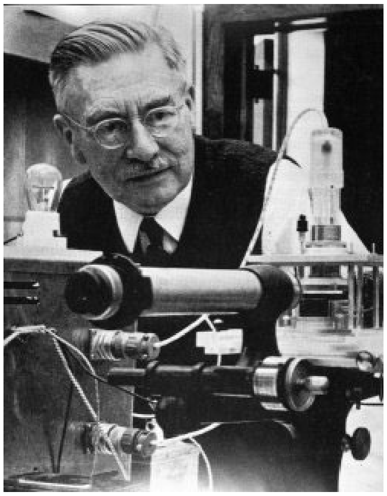


Figure 7.39 Peter Debye

How dipole moments are measured

When a solution of polar molecules is placed between two oppositely-charged plates, they will tend to align themselves along the direction of the field. This process consumes energy which is returned to the electrical circuit when the field is switched off, an effect known as electrical *capacitance.*

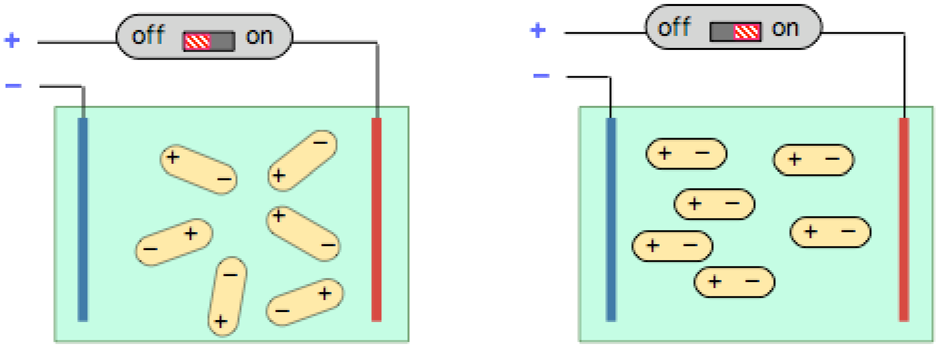


Figure 7.40 polar and nonpolar molecules in charged field

Measurement of the capacitance of a gas or solution is easy to carry out and serves as a means of determining the magnitude of the dipole moment of a substance.

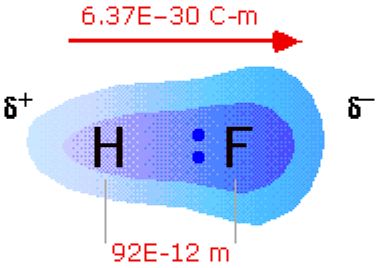


Figure 7.41 polarity of HF molecule

Problem Example 1

Estimate the percent ionic character of the bond in hydrogen fluoride from the experimental data shown at the right.

Solution:

$$\frac{6.37\text{E}{-30}\ \text{C-m}}{92\text{E}{-12}\ \text{m}} = 6.92\ \text{E}{-20}\ \text{C} \quad \text{(charge displaced)}$$

$$\frac{6.92\ \text{E}{-20}\ \text{C}}{1.60\text{E}{-19}\ \text{C/electron}} = 0.43\ \text{(ionic character of bond)}$$

Dipole moments as vector sums

In molecules containing more than one polar bond, the molecular dipole moment is just the vector combination of what can be regarded as individual "bond dipole moments". Being vectors, these can reinforce or cancel each other, depending on the geometry of the molecule; it is therefore not uncommon for molecules containing polar bonds to be nonpolar overall, as in the example of carbon dioxide:

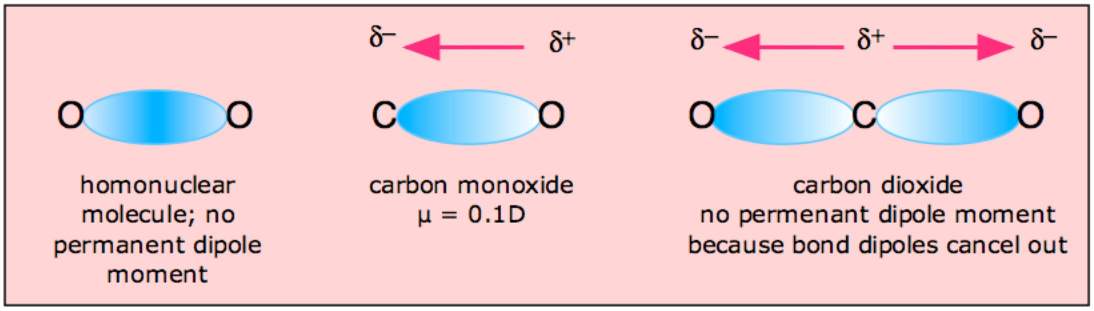
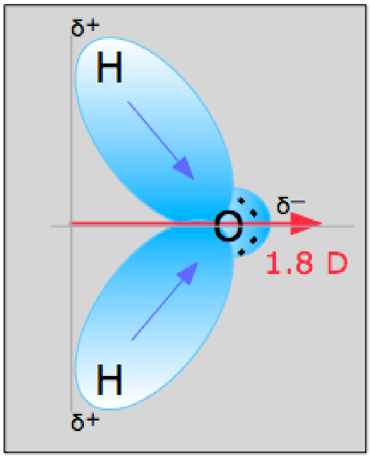


Figure 7.42 Determination of Dipole moment

The zero dipole moment of CO_2 is one of the simplest experimental methods of demonstrating the linear shape of this molecule.



H_2O, by contrast, has a very large dipole moment which results from the two polar H–O components oriented at an angle of 104.5°. The nonbonding pairs on oxygen are a contributing factor to the high polarity of the water molecule.

Figure 7.43 Dipole moment of water

In molecules containing nonbonding electrons or multiple bonds, the electronegativity difference may not correctly predict the bond polarity. A good example of this is carbon monoxide, in which the partial negative charge resides on the carbon, as predicted by its negative formal charge (below.)

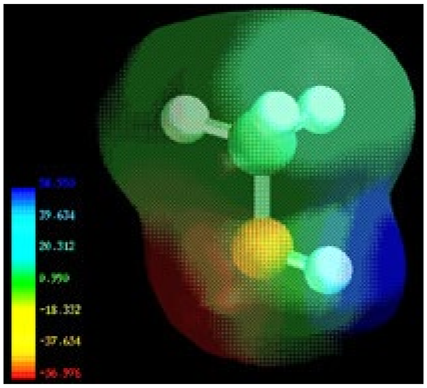


Figure 7.44 Electron Density map in ethanol

Electron densities in a molecule (and the dipole moments that unbalanced electron distributions can produce) are now easily calculated by molecular modelling programs. In this example [source] for methanol CH_3OH, the blue area centered on hydrogen represents a positive charge, the red area centered where we expect the lone pairs to be located represents a negative charge, while the light green around methyl is approximately neutral.

The manner in which the individual bonds contribute to the dipole moment of the molecule is nicely illustrated by the series of chloromethanes:

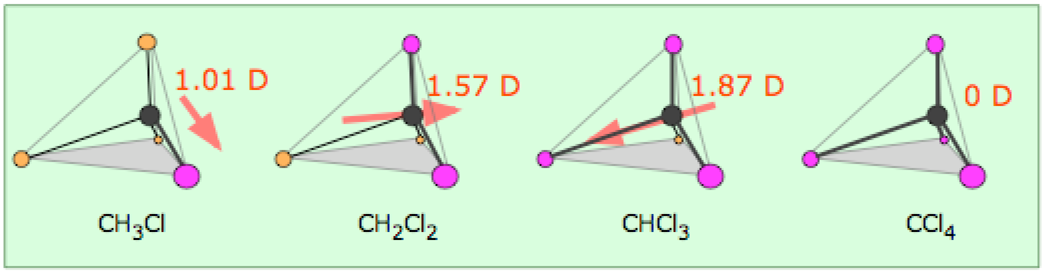


Figure 7.45 Dipole moments of different molecules

(Bear in mind that all four positions around the carbon atom are equivalent in this tetrahedral molecule, so there are only four chloromethane.)

Summary

A covalent bond is the force of attraction that holds together two atoms that share a pair of valence electrons. Covalent bonds form only between atoms of nonmetals.

The two atoms that are held together in a covalent bond may be atoms of the same element or different elements. When atoms of different elements bond together, it forms a covalent compound.

Covalent bonds form because the shared electrons fill each atom's outer energy level and this is the most stable arrangement of electrons.

IV. Lewis Symbols and Structures

What is Lewis Electron Dot Structure?

Lewis Dot Structure is a simple presentation of the overlapping orbitals forming sigma and pi bond. The valence electrons contributing to the bonding (single, double and triple bonds) are presented as dots. Lewis Dot Structure illustrates the distribution of the valence electrons and the octet rule satisfaction to the atoms contributing to the bonding.

Lewis structures extend the concept of the electron dot **diagram** by adding lines between atoms to represent shared pairs in a chemical bond. **Lewis structures** show each atom and its position in the **structure** of the molecule using its chemical **symbol**.

Example Phosphorous and Argon Dot Structures:

Phosphorous has 5 valence electrons and Argon has 8 valence electrons.

Figure 7.46 Lewis Symbol of atoms

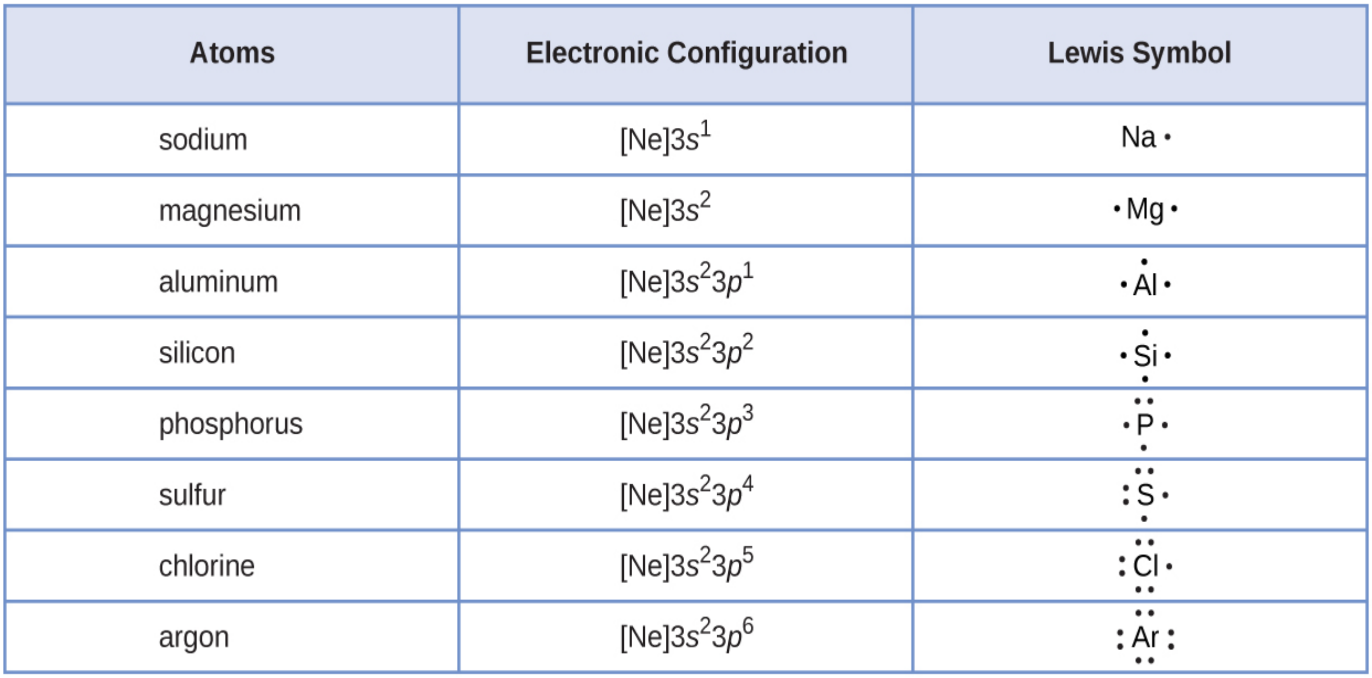
Ref: commons.wikimedia.org/

We use Lewis symbols to describe valence electron configurations of atoms and monatomic ions. A Lewis symbol consists of an elemental symbol surrounded by one dot for each of its valence electrons:

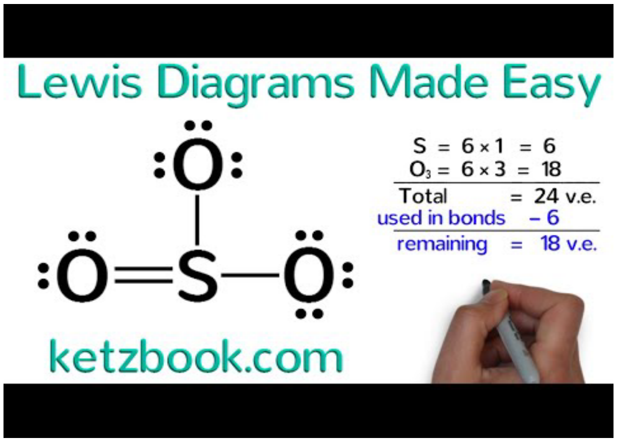
Figure 7.47 Lewis Symbol of Ca

Ref: commons.wikimedia.org/

The following Table shows the Lewis symbols for the elements of the third period of the periodic table. Electron dots are typically arranged in four pairs located on the four "sides" of the atomic symbol.



Atoms	Electronic Configuration	Lewis Symbol
sodium	$[\text{Ne}]3s^1$	$\text{Na}\cdot$
magnesium	$[\text{Ne}]3s^2$	$\cdot\text{Mg}\cdot$
aluminum	$[\text{Ne}]3s^23p^1$	$\cdot\overset{\cdot}{\text{Al}}\cdot$
silicon	$[\text{Ne}]3s^23p^2$	$\cdot\overset{\cdot}{\underset{\cdot}{\text{Si}}}\cdot$
phosphorus	$[\text{Ne}]3s^23p^3$	$\cdot\overset{\cdot\cdot}{\underset{\cdot}{\text{P}}}\cdot$
sulfur	$[\text{Ne}]3s^23p^4$	$:\overset{\cdot\cdot}{\underset{\cdot}{\text{S}}}\cdot$
chlorine	$[\text{Ne}]3s^23p^5$	$:\overset{\cdot\cdot}{\underset{\cdot\cdot}{\text{Cl}}}\cdot$
argon	$[\text{Ne}]3s^23p^6$	$:\overset{\cdot\cdot}{\underset{\cdot\cdot}{\text{Ar}}}:$



Reference: https://www.youtube.com/watch?v=cIuXl7o6mAw&vl=en

How to Draw Lewis Electron Dot Structure?

A Lewis electron dot structure describes the bonding atoms, the number of bonds in the molecule, and the lone pairs left in the bonding atoms.

The general steps are given below:

a) First, the total number of valence electrons present in the molecule is calculated by adding the individual valencies of each atom.
b) If the molecule is an anion, extra electrons ***(number of electrons added = the magnitude of negative charge)*** are added to the Lewis dot structure.
c) When cationic molecules are considered, electrons are subtracted from the total count in order to make up for the positive charge.
d) The least electronegative atom is made the central atom of the molecule or ion.
e) The atoms are now connected via single bonds.
f) Now, the lone pairs of electrons are assigned to each atom belonging to the molecule. Commonly, the lone pairs are assigned to the most electronegative atoms first.
g) Once the lone pairs are assigned, if every atom does not have an octet configuration, a double or triple bond must be drawn to satisfy the octet valency of each atom.
h) If required, a ***lone pair can be converted into a bond pair in order to satisfy the octet rule for two atoms.***

It is important to note that only the valence electrons are considered while drawing Lewis dot structures and the electrons that do not belong to the outermost shell are ignored. Examples are shown below.

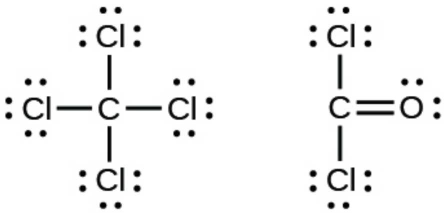
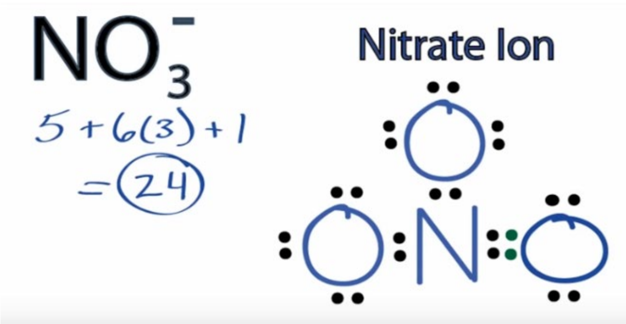


Figure 7.48 Lewis Structure of covalent molecules

Ref: commons.wikimedia.org/

After reviewing all these rules, the Lewis Dot Structure of NO_3^- will be written as shown below:

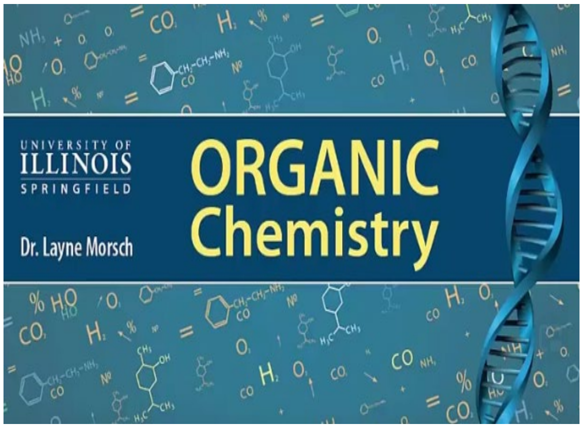


Reference: https://www.youtube.com/watch?v=toXtRCEUBKU

Lewis Structure Examples

The Lewis electron dot structures of a few molecules are illustrated in this subsection.

The video below illustrates the Lewis Dot structure of some organic and inorganic compounds:



https://youtu.be/3nAfsS56yNc

1. Lewis Structure of CO_2

- The central atom of this molecule is carbon.
- ***Oxygen contains 6 valence electrons*** which form 2 lone pairs. Since it is bonded to only one carbon atom, it must form a double bond.
- ***Carbon contains four valence electrons***, resulting in zero lone pairs. Therefore, it is doubly bonded to each **oxygen atom.**

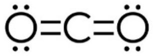


Figure 7.49 Lewis Dot Structure of CO_2

Ref: commons.wikimedia.org/

2. Lewis Structure of O_2

- An atom of ***oxygen contains 6 electrons in the valence shell.***
- Four of the **valence electrons** exist in lone pairs, implying that the oxygen atom must participate in two single bonds or one double bond in order to attain an octet configuration.
- Since there are only two oxygen atoms in an O_2 molecule, the atoms form a double bond resulting in the following Lewis electron dot structure.

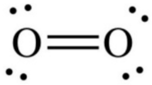


Figure 7.50 Lewis Dot Structure of O_2

Ref: commons.wikimedia.org/

3. Lewis Structure of CO (Carbon Monoxide)

- A carbon monoxide molecule consists of one carbon atom and one oxygen atom.
- The ***carbon atom requires four electrons to obtain octet configuration whereas the oxygen atom requires two.***
- Therefore, the valency is satisfied via the donation of a lone pair of electrons for bonding by the oxygen atom.
- The resulting Lewis electron dot structure displays a **triple bond** connecting a carbon and an oxygen atom, each holding a lone pair of electrons.

Figure 7.51 Lewis Dot Structure of CO

Ref: commons.wikimedia.org/

The Octet Rule Within Covalent Bonds

The octet rule is a chemical rule of thumb that reflects the observation that main group elements tend to bond in such a way that each atom has eight electrons in its valence shell, giving it the same electronic configuration as a noble gas.

The octet rule dictates that atoms are most stable when their valence shells are filled with eight electrons. It is based on the observation that the atoms of the main group elements tend to participate in chemical bonding in such a way that each atom of the resulting molecule has eight electrons in the valence shell. The octet rule is only applicable to the main group elements.

The molecules of the halogens, oxygen, nitrogen, and carbon are known to obey the octet rule. In general, the elements that obey this rule include the **s-block elements** and the p-block elements (with the exception of hydrogen, helium, and lithium).

The octet rule can be observed in the bonding between the carbon and oxygen atoms in a carbon dioxide molecule, as illustrated via a Lewis dot structure below.

Figure 7.52 The Octet Rule

The shared electrons fulfil the valency requirements of both the bonded atoms. Thus, it can be noted that both the oxygen atoms and the carbon atom have an octet configuration in the CO_2 molecule.

Upon observing that the noble gases were chemically inert, the electronic theory of valency was proposed by the German physicist Walther Kossel and the American chemist Gilbert Lewis. It was based on the tendency of atoms to assume the most stable state possible.

Illustrated below here for carbon in CCl_4 (carbon tetrachloride) and silicon in SiH_4 (silane). Because hydrogen only needs two electrons to fill its valence shell, it is an exception to the octet rule. The transition elements and inner transition elements also do not follow the octet rule:

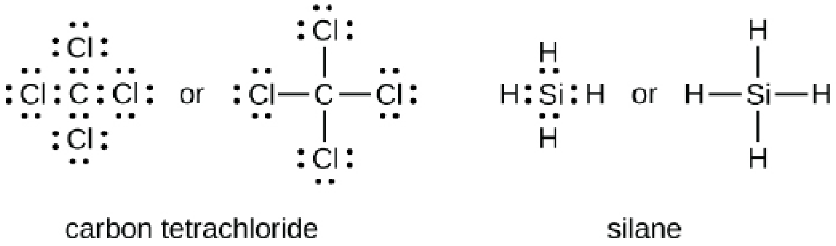
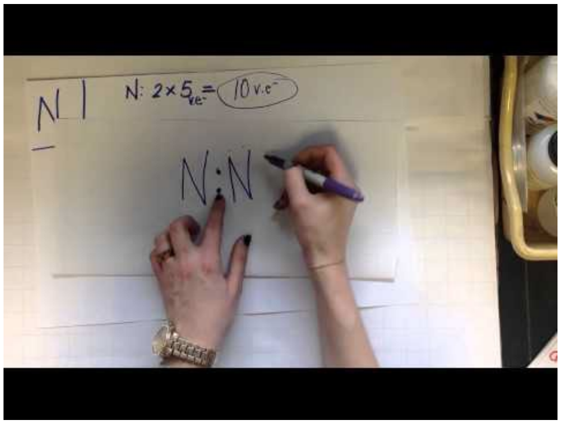


Figure 7.53 Lewis Dot structures

Ref: commons.wikimedia.org/

Lewis Structures: Single, Double & Triple Bonds

A **Lewis dot structure** can be represented by either two dots or by a line between two atoms when there is a chemical **bond** - two lines for **double bond** and **three** lines for a **triple bond**. ... Connect the atoms by electron pair **bonds** so that each atom has a full octet.



Reference: https://www.youtube.com/watch?v=P5v7m-3WArw

So, in definition, Single Bond: "A covalent bond between two atoms that is formed by one bonding pair of electrons." Double Bond: "A multiple covalent bond between two atoms that is formed by two bonding electron pairs. Triple Bond: "A multiple covalent bond between two atoms that is formed by three bonding pairs of electrons.

Multiple Covalent Bond: "more than one bond between atoms, formed by the sharing of more than one electron from each atom. Can be either a double bond or triple bond."

Examples:

A **double bond**

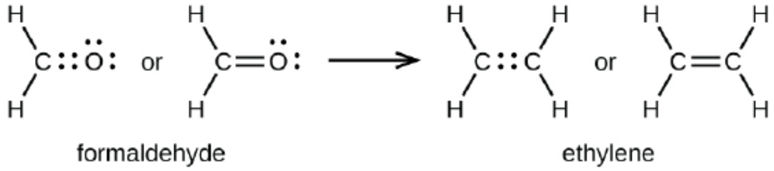


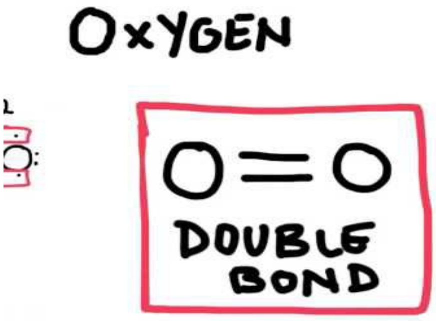
Figure 7.54 Double bond

Ref: commons.wikimedia.org

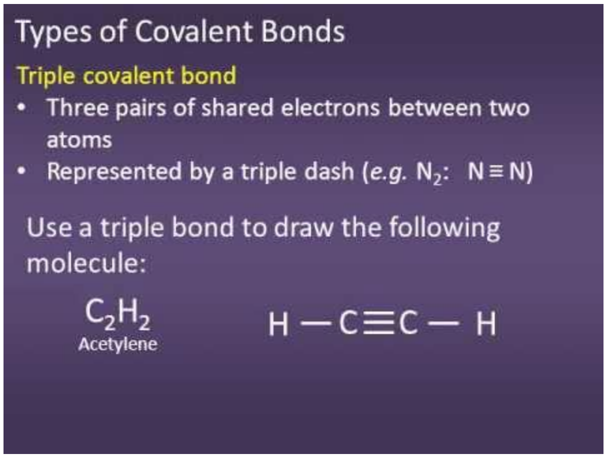
A **triple bond**

Figure 7.55 Lewis Dot structures

Ref: commons.wikimedia.org



Reference: https://www.youtube.com/watch?v=aG3di-2Pxmo


Types of Covalent Bonds

Triple covalent bond

- Three pairs of shared electrons between two atoms
- Represented by a triple dash (*e.g.* N_2: $N \equiv N$)

Use a triple bond to draw the following molecule:

C_2H_2 Acetylene $H-C \equiv C-H$

Reference: https://www.youtube.com/watch?v=SkyrRxtGo-A

Writing Lewis Structures with the Octet Rule

For individual atoms, the **Lewis structure** is drawn by placing a **dot** around the atom for each valence electron available. **Octet rule** states that in forming compounds, atoms gain, lose or share electrons to give a stable electron configuration characterized by eight valence electrons.

For very simple molecules and molecular ions, we can write the Lewis structures by merely pairing up the unpaired electrons on the constituent atoms. See these examples:

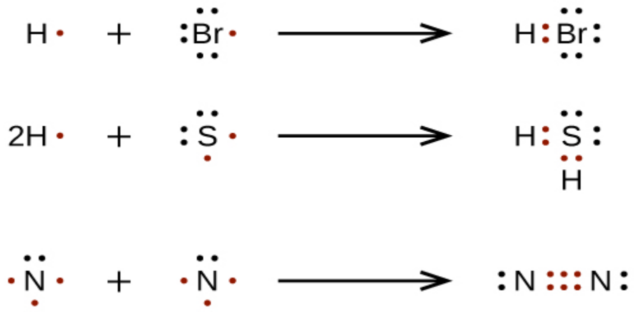
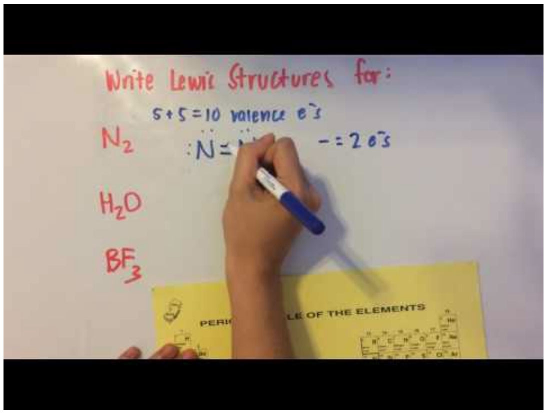


Figure 7.56 Satisfying Octet Rule using Lewis Dot structures

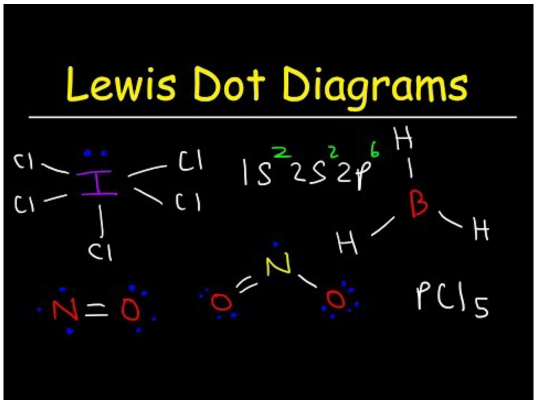
Ref: commons.wikimedia.org

For more complicated molecules and molecular ions, it is helpful to follow the step-by-step procedure outlined here:

1. Determine the total number of valence (outer shell) electrons. For cations, subtract one electron for each positive charge. For anions, add one electron for each negative charge.
2. Draw a skeleton structure of the molecule or ion, arranging the atoms around a central atom. (Generally, the least electronegative element should be placed in the center.) Connect each atom to the central atom with a single bond (one electron pair).
3. Distribute the remaining electrons as lone pairs on the terminal atoms (except hydrogen), completing an octet around each atom.
4. Place all remaining electrons on the central atom.
5. Rearrange the electrons of the outer atoms to make multiple bonds with the central atom in order to obtain octets wherever possible.



Reference: https://www.youtube.com/watch?v=gTSXzAYcP4g



Reference: https://www.youtube.com/watch?v=96L6_IwyHRM

Bonding and nonbonding electrons: lone pairs

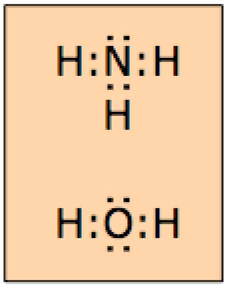


Figure 7.57 Bonding and nonbonding electrons

In many molecules, not all of the electron pairs comprising the octet are shared between atoms. The unshared electron pairs are often called ***lone pairs***. Although lone pairs are not directly involved in bond formation, they should always be shown in Lewis formulas; we will see later that they have an important role to play in determining the shape of the molecule.

Deviation from the Octet Rule

Expanded octets

As mentioned previously, the octet rule works best for the elements in the second period (Li through F) of the periodic table. The reason for this is that electrons, whether shared or not, must be contained in orbitals, and the energies of electrons in such orbitals must be relatively low; otherwise, there would be no energetic advantage in forming a bond in the first place— the atoms would be better off by themselves.

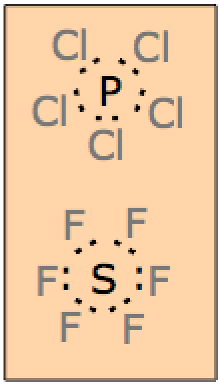


Figure 7.58 Lewis Dot structures

For the second- and third-period elements, the n=2 and n=3 s^2p^6 sets comprise the octet. Some of the third-period elements (Si, P, S, and Cl) can bond to more than four atoms, and thus need to involve more than the four pairs of electrons available in an s^2p^6 octet. This is possible because at n=3, an additional set of *d orbitals* can exist. Although their energies are higher (ordinarily higher than the 4*s* orbitals), they can participate in the valence shells of these atoms.

Examples of molecules in which the n=3 central atom contains an expanded octet are the phosphorus pentahalides and sulfur hexafluoride.

Similarly, for atoms in the fourth period and beyond, higher *d* orbitals can sometimes be used to accommodate additional shared pairs beyond the octet . If you review a diagram showing the relative energies of the different kinds of atomic orbitals (see here, for example), you will notice that all the energy gaps become smaller as the principal quantum number increases, so the energetic cost of using these higher orbitals becomes smaller.

A multivalent molecule is a molecule that has atoms that can violate the octet rule and have more than eight electrons in their valence shells when these atoms are combining to form a covalent bonding.

Examples of these multi valent also called hypervalent molecules are given below:

Phosphorus pentachloride (PCl_5)

sulfur hexafluoride (SF_6)

chlorine trifluoride (ClF_3)

triiodide ion (I_3^-)

The elements in the second period of the periodic table (with the principal energy level n = 2) have the valence electrons orbitals s^2p^6 and there are no d orbitals available and hence these elements strictly obey the octet rule without any deviations. These elements are nonmetals i.e. C, N, O and F.

With the principal energy level n = 3 elements such as Si, P, S and C can bond more that four atoms to make a covalent bond and therefore such elements can violate the octet rule.

The reason behind this violation or exception to the octet rule is that these elements have d sublevels. These d sublevel or sub orbitals are empty and have higher energy that the 4s orbitals in general but in the reality the difference between 3d and 4s energies are small and hence the 3d orbitals can accommodate more electrons.

The 3d orbitals do participate in the forming the covalent bonding and in this process the octet rule is expanded or violated.

Below are examples of such expansion or violation:

Reference: https://courses.lumenlearning.com/boundless-chemistry/chapter/exceptions-to-the-octet-rule/

The pm is a unit of measuring the length of the bond in Pico meter (10^{-12}).

Both phosphorous and sulfur are violating the octet rule:

Multiple bonds

If one pair of electrons shared between two atoms constitutes a chemical bond, it seems logical that two or three pairs could be shared to produce double and triple bonds. Such formulations appear quite naturally when the octet rule is applied to elements such as C, O, S, and N.

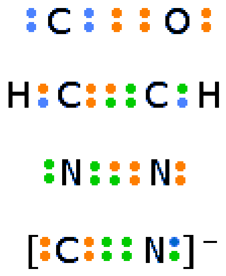


Figure 7.59 Multiple bonds formation

Ref: commons.wikimedia.org

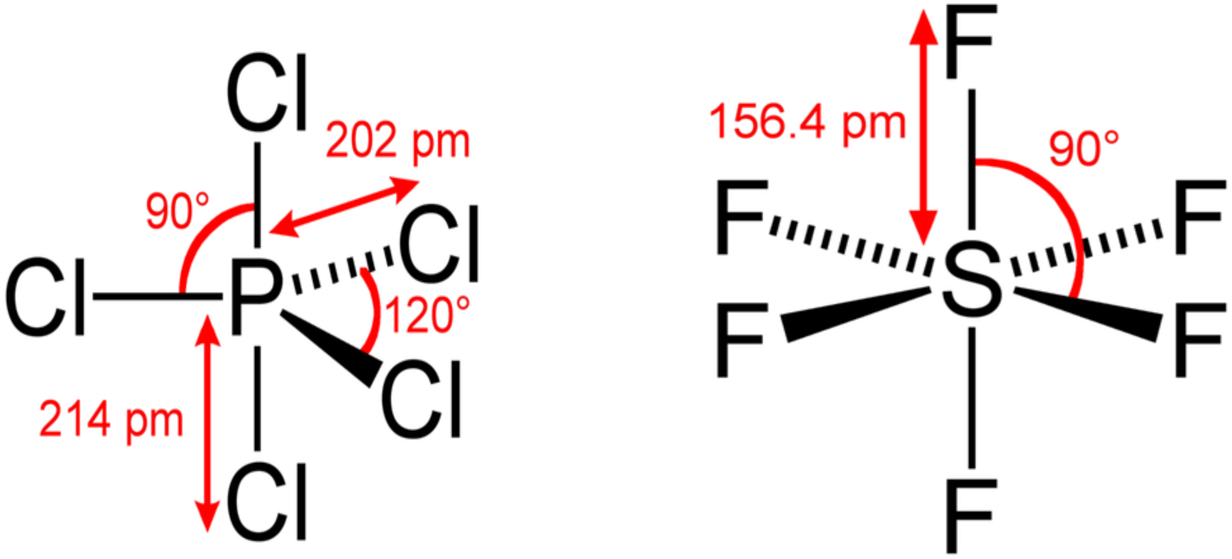
The colors of the electron-dots in this illustration are intended only to help you keep track of the number of electrons contributed by each atom. Because electrons are indistinguishable, it makes no sense to identify a given electron-dot with a given atom.

Since multiple bonds place more electron density between the two nuclei, the latter are held toward each other more closely and tightly; multiple bonds are therefore shorter and stronger than single bonds.

Can there be bonds of higher order than three? No one thought so for a long time, but beginning in the 1960s, experiments and theoretical computations began to reveal that this just might be possible; some molecules just don't follow the rules!

bond type	bonded atoms	molecules	when/who
quadruple	Re::::Re	$[Re_2Cl_8]^{2-}$	1964 F. Albert Cotton, Texas A&M University
quintuple	Cr:::::Cr	RCrCrR (R=large organic group)	2005 Philip Power, U of California, Davis
sextuple	W::::::W	W_2	2006 (Roos, Gagliardi, Borin, U of São Paulo)

Adding to the fun, a 2006 article presented evidence that the carbon atom in $C(PPh_3)_2$ (where Ph stands for a benzene ring) has two lone pair electrons, but no electrons connected to the bonded groups—thus introducing the concept of a "zero-uple" bond.



PCl_5: Phosphorous carries 10 valence electrons combined
SF_6: Sulfur carries 12 valence electrons combined

Figure 7.60 Exception to octet rule

Ref: commons.wikimedia.org

V. Formal Charges and Resonance

In a Lewis structure, formal charges can be assigned to each atom by treating each bond as if one-half of the electrons are assigned to each atom. These hypothetical formal charges are a guide to determining the most appropriate Lewis structure. A structure in which the formal charges are as close to zero as possible is preferred. Resonance occurs in cases where two or more Lewis structures with identical arrangements of atoms but different distributions of electrons can be written. The actual distribution of electrons (the resonance hybrid) is an average of the distribution indicated by the individual Lewis structures (the resonance forms).

Although the total number of valence electrons in a molecule is easily calculated, there is not aways a simple and unambiguous way of determining how many reside in a particular bond or as non-bonding pairs on a particular atom. For example, one can write valid Lewis octet structures for carbon monoxide showing either a double or triple bond between the two atoms, depending on how many nonbonding pairs are placed on each: **C::O:::** and **:C:::O:** (see Problem Example 3 below). The choice between structures such as these is usually easy to make on the principle that the more electronegative atom tends to surround itself with the greater number of electrons. In cases where the distinction between competing structures is not all that clear, an arbitrarily-calculated quantity known as the ***formal charge*** can often serve as a guide.

The formal charge on an atom is the electric charge it would have if all bonding electrons were shared equally with its bonded neighbors.

How to calculate the formal charge on an atom in a molecule

The formal charge on an atom is calculated by the following formula:

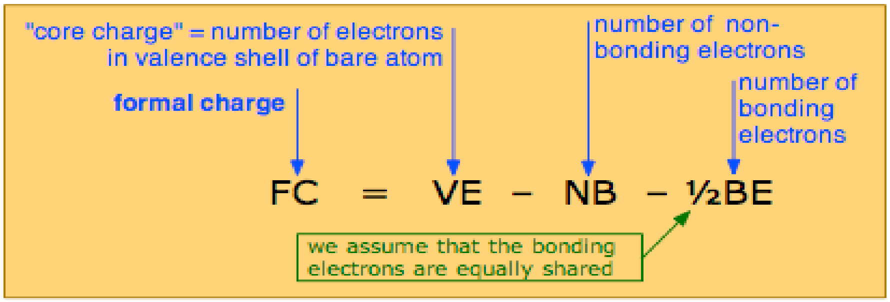


Figure 7.61 Formal Charge calculation

The *core charge* referred to in this diagram is the electric charge the atom would have if all its valence electrons were removed. In simple cases, the formal charge can be worked out visually directly from the Lewis structure, as is illustrated farther on.

Another way of saying this is that **formal charge** results when we take the number of valence electrons of a neutral atom, subtract the nonbonding electrons, and then subtract the number of bonds connected to that atom in the Lewis structure.

Key Equation to calculate formal charge as follows:

formal charge=#valence shell electrons (free atom)−#lone pair electrons−12#bonding electrons

So Knowing the **formal charge** on a particular atom in a structure is an important part of keeping track of the electrons and is important for establishing and predicting the reactivity. The **formal charge** on an atom in a molecule reflects the electron count associated with the atom compared to the isolated neutral atom.

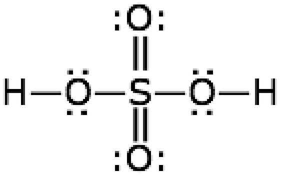


Figure 7.62 Sulfuric Acid H_2SO_4

Ref: commons.wikimedia.org

Problem Example 1

Find the formal charges of all the atoms in the sulfuric acid structure shown here.

Solution: The atoms here are hydrogen, sulfur, and double- and single-bonded oxygens. Remember that a double bond is made up of two electron-pairs.

hydrogen: FC = 1 – 0 – 1 = 0
sulfur: FC = 6 – 0 – 6 = 0
hydroxyl oxygen: FC = 6 – 4 – 2 = 0
double-bonded oxygen: FC = 6 – 4 – 2 = 0

Using formal charge to select the best Lewis structure

The general rule for choosing between alternative structures is that the one involving the *smallest* formal charges is most favored, although the following example shows that this is not always the case.

Problem Example 2

Write out some structures for carbon monoxide CO, both those that do and do not obey the octet rule, and select the "best" on the basis of the formal charges.

Solution:

Structure that obeys the octet rule:

a) For **:C:::O:** Carbon: 4 – 2 – 3 = **–1**; Oxygen: 6 – 2 – 3 = **+1**

Structures that do not obey the octet rule (for carbon):

b) For :C:O::: Carbon: 4 – 2 – 1 = **+1**; Oxygen: 6 – 6 – 1 = **–1**

c) For :C::O:: Carbon: 4 – 2 –2 = **0**; Oxygen: 6 – 4 – 2 = **0**

Comment: All three structures are acceptable (because the formal charges add up to zero for this neutral molecule) and contribute to the overall structure of carbon monoxide, although not equally. Both experiment and more advanced models show that the triple-bonded form *(a)* predominates. Formal charge, which is no more than a bookeeping scheme for electrons, is by itself unable to predict this fact.

In a species such as the thiocyanate ion SCN^- (below) in which two structures having the same minimal formal charges can be written, we would expect the one in which the negative charge is on the more electronegative atom to predominate.

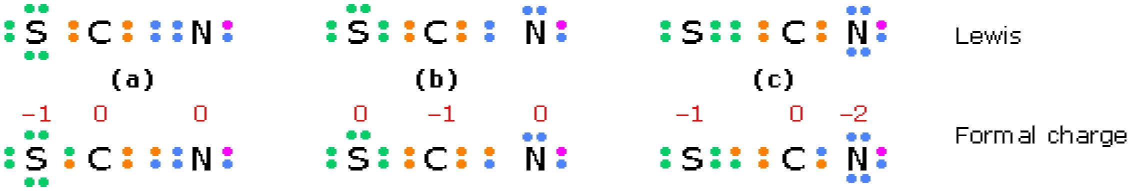


Figure 7.63 Formal Charge

Ref: commons.wikimedia.org

The electrons in the structures of the top row are the valence electrons for each atom; an additional electron (purple) completes the nitrogen octet in this negative ion. The electrons in the bottom row are divided equally between the bonded atoms; the difference between these numbers and those above gives the formal charges.

Formal charge can also help answer the question "where is the charge located?" that is frequently asked about polyatomic ions. Thus by writing out the Lewis structure for the ammonium ion NH_4^+, you should be able to convince yourself that the nitrogen atom has a formal charge of +1 and each of the hydrogens has 0, so we can say that the positive charge is localized on the central atom.

How oxidation numbers are assigned

This is another arbitrary way of characterizing atoms in molecules. In contrast to formal charge, in which the electrons in a bond are assumed to be shared equally, ***oxidation number*** is the electric charge an atom would have if the bonding electrons were assigned exclusively to the more electronegative atom. Oxidation number serves mainly as a tool for keeping track of electrons in reactions in which they are exhanged between reactants, and for characterizing the "combining power" of an atom in a molecule or ion.

The following diagram compares the way electrons are assigned to atoms in calculating formal charge and oxidation number in carbon monoxide.

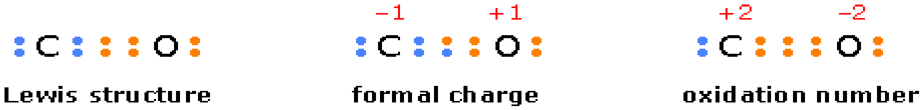
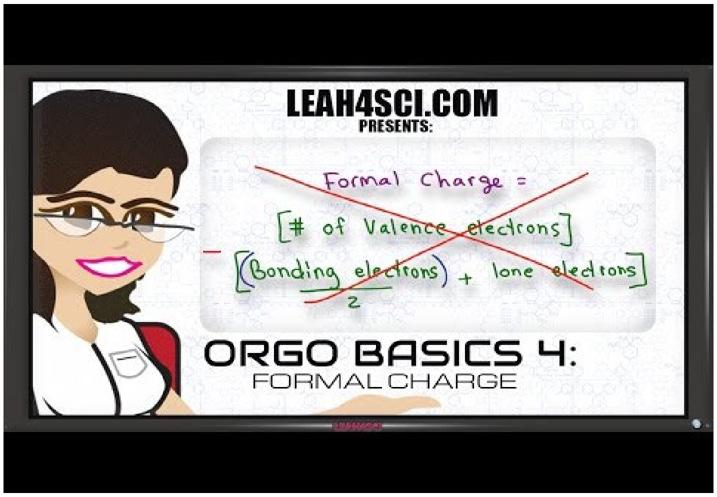


Figure 7.64 Formal Charge vs. Oxidation Number

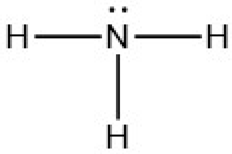
Ref: commons.wikimedia.org

Calculating Formal Charge



Reference: https://youtu.be/J03H472fAKI?t=75

Practice Example #3: , let's calculate the formal charge on the atoms in ammonia (NH_3) whose Lewis structure is as follows:



Ammonia

Figure 7.65 Ammonia NH_3

Ref: commons.wikimedia.org

A neutral nitrogen atom has five valence electrons (it is in group 15). From the Lewis structure, the nitrogen atom in ammonia has one lone pair and three bonds with hydrogen atoms. Substituting into Equation 2.3.1, we obtain

Formal Charge of N = (5 valence e-) - (2 lone pair e-) - (1/2 x 6 bond pair e-) = 0

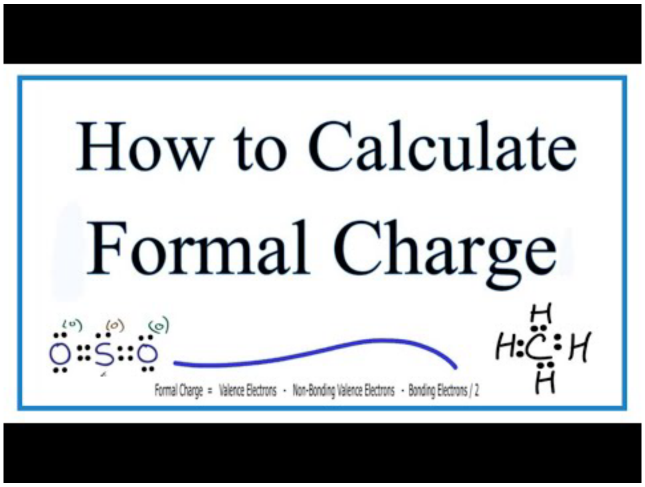
A neutral hydrogen atom has one valence electron. Each hydrogen atom in the molecule has no non-bonding electrons and one bond. Using Equation 2.3.1 to calculate the formal charge on hydrogen, we obtain

Formal Charge of H = (1 valence e-) - (0 lone pair e-) - (1/2 x 2 bond pair e-) = 0

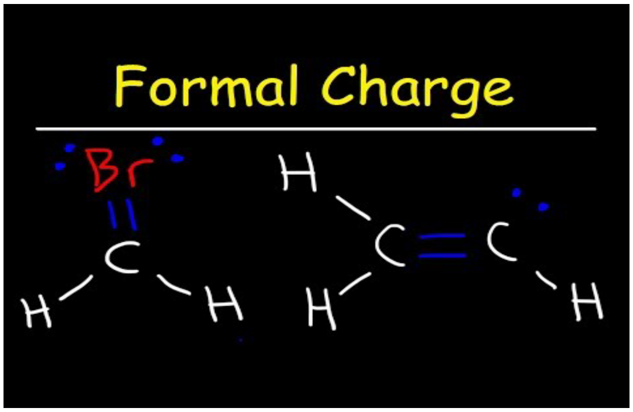
The sum of the formal charges of each atom must be equal to the overall charge of the molecule or ion. In this example, the nitrogen and each hydrogen has a formal charge of zero. When summed the overall charge is zero,

which is consistent with the overall neutral charge of the NH_3 molecule.

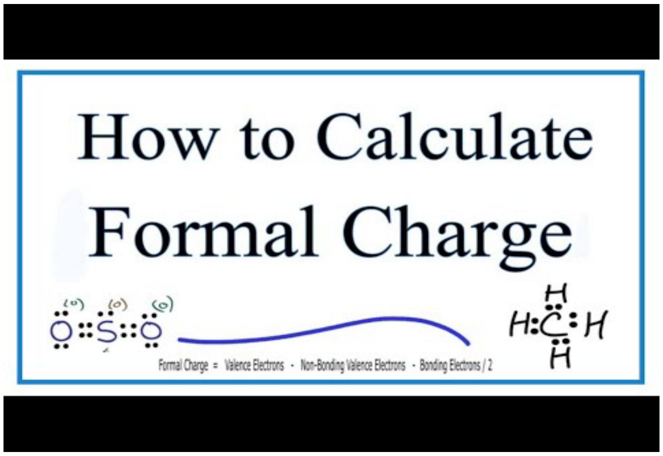
Typically, the structure with the most formal charges of zero on atoms is the more stable Lewis structure. In cases where there MUST be positive or negative formal charges on various atoms, the most stable structures generally have negative formal charges on the more electronegative atoms and positive formal charges on the less electronegative atoms. The next example further demonstrates how to calculate formal charges for polyatomic ions.



Reference: https://www.youtube.com/watch?v=vOFAPlq4y_k



Reference: https://www.youtube.com/watch?v=C2l-76VP8s0



Reference: https://youtu.be/vOFAPlq4y_k

Resonance:

Multiple equivalent structures: resonance

There is a rather large class of molecules for which one has no difficulty writing Lewis structures; in fact, we can write more than one valid structure for a given molecule! Consider, for example, the *nitrate ion* NO_3^-. We can develop a Lewis dot formula satisfying the octet rule as follows:

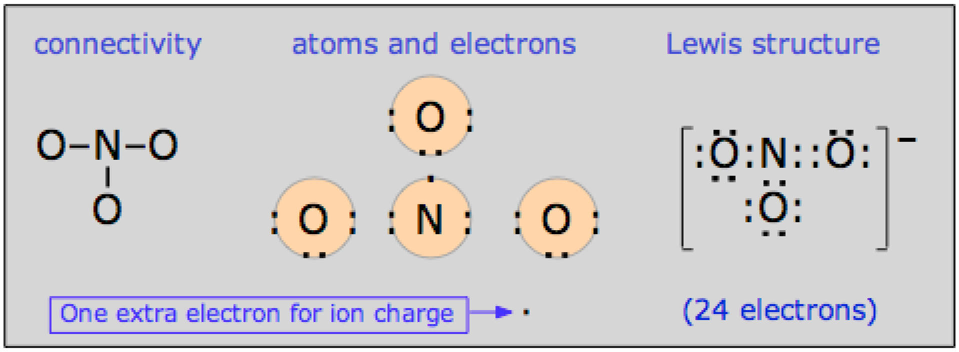


Figure 7.66 Resonance of NO_3^-

According to this structure, the ion contains two N–O single bonds and one N–O double bond. But there is no special reason to place the double bond where it is shown in the diagram above; it could equally well go in either of the other two locations. For this molecule, then, we can write three equally valid structures:

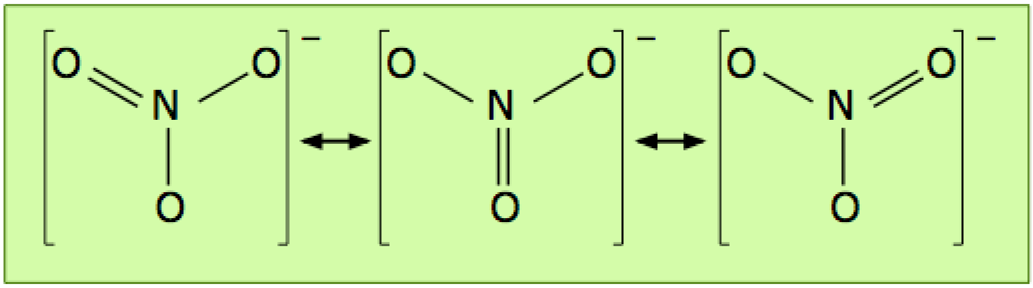


Figure 7.67 Resonating structures of NO_3^-

The double-ended arrows indicate that the nitrate ion is a *superposition* of all three structures, and this is supported by experimental evidence which shows that the three oxygen atoms are chemically identical, that all three bonds have the same length, and that the molecule has trigonal symmetry (meaning that the three oxygens are geometrically equivalent.)

The term ***resonance*** was employed to describe this phenomenon in the 1930's, before chemical bonding became better understood; the three equivalent structures shown above are known as ***resonance hybrids***. The choice of the word "resonance" was unfortunate because it connotes the existence of some kind of dynamic effect that has led to the mistaken idea that the structure is continually alternating between the three possibilities.

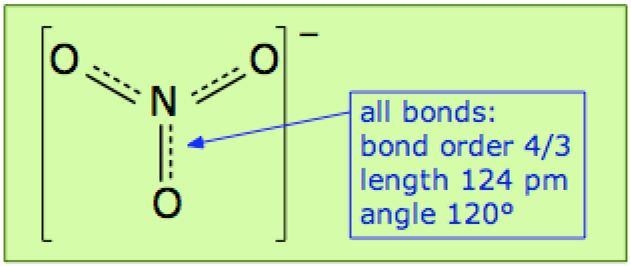


Figure 7.68 Effect of resonance on NO_3^- ion

In actual fact, the nitrate ion has only *one* structure in which the electrons spread themselves evenly so as to make all three N–O links into "1-1/3 bonds"; we describe them as having a ***bond order*** of 4/3. The preferred way of depicting a molecule that has more than one equivalent bonding structure is to use dashed lines to indicate the "fractional" bonds as shown here.

Very similar structures can be written for sulfur trioxide SO_3, and for the carbonate ion CO_3^{2-}.

In writing out resonance structures, it is important to bear in mind that only the electron pairs can be moved around; the atoms must retain the same connectivity. In some cases it is necessary to move electrons to locations that would produce a positive charge on one atom and a negative charge on the other. Since the separation of electric charge always costs energy, such resonance forms will tend to be less stabilizing and will not be as important contributors to the overall structure as those in where there is no charge separation.

Since electrons in molecules tend to arrange themselves into configurations that give the lowest possible energy, it is not surprising that the resonance hybrid represents a more stable (i.e., strongly bound) molecule than does any one of the contributing structures.

There is a good quantum-mechanical rationale for this; according to the Heisenberg uncertainty principle, the energy of the electron will be more uncertain as its position is more exactly specified. Since energies cannot be negative, the more "uncertain" the energy can be, the higher it can be. If an electron is spread out over two or three bonds in the hybrid instead of being confined to the space between only two atoms, its exact location is much less exactly known, and so its energy will be less uncertain, and therefore lower.

Resonance structures of carboxylic acids

This idea is embodied in the statement you will often see, particularly in the older literature, that a given structure "is stabilized by resonance". This jargon has been used, for example, to explain the acidity of the -COOH group found in organic acids. Dissociation of a carboxylic acid such as formic acid yields a carboxylate ion –COO⁻ which can be represented by two equivalent structures. These are more realistically interpreted as a single structure in which the C–O bond order is 1.5:

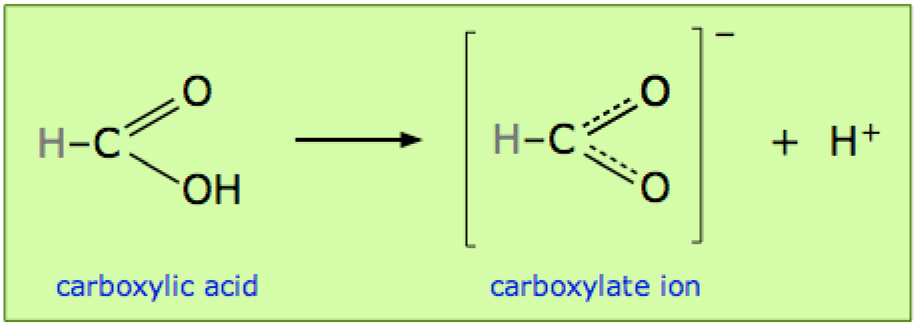


Figure 7.69 Effect of resonance on NO_3^- ion

The idea is that resonance is only possible when the proton has been lost, and that the lower energy of the "resonating" structure provides the driving force for the loss of the proton, and thus is the source of the acidity carboxylic group. (By the way, this view of the cause of carboxylic acidity has been criticized; other factors that may well be more important are also involved.)

Resonance structures of the benzene ring

See here for a summary of the various structures that have been proposed for benzene over the years.

Perhaps the most well known molecule whose structure must be represented as a resonance hybrid is benzene, C_6H_6. The structure of this molecule had long been something of a mystery, in that it was difficult to understand how this formula could be consistent with the well-established tetravalence of carbon in organic compounds. The breakthrough came in 1865 when the German chemist August Kekulé proposed that the molecule is based on a hexagonal ring of carbon atoms as shown at the left below.

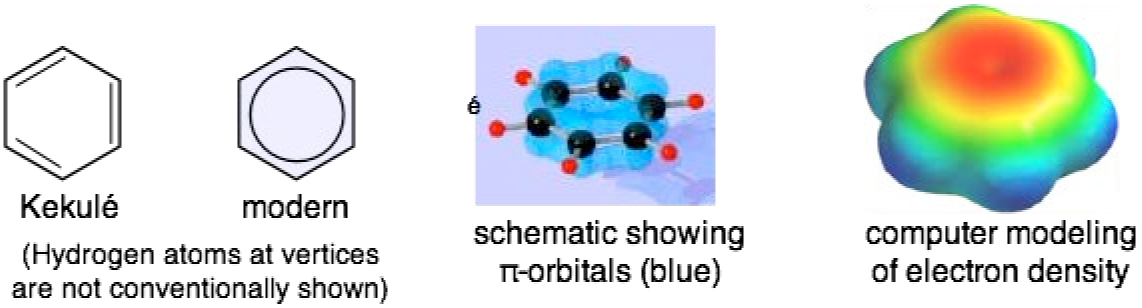


Figure 7.70 Resonating Structures of Benzene

However, this structure is not consistent with the chemistry of benzene, which does not undergo the reactions that would be expected of a molecule containing carbon-carbon double bonds. Such compounds are normally quite reactive, while benzene, in contrast, tends to be rather inert to all but the most powerful reagents.

This apparent discrepancy disappeared after the resonance hybrid theory was developed; benzene is regarded as a hybrid of the two structures shown in the center above, and it is often depicted by the structure at the right, in which the circle represents a "half bond", so that the ***bond order*** of each C–C bond is 1.5. Bond length measurements are entirely consistent with this interpretation; they are almost exactly halfway between the values found in compounds known to contain single and double bonds.

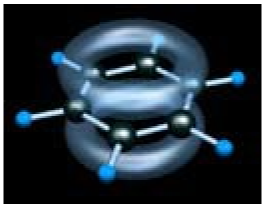


Figure 7.71 3D shape of Benzene

A more realistic representation of the benzene molecule shows the two components of its bonds. The "sticks" joining adjacent carbons constitute "half" of the carbon-carbon bonding, while the circular charge clouds above and below the ring together make up the other "half". The details of this bonding arrangement are discussed in the section on the hybrid orbital model of bonding.

Some apparent violations of the Octet Rule

Electron structures without molecules

Although there are many violations of the octet rule, most electron dot structures that one can write down in accordance with this rule and its general scope of validity correspond to molecules that actually exist. Sometimes, however, we are surprised to find that the molecules corresponding to an apparently reasonable Lewis formula are not known.

In some cases, this has been shown to be a consequence of the very high chemical reactivity of the molecules. Thus hypofluorous acid, HOF, has never been isolated, although its chlorine analog is well known. It was not until 1967 that its short-lived presence was detected spectroscopically. It is now believed that the molecule is stable, but that the products obtained when it reacts with itself are so much more stable that it decomposes almost as fast as it is formed:

$$2HOF(g) \rightarrow 2HF(g) + O_2(g)$$

Other molecules having proper Lewis structures but no apparent existence may be stable only at very low temperatures; examples are O_4 and H_2O_4.

The fluorate ion, FO_3^-, has also never been detected, even though analogs containing the other halogen elements are well known. The problem here may well lie with the very small fluorine atom, which would allow the oxygens to approach so closely that they would repel each other.

Small size is also suggested as the reason for the non-existence of the nitrogen analogs of the sulfate and sulfite ions. These would have the formulas NO_4^{3-} and NO_3^{2-}. Here, the problem is believed to be the high *charge density*: it costs a lot of energy to squeeze this much electric charge in such a small volume. Sulfur, having a larger radius, forms larger ions having lower charge densities, and the total charge would also be only –2 instead of –3.

Molecules without proper Lewis electron structures

There are also examples of molecules whose existence is beyond question, but for which no satisfactory Lewis structures can be written. Two examples are the *triiodide ion* I_3^-, and the *bifluoride ion* HF_2^-.

The **triiodide ion** $[I–I–I]^-$ is a well known species found in aqueous solutions containing iodine and iodide ions:

$$I_2 + I^- \rightarrow I_3^-$$

The **bifluoride ion** $[F–H–F]^-$ is formed in a rather similar way in hydrofluoric acid solutions containing fluoride ion:

$$HF + F^- \rightarrow HF_2^-$$

Try writing electron-dot structures for these two species, and you will see the problem!

Molecules with unpaired electrons

As you know, electrons tend to pair up in atoms and molecules so that their spins cancel out. If this does not happen— either because there is an uneven number of electrons or it is energetically unfavorable, then the species is said to be ***paramagnetic***. Paramagnetic substances are attracted to a magnetic field, but unlike ferromagnetic materials such as iron, they do not retain their magnetic properties (act as magnets) in the absence of an applied field. Most molecules posses an even number of electrons and are diamagnetic.

Dioxygen

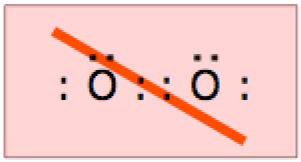


Figure 7.72 Lewis Dot structure of Dioxygen

The most abundant paramagnetic molecule in our world is the ordinary oxygen molecule which has twelve electrons. It is easy to write a proper Lewis structure for O_2 that places an octet around each oxygen atom and a double bond between them. However, it takes only a simple experiment to show that the electrons in dioxygen cannot all be arranged in pairs: if you place a magnet near some liquid oxygen, the liquid will be drawn to the magnet. This can only mean one thing: there are at least two unpaired electrons in the O_2 molecule. A more careful experiment shows that this number is exactly two. Are they in the bond or are they non-bonding electrons? You can decide this by sketching out a few possible structures.

The paramagnetism of oxygen is an anomaly in terms of the Lewis theory, although it is predicted by a more comprehensive theory that we will look at later. There are, however, a few other molecules that we would expect to be paramagnetic simply because they contain an odd number of valence electrons.

Nitric oxide and nitrogen dioxide

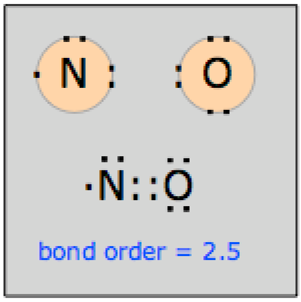


Figure 7.73 Lewis Dot structure of NO

Nitrogen, having five valence electrons, forms two well-known odd-electron molecules with oxygen. **Nitric oxide**, NO, a colorless, odorless, paramagnetic gas, is the simplest stable odd-electron molecule known. It is clear that no structure conforming to the octet rule is possible. The Lewis structure shown here is somewhat misleading; chemical and physical evidence suggest that the unpaired electron is not localized on the nitrogen atom, but extends over the entire molecule.

For example, if the structure were really ·NO, then we would expect the molecule to readily form a dimer ON:NO, but this is not observed. Bond-length measurements indicate that the N–O bond order is 2.5.

Nitric oxide has a remarkably rich chemistry. Until recently, its most famous role was as a precursor to photochemical smog. (The oxide is formed when fuels such as gasoline are burned at high temperatures in the presence of air.)

In the 1980s, to the surprise of almost everyone, NO was identified as an essential component of the signalling pathway of the mamallian cardiovascular system. As such, it provides a means by which cells communicate with one another. Other signalling molecules tend to be far more complicated, and no one would have expected a "free radical" molecule to have other than a damaging effect on the body.

Nitrogen dioxide is also an odd-electron molecule. In contrast to NO, the odd electron in NO_2 appears to be somewhat local to the nitrogen atom. As a consequence, the dimerization equilibrium

$$\rightleftharpoons$$

is so facile that neither gas can be retained in pure form at ordinary temperatures. Because two equivalent Lewis structures can be written, NO_2 is a resonance hybrid in which the N–O bond order is 1.5.

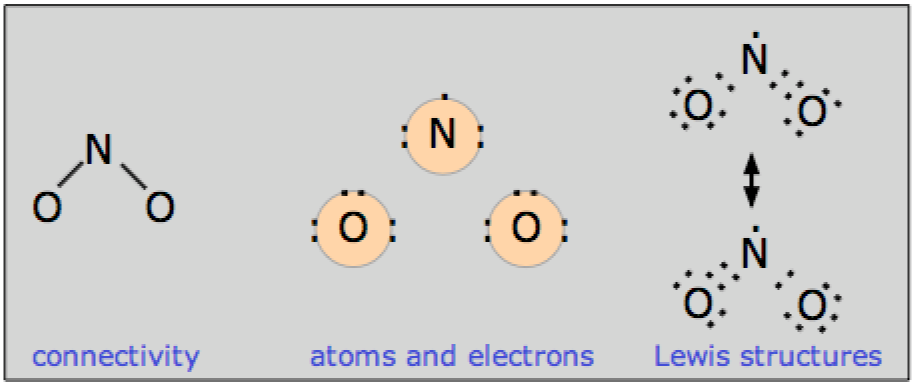


Figure 7.74 Lewis Dot structure of NO_2

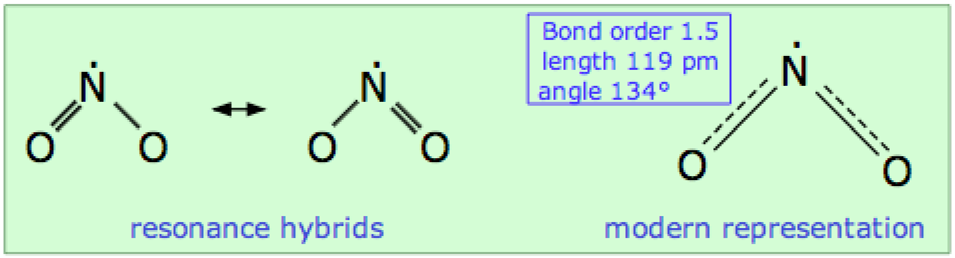
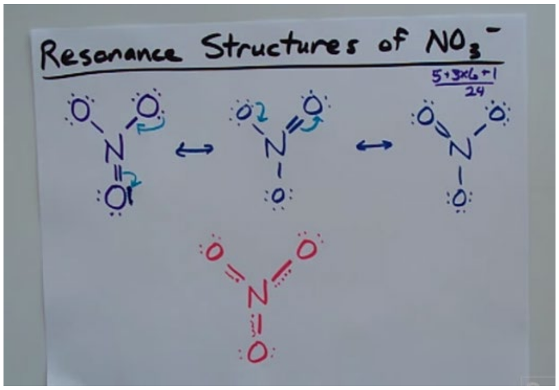


Figure 7.75 Resonating structure of NO_2

More than one non-equivalent structure

It sometimes happens that the octet rule can be satisfied by arranging the electrons in different ways. For example, there are three different ways of writing valid electron dot structures for the thiocyanate ion SCN^-. Some of these structures are more realistic than others; to decide among them, you need to know something about the concepts of *formal charge* and *electronegativity*. These topics are discussed in the lesson that follows this one, where examples of working out such structures are given.

The video below illustrates this effect:



https://www.youtube.com/watch?v=QqEgdc8mnqY

Key Concepts and Summary

In a Lewis structure, formal charges can be assigned to each atom by treating each bond as if one-half of the electrons are assigned to each atom. These hypothetical formal charges are a guide to determining the most appropriate Lewis structure. A structure in which the formal charges are as close to zero as possible is preferred. Resonance occurs in cases where two or more Lewis structures with identical arrangements of atoms but different distributions of electrons can be written. The actual distribution of electrons (the resonance hybrid) is an average of the distribution indicated by the individual Lewis structures (the resonance forms).

VI. Strengths of Ionic and Covalent Bonds

A bond's strength describes how strongly each atom is joined to another atom, and therefore how much energy is required to break the bond between the two atoms. In this section, you will learn about the bond strength of covalent bonds, and then compare that to the strength of ionic bonds, which is related to the lattice energy of a compound.

A bond's strength describes how strongly each atom is joined to another atom, and therefore how much energy is required to break the bond between the two atoms.

It is essential to remember that energy must be added to break chemical bonds (an endothermic process), whereas forming chemical bonds releases energy (an exothermic process). In the case of H_2, the covalent bond is very strong; a large amount of energy, 436 kJ, must be added to break the bonds in one mole of hydrogen molecules and cause the atoms to separate:

$$H_2(g) \longrightarrow 2H(g) \qquad \text{bond energy} = 436 \text{ kJ}$$

Conversely, the same amount of energy is released when one mole of H_2 molecules forms from two moles of H atoms:

$$2H(g) \longrightarrow H_2(g) \qquad \text{bond energy} = \text{-}436 \text{ kJ}$$

Reference: https://www.youtube.com/watch?v=5AObIYlknBc

Bond Strength: Covalent Bonds

The **strength** of a **bond** between two atoms increases as the number of electron pairs in the **bond** increases. Generally, as the **bond strength** increases, the **bond** length decreases.

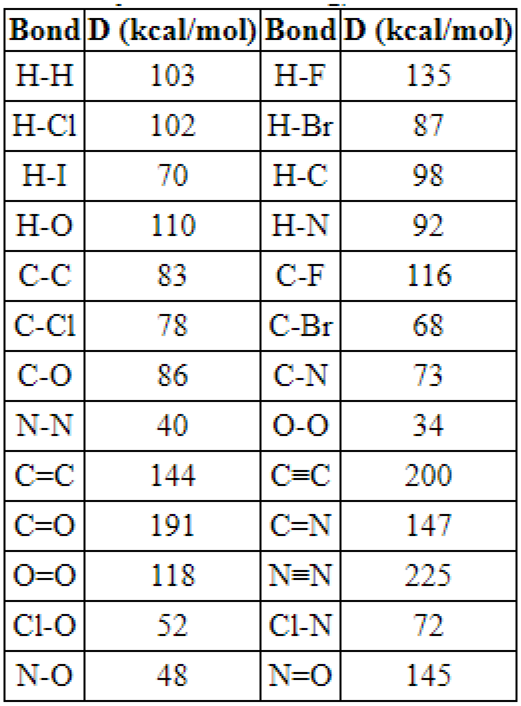
Stable molecules exist because covalent bonds hold the atoms together. We measure the strength of a covalent bond by the energy required to break it, that is, the energy necessary to separate the bonded atoms. Separating any pair of bonded atoms requires energy. The stronger a bond, the greater the energy required to break it.

Strengths of Covalent Bonds

Bond dissociation energy or bond energy is the energy required to break a bond. Usually we mean bond dissociation enthalpy, the enthalpy change for this reaction:
A—B → A(g) + B(g)
For example, H—Cl → H•(g) + Cl•(g)
The • represents an unpaired electron, called a **radical**. When measuring the bond enthalpy, we break the bond so that half the bonding electrons go to each atom. Breaking a bond is always an endothermic process, so the bond energy is always positive. We use the symbol D(A—B) to represent the bond enthalpy of an A—B bond.

Bond energy is similar, but is the average energy required to break all the bonds in a molecule. For instance, C-H bond energy is the enthalpy of atomization of methane divided by 4. This is different from the energy required to break the first C-H bond in CH_4 because breaking the second bond might be easier or harder than breaking the first.

Some approximate average bond enthalpies, in kcal/mol (use this table to get a sense of which bonds are relatively weak or strong)



Bond	D (kcal/mol)	Bond	D (kcal/mol)
H-H	103	H-F	135
H-Cl	102	H-Br	87
H-I	70	H-C	98
H-O	110	H-N	92
C-C	83	C-F	116
C-Cl	78	C-Br	68
C-O	86	C-N	73
N-N	40	O-O	34
C=C	144	C≡C	200
C=O	191	C=N	147
O=O	118	N≡N	225
Cl-O	52	Cl-N	72
N-O	48	N=O	145

How do we measure?

As you might guess from the discussion above about bond energy vs. bond dissociation energy, it's actually quite complicated to measure these! There are a lot of complications to consider, and you can't always measure directly the heat of reaction that you want.

Why does it matter?

Having a general knowledge of bond strengths lets us understand the structures of molecules and predict reactions. For instance, when we guess the arrangement of atoms to make a Lewis structure, we will probably do better if we avoid making weak bonds. N-N and O-O single bonds are pretty weak, so usually we try not to put them in Lewis structures, unless nothing else makes sense. The structure will be better if we can make a multiple bond or put some other atom in between.

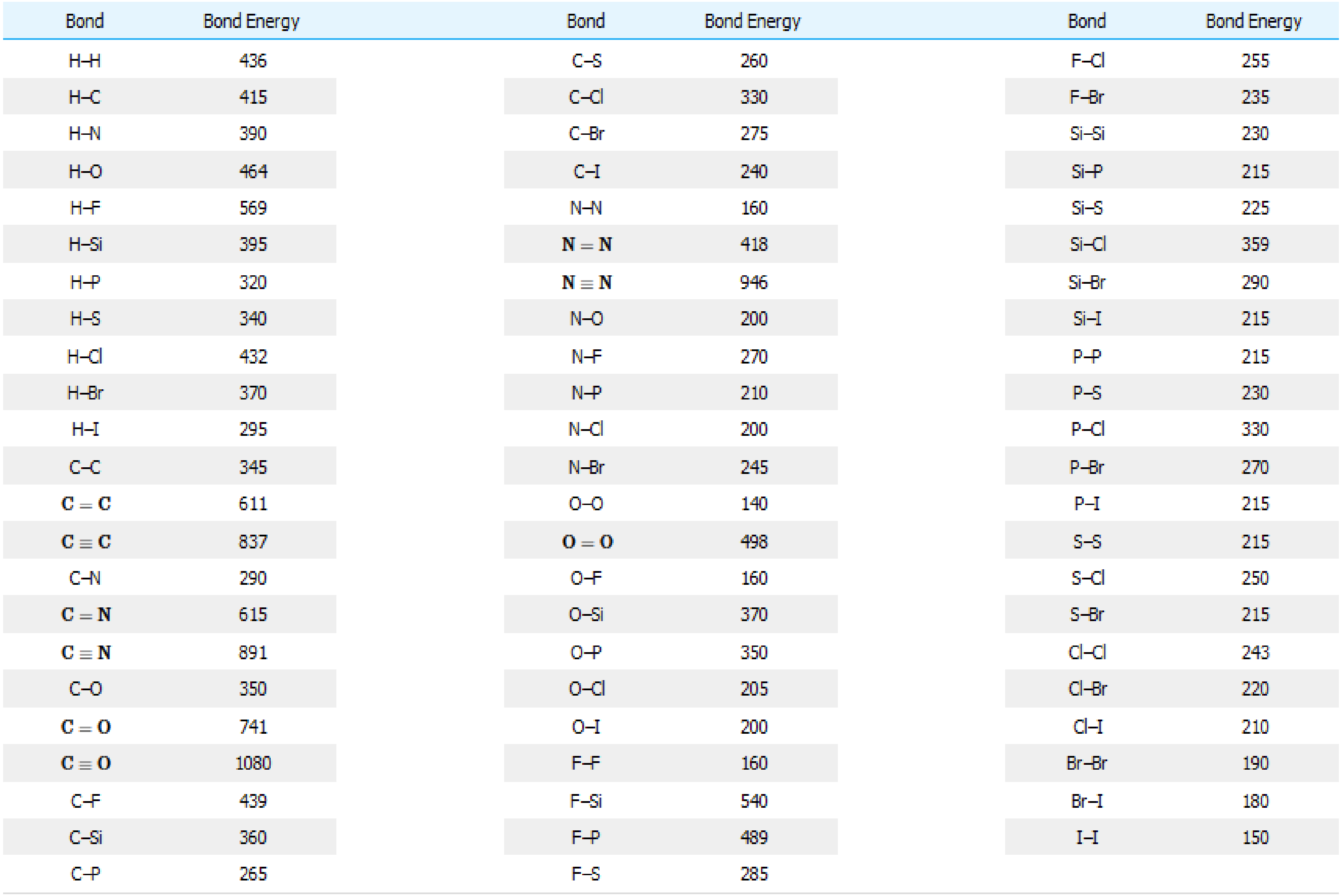
We can also use bond strength knowledge to predict what direction reactions will go and how fast they will go. If the product has stronger bonds than the reactants, the reaction is likely to be exothermic, and exothermic reactions often go forward. If the reactant has strong bonds, you might need to use a lot of energy to get the reaction started, even if it is exothermic. Combustion reactions are an example: C-C and C-H bonds are pretty strong, so we need a spark or a match to start the burning.

Another example is "nitrogen fixation": we need N to make proteins and other important molecules in our bodies, but it is very hard to get N from N_2 because of the strong triple bond. This is why we have to use fertilizer in agriculture, and making nitrogen fertilizer uses roughly 1% of the world's energy. Another example is teflon or PTFE, which makes a very slippery and non-reactive coating that is used in non-stick pans, containers for reactive chemicals, etc. PTFE has only C-C and C-F bonds, both of which are very strong, so it doesn't easily react even at high temperature when you cook with it. In contrast, if a reactant has some very weak bonds, it might be very easy to start a reaction. For instance, hydrogen peroxide (HOOH) can be used as a bleach or disinfectant because the weak O-O single bond can easily break, helping it oxidize whatever is nearby. Hydrogen peroxide and hydrazine (N_2H_4) can both be used as rocket fuel because they react easily and exothermically (they have weak bonds, and they form products with stronger bonds).

The strength of a bond between two atoms increases as the number of electron pairs in the bond increases. Generally, as the bond strength increases, the bond length decreases. Thus, we find that triple bonds are stronger and shorter than double bonds between the same two atoms; likewise, double bonds are stronger and shorter than single bonds between the same two atoms. Average bond energies for some common bonds appear in the following Table-1, and a comparison of bond lengths and bond strengths for some common bonds appears in the following Table-2. When one atom bonds to various atoms in a group, the bond strength typically decreases as we move down the group. For example, C–F is 439 kJ/mol, C–Cl is 330 kJ/mol, and C–Br is 275 kJ/mol.

Table-1 Bond Energies (kJ/mol)

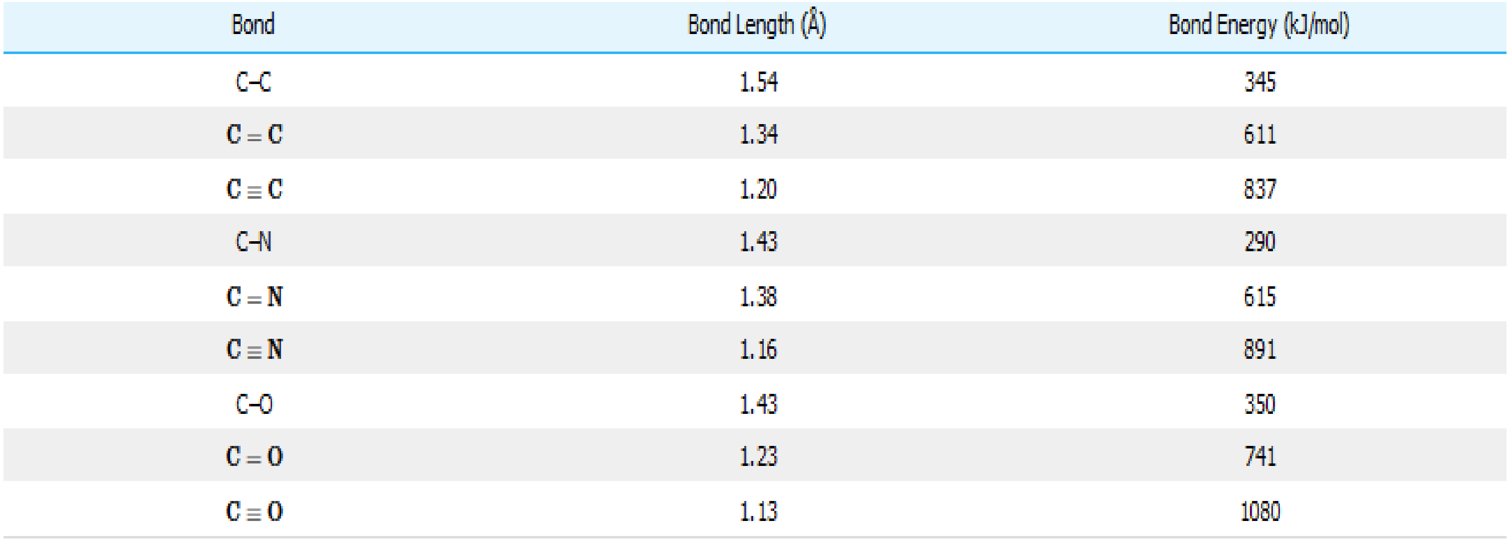
Reference:
https://chem.libretexts.org/Courses/University_of_Kentucky/UK%3A_General_Chemistry/07%3A_Chemical_Bonding_and_Molecular_Geometry/7.5%3A_Strengths_of_Ionic_and_Covalent_Bonds



Bond	Bond Energy	Bond	Bond Energy	Bond	Bond Energy
H–H	436	C–S	260	F–Cl	255
H–C	415	C–Cl	330	F–Br	235
H–N	390	C–Br	275	Si–Si	230
H–O	464	C–I	240	Si–P	215
H–F	569	N–N	160	Si–S	225
H–Si	395	**N = N**	418	Si–Cl	359
H–P	320	**N ≡ N**	946	Si–Br	290
H–S	340	N–O	200	Si–I	215
H–Cl	432	N–F	270	P–P	215
H–Br	370	N–P	210	P–S	230
H–I	295	N–Cl	200	P–Cl	330
C–C	345	N–Br	245	P–Br	270
C = C	611	O–O	140	P–I	215
C ≡ C	837	**O = O**	498	S–S	215
C–N	290	O–F	160	S–Cl	250
C = N	615	O–Si	370	S–Br	215
C ≡ N	891	O–P	350	Cl–Cl	243
C–O	350	O–Cl	205	Cl–Br	220
C = O	741	O–I	200	Cl–I	210
C ≡ O	1080	F–F	160	Br–Br	190
C–F	439	F–Si	540	Br–I	180
C–Si	360	F–P	489	I–I	150
C–P	265	F–S	285		

Table-2 Average Bond Lengths and Bond Energies for Some Common Bonds.

References:
https://chem.libretexts.org/Courses/University_of_Kentucky/UK%3A_General_Chemistry/07%3A_Chemical_Bonding_and_Molecular_Geometry/7.5%3A_Strengths_of_Ionic_and_Covalent_Bonds



Bond	Bond Length (Å)	Bond Energy (kJ/mol)
C–C	1.54	345
C = C	1.34	611
C ≡ C	1.20	837
C–N	1.43	290
C = N	1.38	615
C ≡ N	1.16	891
C–O	1.43	350
C = O	1.23	741
C ≡ O	1.13	1080

We can use bond energies to calculate approximate enthalpy changes for reactions where enthalpies of formation are not available. Calculations of this type will also tell us whether a reaction is exothermic or endothermic.

- An **exothermic reaction** (ΔH negative, heat produced) results when the bonds in the products are stronger than the bonds in the reactants.
- An **endothermic reaction** (ΔH positive, heat absorbed) results when the bonds in the products are weaker than those in the reactants.

The enthalpy change, ΔH, for a chemical reaction is approximately equal to the sum of the energy required to break all bonds in the reactants (energy "in", positive sign) plus the energy released when all bonds are formed in the products (energy "out," negative sign). This can be expressed mathematically in the following way:

$$\Delta H = \sum D_{\text{bonds broken}} - \sum D_{\text{bonds formed}}$$

In this expression, the symbol ΣΣ means "the sum of" and D represents the bond energy in kilojoules per mole, which is always a positive number. The bond energy is obtained from a table and will depend on whether the particular bond is a single, double, or triple bond. Thus, in calculating enthalpies in this manner, it is important that we consider the bonding in all reactants and products. Because D values are typically averages for one type of bond in many different molecules, this calculation provides a rough estimate, not an exact value, for the enthalpy of reaction.

Consider the following reaction:

$$H_{2\,(g)} + Cl_{2\,(g)} \longrightarrow 2\,HCl_{(g)}$$

Or

$$H\text{–}H_{(g)} + Cl\text{–}Cl_{(g)} \longrightarrow 2\,H\text{–}Cl_{(g)}$$

To form two moles of HCl, one mole of H–H bonds and one mole of Cl–Cl bonds must be broken. The energy required to break these bonds is the sum of the bond energy of the H–H bond (436 kJ/mol) and the Cl–Cl bond (243 kJ/mol). During the reaction, two moles of H–Cl bonds are formed (bond energy = 432 kJ/mol), releasing 2 × 432 kJ; or 864 kJ. Because the bonds in the products are stronger than those in the reactants, the reaction releases more energy than it consumes:

$$\begin{aligned} \Delta H &= \sum D_{\text{bonds broken}} - \sum D_{\text{bonds formed}} \\ \Delta H &= [D_{H-H} + D_{Cl-Cl}] - 2D_{H-Cl} \\ &= [436 + 243] - 2(432) = -185\ \text{kJ} \end{aligned}$$

This excess energy is released as heat, so the reaction is exothermic. where it gives a value for the standard molar enthalpy of formation of HCl(g), ΔH∘fΔHf∘, of –92.307 kJ/mol. Twice that value is –184.6 kJ, which agrees well with the answer obtained earlier for the formation of two moles of HCl.

Lengths of chemical bonds

The length of a chemical bond the distance between the centers of the two bonded atoms (the ***internuclear distance***.) Bond lengths have traditionally been expressed in Ångstrom units, but picometers are now preferred (1Å = 10^{-8} cm = 100 pm.) Bond lengths are typically in the range 1-2 Å or 100-200 pm. Even though the bond is vibrating, equilibrium bond lengths can be determined experimentally to within ±1 pm.

bond	Ave. Length	Ave. Energy/kJ mol^{-1}
H—H	74 pm	432
H—C	109 pm	415
H—N	101	390
H—O	96	460
H—Cl	127	428
H—Br	141	362
C—C	154	345
C=C	133	615
C≡C	120	835
N≡N	110	942
Cl—Cl	199	240
Br—Br	228	190
I—I	267	149

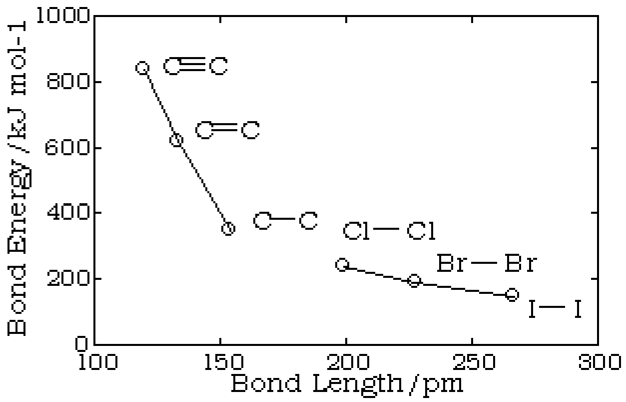


Figure 7.76 Bond energy vs. Bond Length

Bond lengths depend mainly on the sizes of the atoms, and secondarily on the bond strengths, the stronger bonds tending to be shorter. Bonds involving hydrogen can be quite short; The shortest bond of all, H–H, is only 74 pm. Multiply-bonded atoms are closer together than singly-bonded ones; this is a major criterion for experimentally determining the *multiplicity* of a bond. This trend is clearly evident in the above plot which depicts the sequence of carbon-carbon single, double, and triple bonds.

The most common method of measuring bond lengths in solids is by analysis of the diffraction or scattering of X-rays when they pass through the regularly-spaced atoms in the crystal. For gaseous molecules, neutron- or electron-diffraction can also be used.

The complete structure of a molecule requires a specification of the coordinates of each of its atoms in three-dimensional space. This data can then be used by computer programs to construct *visualizations* of the molecule as discussed above. One such visualization of the **water molecule**, with bond distances and the HOH bond angle superimposed on a space-filling model, is shown here. (It is taken from an excellent reference source on water). The colors show the results of calculations that depict the way in which electron charge is distributed around the three nuclei.

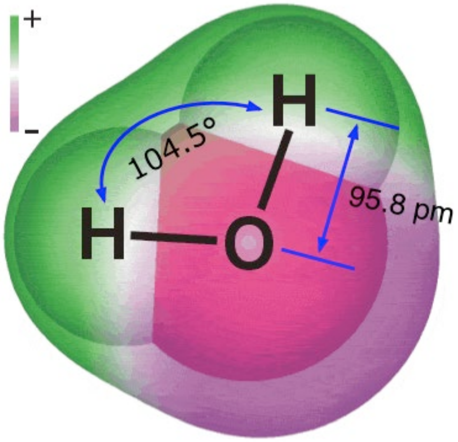


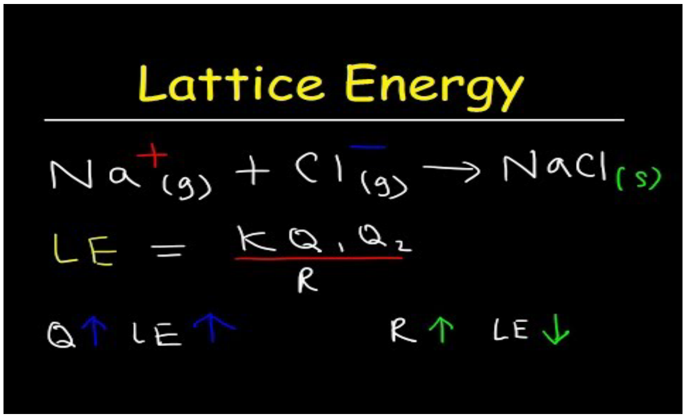
Figure 7.77 Water Molecule

Ionic Bond Strength and Lattice Energy

Multiple **bonds** are stronger than single **bonds** between the same atoms. For **ionic bonds**, the **lattice energy** is the **energy** required to separate one mole of a **compound** into its gas phase **ions**. **Lattice energy** increases for **ions** with higher charges and shorter distances between **ions**.

Ions are atoms or molecules which are electrically charged. **Cations** are positively charged and **anions** are negatively charged. Ions form when atoms gain or lose valence electrons. Since electrons are negatively charged, an atom that loses one or more electrons will become positively charged; an atom that gains one or more electrons becomes negatively charged. **Ionic bonding** is the attraction between positively- and negatively-charged ions. These oppositely charged ions attract each other to form ionic networks, or **lattices**. Electrostatics explains why this happens: opposite charges attract and like charges repel. When many ions attract each other, they form large, ordered, crystal lattices in which each ion is surrounded by ions of the opposite charge. Generally, when metals react with non-metals, electrons are transferred from the metals to the non-metals. The metals form positively-charged ions and the non-metals form negatively-charged ions.

The properties of ionic compounds follow from the orderly crystal lattice arrangement of tightly bonded charged particles that make them up. Ionic compounds tend to have high melting and boiling points, because the attraction between ions in the lattice is very strong. Moving ions out of the lattice disrupts the structure, so ionic compounds tend to be brittle rather than malleable. Ionic compounds do not conduct electricity in the solid state because ions are not free to move around the lattice; however, when ionic compounds are dissolved, they may *dissociate* into individual ions which move freely through the solution and therefore conduct electricity well.



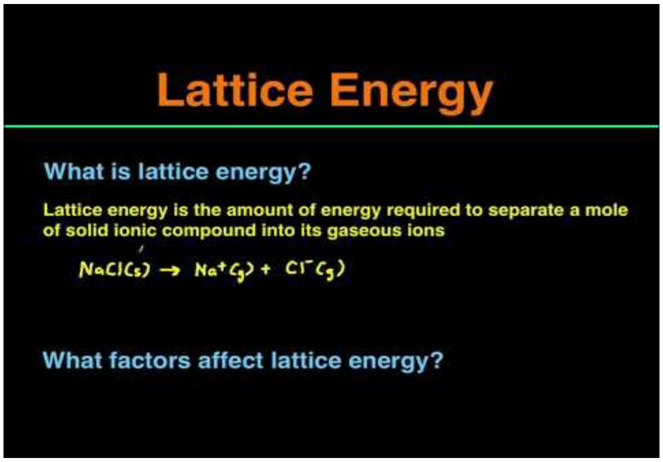
Lattice Energy

$Na^+_{(g)} + Cl^-_{(g)} \rightarrow NaCl_{(s)}$

$LE = \frac{KQ_1Q_2}{R}$

$Q\uparrow \; LE\uparrow \qquad R\uparrow \; LE\downarrow$

Reference: https://www.youtube.com/watch?v=I61-N0GuSx8



Lattice Energy

What is lattice energy?

Lattice energy is the amount of energy required to separate a mole of solid ionic compound into its gaseous ions

$NaCl_{(s)} \rightarrow Na^+_{(g)} + Cl^-_{(g)}$

What factors affect lattice energy?

Reference: https://www.youtube.com/watch?v=jIyIhTzA4xI

EXAMPLE

Lattice Energy Comparisons

The precious gem ruby is aluminum oxide, Al_2O_3, containing traces of Cr^{3+}. The compound Al_2Se_3 is used in the fabrication of some semiconductor devices. Which has the larger lattice energy, Al_2O_3 or Al_2Se_3?

Solution

In these two ionic compounds, the charges Z^+ and Z^- are the same, so the difference in lattice energy will depend upon Ro. The O^{2-} ion is smaller than the Se^{2-} ion. Thus, Al_2O_3 would have a shorter interionic distance than Al_2Se_3, and Al_2O_3 would have the larger lattice energy.

Check Your Learning

Zinc oxide, ZnO, is a very effective sunscreen. How would the lattice energy of ZnO compare to that of NaCl?

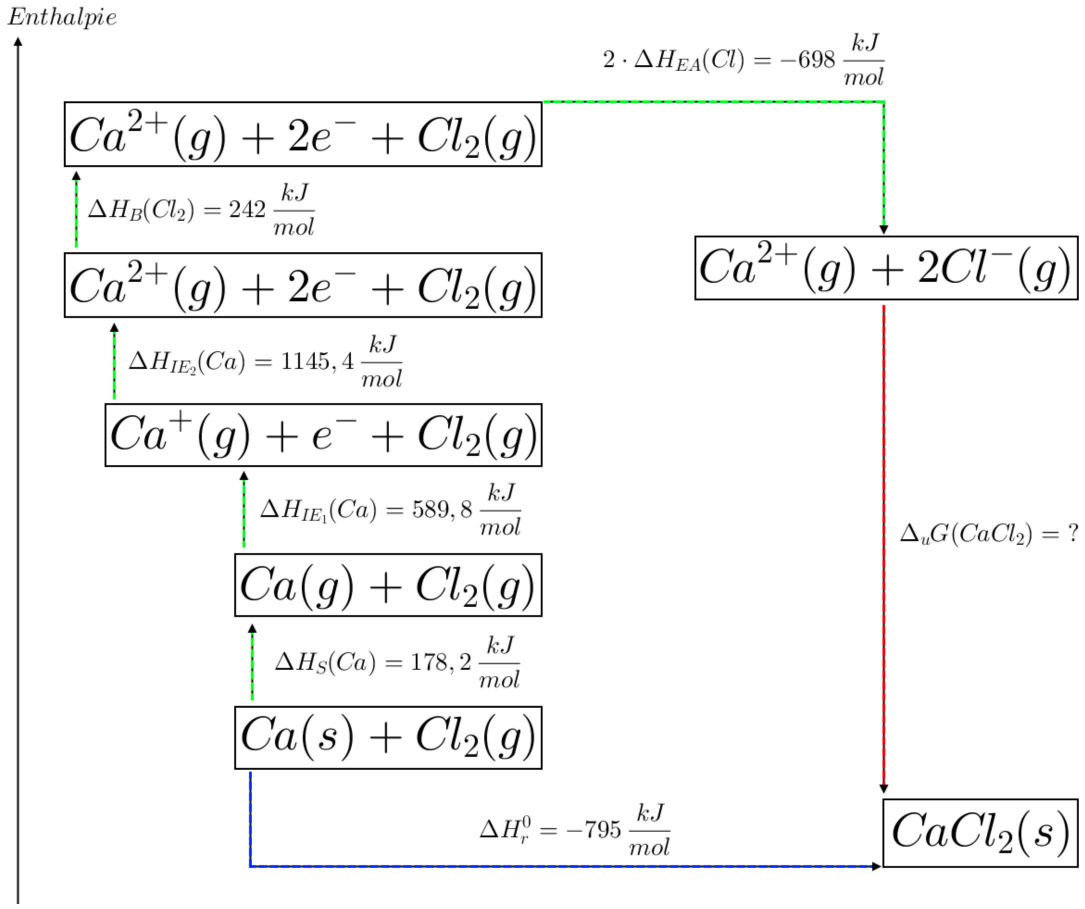
Answer: ZnO would have the larger lattice energy because the Z values of both the cation and the anion in ZnO are greater, and the interionic distance of ZnO is smaller than that of NaCl.

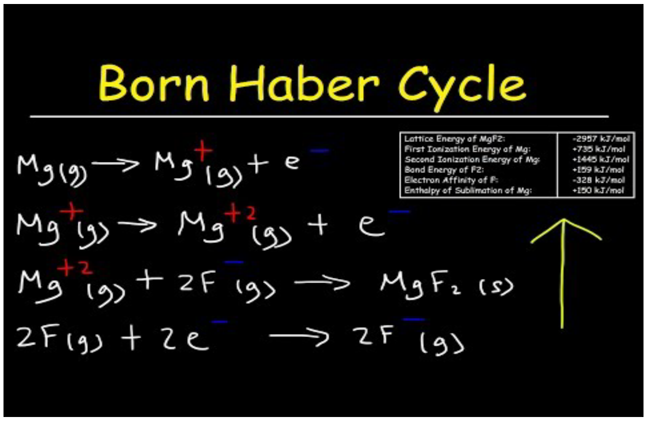
The Born-Haber Cycle

Born Haber cycle is a **cycle** of enthalpy change of process that leads to the formation of a solid crystalline ionic compound from the elemental atoms in their standard state and of the enthalpy of formation of the solid compound such that the net enthalpy becomes zero.

It is not possible to measure lattice energies directly. However, the lattice energy can be calculated using the equation given in the previous section or by using a thermochemical cycle. The **Born-Haber cycle** is an application of Hess's law that breaks down the formation of an ionic solid into a series of individual steps:

- $\Delta H f°$, the standard enthalpy of formation of the compound
- *IE*, the ionization energy of the metal
- *EA*, the electron affinity of the nonmetal
- $\Delta Hs°$, the enthalpy of sublimation of the metal
- *D*, the bond dissociation energy of the nonmetal
- ΔHlattice, the lattice energy of the compound





Born Haber Cycle

$Mg_{(g)} \rightarrow Mg^{+}_{(g)} + e^-$

$Mg^{+}_{(g)} \rightarrow Mg^{+2}_{(g)} + e^-$

$Mg^{+2}_{(g)} + 2F^-_{(g)} \rightarrow MgF_2\,(s)$

$2F_{(g)} + 2e^- \rightarrow 2F^-_{(g)}$

Lattice Energy of MgF2:	-2957 kJ/mol
First Ionization Energy of Mg:	+735 kJ/mol
Second Ionization Energy of Mg:	+1445 kJ/mol
Bond Energy of F2:	+159 kJ/mol
Electron Affinity of F:	-328 kJ/mol
Enthalpy of Sublimation of Mg:	+150 kJ/mol

Reference: https://www.youtube.com/watch?v=DI-bwx8r3r8

VII. Molecular Structure and Polarity

VSEPR Theory

The premise of the **VSEPR theory** is that electron pairs located in bonds and lone pairs repel each other and will therefore adopt the geometry that places electron pairs as far apart from each other as possible.

In 1956, British scientists R.J. Gillespie and R.S. Nyholm recognized that the current model for explaining bond angles did not work well. The theory at that time relied on hybrid orbitals to explain all aspects of bonding. The problem was that the theory gave incorrect prediction of bond angles for many compounds. They developed a new approach based on earlier work by other scientists that incorporated a consideration of electron pairs in predicting three-dimensional structure.

The **valence shell** is the outermost electron-occupied shell of an atom. The valence shell holds the electrons that are involved in bonding and are the electrons shown in a Lewis structure. The acronym VSEPR stands for the **valence-shell electron pair repulsion** model. The model states that electron pairs will repel each other such that the shape of the molecule will adjust so that the valence electron-pairs stay as far apart from each other as possible. Molecules can be systematically classified according to the number of bonding pairs of electrons as well as the number of nonbonding or lone pairs around the central atom. For the purposes of the VSEPR model, a double or triple bond is no different in terms of repulsion than a single bond. It is important to note here that shape of the molecule is determined by electronic arrangement of central atom only!

So in summary, VSEPR theory allows more accurate predictions of molecular shape by predicting the arrangement of electron pairs around each central atom and, usually, the correct arrangement of atoms in a molecule. We should understand, however, that the theory only considers electron-pair repulsions. Other interactions, such as nuclear-nuclear repulsions and nuclear-electron attractions, are also involved in the final arrangement that atoms adopt in a particular molecular structure.

VSEPR theory predicts the order of repulsions and an order of the amount of space occupied by different electron pairs. The order of electron-pair repulsions from greatest to least repulsion is:

lone pair-lone pair > lone pair-bonding pair > bonding pair-bonding pair

As a simple example of VSEPR theory, let us predict the structure of a gaseous BeF_2 molecule. The Lewis structure of BeF_2 as in the following Figure shows only two electron pairs around the central beryllium atom. With two bonds and no lone
pairs of electrons on the central atom, the bonds are as far apart as possible, and the electrostatic repulsion between these regions of high electron density is reduced to a minimum when they are on opposite sides of the central atom. The bond angle is 180°.

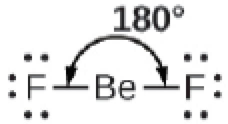


Figure 7.78: BeF_2

Ref: commons/Wikimedia.org/

In the above Figure, the BeF2 molecule adopts a linear structure in which the two bonds are as far apart as possible, on opposite sides of the Be atom.

Carbon dioxide, CO_2

In the CO_2 molecule, each oxygen is double bonded to the central carbon, as the Lewis structure on the left shows. VSEPR predicts that the molecule will be **linear** because that's the configuration that moves the C=O bonds as far apart as possible.

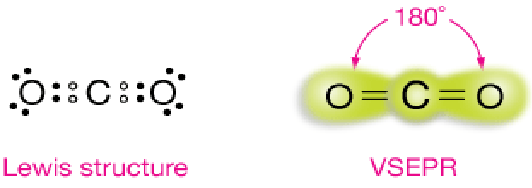


Figure 7.79 Linear CO_2 molecule

The actual picture is really more like that shown on the right, because each oxygen atom has two lone electron pairs.

Notice that even these lone pairs, which don't really contribute to what we think of as the structure of the molecule, orient in such a way as to maximize the distance between them. Notice the similarity between the left-most two lone pairs and the C atom, and the shape of BF_2.

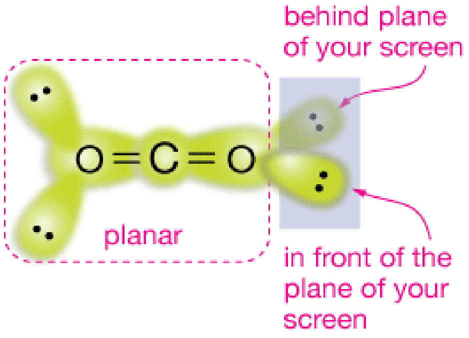


Figure 7.80 Electronic Geometry of CO_2 molecule

Generally, when we speak of the structure of a molecule, we're talking about the location of the nuclei of atoms, but we even have to be careful there for two reasons: (1) All atoms move all of the time, so we're always talking about *average* positions of atoms as they vibrate, and (2) those lone pairs can be big factors in determining the shape and properties of a molecule.

The table below shows the basic electron-pair geometries predicted by VSEPR theory maximize the space around any region of electron density:

References:
https://chem.libretexts.org/Bookshelves/General_Chemistry/Book%3A_Chemistry_(OpenSTAX)/07%3A_Chemical_Bonding_and_Molecular_Geometry/7.6%3A_Molecular_Structure_and_Polarity

Molecular structure describes the location of the atoms, not the electrons. We differentiate between these two situations by naming the geometry that includes all electron pairs the electron-pair geometry. The **structure** that includes only the placement of the atoms in the **molecule** is called the **molecular structure**.

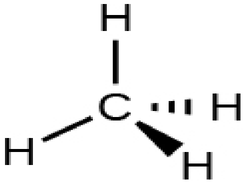
A whole **molecule** may also have a separation of charge, depending on its **molecular structure** and the **polarity** of each of its bonds. If such a charge separation exists, the **molecule** is said to be a polar **molecule** (or dipole); otherwise the **molecule** is said to be nonpolar.

It is important to note that electron-pair geometry around a central atom is *not* the same thing as its molecular structure. Molecular structure describes the location of the *atoms*, not the electrons.

We differentiate between these two situations by naming the geometry that includes *all* electron pairs the **electron-pair geometry**. The number of regions surrounding central atom is called "**Electron Group Geometry**" or **Steric Number (SN)**. This includes arrangement derived using Lewis structure including bond pairs and lone pairs.

The structure that includes only the placement of the atoms in the molecule is called the **molecular structure**. The electron-pair geometries will be the same as the molecular structures when there are no lone electron pairs around the central atom, but they will be different when there are lone pairs present on the central atom.

For example, the methane molecule, CH_4, which is the major component of natural gas, has four bonding pairs of electrons around the central carbon atom; the electron-pair geometry is tetrahedral, as is the molecular structure in the following Figure-A below.



Methane

Figure 7.81 Electronic Geometry of CH_4 molecule

The above Figure-A showing the molecular structure of Methane (CH_4). The molecule structure is shown with tetrahedral arrangement of the hydrogen atoms.

VSEPR structures like this one are often drawn using the wedge and dash notation, in which solid lines represent bonds in the plane of the page, solid wedges represent bonds coming up out of the plane, and dashed lines represent bonds going down into the plane.

On the other hand, the ammonia molecule, NH_3, also has four electron pairs associated with the nitrogen atom, and thus has a tetrahedral electron-pair geometry. One of these regions, however, is a lone pair, which is not included in the molecular structure, and this lone pair influences the shape of the molecule (Figure-B).

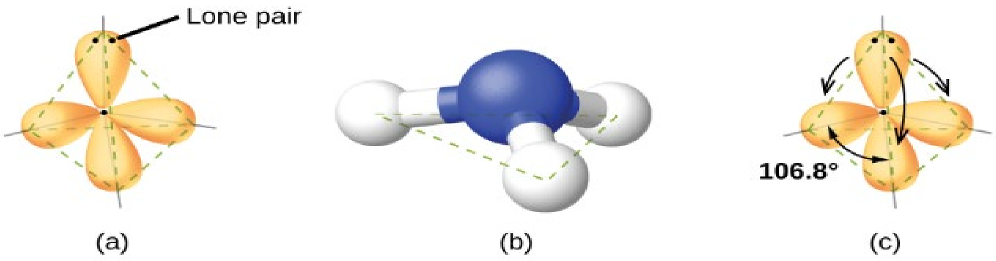
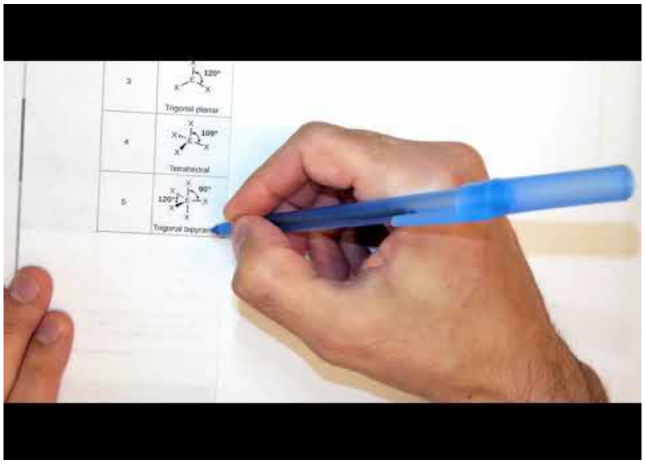
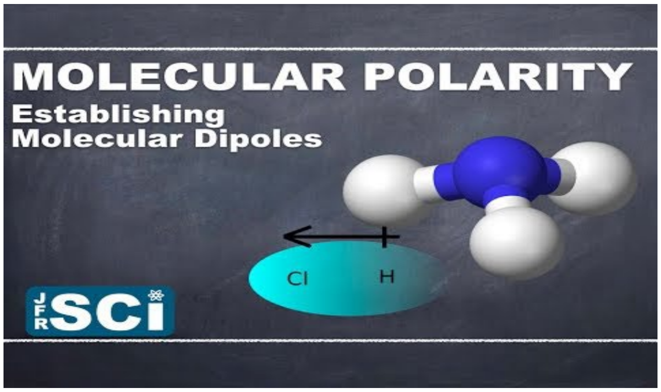


Figure 7.82 Electronic Geometry of NH_3 molecule

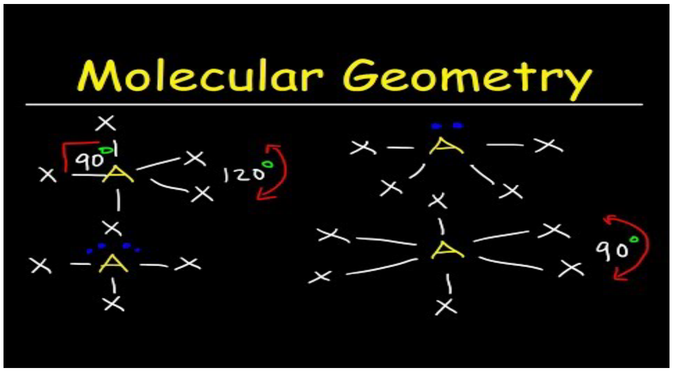
Figure 7.82(a) The electron-pair geometry for the ammonia molecule is tetrahedral with one lone pair and three single bonds. (b) The trigonal pyramidal molecular structure is determined from the electron-pair geometry. (c) The actual bond angles deviate slightly from the idealized angles because the lone pair takes up a larger region of space than do the single bonds, causing the HNH angle to be slightly smaller than 109.5°.



Reference: https://youtu.be/0SJ0oprIhTU



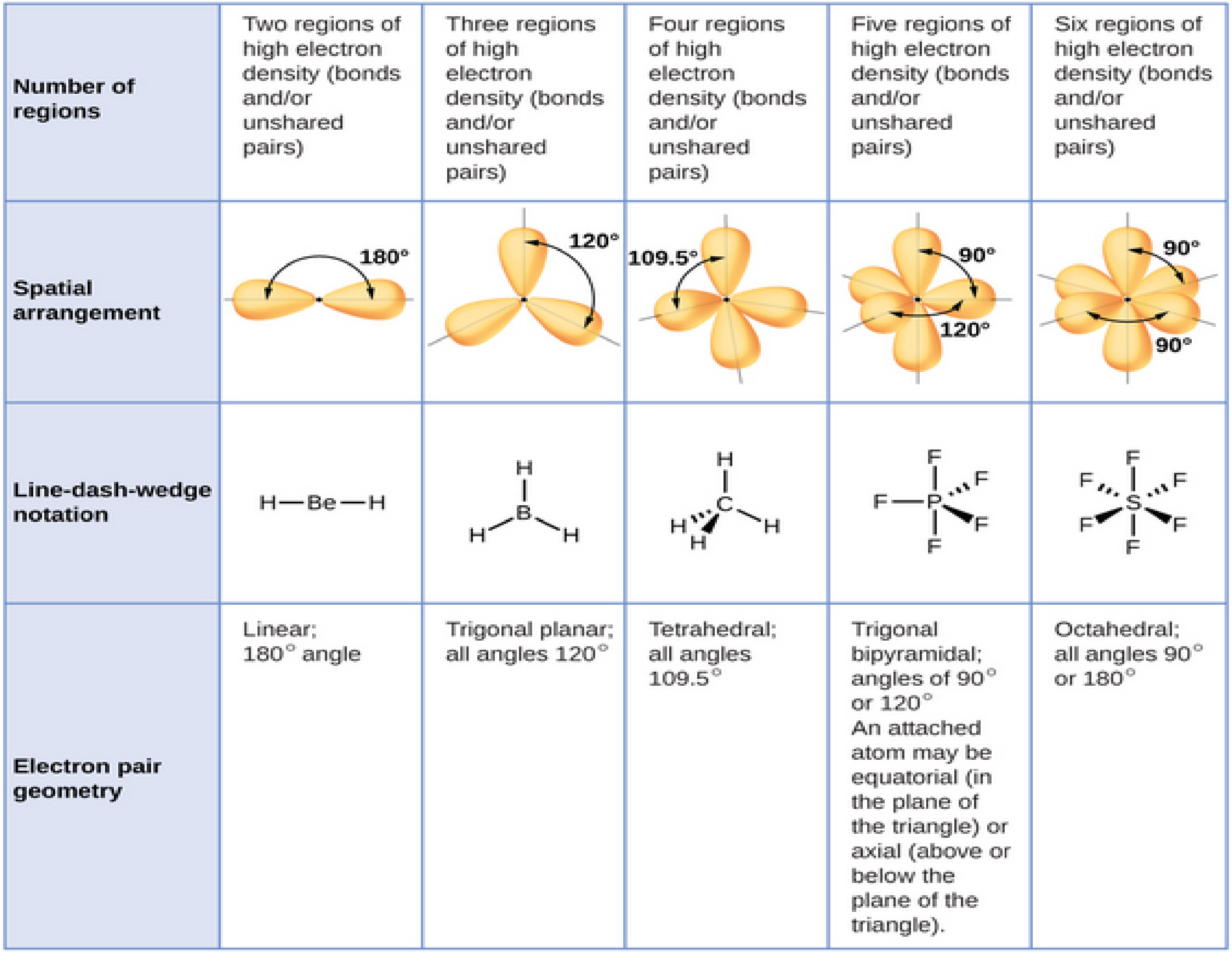
Reference: https://www.youtube.com/watch?v=bBYlyqb7aOI



Reference: https://www.youtube.com/watch?v=_Cw0_cJzkSI&t=17s

Figure 7.83 VSEPR Chart

Ref: www.openstax.org/

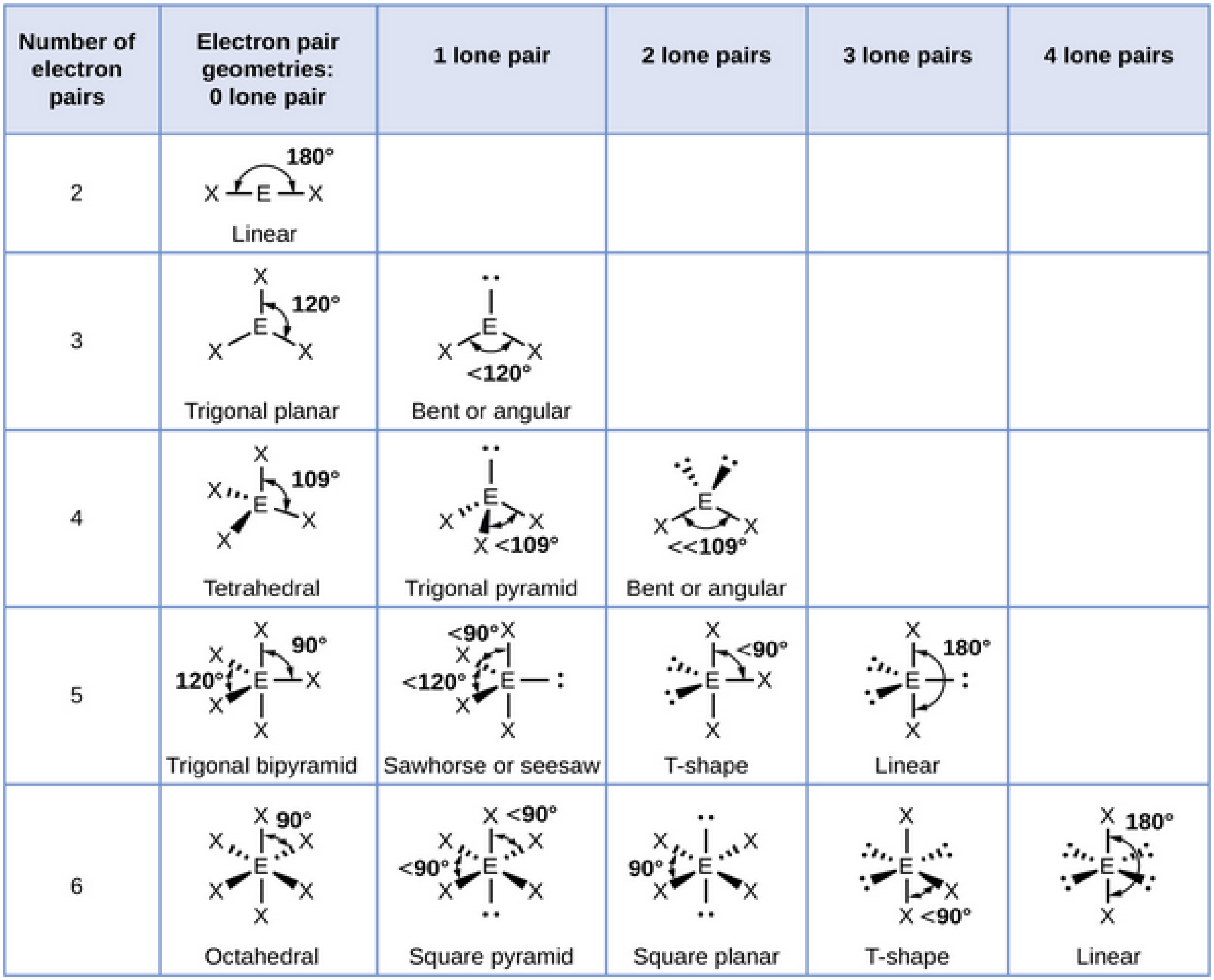


Number of regions	Two regions of high electron density (bonds and/or unshared pairs)	Three regions of high electron density (bonds and/or unshared pairs)	Four regions of high electron density (bonds and/or unshared pairs)	Five regions of high electron density (bonds and/or unshared pairs)	Six regions of high electron density (bonds and/or unshared pairs)
Spatial arrangement	180°	120°	109.5°	90° 120°	90° 90°
Line-dash-wedge notation	H—Be—H	H B H H	H C H H H	F F—P F F F	F F S F F F F
Electron pair geometry	Linear; 180° angle	Trigonal planar; all angles 120°	Tetrahedral; all angles 109.5°	Trigonal bipyramidal; angles of 90° or 120° An attached atom may be equatorial (in the plane of the triangle) or axial (above or below the plane of the triangle).	Octahedral; all angles 90° or 180°

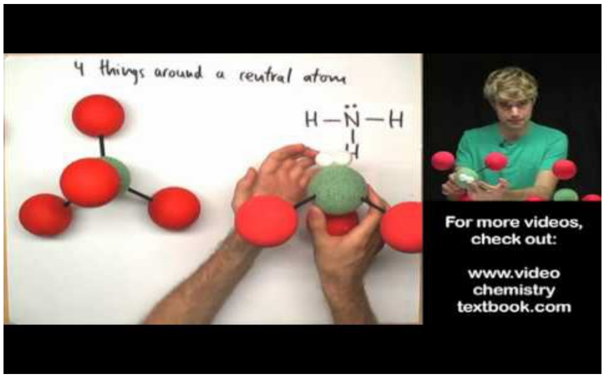
Also, the table below illustrates the molecular structures which are identical to the electron-pair geometries when there are no lone pairs present at the central atom (column number 1).

Figure 7.84 VSEPR Chart

Ref: www.openstax.org/

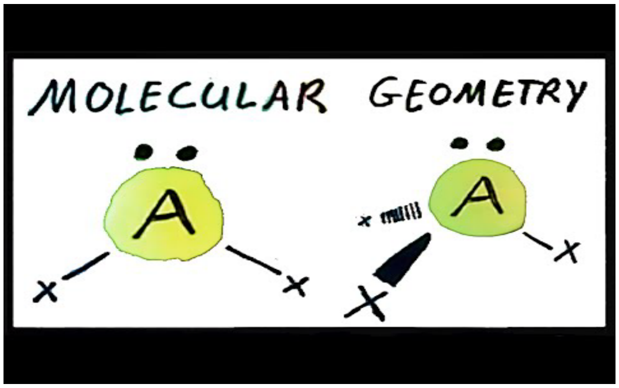


Number of electron pairs	Electron pair geometries: 0 lone pair	1 lone pair	2 lone pairs	3 lone pairs	4 lone pairs
2	180° Linear				
3	120° Trigonal planar	<120° Bent or angular			
4	109° Tetrahedral	<109° Trigonal pyramid	<<109° Bent or angular		
5	90° 120° Trigonal bipyramid	<90° <120° Sawhorse or seesaw	<90° T-shape	180° Linear	
6	90° Octahedral	<90° <90° Square pyramid	90° Square planar	<90° T-shape	180° Linear

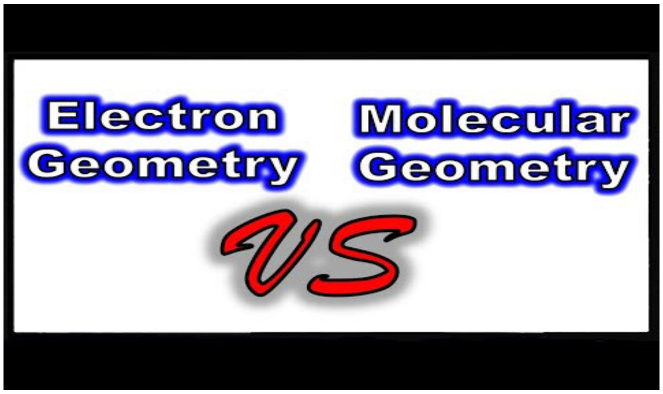


Reference: https://www.youtube.com/watch?v=nxebQZUVvTg

Reference: https://www.youtube.com/watch?v=keHS-CASZfc



Reference: https://www.youtube.com/watch?v=3ZsqcDOBv7g



Reference: https://www.youtube.com/watch?v=v0nzeCpCb3k

Predicting Electron Pair Geometry and Molecular Structure

Thus, **electron pairs** will spread themselves as far from each other as possible to minimize repulsion. Using the **VSEPR** theory, the **electron** bond **pairs** and **lone pairs** on the center atom will help us **predict** the **shape** of a **molecule**. The **shape** of a **molecule** is determined by the location of the nuclei and its **electrons**.

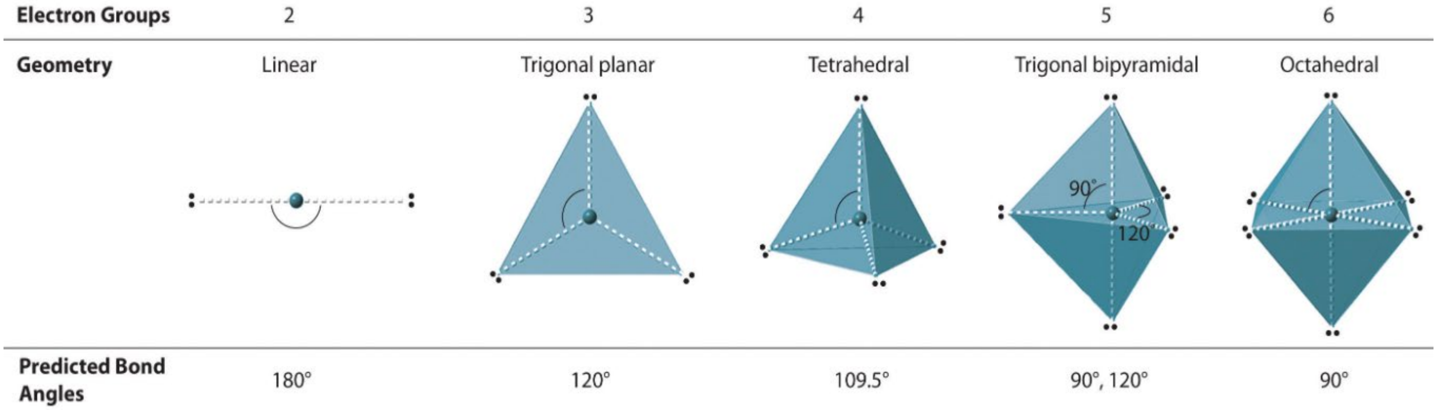
The VSEPR theory is to determine the electron pair geometries and the molecular structures: A model used to predict the shapes of many molecules and polyatomic ions, based on the idea that the lowest-energy arrangement for a compound is the one in which its electron pairs (bonding and nonbonding) are as far apart as possible. (pronounced "vesper"), which can be used to predict the shapes of many molecules and polyatomic ions. Keep in mind, however, that the VSEPR model, like any model, is a limited representation of reality; the model provides no information about bond lengths or the presence of multiple bonds. Following sections of this chapter will connect the VSEPR model to atomic and molecular orbitals.

The VSEPR model can predict the structure of nearly any molecule or polyatomic ion in which the central atom is a nonmetal, as well as the structures of many molecules and polyatomic ions with a central metal atom. The **VSEPR model is *not* a theory; it does not attempt to explain observations. Instead, it is a counting procedure that accurately predicts the three-dimensional structures of a large number of compounds, which cannot be predicted using the Lewis electron-pair approach.**

So Lewis electron structures predict the number and types of bonds, whereas VSEPR can predict the shapes of many molecules and polyatomic ions.

We can use the VSEPR model to predict the geometry of most polyatomic molecules and ions by focusing on only the number of electron pairs around the *central atom*, ignoring all other valence electrons present. According to this model, valence electrons in the Lewis structure form *groups*, which may consist of a single bond, a double bond, a triple bond, a lone pair of electrons, or even a single unpaired electron, which in the VSEPR model is counted as a lone pair. Because electrons repel each other electrostatically, the most stable arrangement of electron groups (i.e., the one with the lowest energy) is the one that minimizes repulsions. Groups are positioned around the central atom in a way that produces the molecular structure with the lowest energy, as illustrated in the following Figure 7.85 A and Figure 7.85 -B.

Figure-A: Common Structures for Molecules and Polyatomic Ions That Consist of a Central Atom Bonded to Two or Three Other Atoms.

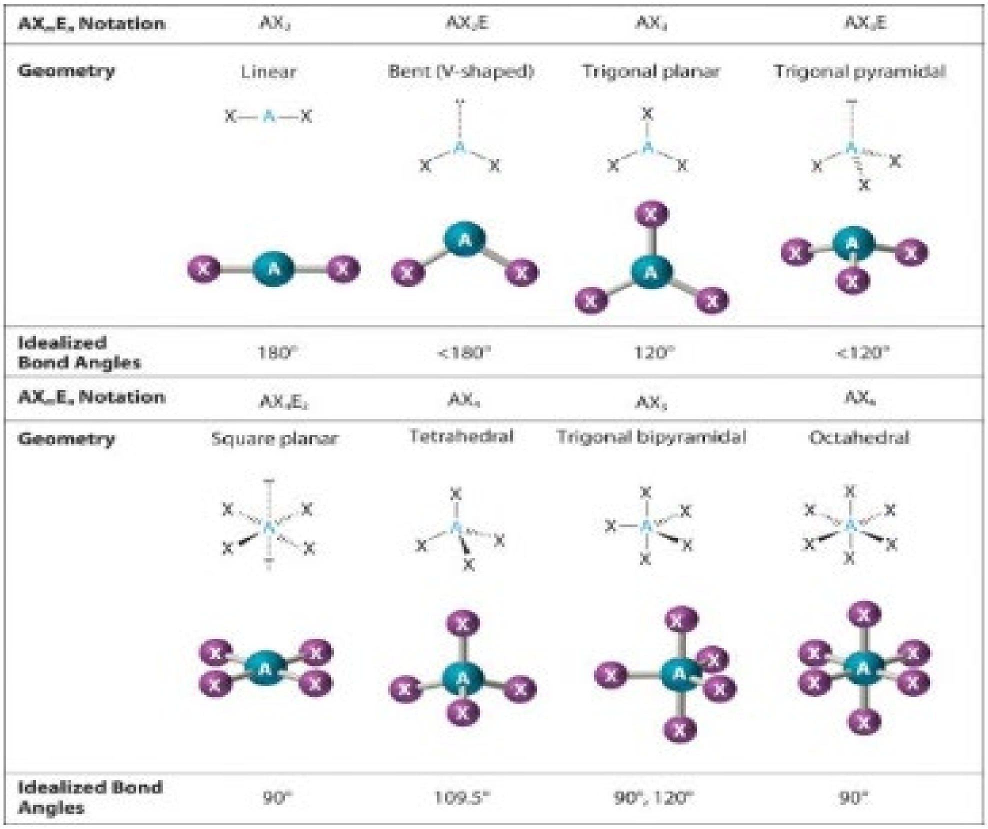


Electron Groups	2	3	4	5	6
Geometry	Linear	Trigonal planar	Tetrahedral	Trigonal bipyramidal	Octahedral
Predicted Bond Angles	180°	120°	109.5°	90°, 120°	90°

Figure-B: Geometries for Species with Two to Six Electron Groups

Ref. www.libretext.org/

The following we will illustrate the several examples, beginning with atoms with two electron groups. We will also summarize the common molecular geometries and idealized bond angles of molecules and ions with two to six electron groups.



AX_mE_n Notation	AX_2	AX_2E	AX_3	AX_3E
Geometry	Linear	Bent (V-shaped)	Trigonal planar	Trigonal pyramidal
Idealized Bond Angles	180°	<180°	120°	<120°
AX_mE_n Notation	AX_4E_2	AX_4	AX_5	AX_6
Geometry	Square planar	Tetrahedral	Trigonal bipyramidal	Octahedral
Idealized Bond Angles	90°	109.5°	90°, 120°	90°

Figure 7.86 AXE groups in VSEPR

Ref. www.libretext.org/

Common Molecular Geometries for Species with Two to Six Electron Groups.

Below we will discuss each type of electron pair Geometry and molecular shape more in detail.

Trigonal molecules

In an AX_3 molecule such as BF_3, there are three regions of electron density extending out from the central atom. The repulsion between these will be at a minimum when the angle between any two is (360° ÷ 3) = 120°. This requires that all four atoms be in the same plane; the resulting shape is called ***trigonal planar***, or simply *trigonal*.

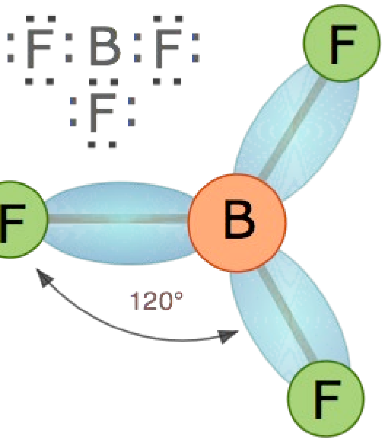


Figure 7.87 Shape of BF_3 molecule

Tetrahedral coordination

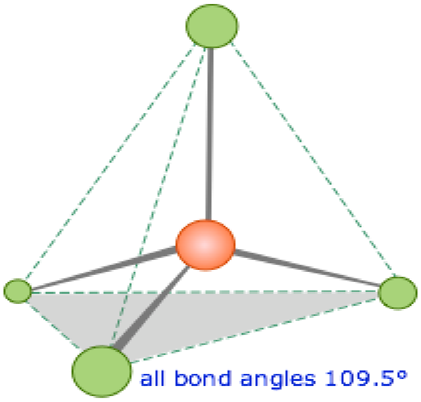


Figure 7.88 Tetrahedral CH_4 molecule

Methane, CH_4, contains a carbon atom bonded to four hydrogens. What bond angle would lead to the greatest possible separation between the electron clouds associated with these bonds? In analogy with the preceding two cases, where the bond angles were 360°/2=180° and 360°/3=120°, you might guess 360°/4=90°; if so, you would be wrong. The latter calculation would be correct if all the atoms were constrained to be in the same plane (we will see cases where this happens later), but here there is no such restriction. Consequently, the four equivalent bonds will point in four **geometrically equivalent directions** in three dimensions corresponding to the four corners of a ***tetrahedron*** centered on the carbon atom. The angle between any two bonds will be 109.5°.

This is called ***tetrahedral coordination***.

> This is the most important coordination geometry in Chemistry: it is imperative that you be able to sketch at least a crude perspective view of a tetrahedral molecule.

It is interesting to note that the tetrahedral coordination of carbon in most of its organic compounds was worked out in the nineteenth century on purely geometrical grounds and chemical evidence, long before direct methods of determining molecular shapes were developed.

For example, it was noted that there is only one dichloromethane, CH_2Cl_2.

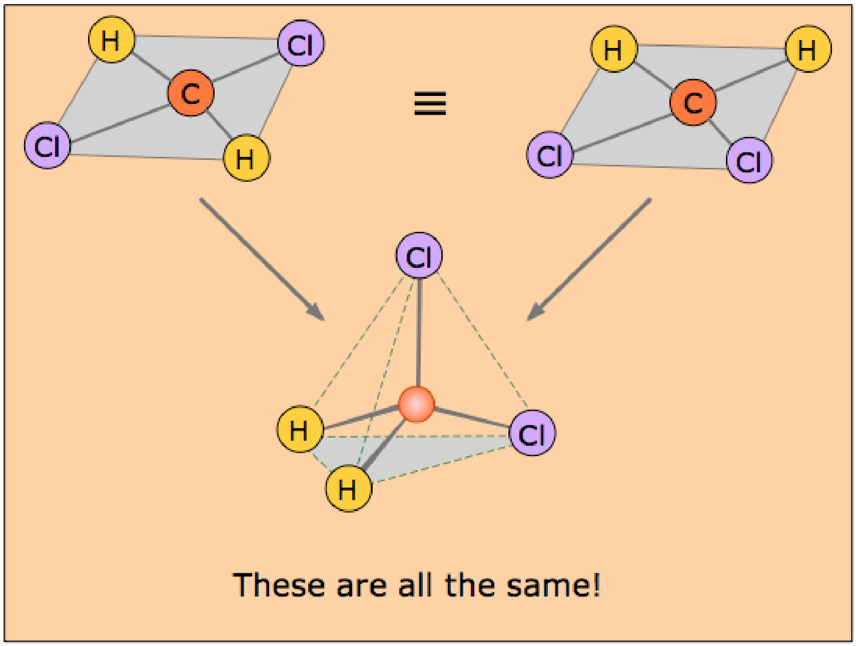


Figure 7.89 Shape of CH_2Cl_2

If the coordination around the carbon were square, then there would have to be two isomers of CH_2Cl_2, as shown in the pair of structures here. The distances between the two chlorine atoms would be different, giving rise to differences in physical properties would allow the two isomers to be distinguished and separated.

The existence of only one kind of CH_2Cl_2 molecule means that all four positions surrounding the carbon atom are geometrically equivalent, which requires a tetrahedral coordination geometry. If you study the tetrahedral figure closely, you may be able to convince yourself that it represents the connectivity shown on both of the "square" structures at the top. A three-dimensional ball-and-stick mechanical model would illustrate this very clearly.

Tetrahedrally-coordinated carbon chains

Carbon atoms are well known for their tendency to link together to form the millions of organic molecules that are known. We can work out the simpler hydrocarbon chains by looking at each central atom separately. Thus the hydrocarbon *ethane* is essentially two CH_3 tetrahedra joined end-to-end. Similar ***alkane*** chains having the general formula $H_3C–(CH_2)_n–CH_3$ (or C_nH_{2n+2}) can be built up; a view of *pentane*, C_5H_{12}, is shown below.

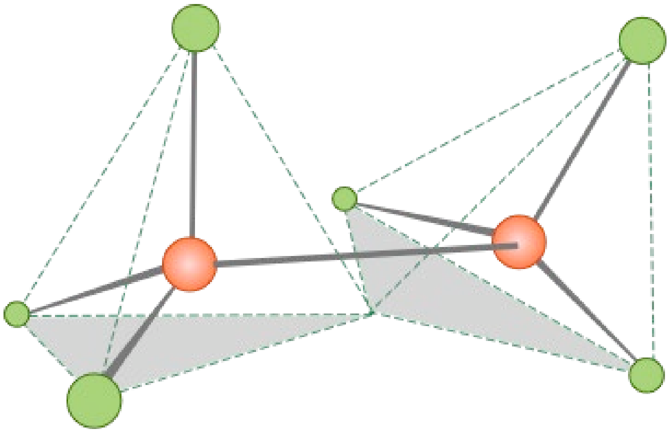


Figure 7.90 Tetrahedral chain of carbon atoms

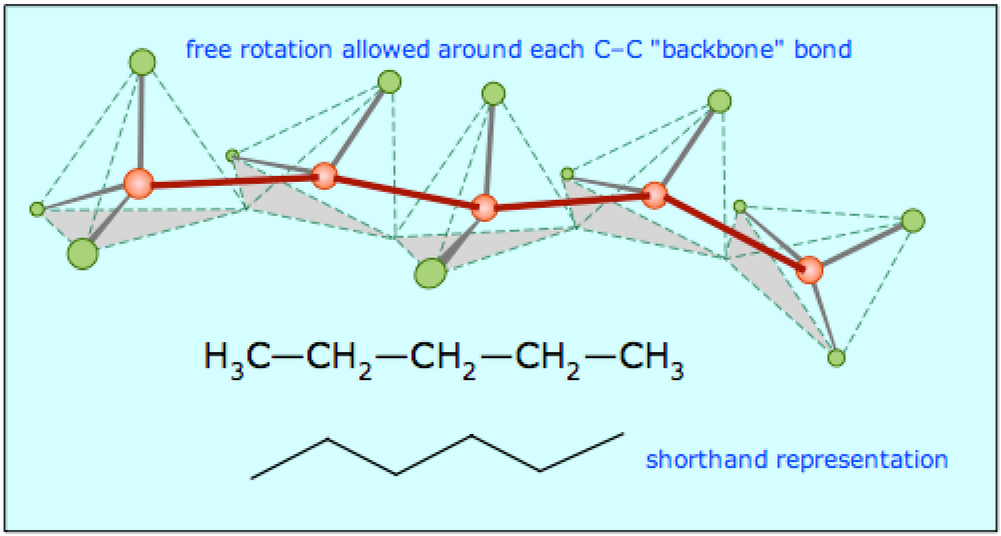


Figure 7.91 shape of long chain carbon atoms

Notice that these "straight chain hydrocarbons" (as they are often known) have a carbon "backbone" structure that is not really straight, as is illustrated by the zig-zag figure that is frequently used to denote hydrocarbon structures.

Coordination geometry and molecular geometry

Coordination number refers to the number of electron pairs that surround a given atom; we often refer to this atom as the ***central atom*** even if this atom is not really located at the geometrical center of the molecule. If all of the electron pairs surrounding the central atom are shared with neighboring atoms, then the ***coordination geometry*** is the same as the ***molecular geometry***. The application of VSEPR theory then reduces to the simple problem of naming (and visualizing) the geometric shapes associated with various numbers of points surrounding a central point (the central atom) at the greatest possible angles. Both classes of geometry are named after the shapes of the imaginary geometric figures (mostly regular solid polygons) that would be centered on the central atom and would have an electron pair at each vertex.

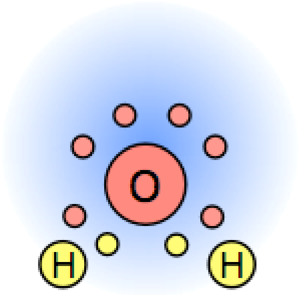
If one or more of the electron pairs surrounding the central atom is not shared with a neighboring atom (that is, if it is a lone pair), then the molecular geometry is simpler than the coordination geometry, and it can be worked out by inspecting a sketch of the coordination geometry figure.

Tetrahedral coordination with lone pairs

In the examples we have discussed so far, the shape of the molecule is defined by the coordination geometry; thus the carbon in methane is tetrahedrally coordinated, and there is a hydrogen at each corner of the tetrahedron, so the molecular shape is also tetrahedral.

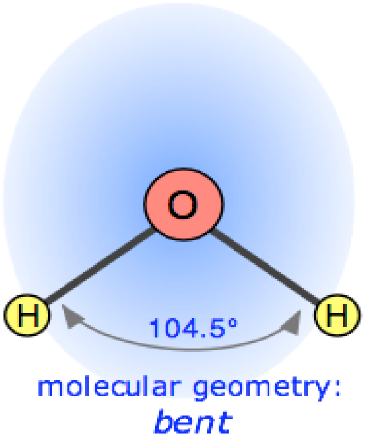
It is common practice to represent bonding patterns by "generic" formulas such as AX_4, AX_2E_2, etc., in which "X" stands for bonding pairs and "E" denotes lone pairs. (This convention is known as the "AXE method")

The bonding geometry will not be tetrahedral when the valence shell of the central atom contains nonbonding electrons, however. The reason is that the ***nonbonding electrons*** are also in orbitals that occupy space and repel the other orbitals. This means that in figuring the coordination number around the central atom, we must count both the bonded atoms and the nonbonding pairs.



The water molecule: AX_2E_2

Figure 7.92 water molecule shape



In the water molecule, the central atom is O, and the Lewis electron dot formula predicts that there will be two pairs of nonbonding electrons. The oxygen atom will therefore be tetrahedrally coordinated, meaning that it sits at the center of the tetrahedron as shown below. Two of the coordination positions are occupied by the shared electron-pairs that constitute the O–H bonds, and the other two by the non-bonding pairs. Thus although the oxygen atom is tetrahedrally coordinated, the bonding geometry (shape) of the H_2O molecule is described as ***bent.***

Figure 7.93 bent shape of water

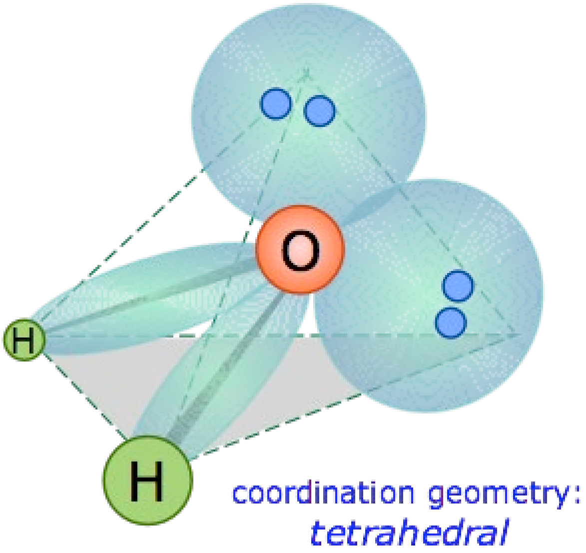


Figure 7.94 Tetrahedral Electronic Geometry of Water

There is an important difference between bonding and non-bonding electron orbitals. Because a nonbonding orbital has no atomic nucleus at its far end to draw the electron cloud toward it, the charge in such an orbital will be concentrated closer to the central atom. As a consequence, nonbonding orbitals exert more repulsion on other orbitals than do bonding orbitals. Thus in H_2O, the two nonbonding orbitals push the bonding orbitals closer together, making the H–O–H angle 104.5° instead of the tetrahedral angle of 109.5°.

Although the water molecule is electrically neutral, it is not electrically *uniform*; the non-bonding electrons create a higher concentration of negative charge (blue color) at the oxygen end, making the hydrogen side relatively positive (red).

This image was produced by a computer simulation based on the more complete molecular orbital model that we describe in the next lesson.

This charge unbalance gives rise to many of the so-called *anomalous properties of water*.

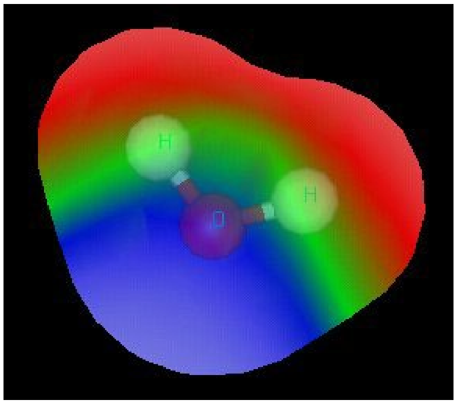


Figure 7.95 Charge Density of water

Ammonia: AX_3E

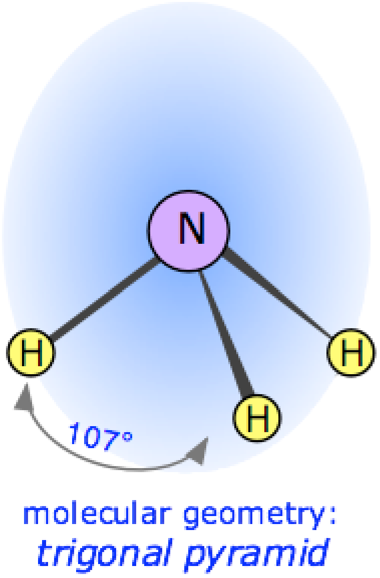
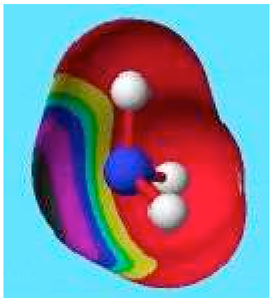


Figure 7.96 Shape of ammonia, NH_3



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The electron-dot structure of NH_3 places one pair of nonbonding electrons in the valence shell of the nitrogen atom. This means that there are three bonded atoms and one lone pair, for a coordination number of four around the nitrogen, the same as occurs in H_2O. We can therefore predict that the three hydrogen atom will lie at the corners of a tetrahedron centered on the nitrogen atom. The lone pair orbital will point toward the fourth corner of the tetrahedron, but since that position will be vacant, the NH_3 molecule itself cannot be tetrahedral. Instead, it assumes a ***pyramidal*** shape. More precisely, the shape is that of a ***trigonal pyramid*** (i.e., a pyramid having a triangular base). The hydrogen atoms are all in the same plane, with the nitrogen above (or below, or to the side; molecules of course don't know anything about "above" or "below"!) The fatter orbital containing the non-bonding electrons pushes the bonding orbitals together slightly, making the H–N–H bond angles about 107°.

Central atoms with five bonds

Compounds of the type AX_5 are formed by some of the elements in Group 15 of the periodic table; PCl_5 and AsF_5 are examples.

In what directions can five electron pairs arrange themselves in space so as to minimize their mutual repulsions? In the cases of coordination numbers 2, 3, 4, and 6, we could imagine that the electron pairs distributed themselves as far apart as possible on the surface of a sphere; for the two higher numbers, the resulting shapes correspond to the regular polyhedron having the same number of sides.

The problem with coordination number 5 is that there is no such thing as a regular polyhedron with five vertices.

In 1758, the great mathematian Euler proved that there are only five regular convex polyhedra, known as the platonic solids: tetrahedron (4 triangular faces), octahedron (6 triangular faces), icosahedron (20 triangular faces), cube (6 square faces), and dodecahedron (12 pentagonal faces). Chemical examples of all are known; the first icosahedral molecule, LaC_{60} (in which the La atom has 20 nearest C neighbors) was prepared in 1986.

Besides the five regular solids, there can be 15 semi-regular isogonal solids in which the faces have different shapes, but the vertex angles are all the same. These geometrical principles are quite important in modern structural chemistry.

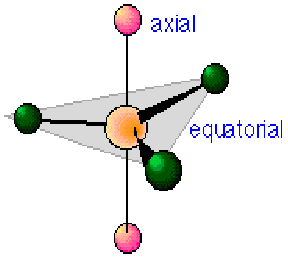


Figure 7.98 Electronic Geometry of Trigonal Bipyramidal

The shape of PCl_5 and similar molecules is a ***trigonal bipyramid***. This consists simply of two triangular-base pyramids joined base-to-base. Three of the chlorine atoms are in the plane of the central phosphorus atom (*equatorial* positions), while the other two atoms are above and below this plane (*axial* positions). Equatorial and axial atoms have different geometrical relationships to their neighbors, and thus differ slightly in their chemical behavior.

In 5-coordinated molecules containing lone pairs, these non-bonding orbitals (which you will recall are closer to the central atom and thus more likely to be repelled by other orbitals) will preferentially reside in the equatorial plane. This will place them at 90° angles with respect to no more than two axially-oriented bonding orbitals.

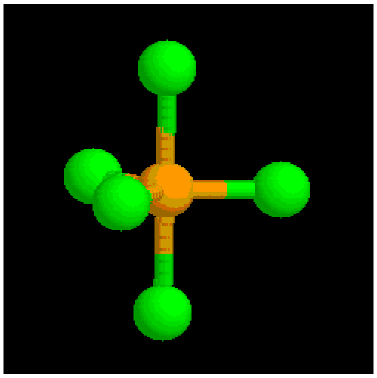


Figure 7.99 Ball and Stick model of Trigonal Bipyramidal grometry

Using this reasoning, we can predict that an AX_4E molecule (that is, a molecule in which the central atom A is coordinated to four other atoms "X" and to one nonbonding electron pair) such as SF_4 will have a "see-saw" shape; substitution of more nonbonding pairs for bonded atoms reduces the triangular bipyramid coordination to even simpler molecular shapes, as shown below.

Figure 7.100 lone pairs in Trigonal bipyramidal geometry

Octahedral coordination

Just as four electron pairs experience the minimum repulsion when they are directed toward the corners of a tetrahedron, six electron pairs will try to point toward the corners of an ***octahedron***. An octahedron is not as complex a shape as its name might imply; it is simply two square-based pyramids joined base to base. You should be able to sketch this shape as well as that of the tetrahedron.

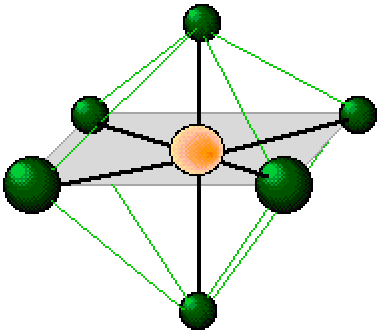


Figure 7.101 Electronic Geometry of Octahedral

Ref: https://www.chem1.com/acad/webtext/chembond/index.html

The shaded plane shown in this octahedrally-coordinated molecule is only one of three equivalent planes defined by a four-fold symmetry axis. All the ligands are geometrically equivalent; there are no separate axial and equatorial positions in an AX_6 molecule. Click here to see an image that shows the symmetry of the octahedron in more detail.

At first, you might think that a coordination number of six is highly unusual; it certainly violates the octet rule, and there are only a few molecules (SF_6 is one) where the central atom is hexavalent. It turns out, however, that this is one of the most commonly encountered coordination numbers in inorganic chemistry. There are two main reasons for this:

- Many transition metal ions form coordinate covalent bonds with lone-pair electron donor atoms such as N (in NH_3) and O (in H_2O). Since transition elements can have an outer configuration of $d^{10}s^2$, up to six electron pairs can be accommodated around the central atom. A coordination number of 6 is therefore quite common in transition metal hydrates, such as $Fe(H_2O)_6^{3+}$.

- Although the central atom of most molecules is bonded to fewer than six other atoms, there is often a sufficient number of lone pair electrons to bring the total number of electron pairs to six.

Octahedral coordination with lone pairs

There are well known examples of 6-coordinate central atoms with 1, 2, and 3 lone pairs. Thus all three of the molecules whose shapes are depicted below possess octahedral coordination around the central atom. Note also that the orientation of the shaded planes shown in the two rightmost images are arbitrary; since all six vertices of an octahedron are identical, the planes could just as well be drawn in any of the three possible vertical orientations.

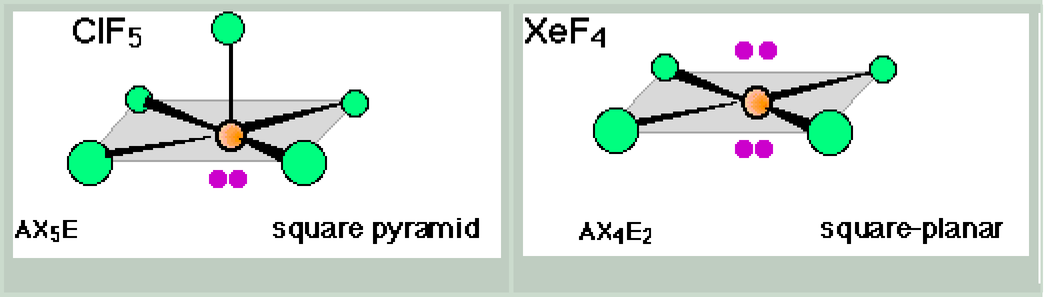
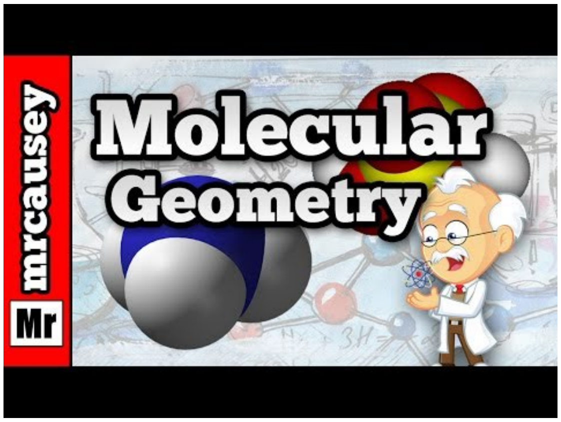
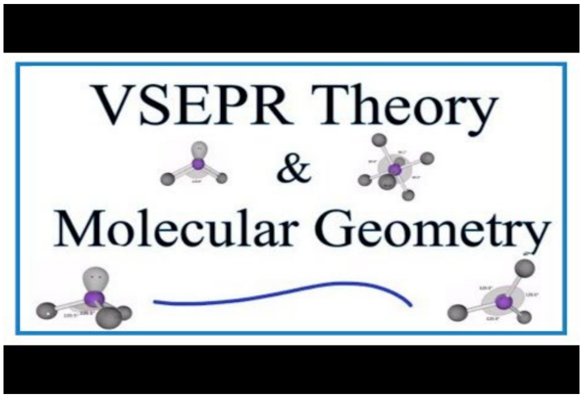


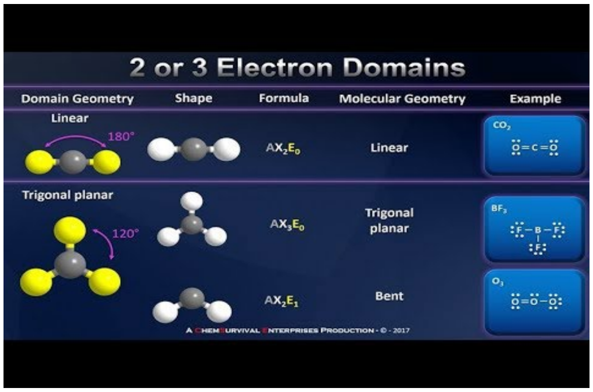
Figure 7.102 Lone pairs of Octahedral Geometry



Reference: https://www.youtube.com/watch?v=-pq2wum1uDc



Reference: https://www.youtube.com/watch?v=Moj85zwdULg



2 or 3 Electron Domains

Domain Geometry	Shape	Formula	Molecular Geometry	Example
Linear 180°		AX_2E_0	Linear	CO_2 $O=C=O$
Trigonal planar 120°		AX_3E_0	Trigonal planar	BF_3 $F-B-F$, F
		AX_2E_1	Bent	O_3 $O=O-O$

A ChemSurvival Enterprises Production - © - 2017

Reference: https://www.youtube.com/watch?v=umwN74a0A2g

Following CLASSROOM ACTIVITY has been adapted from Phet simulation: https://phet.colorado.edu

It's All in the Shape: Discovering Molecular Geometry

Structure begets function. How molecules behave or interact with one another or other molecules is an important part of chemistry. Molecular structure controls properties such as solubility or boiling point. So let's explore the simple world of molecular geometry.

It would be helpful to build some molecular models. If you have some toothpicks and clay, playdough, or gummy bears, you can make some models - the clay or gummy bear will be the central atom and the toothpicks will represent the electron pairs.

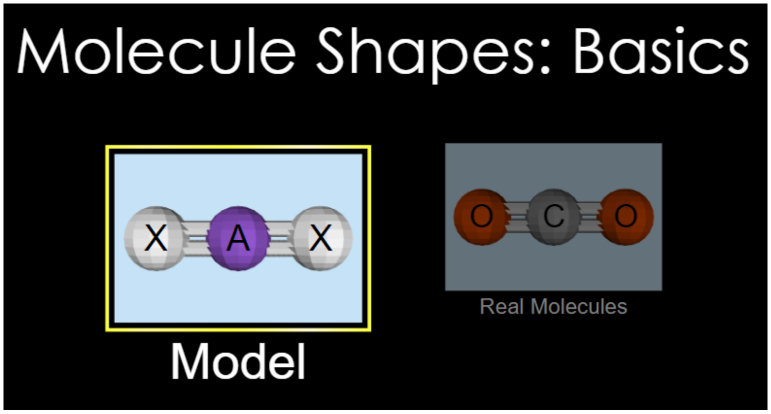
Predict the geometry for the three situations given in the table below. How do you think electron pairs will behave towards each other? This behavior will control how they arrange around a central atom depending on the number of electron pairs.

Number of **electron pairs** around central atom	Predict a possible arrangement - sketch it!	What is the angle between the electron pairs?	Are all the angles the same? If not, point out the differences.
2 pairs			
3 pairs			

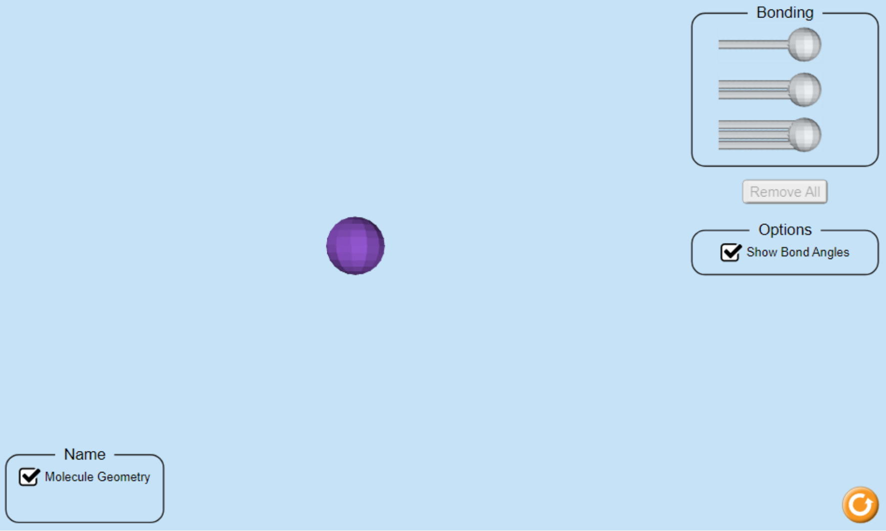
4 pairs			

Beware of molecular roadkill (flattened molecules)!!!
Now electron pairs are repulsive to each other; hence, they minimize repulsion by maximizing distance. They want to get away from each other! This is the basis of valence shell electron-pair repulsion theory or VSEPR. Let's see how well your predictions came out above and add two more geometries to the list. Go to the following PhET html5 simulation:

https://phet.colorado.edu/sims/html/molecule-shapes-basics/latest/molecule-shapes-basics_en.html



Click on the Model box as shown above. When the screenshot below opens, follow the instructions below.



☑ Show Bond Angles

☑ Molecule Geometry

2. Check the Show Bond Angles Option
3. Check the Name Molecular Geometry

Now if you click the single bond (top entity in the Bonding box (upper right corner), you can build the geometries in the table below around the central purple atom. **WATCH carefully** as you do this and you will see repulsion in action!!! If you click and hold in the space away from the boxes, you can rotate the molecule to examine the bond angles and general shape.

Number of **electron pairs** around central atom	Sketch the arrangement of the atoms	What is the angle between the electron pairs?	Are all the angles the same? If not, point out the differences.
2 pairs Name of molecular geometry:			
3 pairs Name of molecular geometry:			
4 pairs Name of molecular geometry:			
5 pairs Name of molecular geometry:			
6 pairs Name of molecular geometry:			

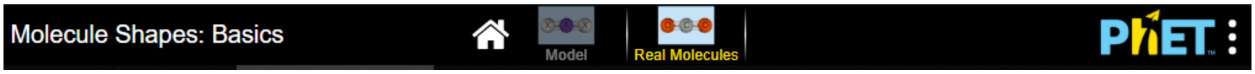
Draw the Lewis dot structures for the molecules below.

$BeCl_2$ BF_3 CH_4

PCl_5 SF_6

The number of electron pairs **on the central atom**, first atom in each formula above, determines the molecular geometry. Predict and illustrate the molecular geometries of the structures above.

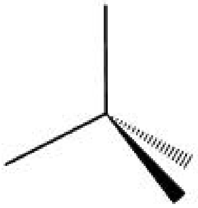
Click on the Real Molecules box at the bottom of the screen.

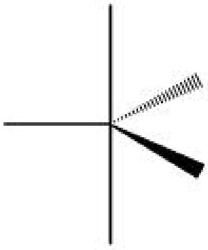


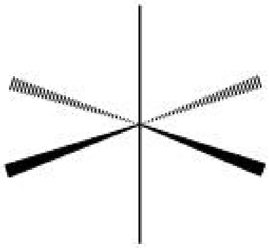
Check your predictions for the molecules. Did you get the correct answers? Revise your illustration if needed. Some help with illustrations is on the next page!

To help with the illustration of the geometries, wedge diagrams, which are used in organic chemistry, are introduced below. The solid triangular shape is in front of the plane of the paper and the dashed triangular shape is in back of the plane of the paper.

Wedge Diagrams for Three Deminsional Geometries

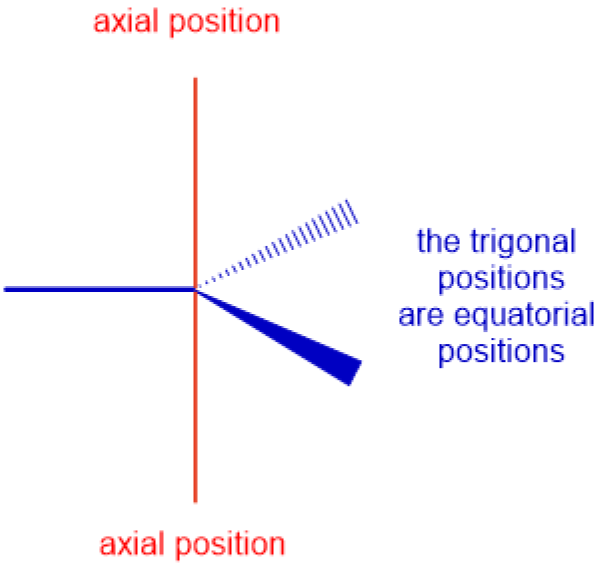

tetrahedral


trigonal bipyramidal


octahedral

On these three geometries, are there any opposite positions (place where atoms are 180° apart)? Circle them.

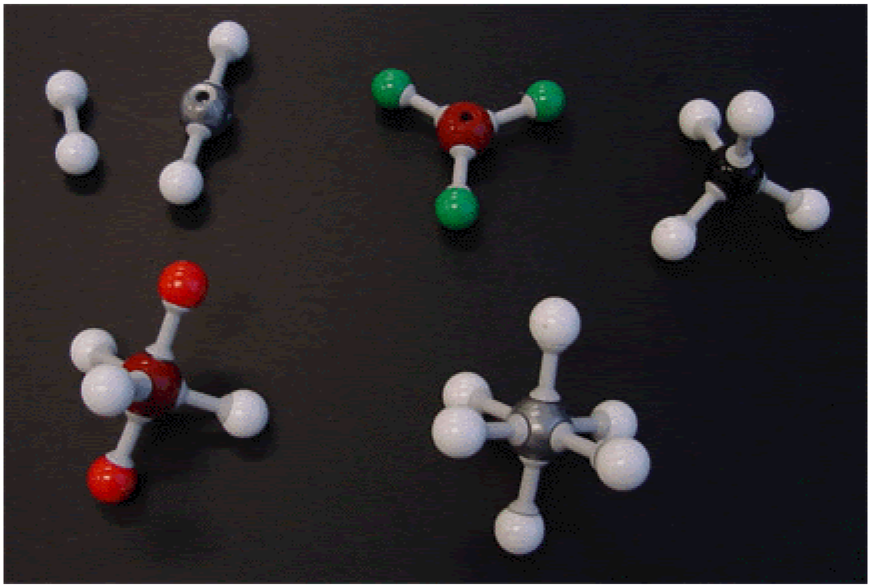
The trigonal bipyramidal geometry (tbp) needs a little further explanation before we go on. This geometry has two distinct positions - axial (180° apart) and equatorial (120° apart). This will be important later.



Here is a Google Slide with four movies (<30 seconds each) rotating the various geometries, click the present button in the upper right and then click on the short movies to view. Click here

Wedge diagrams created in **ChemSketch**.

Here are models of the ideal geometries that were just explored.



Source: https://www.indigoinstruments.com/molecular_models/molymod/

For the following molecules, draw the Lewis dot structure and determine the geometry, and sketch the molecules with all atoms identified using wedge diagrams if needed.

SiH_4 $AlCl_3$

SeF_6 AsF_5

Let's do a little carbon chemistry, where you will run across double and triple bonds. Multiple bonds are counted as one pair of electrons, so a single, double, or triple bond counts as one pair.

Determine the geometry of each carbon in the structures below. Start with drawing the Lewis dot structures for each molecule.

CO_2 H_2CO $H_2C{=}CH_2$ $HC{\equiv}CH$ CO

Draw the 3D structure of acetic acid, CH_3COOH (first carbon is tetrahedral, second carbon is trigonal planar).

Determine the molecular geometry for the following three molecules:

CH_4 NH_3 H_2O

What is different about ammonia and water compared to methane?

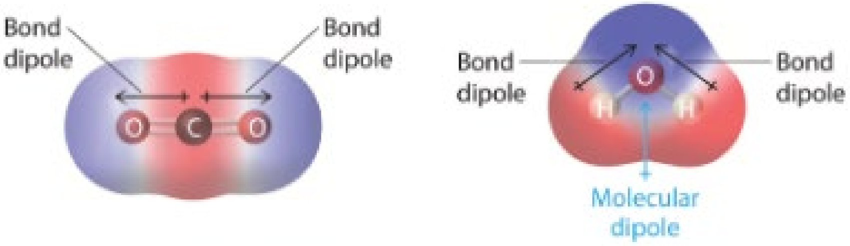
Molecular Polarity and Dipole Moment

They can occur between two ions in an ionic bond or between atoms in a covalent bond; **dipole** moments arise from differences in electronegativity. The larger the difference in electronegativity, the larger the dipole moment. ... The dipole moment is a measure of the **polarity** of the **molecule**.

Not only bonds can have dipole moments, however. A whole molecule may also have a separation of charge, depending on its molecular structure and the polarity of each of its bonds. If such a charge separation exists, the molecule is said to be a polar molecule (or dipole); otherwise the molecule is said to be nonpolar. The dipole moment measures the extent of net charge separation in the molecule as a whole. We determine the dipole moment by adding the bond moments in three-dimensional space, taking into account the molecular structure.

For diatomic molecules, there is only one bond, so its bond dipole moment determines the molecular polarity. Homonuclear diatomic molecules such as Br_2 and N_2 have no difference in electronegativity, so their dipole moment is zero. For heteronuclear molecules such as CO, there is a small dipole moment. For HF, there is a larger dipole moment because there is a larger difference in electronegativity.

In more complex molecules with polar covalent bonds, the three-dimensional geometry and the compound's symmetry determine whether there is a net dipole moment. The dipole moment of a molecule is the *vector sum* of the dipole moments of the individual bonds in the molecule. If the individual bond dipole moments cancel one another, there is no net dipole moment. Such is the case for CO_2, a linear molecule (Figure below). Each C–O bond in CO_2 is polar, yet experiments show that the CO_2 molecule has no dipole moment. Because the two C–O bond dipoles in CO_2 are equal in magnitude and oriented at 180° to each other, they cancel. As a result, the CO_2 molecule has no *net* dipole moment even though it has a substantial separation of charge. In contrast, the H_2O molecule is not linear it is bent in three-dimensional space, so the dipole moments do not cancel each other. Thus a molecule such as H_2O has a net dipole moment. We expect the concentration of negative charge to be on the oxygen, the more electronegative atom, and positive charge on the two hydrogens. This charge polarization allows H_2O to hydrogen-bond to other polarized or charged species, including other water molecules.



(a) No net dipole moment (b) Net dipole moment

Figure7.103 Above: *How Individual Bond Dipole Moments Are Added Together to Give an Overall Molecular Dipole Moment for Two Triatomic Molecules with Different Structures. (a) In CO_2, the C–O bond dipoles are equal in magnitude but oriented in opposite directions (at 180°). Their vector sum is zero, so CO_2 therefore has no net dipole. (b) In H_2O, the O–H bond dipoles are also equal in magnitude, but they are oriented at 104.5° to each other. Hence the vector sum is not zero, and H_2O has a net dipole moment.*

Reference: https://courses.lumenlearning.com/suny-mcc-organicchemistry/chapter/dipole-moments/

In the following OCS molecule has a structure similar to CO_2, but a sulfur atom has replaced one of the oxygen atoms. To determine if this molecule is polar, we draw the molecular structure. VSEPR theory predicts a linear molecule:

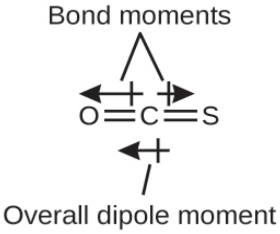


Figure 7.104 Molecular Polarity of OCS

Chloromethane, CH_3Cl, is another example of a polar molecule. Although the polar C–Cl and C–H bonds are arranged in a tetrahedral geometry, the C–Cl bonds have a larger bond moment than the C–H bond, and the bond moments do not completely cancel each other. All of the dipoles have a upward component in the orientation shown, since carbon is more electronegative than hydrogen and less electronegative than chlorine:

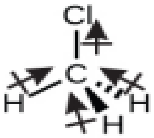
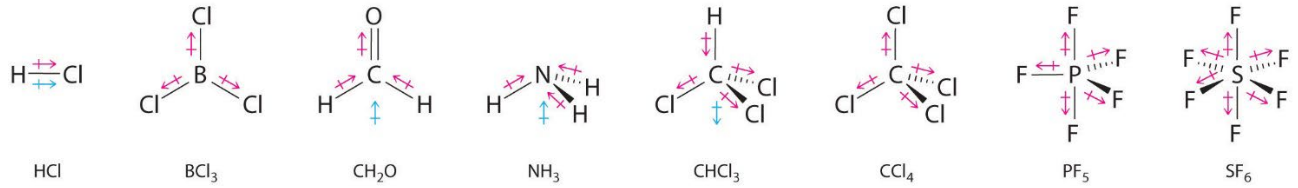


Figure 7.105 Molecular Polarity of CH_4

Other examples of molecules with polar bonds are shown in the following Figures. In molecular geometries that are highly symmetrical (most notably tetrahedral and square planar, trigonal bipyramidal, and octahedral), individual bond dipole moments completely cancel, and there is no net dipole moment. Although a molecule like $CHCl_3$ is best described as tetrahedral, the atoms bonded to carbon are not identical. Consequently, the bond dipole moments cannot cancel one another, and the molecule has a dipole moment. Due to the arrangement of the bonds in molecules that have V-shaped, trigonal pyramidal, seesaw, T-shaped, and square pyramidal geometries, the bond dipole moments cannot cancel one another. Consequently, molecules with these geometries always have a nonzero dipole moment.



Figures 7.106 *show Molecules with Polar Bonds. Individual bond dipole moments are indicated in red. Due to their different three-dimensional structures, some molecules with polar bonds have a net dipole moment (HCl, CH_2O, NH_3, and $CHCl_3$), indicated in blue, whereas others do not because the bond dipole moments cancel (BCl_3, CCl_4, PF_5, and SF_6).*

In brief, to summarize, to be polar, a molecule must:

1. Contain at least one polar covalent bond.
2. Have a molecular structure such that the sum of the vectors of each bond dipole moment does not cancel.

Properties of Polar Molecules

Polar molecules occur when there is an **electronegativity** difference between the bonded atoms. Nonpolar molecules occur when electrons are shared equal between atoms of a diatomic molecule or when polar bonds in a larger molecule cancel each other out. Following Phet Simulation activity may help to understand better.

Molecule polarity is illustrated in a Phet simulation activity below:

https://phet.colorado.edu/en/simulation/molecule-polarity

In the simulation above, the students can explore:

Predict how changing electronegativity will affect the bond polarity.

Explain the relationship between the bond dipoles and the molecular dipole.

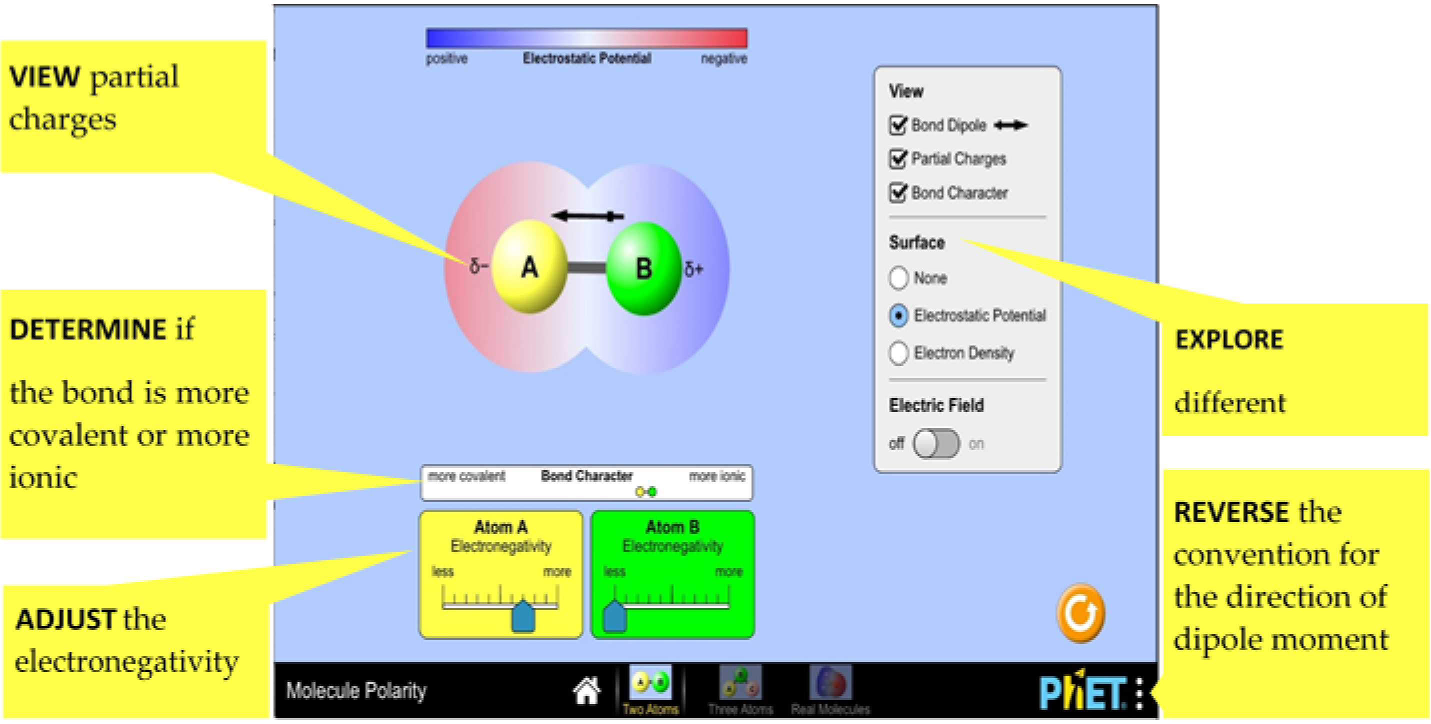
Determine if a non-polar molecule can contain polar bonds.

Describe how the ABC bond angle effects the molecular dipole.

Compare the behavior of non-polar and polar molecules in an external electric field.

Two Atoms Screen

Change the electronegativity of the atoms, view the resulting electrostatic potential or electron density, and predict the bond polarity.



VIEW partial charges

DETERMINE if the bond is more covalent or more ionic

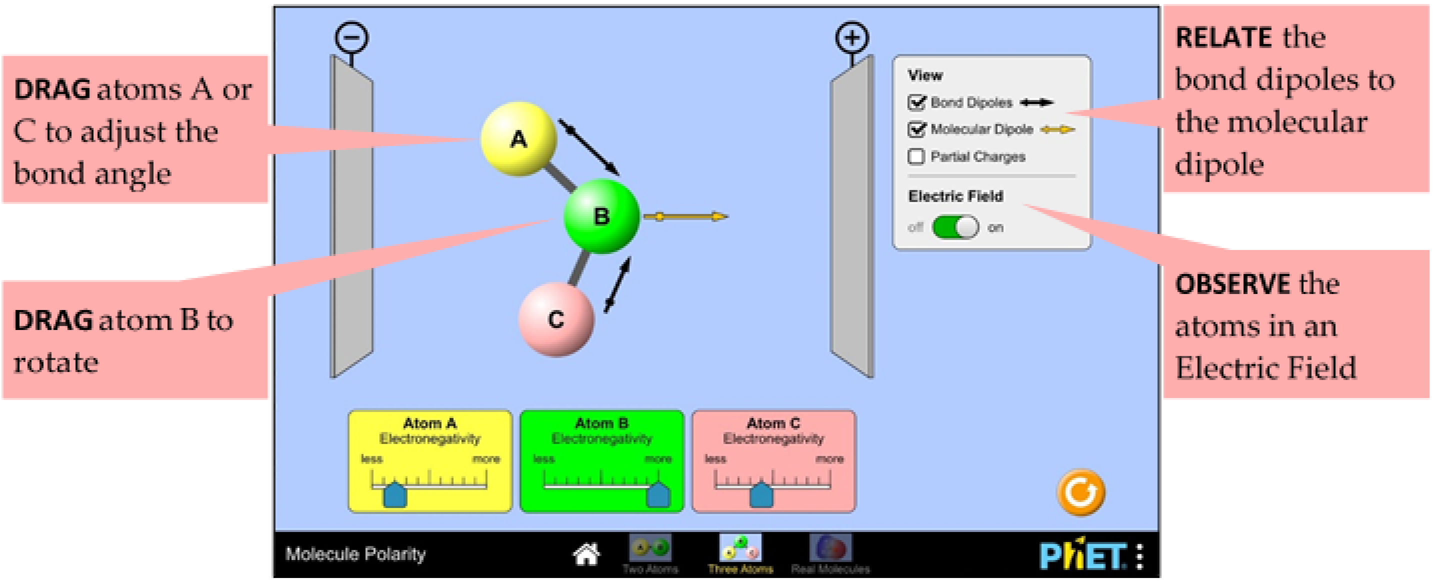
ADJUST the electronegativity

EXPLORE different

REVERSE the convention for the direction of dipole moment

Three Atoms Screen

Explore the relationship between the bond dipoles and the molecular dipole, and observe the molecule in an electric field.



View

☑ Bond Dipoles

☑ Molecular Dipole

☐ Partial Charges

Electric Field off ● on

DRAG atoms A or C to adjust the bond angle

DRAG atom B to rotate

RELATE the bond dipoles to the molecular dipole

OBSERVE the atoms in an Electric Field

Simulation conclusions:

The electronegativity slider ranges from 2 to 4, but the value is never displayed. The resulting electronegativity difference between two bonded atoms varies from 0 to 2.

Bond dipoles are parallel to the bond axis, and their length is linearly proportional to the difference in electronegativity. Note that this is a simplification; in reality, the dipole is not influenced solely by electronegativity.

The molecular dipole is the vector sum of the bond dipoles. In the Two Atoms screen, the molecular dipole is not shown, as it is equivalent to the bond dipole. In the Three Atoms screen, manipulating electronegativity results in an understanding of summing vector magnitudes, while manipulating bond angles results in an understanding of summing vector angles.

The magnitude of an atom’s partial charge is linearly proportional to the electronegativity difference between the bonded pair. If an atom has a higher electronegativity than the atom at the other end of the bond, then the partial charge’s sign is negative; otherwise it is positive. For atoms that participate in more than one bond (e.g., atom B in the “Three Atoms” screen), net partial charge is the sum of the partial charges contributed by each bond.

The electrostatic potential and electron density are linearly proportional to the electronegativity difference set by the sliders. These surfaces are not implemented for the triatomic molecule in the Three Atoms screen, because the manipulation of bond angles results in undefinable surfaces.

The Three Atoms screen allows for students to change the bond angle between the outer atoms C). The AB and BC bonds are treated independently, and the model does not allow for these atoms to repel each other. To explore how atoms would repel one another when the bond angles are changed.

Follow Up Questions:

1. Explain how the polarity of a molecule is related to the electronegativity of the atoms within the molecule. Use your knowledge gained from the previous chapters.

- In general, in chemistry, polarity refers to the distribution of electric charge around atoms, chemical groups, or molecules.
- Polar molecules occur when there is an electronegativity difference between the bonded atoms.
- Nonpolar molecules occur when electrons are shared equal between atoms of a diatomic molecule or when polar bonds in a larger molecule cancel each other out.

Examples of polar molecules include:

Water - H_2O

Hydrogen sulfide - H_2S

Ammonia - NH_3

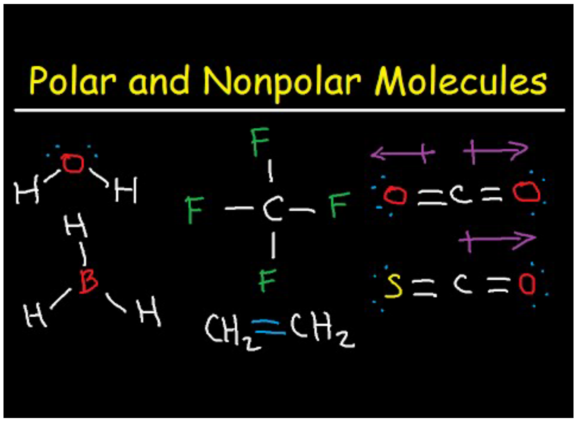
Ethanol - C_2H_6O

Sulfur dioxide - SO_2

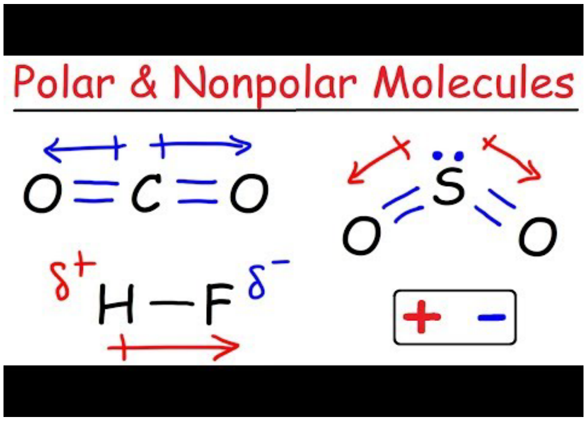
Examples of nonpolar molecules include:

- Any of the noble gasses: He, Ne, Ar, Kr, Xe (These are atoms, not technically molecules.)
- Any of the homonuclear diatomic elements: H_2, N_2, O_2, Cl_2 (These are truly nonpolar molecules.)
- Carbon dioxide - CO_2
- Benzene - C_6H_6
- Carbon tetrachloride - CCl_4
- Methane - CH_4
- Ethylene - C_2H_4
- Hydrocarbon liquids, such as gasoline and toluene
- Most organic molecules

Reference: Pauling, L. (1960). The Nature of the Chemical Bond *(3rd ed.). Oxford University Press. pp. 98–100. ISBN 0801403332.*



Reference: https://www.youtube.com/watch?v=SiZXRScxbl0&t=2s

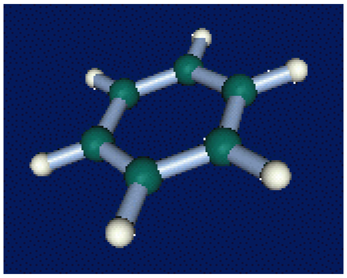


Reference: https://youtu.be/4ykSzY1_4vI

SUPPLEMENTAL

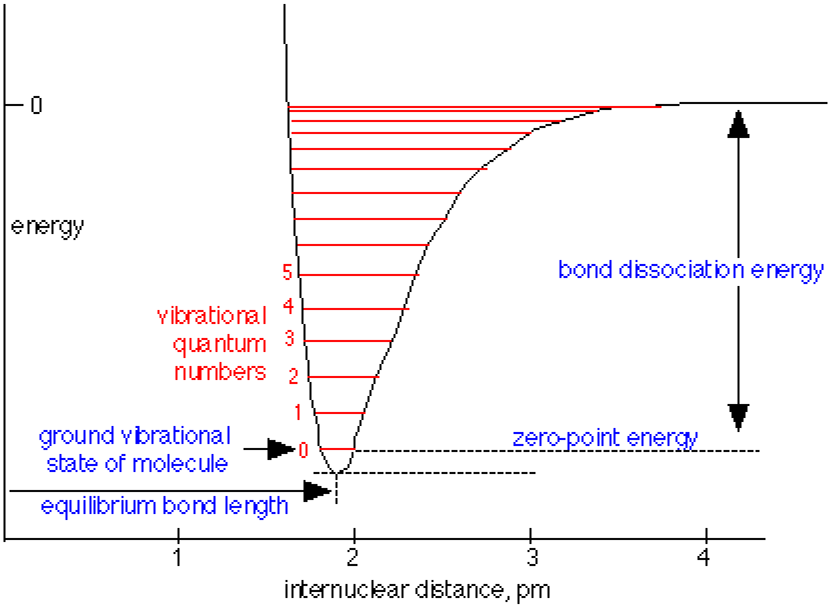
****

Research Based Information: Bond stretching and infrared absorption



[source]

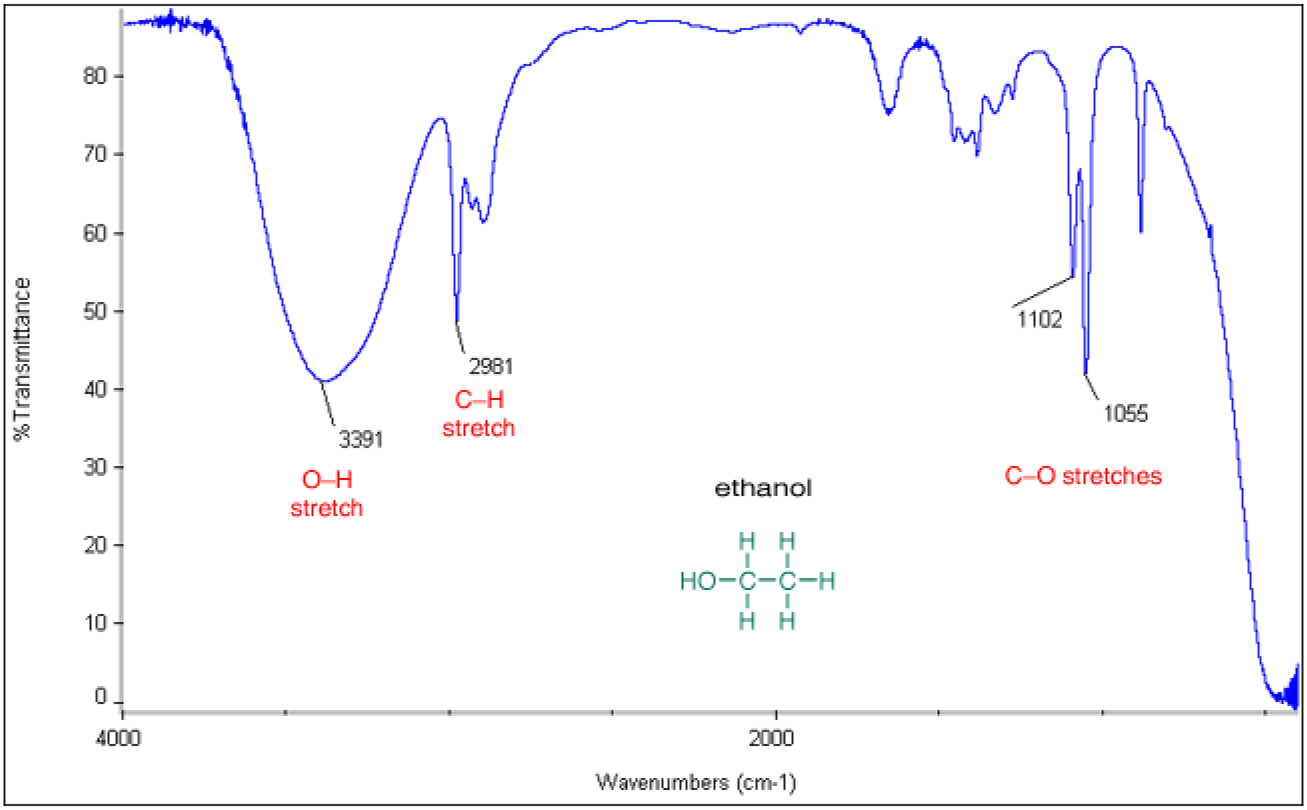
When an atom is displaced from its equilibrium position in a molecule, it is subject to a restoring force which increases with the displacement. A spring follows the same law (Hooke's law); a chemical bond is therefore formally similar to a spring that has weights (atoms) attached to its two ends. A mechanical system of this kind possesses a natural vibrational frequency which depends on the masses of the weights and the stiffness of the spring. These vibrations are initiated by the thermal energy of the surroundings; chemically-bonded atoms are never at rest at temperatures above absolute zero.



On the atomic scale in which all motions are *quantized*, a vibrating system can possess a series of vibrational frequencies, or *states*. These are depicted by the horizontal lines in the potential energy curve shown here. Notice that the very bottom of the curve does not correspond to an allowed state because at this point the positions of the atoms are precisely specified, which would violate the uncertainty principle. The lowest-allowed, or *ground* vibrational state is the one denoted by 0, and it is normally the only state that is significantly populated in most molecules at room temperature. In order to jump to a higher state, the molecule must absorb a photon whose energy is equal to the distance between the two states.

For ordinary chemical bonds, the energy differences beween these natural vibrational frequencies correspond to those of ***infrared light***. Each wavelength of infrared light that excites the vibrational motion of a particular bond will be absorbed by the molecule. In general, the stronger the bond and the lighter the atoms it connects, the higher will be its natural stretching frequency and the shorter the wavelength of light absorbed by it. Studies on a wide variety of molecules have made it possible to determine the wavelengths absorbed by each kind of bond (See here for a brief list.) By plotting the degree of absorption as a function of wavelength, one obtains the ***infrared spectrum*** of the molecule which allows one to "see" what kinds of bonds are present.

Infrared spectrum of alcohol The low points in the plot below indicate the frequencies of infrared light that are absorbed by ethanol (ethyl alcohol),
CH_3CH_2OH. Notice how stretching frequencies involving hydrogen are higher, reflecting the smaller mass of that atom. Only the most prominent absorption bands are noted here.



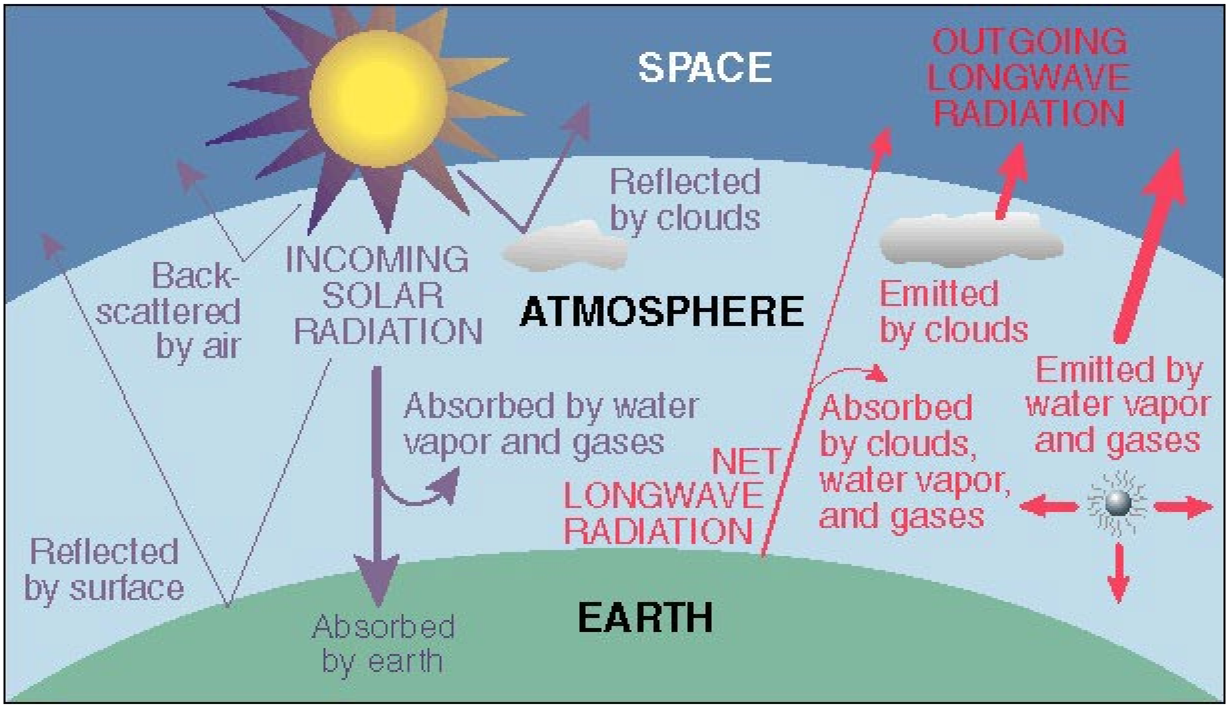
Now that you know something about bond stretching vibrations, you can impress your friends by telling them **why water is blue**

Actual infrared spectra are complicated by the presence of more complex motions (stretches involving more than two atoms, wagging, etc.), and absorption to higher quantum states (overtones), so infrared spectra can become quite complex. This is not necessarily a disadvantage, however, because such spectra can serve as a "fingerprint" that is unique to a particular molecule and can be helpful in identifying it. Largely for this reason, infrared spectrometers are standard equipment in most chemistry laboratories.

Infrared absorption and the greenhouse effect

The aspect of bond stretching and bending frequencies that impacts our lives most directly is the way that some of the gases of the atmosphere absorb infrared light and thus affect the heat balance of the Earth. Owing to their symmetrical shapes, the principal atmospheric components N_2 and O_2 do not absorb infrared light, but the minor components water vapor and carbon dioxide are strong absorbers, especially in the long-wavelength region of the infrared. Absorption of infrared light by a gas causes its temperature to rise, so any source of infrared light will tend to warm the atmosphere; this phenomenon is known as the ***greenhouse effect***.

The incoming radiation from the Sun (which contains relatively little long-wave infrared light) passes freely through the atmosphere and is absorbed by the Earth's surface, warming it up and causing it to re-emit some of this energy as long-wavelength infrared. Most of the latter is absorbed by the H_2O and CO_2 , the major greenhouse gasis in the unpolluted atmosphere, effectively trapping the radiation as heat. Thus the atmosphere is heated by the Earth, rather than by direct sunlight. Without the “***greenhouse gases***” in the atmosphere, the Earth's heat would be radiated away into space, and our planet would be too cold for life.



Radiation balance of the Earth In order to maintain a constant average temperature, the quantity of radiation (sunlight) absorbed by the surface must be exactly balanced by the quantity of long-wavelength infrared emitted by the surface and atmosphere and radiated back into space. Atmospheric gases that absorb this infrared light (depicted in red on the right part of this diagram) partially block this emission and become warmer, raising the Earth's temperature. This diagram is from the U. of Oregon Web page referenced below.

Since the beginning of the Industrial Revolution in the 19th century, huge quantities of additional greenhouse gases have been accumulating in the atmosphere. Carbon dioxide from fossil fuel combustion has been the principal source, but intensive agriculture also contributes significant quantities of methane (CH_4) and nitrous oxide (N_2O) which are also efficient far-infrared absorbers. The measurable increase in these gases is believed by many to be responsible for the increase in the average temperature of the Earth that has been noted over the past 50 years— a trend that could initiate widespread flooding and other disasters if it continues.

Links on the greenhouse effect and global warming:
University of Oregon Global Warming page
U.S. EPA Global Warming site

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WORKSHEET WITH ANSWERS

Q 1: Ionic bonds form when ions share electrons.

A- True
B- False

Answer: B

Q 2: Ionic bonds form only between atoms of nonmetals.

A- True

B- False

Answer: B

Q 3: When metallic elements become ions they:

A- Gain electrons
B- Become positively charged
C- Become negatively charged
D- Have no charge

Answer: B

Q 4: Which two elements could form an ionic compound?

A- #6 carbon and #8 oxygen
B- #1 hydrogen and #7 nitrogen
C: #3 lithium and #9 fluorine
D- #5 boron and #10 neon

Answer: C

Q 5: Which of the following compounds is not an ionic compound?

A- barium oxide
B- lithium oxide
C- carbon dixoide
D- calcium chloride

Answer: C

Q 6: What is a chemical bond that involves sharing a pair of electrons between atoms in a molecule?

A- A Cation

B- An anion

C- A Covalent bond

D- An ionic bond

Answer: C

Q 7: Covalent chemical bonds where two lobes of one involved electron orbital overlap two lobes of the other is a:

A- Ionic bond

B- Covalent bond

C- Sigma bond

D- Pi bond

Answer: D

Q 8: A chemical bond in which one atom loses an electron to form a positive ion and the other atom gains an electron to form a negative ion is a (an):

A- Cation

B- Ionic bond

C- Covalent bond

Answer: B

Q 9: A positively charged ion:

A- Sigma bond

B- Pi bond

C- Anion

D- Cation

Answer: D

Q 10: Electron-dot diagrams or Electron-dot structures:

A- Lewis Dot structure

B- An ion

C- Electronegativity

D- An anion

Answer: A

Q 10: The valence electrons of representative elements are

(a) in s orbitals only.
(b) located in the outermost occupied major energy level.
(c) located closest to the nucleus.
(d) located in d orbitals.
(e) located in the innermost occupied shell.

Answer: b

Q 11: Which one of the formulas for ionic compounds below is **incorrect**?

(a) $SrCl_2$
(b) Cs_2S
(c) $AlCl_3$
(d) Al_3P_2
(e) CaSe

Answer: d

Q 12: Which is classified as nonpolar covalent?

(a) the H-I bond in HI
(b) the H-S bond in H_2S
(c) the P-Cl bond in PCl_3
(d) the N-Cl bond in NCl_3
(e) the N-H bond in NH_3

Answer: d

Q 12: What is the total number of electrons in the correct Lewis dot formula of the sulfite ion?

(a) 8
(b) 24
(c) 26
(d) 30
(e) 32

Answer: c

Q 13: In the Lewis structure for the OF_2 molecule, the number of lone pairs of electrons around the central oxygen atom is

(a) 0
(b) 1
(c) 2
(d) 3
(e) 4

Answer: c

Q 14: The electronic structure of the SO_2 molecule is best represented as a resonance hybrid of ____ equivalent structures.

(a) 2
(b) 3
(c) 4
(d) 5
(e) This molecule does not exhibit resonance.

Answer: a

Q 14: Draw one of the resonance structures of SO_3. The formal charge of S is

(a) +2
(b) +1
(c) 0
(d) -1
(e) -2

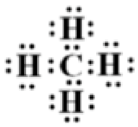
Answer: a

Q 15: Which one of the following violates the octet rule?

(a) PCl_3
(b) CBr_4
(c) NF_3
(d) OF_2
(e) AsF_5

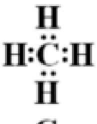
Answer: e

Q 16: Choose the electron dot diagram that correctly shows the bonding in methane CH_4.



A

B



C

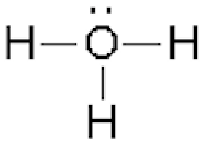
D

1- A
2- B
3- C

4- D

Answer: C

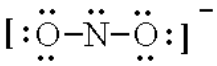
Q 17: What is the formal charge on oxygen for the hydronium ion H_3O^+?



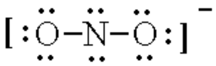
A- +3
B- -2
C- +1
D- -3
E- 0

Answer: C

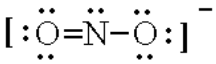
Q 18: Choose the electron dot diagram that correctly shows the bonding for the nitrite ion, NO_2^-:



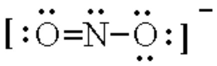
A



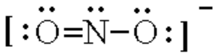
B



C



D



E

1- A
2- B
3- C
4- D
5- E

Answer: D

Q 19: Draw the best electron dot structure for the sulfate ion SO_4^{2-} that follows the octet rule. What is the formal charge on sulfur in this structure?

A- 0

B- -1

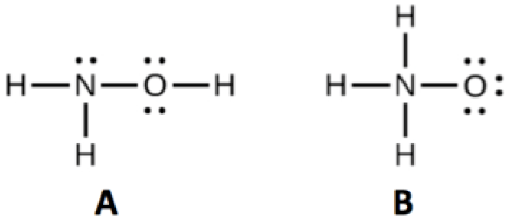
C- -2

D- +1

E- +2

Answer: E

Q 20: Are A and B resonance structures of each other?



- A- Yes
- B- No
- C- Cannot be determined from the information given

Answer: B

Q 21: How many (total) reasonable resonance structures can be drawn for the carbonate ion (CO_3^{2-})?

A- 1

B- 2

C- 3

D-4

E- None

Answer: C

Q 22: Resonance structures differ by ___________.

A- number and placement of electrons
B- number of electrons only
C- placement of atoms only
D- number of atoms only
E- placement of electrons only

Answer: E

Q 23: A water molecule (H_2O) is an example of a covalent bond because _____.

A- The hydrogen gains an electron an the oxygen loses one.
B- Electrons are shared btween the hydrogen and oxygen
C- They do not form a Neutral goup of atoms.

D- Hydrogen and oxygen are both negative ions.

Answer: B

Q 24: Ionic bonds form between what types of elements?

A- Metal to Metal
B- Metal to Nonmetal
C-Nonmetal to Nonmetal

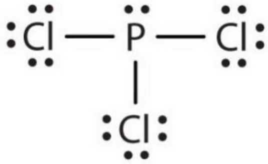
Answer: B

Q 25: Covalent bonds form between what types of elements?

A- Metal to Nonmetal
B- Nonmetal to Nonmetal
C- Metal to Metal

Answer: B

Q 26: Is this molecule polar or non-polar?

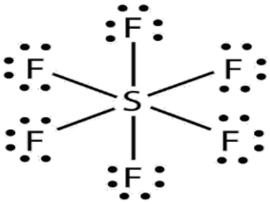


A- Polar

B- Non-Polar

Answer: A

Q 27: Is this molecule polar or non-polar?



A- Polar

B- Non-Polar

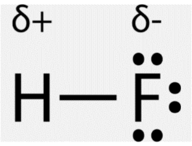
Answer: B

Q 28: In covalent bonds, electrons are ____________.

A- transferred
B- gained
C- lost
D- shared

Answer: D

Q 29: In this Lewis structure, the symbol above F means...



A- electrons are being transferred to Fluorine
B- electrons are less attracted to F than H
C- electrons are more attracted to F than H
D- Fluorine has formed a cation

Answer: C

Q 30: Which molecule contains bonds of GREATER polarity?

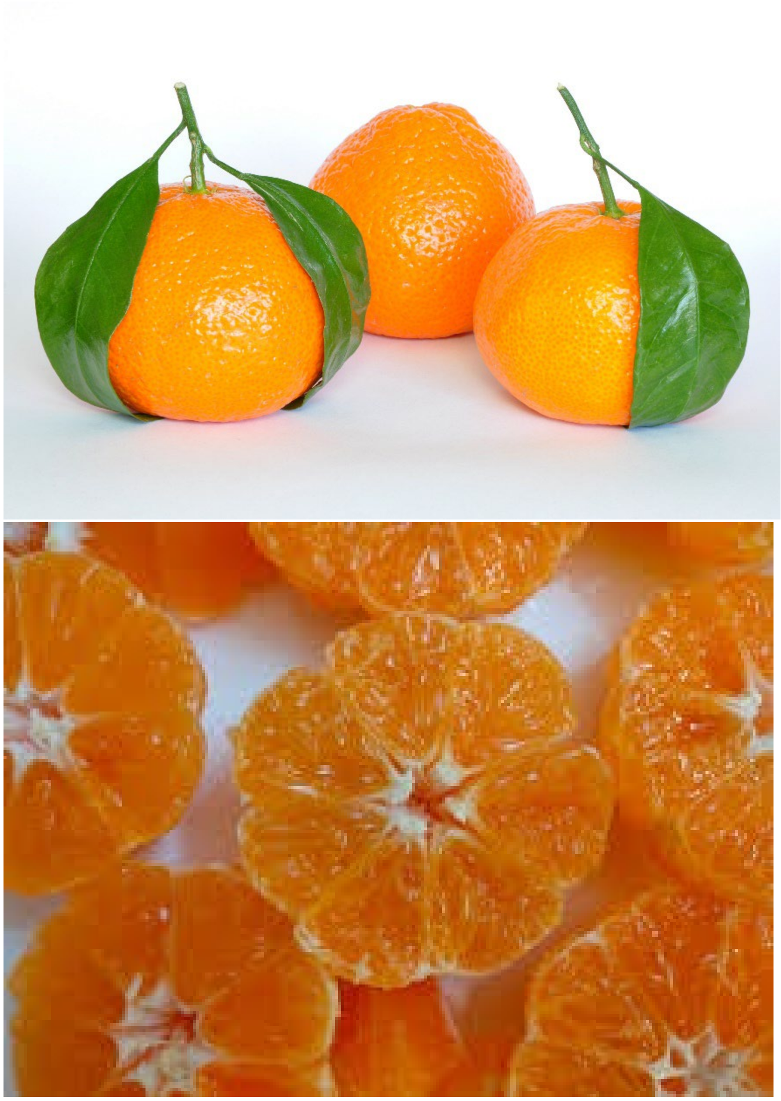
A- H_2O
B- OF_2

Answer: A

ADVANCED THEORIES OF CHEMICAL BONDING

Key Concepts:

8.1 Valence bond Theory
8.2 Hybridization
8.3 Orbital Overlaps & Types of Bonds
8.4 Molecular Orbital Theory
8.5 Magnetism & MO theory



Mandarin oranges resembles orbital lobes

I. VALENCE BOND (VB) THEORY

Nothing is perfect! Haven't you heard it too many times in your life? Yeah, and it's true! This belief applies to chemistry as well. If you thought that the Lewis theory explained all about compounds and molecules, you are wrong! It failed to explain many concepts and that is why we have the Valence Bond Theory. Here, we will read more about the valence bond theory and also look at its limitations. Yes, even this theory isn't perfect guys! Let's learn why.

As useful and appealing as the concept of the ***shared-electron pair bond*** is, it raises a somewhat troubling question that we must sooner or later face: what is the nature of the **orbitals** in which the shared electrons are contained? Up until now, we have been tacitly assuming that each valence electron occupies the same kind of atomic orbital as it did in the isolated atom. As we shall see below, his assumption very quickly leads us into difficulties.

1 Why atomic orbitals don't work for molecules

Consider how we might explain the bonding in a compound of divalent beryllium, such as beryllium hydride, BeH_2. The beryllium atom, with only four electrons, has a configuration of $1s^22s^2$. Note that the two electrons in the $2s$ orbital have opposite spins and constitute a stable pair that has no tendency to interact with unpaired electrons on other atoms.

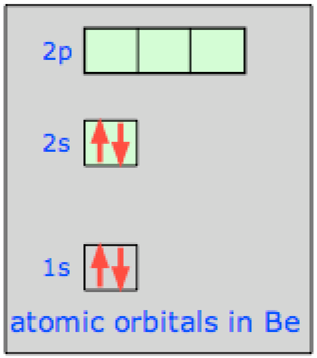


Figure 8.1 Atomic Orbitals in Be

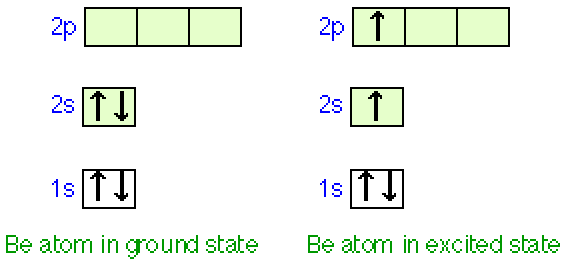


Figure 8.2 Excited energy levels of Be

The only way that we can obtain two unpaired electrons for bonding in beryllium is to promote one of the 2*s* electrons to the 2*p* level. However, the energy required to produce this excited-state atom would be sufficiently great to discourage bond formation. It is observed that Be does form reasonably stable bonds with other atoms. Moreover, the two bonds in BeH_2 and similar molecules are completely equivalent; this would not be the case if the electrons in the two bonds shared Be orbitals of different types, as in the "excited state" diagram above.

These facts suggest that it is incorrect to assume that the distribution of valence electrons that are shared with other atoms can be described by atomic-type *s, p*, and *d* orbitals at all.

Remember that these different orbitals arise in the first place from the interaction of the electron with the *single central* electrostatic force field associated with the positive nucleus. An outer-shell electron in a bonded atom will be under the influence of a force field emanating from *two* positive nuclei, so we would expect the orbitals in the bonded atoms to have a somewhat different character from those in free atoms. In fact, as far as valence electrons are concerned, we can throw out the concept of atomic orbital altogether and reassign the electrons to a new set of ***molecular orbitals*** that are characteristic of each molecular configuration. This approach is indeed valid, but we will defer a discussion of it until a later unit.

For now, we will look at a less-radical model that starts out with the familiar valence-shell atomic orbitals, and allows them to combine to form ***hybrid orbitals*** whose shapes conform quite well to the bonding geometry that we observe in a wide variety of molecules.

2 What are hybrid orbitals?

About orbitals: a quick review

First, recall that the electron, being a quantum particle, cannot have a distinct location; the most we can do is define the region of space around the nucleus in which the probability of finding the electron exceeds some arbitrary value, such as 90% or 99%. This region of space is the orbital. Because of the wavelike character of matter, the orbital corresponds to a standing wave pattern in 3-dimensional space which we can often represent more clearly in 2-dimensional cross section. The quantity that is varying ("waving") is a number denoted by ψ (*psi*) whose value varies from point to point according to the wave function for that particular orbital.

Orbitals of all types are simply mathematical functions that describe particular standing-wave patterns that can be plotted on a graph but have no physical reality of their own. Because of their wavelike nature, two or more orbitals (i.e., two or more functions ψ) can be combined both in-phase and out-of-phase to yield a pair of resultant orbitals which, to be useful, must have squares that describe actual electron distributions in the atom or molecule.

The *s,p,d* and *f* orbitals that you are familiar with are the most convenient ones for describing the electron distribution in isolated atoms because assignment of electrons to them according to the usual rules always yields an overall function Ψ^2 that predicts a spherically symmetric electron distribution, consistent with all physical evidence that atoms are in fact spherical. For atoms having more than one electron, however, the *s,p,d,f* basis set is only one of many possible ways of arriving at the same observed electron distribution. We use it not because it is unique, but because it is the simplest.

In the case of a molecule such as BeH_2, we know from experimental evidence that the molecule is linear and therefore the electron density surrounding the central atom is no longer spherical, but must be concentrated along two directions 180° apart, and we need to construct a function Ψ^2 having these geometrical properties. There are any number of ways of doing this, but it is convenient is to use a particular set of functions ψ (which we call ***hybrid orbitals***) that are constructed by combining the atomic *s,p,d,* and *f* functions that are already familiar to us.

You should understand that *hybridization is not a physical phenomenon*; it is merely a *mathematical operation* that combines the atomic orbitals we are familiar with in such a way that the new (hybrid) orbitals possess the geometric and other properties that are reasonably consistent with what we observe in a wide range (but certainly not in all) molecules. In other words, hybrid orbitals are *abstractions* that describe reality fairly well in certain classes of molecules (and fortunately, in much of the very large class of organic substances) and are therefore a useful means of organizing a large body of chemical knowledge... but they are far from infallible.

This approach, which assumes that the orbitals remain more or less localized on one central atom, is the basis of the theory which was developed in the early 1930s, mainly by ***Linus Pauling***.

Figure 8.3 Linus Pauling

Linus Pauling (1901-1994) was the most famous American chemist of the 20th century and the author of the classic book *The Nature of the Chemical Bond*. His early work pioneered the application of X-ray diffraction to determine the structure of complex molecules; he then went on to apply quantum theory to explain these observations and predict the bonding patterns and energies of new molecules.

(His short and lucid 1928 article updating Lewis' theory of the shared-electron covalent bond can be seen here.) Pauling, who spent most of his career at Cal Tech, won the Nobel Prize for Chemistry in 1954 and the Peace Prize in 1962.

"In December 1930 Pauling had his famous 'breakthrough' where, in a rush of inspiration, he '*stayed up all night, making, writing out, solving the equations, which were so simple that I could solve them in a few minutes*'. This flurry of calculations would eventually become the first of Pauling's germinal series of papers on the nature of the chemical bond. '*I just kept getting more and more euphorious as time went by*', Pauling would recall. " [source]

Although the hybrid orbital approach has proven very powerful (especially in organic chemistry), it does have its limitations. For example, it predicts that both H_2O and H_2S will be tetrahedrally coordinated bent molecules with bond angles slightly smaller than the tetrahedral angle of 109.5° owing to greater repulsion by the nonbonding pair. This description fits water (104.5°) quite well, but the bond angle in hydrogen sulfide is only 92°, suggesting that atomic *p* orbitals (which are 90° apart) provide a better description of the electron distribution about the sulfur atom than do sp^3 hybrid orbitals.

The hybrid orbital model is simple to apply and understand, but it is best regarded as one special way of looking at a molecule that can often be misleading. Another viewpoint, called the *molecular orbital theory*, offers us a complementary perspective that it is important to have if we wish to develop a thorough understanding of chemical bonding in a wider range of molecules.

Constructing hybrid orbitals

Below: "Constructive" and "destructive" combinations of 2*p* and 2*s* wave functions (line plots) give rise to the *sp* hybrid function shown at the right.
The solid figures depict the corresponding probability functions ψ^2.

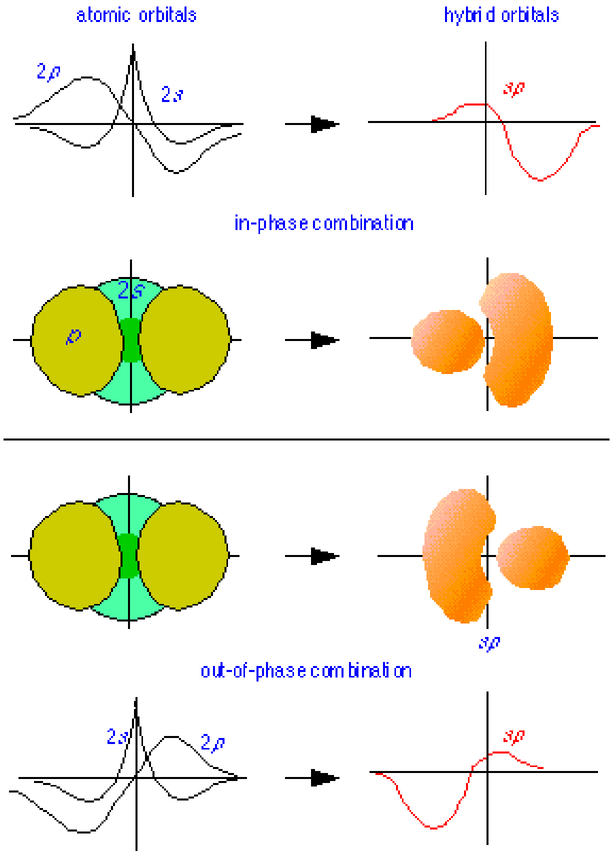


Figure 8.4 Combination of Atomic Orbitals

Hybrid orbitals are constructed by combining the ψ functions for atomic orbitals. Because wave patterns can combine both constructively and destructively, a pair of atomic wave functions such as the *s*- and *p*- orbitals shown at the left can combine in two ways, yielding the *sp hybrids* shown.

Two central theme of VB theory:

1. Opposing spins of the electron pair: According to the exclusion principle, the space formed by the overlapping orbitals has a maximum capacity of two electrons that must have opposite spins. When the molecule of H_2 forms for instance, electrons of two H atoms occupy the overlapping 1s orbitals and have opposite spins.

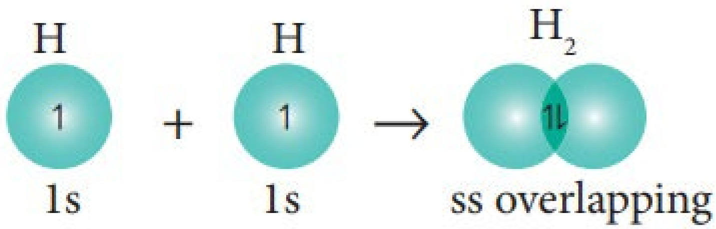


Fig 10. 18 Formation of hydrogen molecule

Figure 8.5 Overlap of H-atomic orbitals

Ref: Commons.wikimedia.org/

2. Maximum overlap of bonding orbitals: The greater the orbital overlap, the stronger the bond. The extent of overlap depends on the shape and energy of the orbitals. In the HF bond, for example, the 1s orbital of H overlaps the half-filled 2p orbital of F along the long axis of the orbital. Bond formed in any other direction would be weaker.

In this theory, Molecules are visualized as a group of atoms sharing electron pairs between atomic orbitals. Hybrid orbitals which are combinations of the native atomic orbitals, are required to explain molecular structure.

II. HYBRIDIZATION

A) Sp3 hybridization

VB theory proposes that one s and all three p-orbitals of the central atom mix and form four sp3 hybrid orbitals, which point toward the vertices of a tetrahedron. In methane CH_4, the central C atom is sp3 hybridized. Its four valence electrons half-fill the four sp3 hybrids, which overlap the half-filled 1s orbitals of the four H atoms and form four C-H bonds.

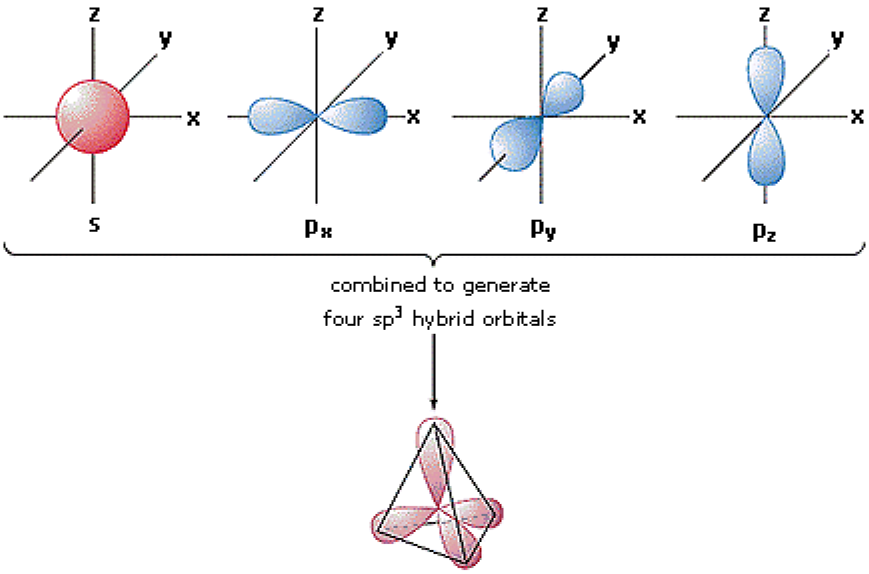


Figure 8.6 Overlap of s-p atomic orbitals

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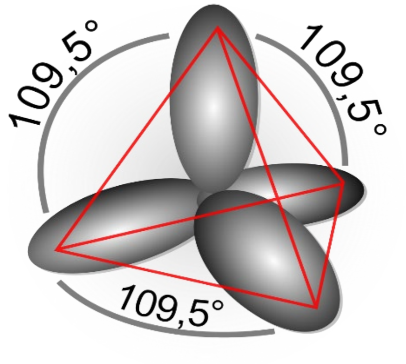

Figure 8.7 sp3 hybrid orbital shape

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Here is the electronic distribution

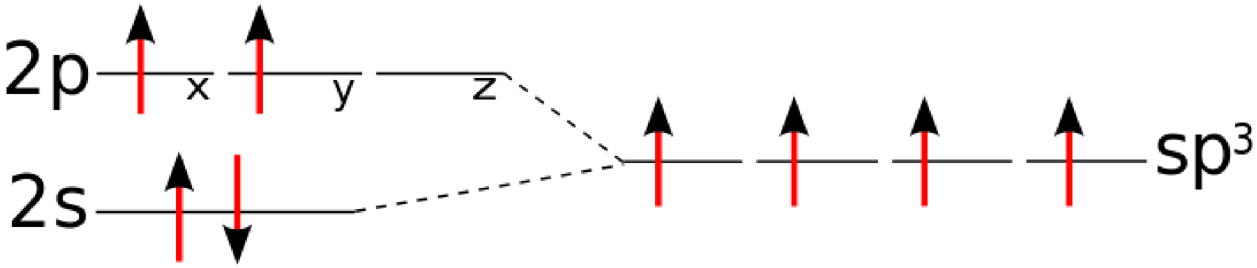

Figure 8.8 Electronic arrangement in sp3 hybrid orbital

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CH_4 hybridization:

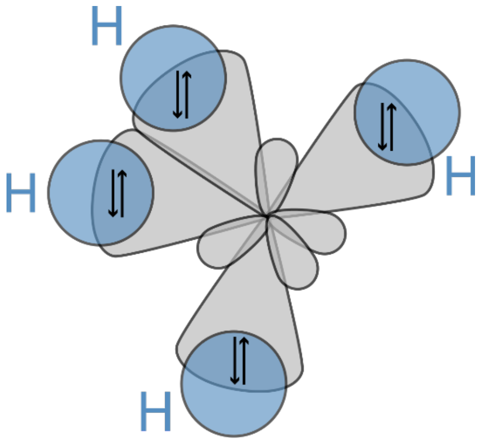

Figure 8.9 Electronic arrangement in Hybrid Orbitals of Methane

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Tetrahedral (sp^3) hybridization

Let us now look at several tetravalent molecules, and see what kind of hybridization might be involved when four outer atoms are bonded to a central atom. Perhaps the commonest and most important example of this bond type is methane, CH_4.

In the ground state of the free carbon atom, there are two unpaired electrons in separate 2*p* orbitals. In order to form four bonds (tetravalence), need four unpaired electrons in four separate but equivalent orbitals. We assume that the single 2*s*, and the three 2*p* orbitals of carbon mix into four sp^3 hybrid orbitals which are chemically and geometrically identical; the latter condition implies that the four hybrid orbitals extend toward the corners of a tetrahedron centered on the carbon atom.

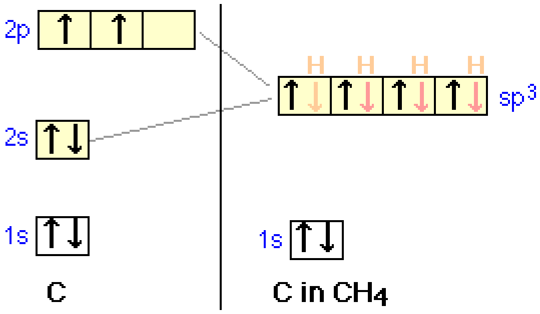
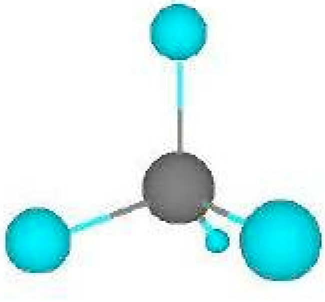


Figure 8.10 Formation of Hybrid Orbitals of Methane

Ref: Commons.wikimedia.org/

Methane is the simplest hydrocarbon; the molecule is approximately spherical, as is shown in the space-filling model:



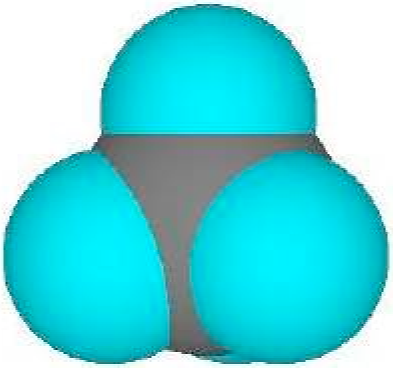


Figure 8.11(a) Ball and Stick 3D model of Methane

Figure 8.11(b) Space filling 3D model of Methane

[source]

By replacing one or more of the hydrogen atoms in CH_4 with another sp^3 hybridized carbon fragments, hydrocarbon chains of any degree of complexity can be built up. The simplest of these is ethane:

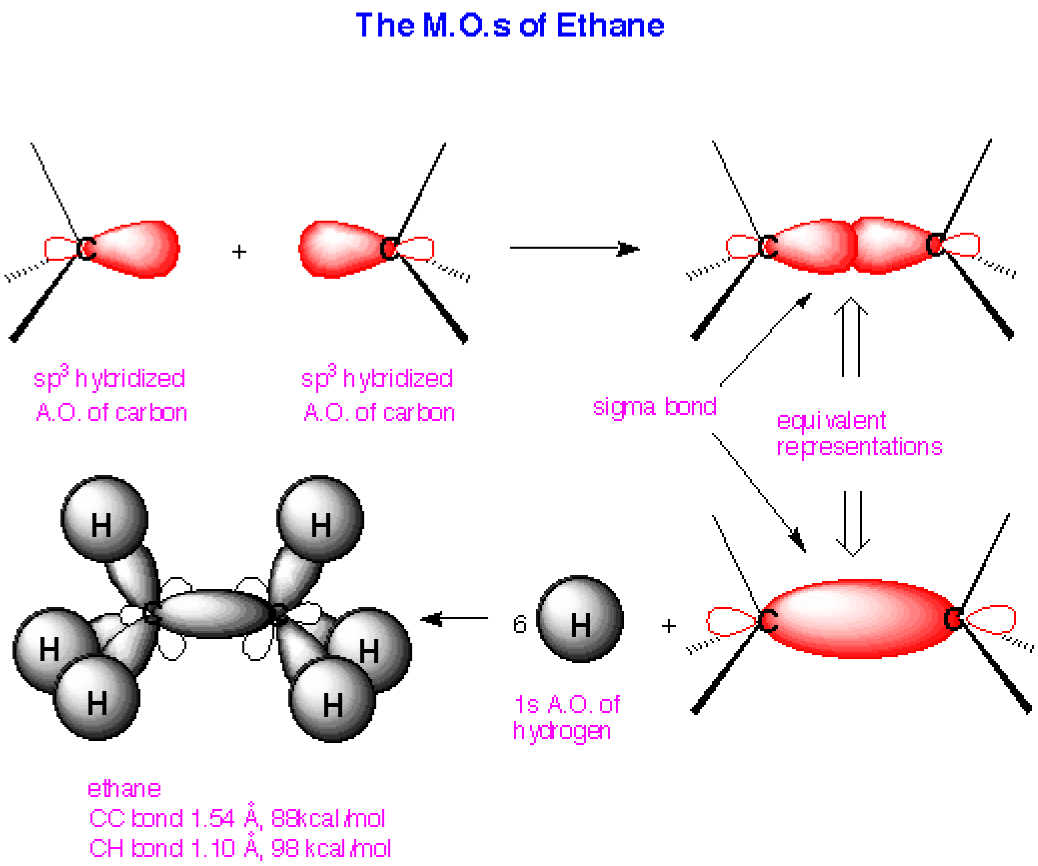


Figure 8.12 Overlapping of sp3 hybrid orbitals in ethane

This shows how an *sp*^{3} orbital on each of two two carbon atoms join (overlap) to form a carbon-carbon bond, and then the remaining carbon *sp*^{3} orbital overlaps with six hydrogen 1s orbitals to form the ethane molecule. [source - Yale U.]

4 Lone pair electrons in hybrid obitals

If lone pair electrons are present on the central atom, these can occupy one or more of the *sp*^{3} orbitals. This causes the molecular geometry to be different from the coordination geometry, which remains tetrahedral.

In the ammonia molecule, for example, the nitrogen atom normally has three unpaired p electrons, but by mixing the 2*s* and 2*p* orbitals, we can create four *sp*^{3}-hybrid orbitals just as in carbon. Three of these can form shared-electron bonds with hydrogen, resulting in ammonia, NH_3.

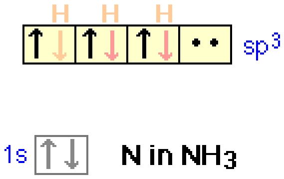


Figure 8.13 Lone pair in ammonia

The fourth of the sp^3 hybrid orbitals contains the two remaining outer-shell electrons of nitrogen which form a non-bonding lone pair. In acidic solutions these can coordinate with a hydrogen ion, forming the ammonium ion NH_4^+.

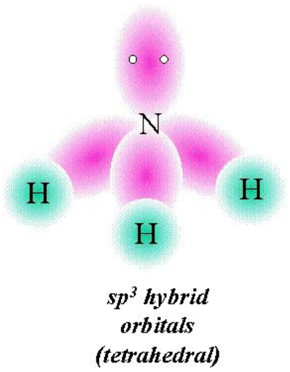


Figure 8.14 sp3 Hybrid Orbitals in ammonia

Although no bonds are formed by the lone pair in NH_3, these electrons do give rise to a charge cloud that takes up space just like any other orbital.

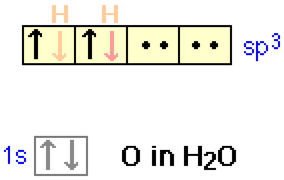


Figure 8.15 Lone pair in water

In the water molecule, the oxygen atom can form four sp^3 orbitals. Two of these are occupied by the two lone pairs on the oxygen atom, while the other two are used for bonding. The observed H-O-H bond angle in water (104.5°) is less than the tetrahedral angle (109.5°); one explanation for this is that the non-bonding electrons tend to remain closer to the central atom and thus exert greater repulsion on the other orbitals, thus pushing the two bonding orbitals closer together.

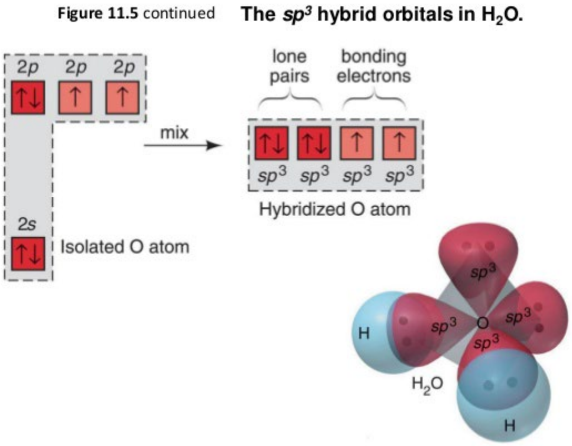
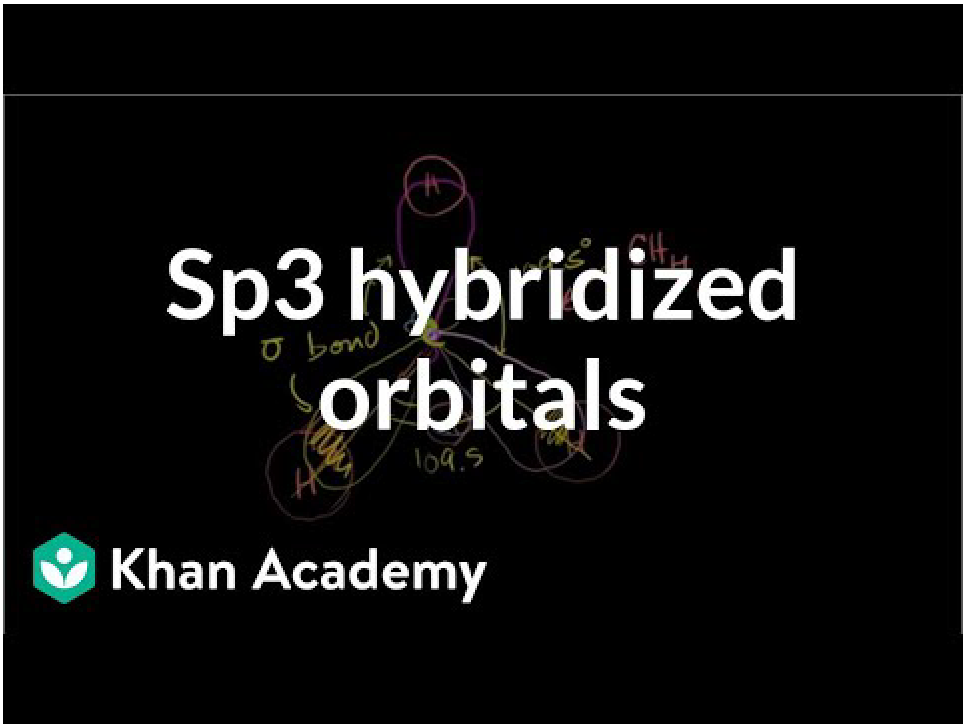


Figure 8.16 Atomic Orbital mixing in water

Ref: commons.wikimedia.org/



B) Sp2 Hybridization:

From an energy standpoint, we can represent the transition from atomic *s*- and *p*-orbitals to an *sp* hybrid orbital in this way:

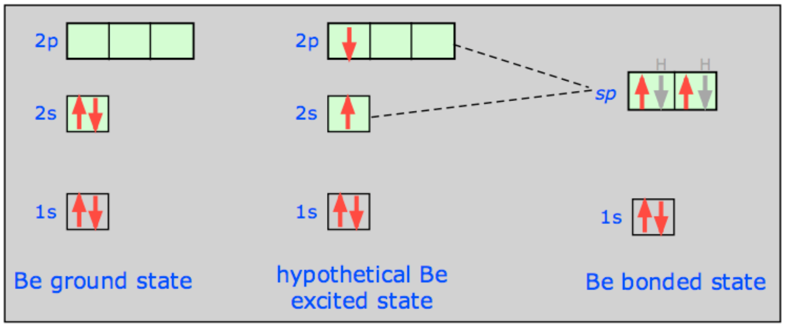


Figure 8.17 Atomic Orbital overlap in sp2 Hybridization

Notice here that 1) the total number of occupied orbitals is conserved, and 2) the two *sp* hybrid orbitals are intermediate in energy between their parent atomic orbitals.

In terms of plots of the actual orbital functions ψ we can represent the process as follows:

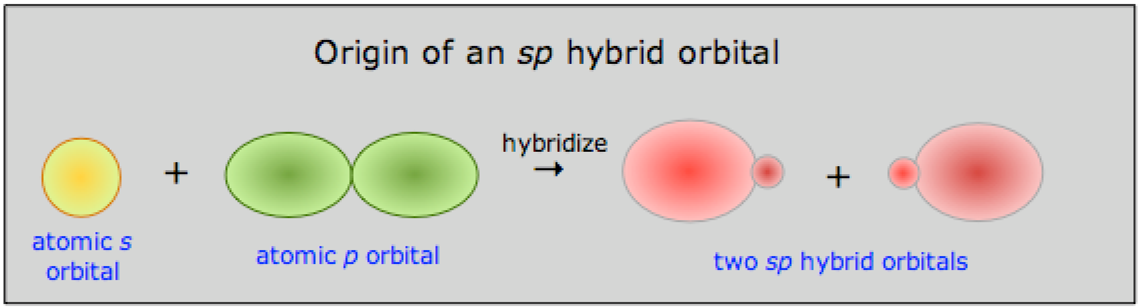


Figure 8.18 Atomic Orbital overlap in sp Hybridization

The probability of finding the electron at any location is given not by ψ, but by ψ^2, whose form is roughly conveyed by the solid figures in this illustration.

In order to rationalize the trigonal planar electron-group arrangement and the shape of the molecules based

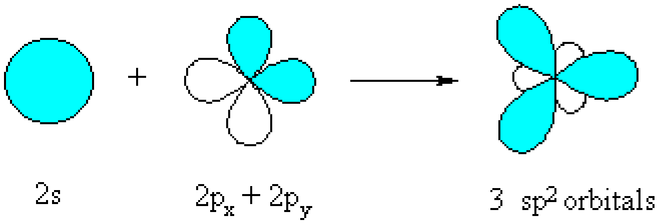


Figure 8.19 Formation of sp2 hybrid Orbital

When one s-orbital mixes with two out three p-orbitals, three sp2 hybrid orbitals are produced and one p orbital remains un-hybridized.

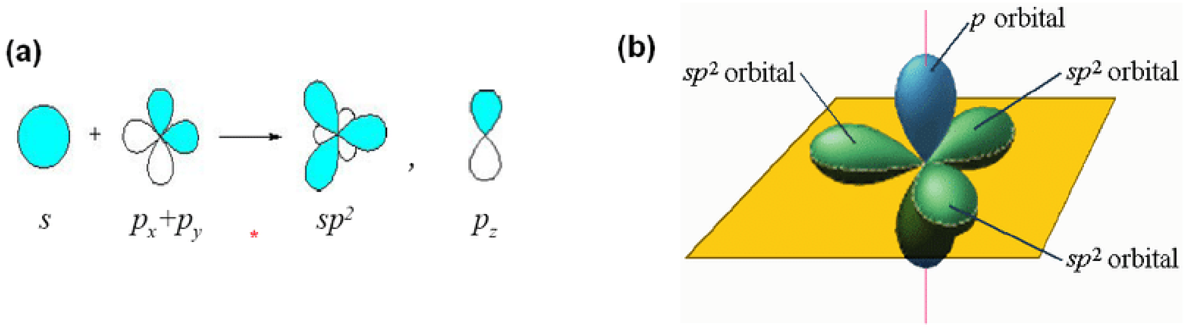


Figure 8.20 3D Arrangement of hybrid Orbitals

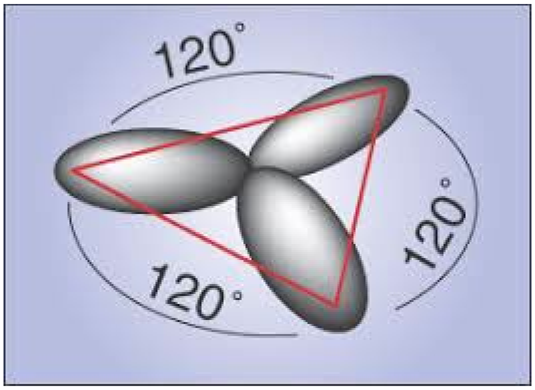


Figure 8.21 Shape of hybrid Orbitals

Example: BF_3

VB Theory proposes that the central B atom in BF_3 molecule is sp2 hybridized. The figure below shows three sp2 hybrid orbitals in the trigonal plane, with the 3rd 2p orbital unhybridized and perpendicular to the plane. Each sp2 hybrid orbital overlaps with 2p orbital of F atom. There are total six valence electrons are present in three sp2 orbitals, 3 from B atom and one from each F atom.

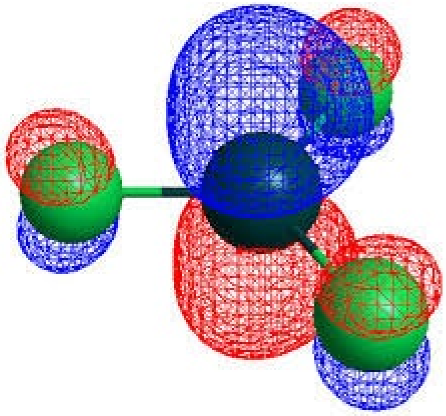


Figure 8.22 3D Shape of hybrid Orbitals in BF_3

Ethylene(C_2H_4) is the example of a molecule where Sp2 hybridization can be observed. Look at the diagram below. VB theory can explain the double nature of the carbon carbon bond in ethylene. Each C atom's four valence electrons half fill its three sp2 orbitals and its unhybridized p orbitals, which lied perpendicular to the sp^2 plane. Two sp2 orbitals from each C forms C-H sigma bond by overlapping 1s orbital of H atom.

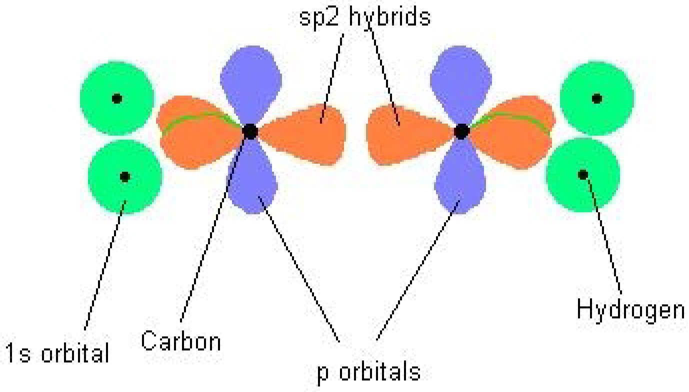


Figure 8.23 sp2 Hybrid Orbitals overlap in C_2H_4

The third sp2 orbital forms a C-C sigma bond with another C because their orientation allows end-to-end overlap. With the σ-bonded C atoms near each other, their half-filled un-hybridized 2p orbitals are close enough to overlap side by side. Such overlap forms π bonds.

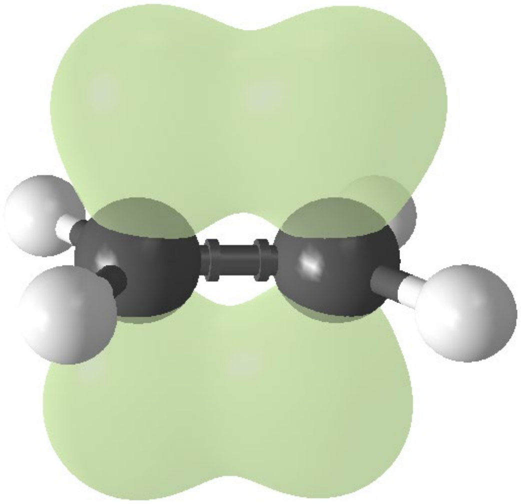
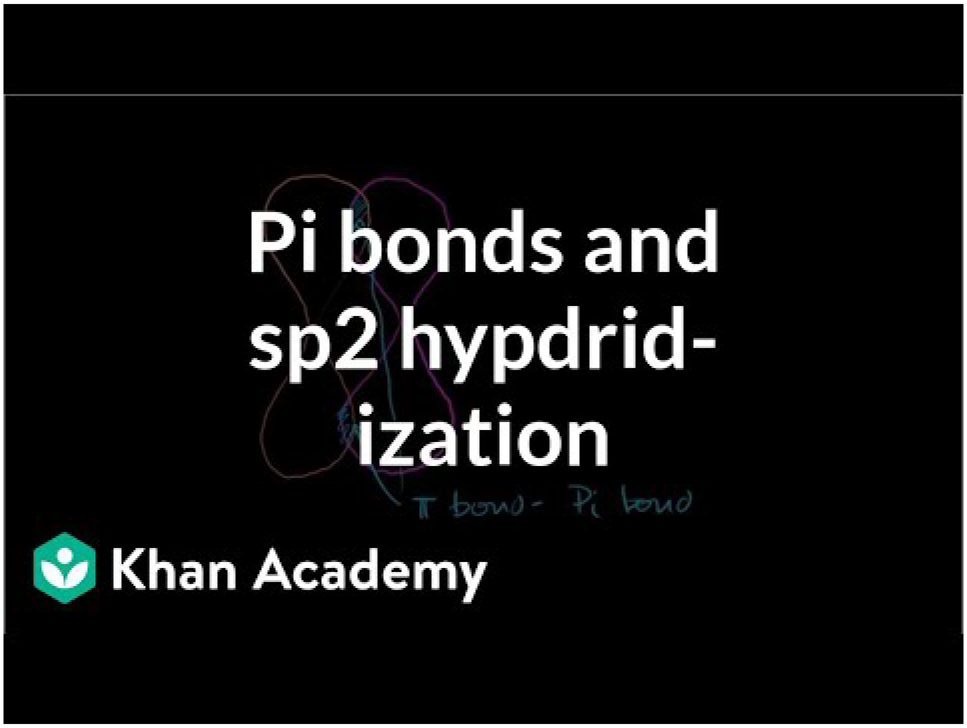


Figure 8.24 Electron Cloud in C_2H_4



Pi bonds and sp2 hypdrid-ization

π bond - Pi bond

Khan Academy

Trigonal (sp^2) hybridization

We can now go on to apply the same ideas to some other simple molecules. In boron trifluoride, for example, we start with the boron atom, which has three outer-shell electrons in its normal or ground state, and three fluorine atoms, each with seven outer electrons. As is shown in this configuration diagram, one of the three boron electrons is unpaired in the ground state. In order to explain the trivalent bonding of boron, we postulate that the atomic *s*- and *p*- orbitals in the outer shell of boron mix to form three equivalent hybrid orbitals. These particular orbitals are called ***sp^2* hybrids**, meaning that this set of orbitals is derived from one s- orbital and two p-orbitals of the free atom.

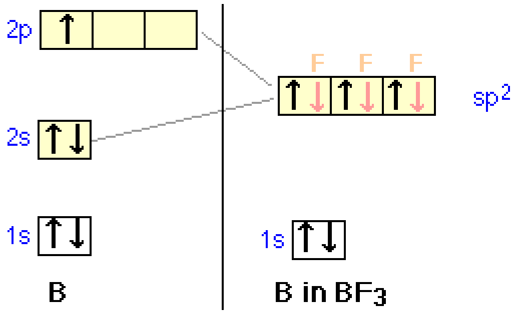
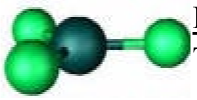


Figure 8.25 Electronic Arrangement in sp2 hybrid orbitals in BF$_3$

This illustration shows how an *s*-orbital mixes with two *p* orbitals to form a set of three sp^2 hybrid orbitals. Notice again how the three atomic orbitals yield the same number of hybrid orbitals.



Boron trifluoride BF_3 is a common example of sp^2 hybridization. The molecule has plane trigonal geometry.

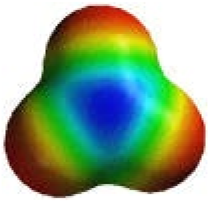


Figure 8.25 3D shape in sp2 hybrid orbitals in BF_3

C) sp hybridization

Hybrids derived from atomic ***s***- and ***p*** orbitals

Digonal bonding: sp-hybrid orbitals

Returning to the example of BeH_2, we can compare the valence orbitals in the free atoms with those in the beryllium hydride molecule as shown here. Of course, the overlap between the hydrogen-1s orbitals and the two lobes of the beryllium sp-hybrid orbitals constitutes the two Be— H "bonds" in this molecule.

Notice that whereas a single *p*-orbital has lobes on both sides of the atom, a single *sp*-hybrid has most of its electron density on one side, with a minor and more spherical lobe on the other side. This minor lobe is centered on the central atom (some textbook illustrations don't get this right.)

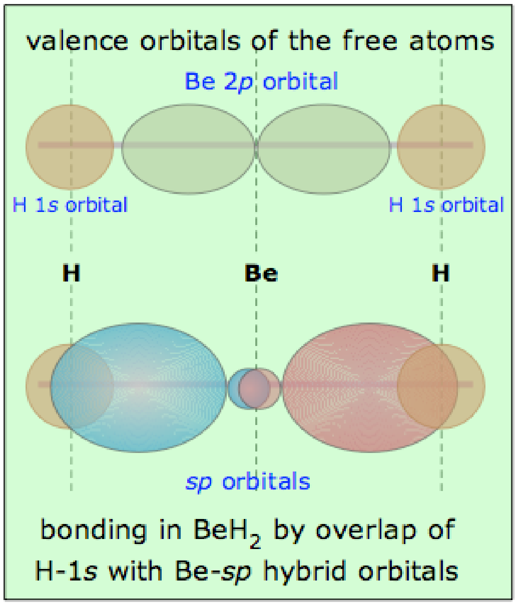


Figure 8.26 Formation of sp Hybrid Orbitals

As far as the *shape* of the molecule is concerned, the result is exactly the same as predicted by the VSEPR model (although hybrid orbital theory predicts the same result in a more fundamental way.) We can expect any central atom that uses *sp*-hybridization in bonding to exhibit linear geometry when incorporated into a molecule.

When two electron groups surround the central atom, we observe a linear shape

Both shape and orientation maximize overlap with the orbital of the other atom in the bond.

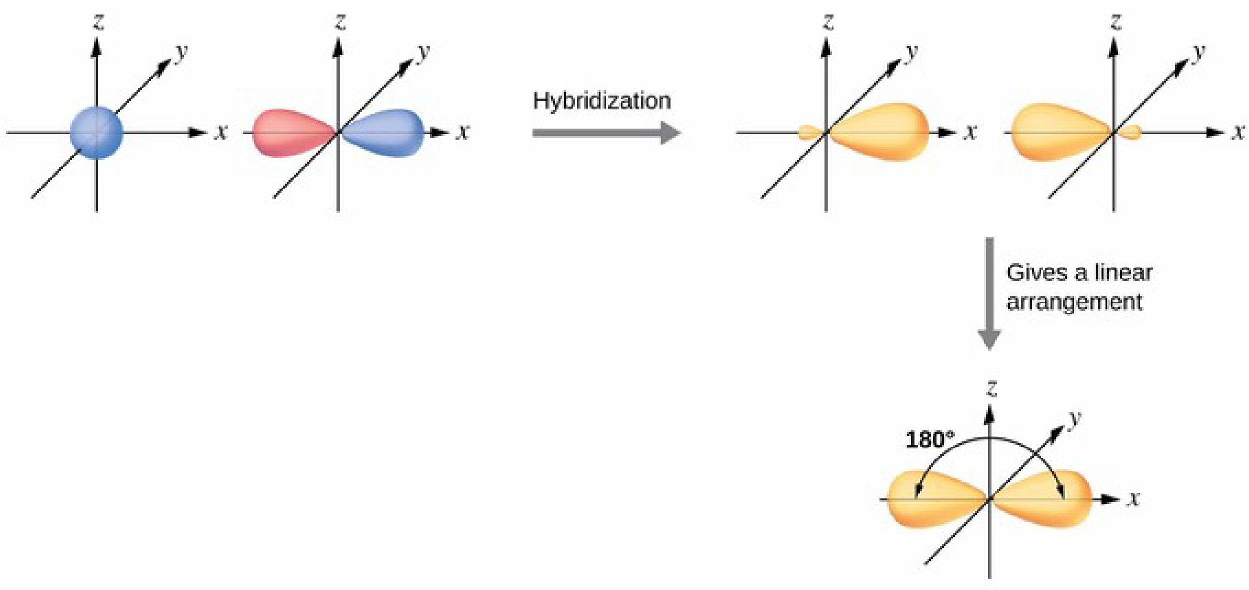


Figure 8.27 Orbital Overlap in sp Hybrid Orbitals

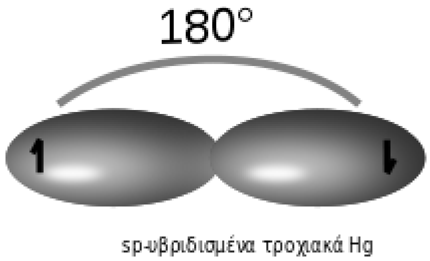


Figure 8.28 3D shape in sp Hybrid Orbitals

Beryllium chloride is one of examples of molecules where the central atom Be is sp hybridized. The 2s and one of the three 2p orbitals of Be mix and form two sp orbitals. These overlap 3p orbitals of two Cl atoms of the four valence electrons-two from Be and one from each Cl-occupy the overlapped orbitals in pairs with opposite spins. The two unhybridized 2p orbitals of Be lie perpendicular to each other and to the bond axes. Thus through hybridization, the paired 2s electrons in the isolated Be atom are distributed into two sp orbitals, which form the two Be-Cl bond.

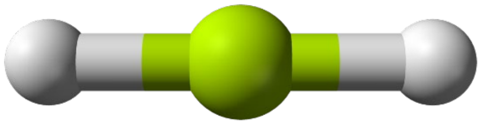


Figure 8.28 3D shape of sp Hybrid Orbitals in $BeCl_2$

Ref: Commons.wikimedia.org/

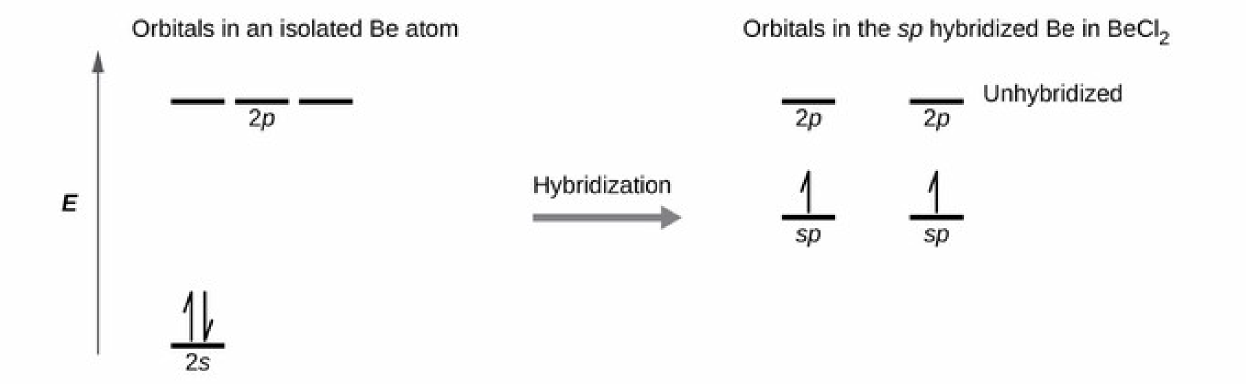


Figure 8.29 3D shape of sp Hybrid Orbitals in $BeCl_2$

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In case of acetylene(C_2H_2),each carbon has two unhybridized p orbitals.

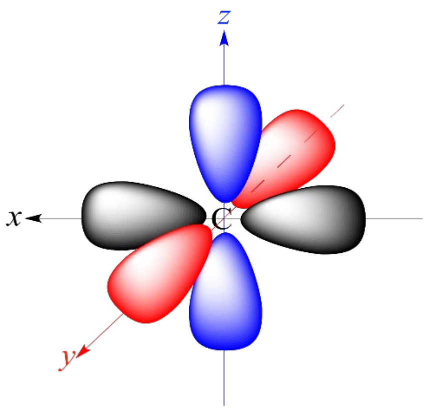

Figure 8.30 3D shape of sp Hybrid Orbitals in C

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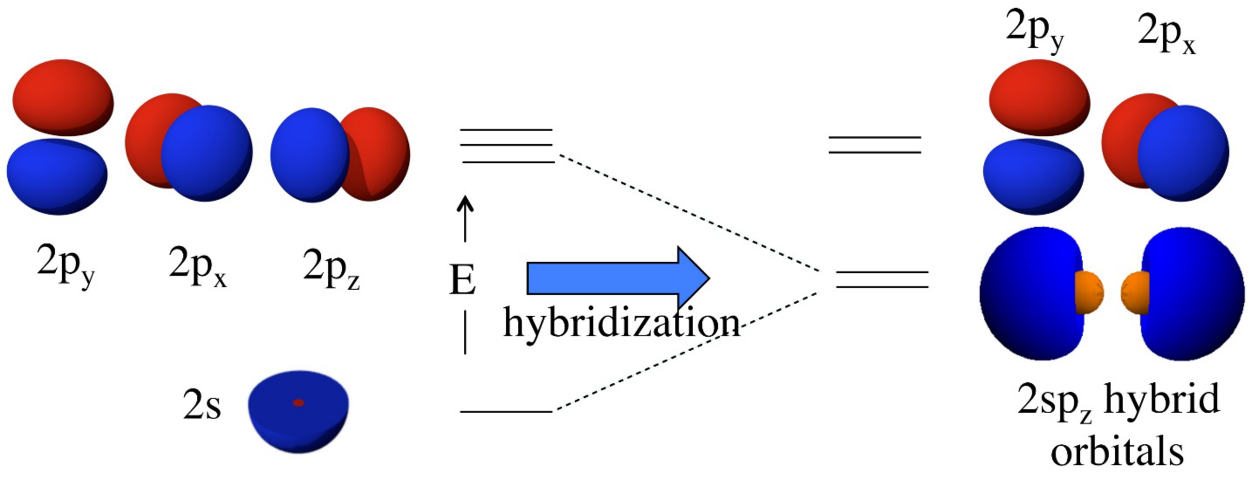

Figure 8.31 Formation of Pi Hybrid Orbitals in C

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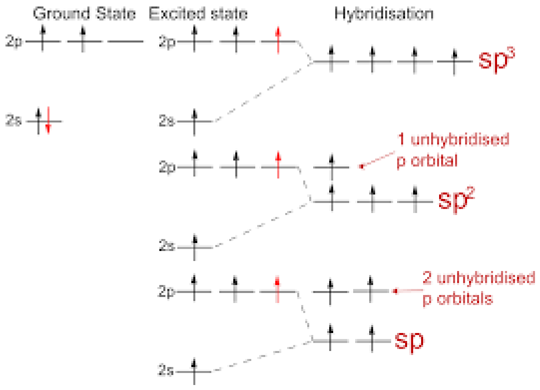

Figure 8.32 Electronic arrangement in different Hybrid Orbitals

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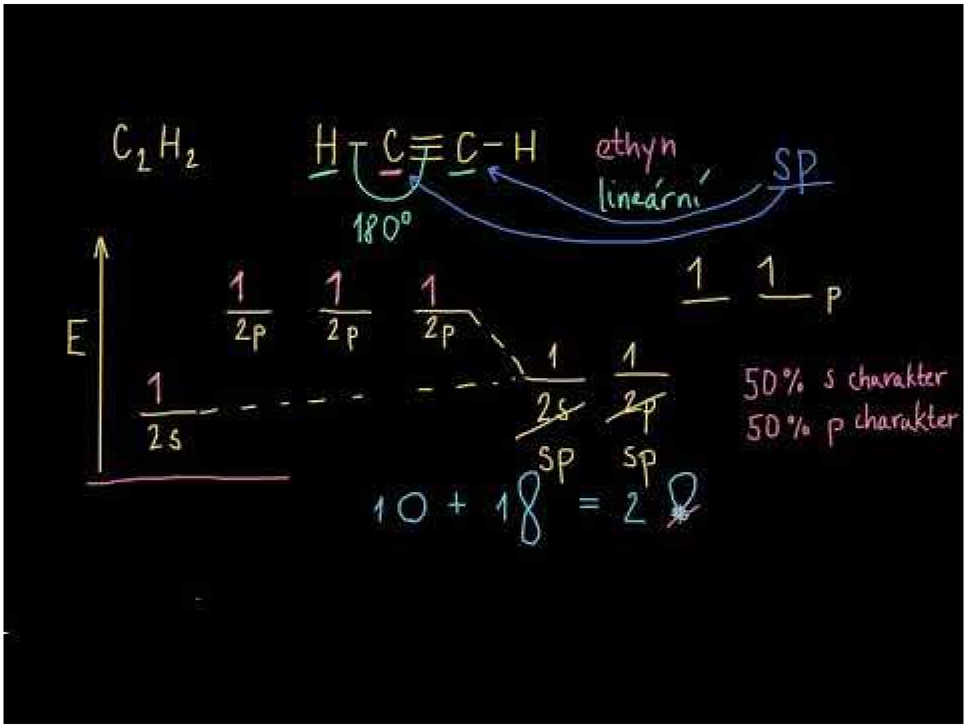

What you should be able to do

1) Make sure you thoroughly understand the following essential ideas which have been presented above.
2) Explain why the sharing of atomic orbitals (as implied in the Lewis model) cannot adequately account for the observed bonding patterns in simple molecules.
3) Sketch out a diagram illustrating how the plots of atomic *s*- and *p*- orbital wave functions give rise to a pair of hybrid orbitals.
4) Draw "orbital box" diagrams showing how combinations of an atomic *s* orbital and various numbers of *p* orbitals create sp, sp^2, and sp^3 hybrid orbitals.
5) Show how hybrid orbitals are involved in the molecules methane, water, and ammonia.

Hybrids involving *d* orbitals

In atoms that are below those in the first complete row of the periodic table, the simple octet rule begins to break down. For example, we have seen that PCl_3 does conform to the octet rule but

PCl_5 does not. We can describe the bonding in PCl_3 very much as we do NH_3: four *sp*^{3}-hybridized orbitals, three of which are shared with electrons from other atoms and the fourth containing a nonbonding pair.

D)Sp^{3}d & sp^{3}d^2 Hybridization

There are five d orbitals that can also take part in hybridization

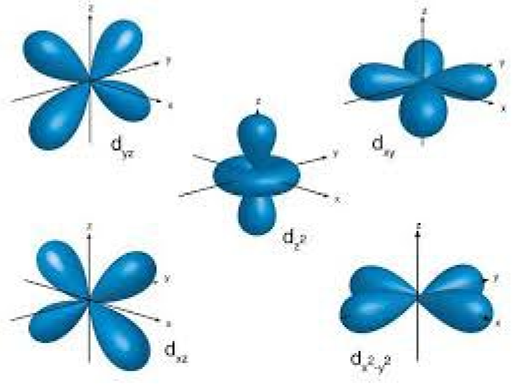

Figure 8.33 d-orbitals

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Sp^{3}d hybridization

Pentagonal bipyramid molecules: *sp*^{3}*d* hybridization

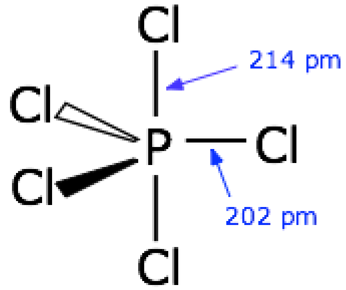


Figure 8.34 sp3d Hybrid Orbitals in PCl_5

Ref: Commons.wikimedia.org

In order to understand the bonding in **phosphorus pentachloride PCl_5**, we have to consider the *d* orbitals in addition to the *s*- and *p* types. When *d* orbitals are energetically close to the outmost *s*- and *p* orbitals, additional hybrid types can be built. In the case of PCl_5 we need five hybrid orbitals, and these can be constructed by adding two *d*-orbital functions to the mathematical mixture of one *s*- and two *p*-orbitals, resulting in five ***sp^3d*** hybrid orbitals directed toward the corners of a trigonal bipyramid, as is predicted by VSEPR theory.

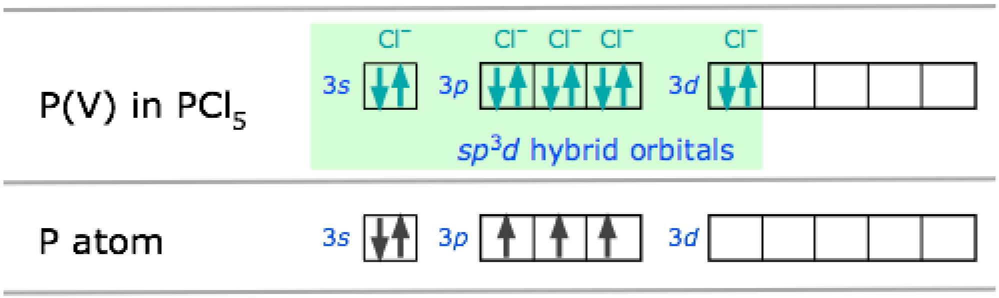
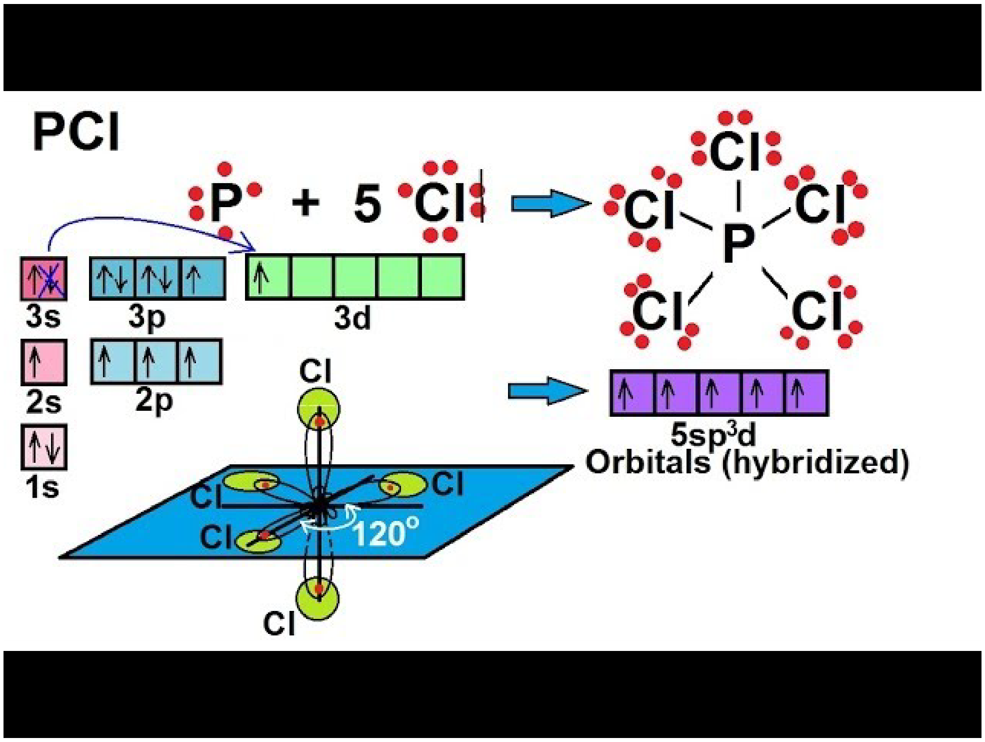


Figure 8.35 Electronic Arrangement of sp3d Hybrid Orbitals in PCl_5

The shapes of molecules with trigonal bipyramidal electron group arrangements are rationalized with VB theory through similar arguments. The difference is that molecules have central atoms from period 3 or higher so that s, p and d orbitals are mixed up to form hybrid orbitals.

For the shape of PCl5, VB model proposes one 3s, three 3p and one of the five 3d orbitals of the central P atom mix and form five sp3d hybrid



E) sp^{3}d^2 hybridization

To rationalize the shape of SF6, the VB model proposes that the one, 3s, the three 3p and two of the five 3d orbitals of the central S atom mix and foem sp3d2 hybrid orbitals which point to the vertices of an octahedron. Each hybrid orbital overlaps a 2p orbital of an F atom, and the six valence electrons of S, together with one from each of the six F atom.

SF6 Hybridization-QUORA

https://www.quora.com/What-is-the-hybridization-of-SF6

Octahedral coordination: *sp*^{3}*d*^{2} hybridization

The molecule **sulfur hexafluoride SF$_6$** exemplifies one of the most common types of *d*-orbital hybridization. The six bonds in this octahedrally-coordinated molecule are derived from mixing six atomic orbitals into a hybrid set. The easiest way to understand how these come about is to imagine that the molecule is made by combining an imaginary S^{6+} ion (which we refer to as the *S(VI) valence state*) with six F$^-$ ions to form the neutral molecule. These now-empty 3*s* and 3*p* orbitals then mix with two 3*d* orbitals to form the *sp*^{3}*d*^{2} hybrids.

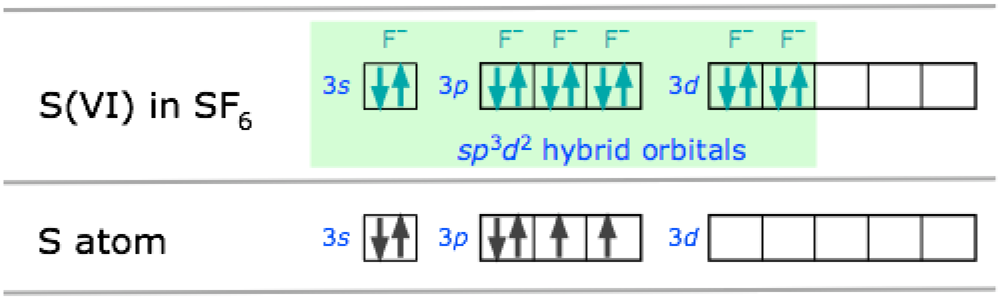


Figure 8.36 Electronic Arrangement of sp3d2 Hybrid Orbitals in SF_6

Some of the most important and commonly encountered compounds, which involve the d orbitals in bonding, are the *transition metal complexes*. The term “complex” in this context means that the molecule is composed of two or more kinds of species, each of which can have an independent existence.

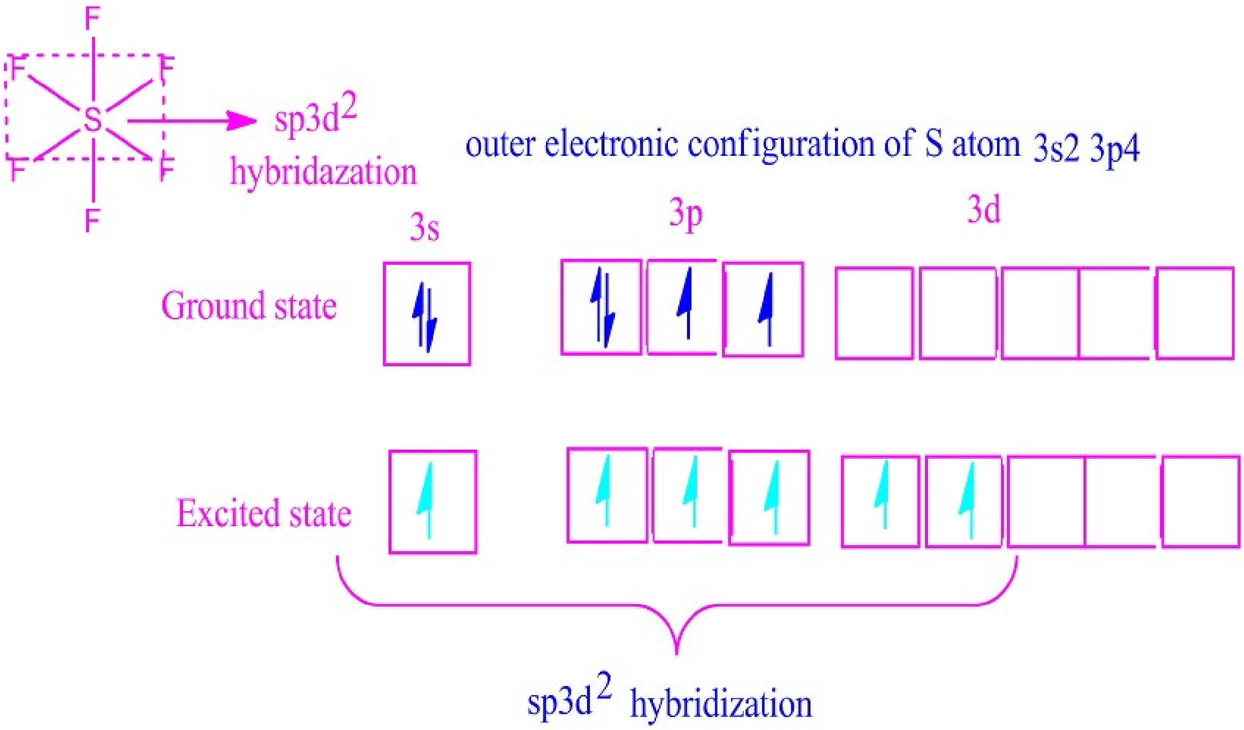


Figure 8.37 Formation of sp3d2 Hybrid Orbitals in PCl_5

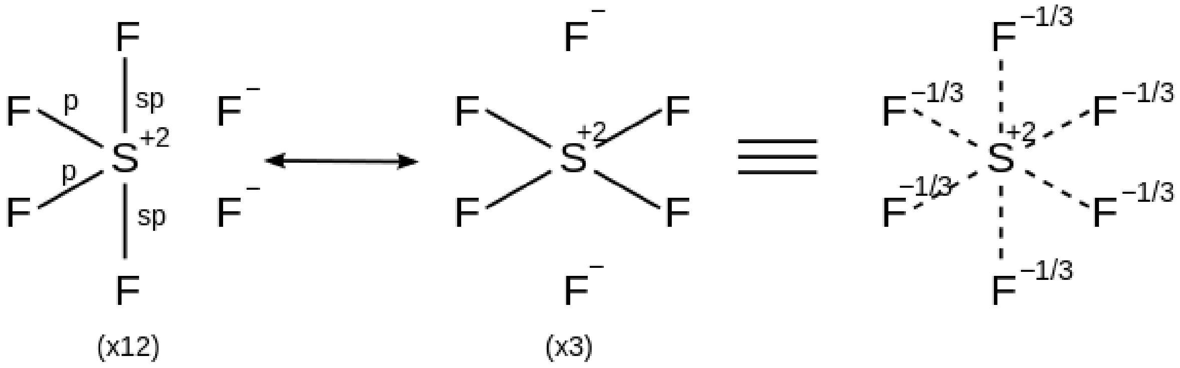


Figure 8.38 Charge distribution of sp3d2 Hybrid Orbitals in SF_6

Ref: Commons.wikimedia.org/

In summary, square planar and square pyramidal molecules have lone pairs in one

Six electron pairs (ortahedral geo)sp3d2

Five electron pairs (trigonal bipyramidal) sp3d

Four electron pair (tetrahedral) sp3

Three electron pair (Trigonal planar) sp2

Two electron pair (linear) sp

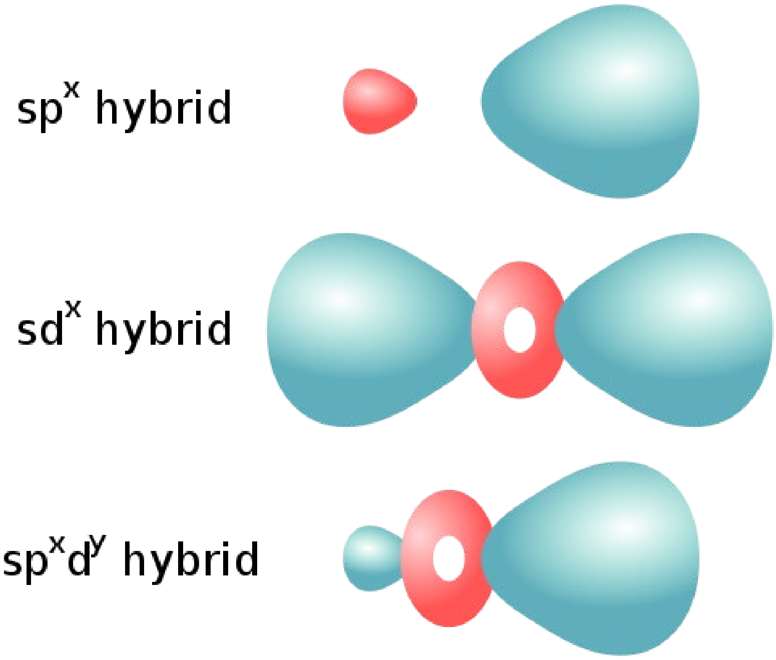


Figure 8.39 Shapes of all Hybrid Orbitals

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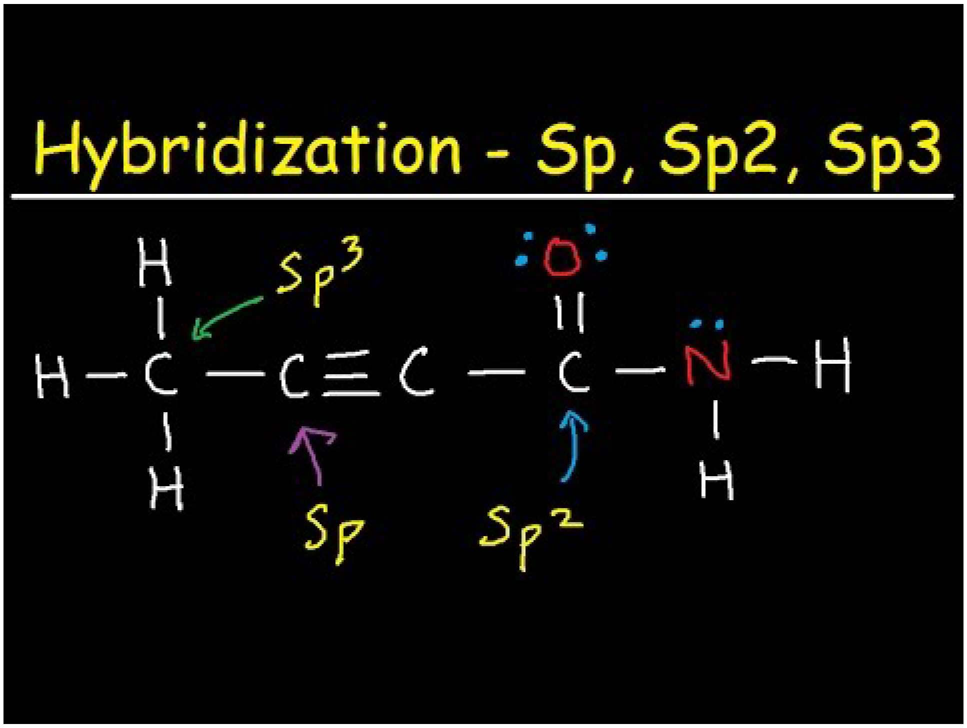
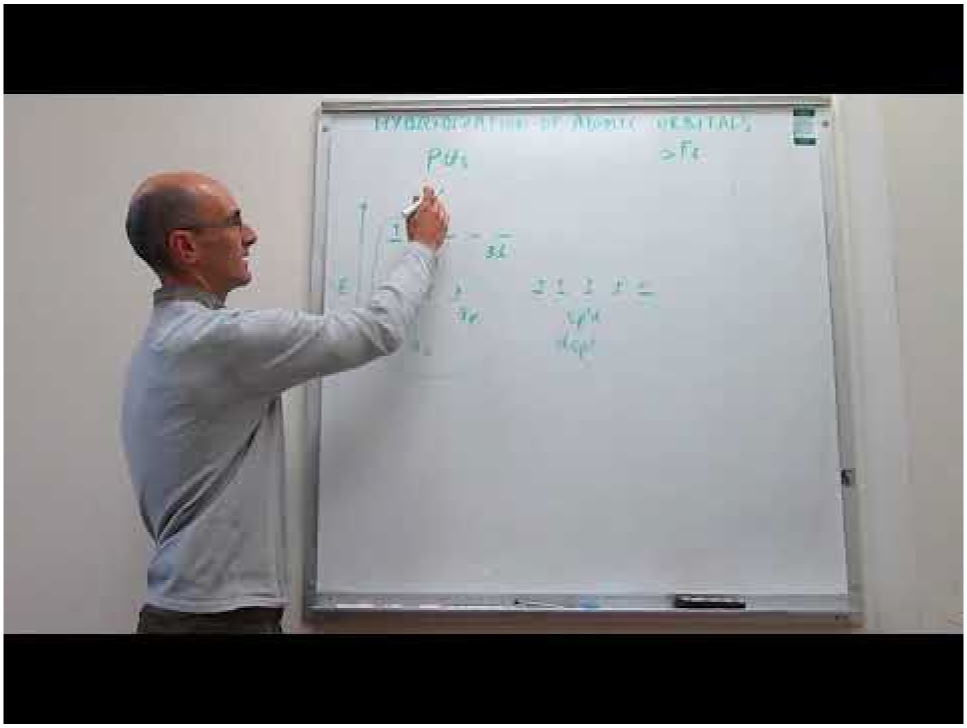
Watch this short video:



The following video is about sp3d and sp3d2 hybridization model.



SUPPLEMENTAL

Hybrid orbitals in molecular ions

There's more to know about hybrid orbitals!

Hybridization can also help explain the existence and structure of many inorganic molecular ions. Consider, for example, electron configurations of zinc in the compounds in the illustrations below.

The tetrachlorozinc ion (top row) is another structure derived from zinc and chlorine. As we might expect, this ion is tetrahedral; there are four chloride ions surrounding the central zinc ion. The zinc ion has a charge of +2, and each chloride ion is –1, so the net charge of the complex ion is –2.

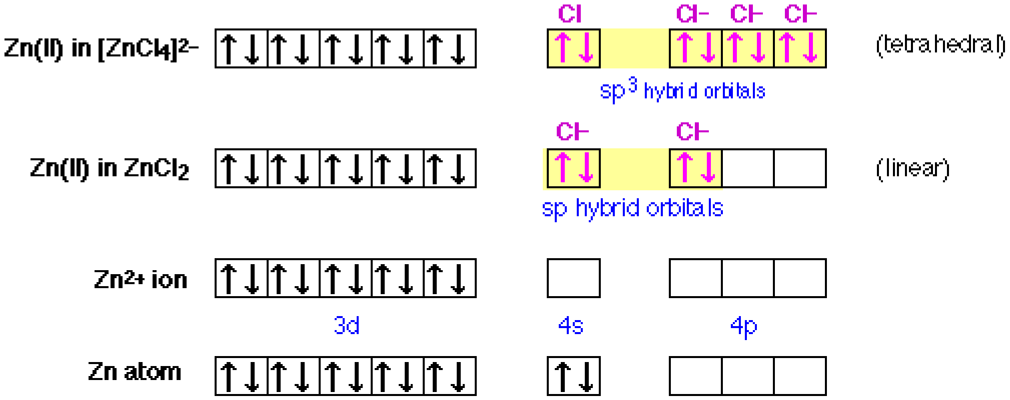


Figure 8.40 Electronic Arrangement in Hybrid Orbitals in transition metal ions

At the bottom is shown the electron configuration of atomic zinc, and just above it, of the divalent zinc ion. Notice that this ion has no electrons at all in its 4-shell. In zinc chloride, shown in the next row up, there are two equivalent chlorine atoms bonded to the zinc. The bonding orbitals are of sp character; that is, they are hybrids of the 4s and one 4p orbital of the zinc atom. Since these orbitals are empty in the isolated zinc ion, the bonding electrons themselves are all contributed by the chlorine atoms, or rather, the chloride ions, for it is these that are the bonded species here. Each chloride ion possesses a complete octet of electrons, and two of these electrons occupy each sp bond orbital in the zinc chloride complex ion. This is an example of a ***coordinate covalent bond***, in which the bonded atom contributes both of the electrons that make up the shared pair.

Square-planar molecules: dsp^2 hybridization

For example, the ions Pt^{2+} and Cl^- can form the ion $[PtCl_4]^{2-}$. To understand the hybridization scheme, it helps to start with the neutral Pt atom, then imagine it losing two electrons to become an ioin, followed by grouping of the two unpaired 5*d* electrons into a single *d* orbital, leaving one vacant.This vacant orbital, along with the 6*s* and two of the 6*p* orbitals, can then accept an electron pair from four chlorines.

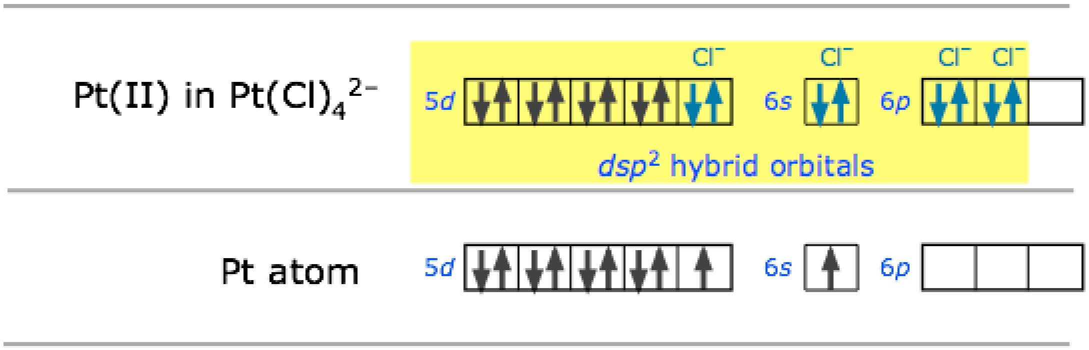


Figure 8.41 Electronic Arrangement in Hybrid Orbitals in $Pt(Cl)_4^-$

All of the four-coordinated molecules we have discussed so far have tetrahedral geometry around the central atom. Methane, CH_4, is the most well known example. It may come as something as a suprise, then, to discover that the **tetrachlorplatinum (II) ion $[PtCl_4]^{2-}$** has an essentially two-dimensional ***square-planar*** configuration. This type of bonding pattern is quite common when the parent central ion (Pt^{2+} in this case) contains only eight electrons in its outmost *d*-subshell.

Octahedral coordination: sp^3d^2 and d^2sp^3

Many of the most commonly encountered transition metal ions accept electron pairs from donors such as CN^- and NH_3 (or lacking these, even from H_2O) to form octahedral coordination complexes. The **hexamminezinc(II)** cation depicted below is typical.

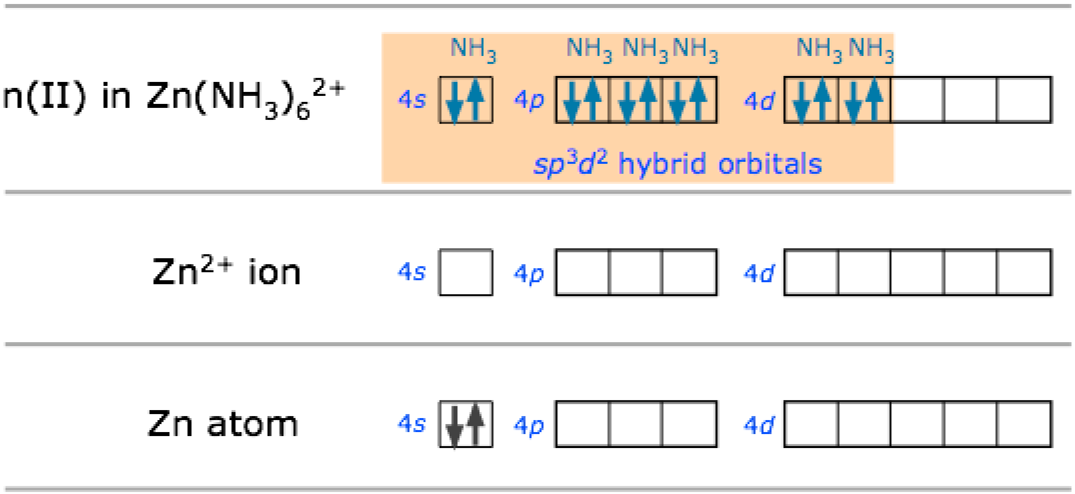


Figure 8.42 Electronic Arrangement in Hybrid Orbitals in $Zn(NH_3)_6^{2+}$

In sp^3d^2 hybridization the bonding orbitals are derived by mixing atomic orbitals having the same principal quantum number ($n = 4$ in the preceding example). A slightly different arrangement, known as d^2sp^3 hybridization, involves *d* orbitals of lower principal quantum number. This is possible because of the rather small energy differences between the *d* orbitals in one "shell" with the *s* and *p* orbitals of the next higher one— hence the term "inner orbital" complex which is sometims used to describe ions such as **hexamminecobalt(III)**, shown below.. Both arrangements produce octahedral coordination geometries.

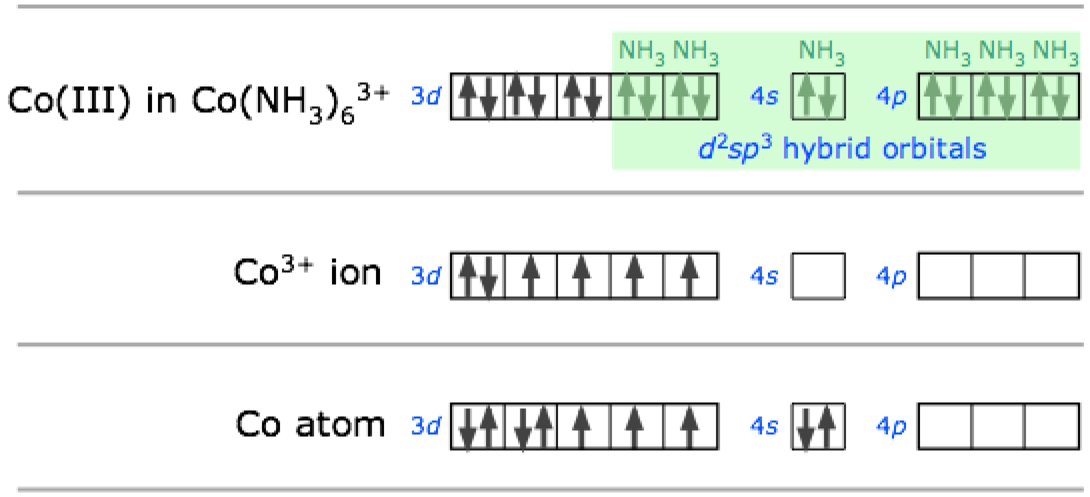


Figure 8.43 Electronic Arrangement in Hybrid Orbitals in $Co(NH_3)_6^{2+}$

In some cases, the same central atom can form either inner or outer complexes depending on the particular ligand and the manner in which its electrostatic field affects the relative energies of the different orbitals. Thus the **hexacyanoiron(II)** ion utilizes the iron 3*d* orbitals, whereas **hexaaquoiron(II)** achieves a lower energy by accecpting two H_2O molecules in its 4*d* orbitals.

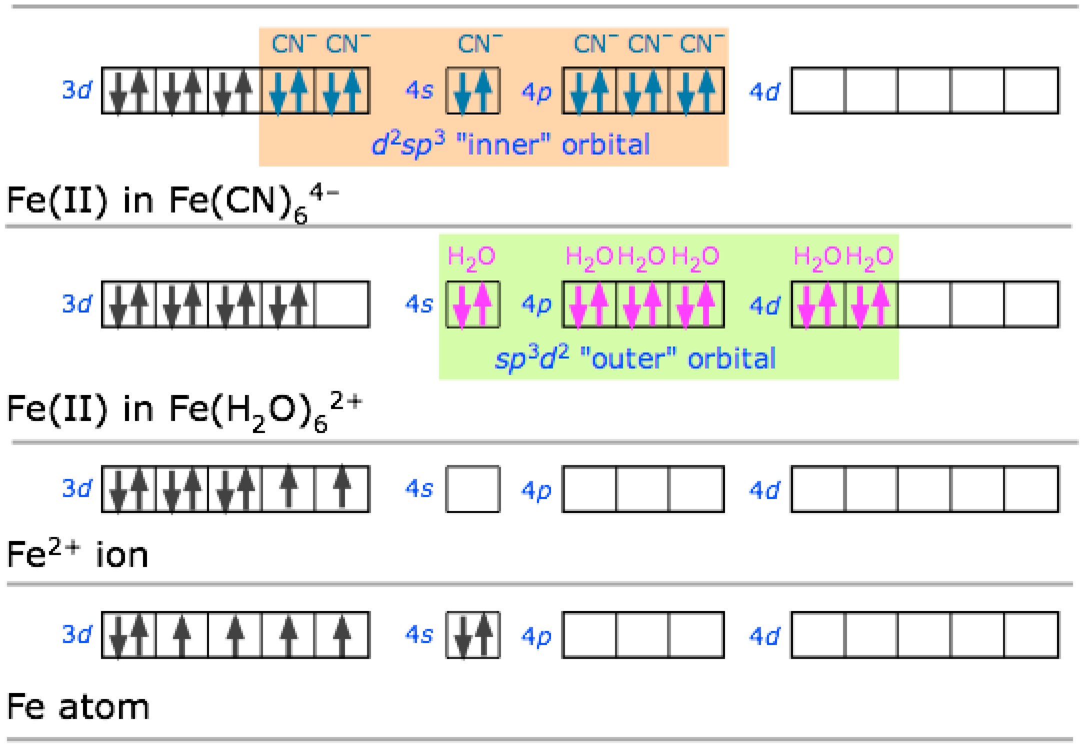


Figure 8.44 Electronic Arrangement in Hybrid Orbitals in Fe ion and complxes

Ref: https://www.chem1.com/acad/webtext/chembond/cb06.html

Although this "inner-outer" hybrid model was instrumental in explaining the properties of transition metal complexes in the first half of the 20th century, it has now been replaced with a more comprehensive model known as ***ligand field theory*** which is introduced in another lesson.

4 Some final remarks about hybrid orbitals

As is the case with any scientific model, the hybridization model of bonding is useful only to the degree to which it can predict phenomena that are actually observed. Most models contain weaknesses that place limits on their general applicability. The need for caution in accepting this particular model is made more apparent when we examine the shapes of the molecules below the first full row of the periodic table. For example, we would expect the bonding in hydrogen sulfide to be similar to that in water, with tetrahedral geometry around the sulfur atom. Experiments, however, reveal that the H–S–H bond angle is only 92°. Hydrogen sulfide thus deviates much more from tetrahedral geometry than does water, and there is no apparent and clear reason why it should. It is certainly difficult to argue that electron-repulsion between the two nonbonding orbitals is pushing the H–S bonds closer together (as is supposed to happen to the H–O bonds in water); many would argue that this repulsion would be less in hydrogen sulfide than in water, since sulfur is a larger atom and is hence less electronegative.

It might be, then, that our model of orbital hybridization into four equivalent sp^3 orbitals does not apply to H_2S. It looks like the "simple" explanation that bonding occurs through two half occupied atomic *p* orbitals 90° apart comes closer to the mark. Perhaps hybridization is not an all-or-nothing phenomenon; perhaps the two 3*p* orbitals are substantially intact in hydrogen sulfide, or are hybridized only slightly. In general, the hybridization model does not work very well with nonmetallic elements farther down in the periodic table, and there is as yet no clear explanation why. We must simply admit that we have reached one of the many points in chemistry where our theory is not sufficiently developed to give a clear and unequivocal answer. This does not detract, however, from the wide usefulness of the hybridization model in elucidating the bond character and bond shapes in the millions of molecules based on first-row elements, particularly of carbon.

Are hybrid orbitals real?

The justification we gave for invoking hybridization in molecules such as BeH_2, BF_3 and CH_4 was that the bonds in each are geometrically and chemically equivalent, whereas the atomic *s*- and *p*-orbitals on the central atoms are not. By combining these into new orbitals of sp, sp^2 and sp^3 types we obtain the required number of completely equivalent orbitals. This seemed easy enough to do on paper; we just drew little boxes and wrote "sp^2" or whatever below them. But what is really going on here?

The full answer is beyond the scope of this course, so we can only offer the following very general explanation. First, recall what we mean by "orbital": a mathematical function ψ having the character of a standing wave whose square ψ^2 is proportional to the probability of finding the electron at any particular location in space. The latter, the *electron density distribution*, can be observed (by X-ray scattering, for example), and in this sense is the only thing that is “real”.

A given standing wave (ψ-function) can be synthesised by combining all kinds of fundamental wave patterns (that is, atomic orbitals) in much the same way that a color we observe can be reproduced by combining different sets of primary colors in various proportions. In neither case does it follow that these original orbitals (or colors) are actually present in the final product. So one could well argue that hybrid orbitals are not “real”; they simply turn out to be convenient for understanding the bonding of simple molecules at the elementary level, and this is why we use them.

An alternative to hybrids: the Bent-Bond model

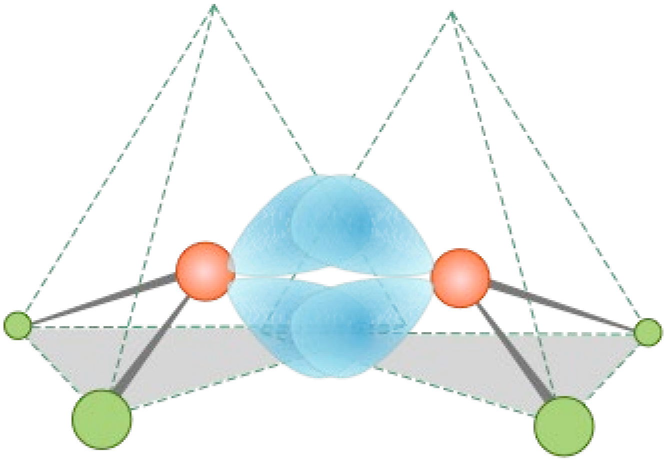


Figure 8.45 Bent-bond model

It turns out, in fact, that the electron distribution and bonding in ethylene can be equally well described by assuming no hybridization at all. The “bent bond” model requires only that the directions of

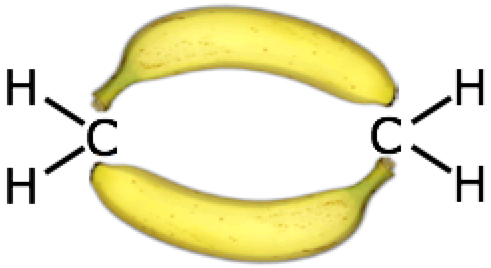


Figure 8.46 Banana Bonds

some of the atomic-*p* orbitals be distorted sufficiently to provide the overlap needed for bonding; these are sometimes referred to as "*banana bonds*".

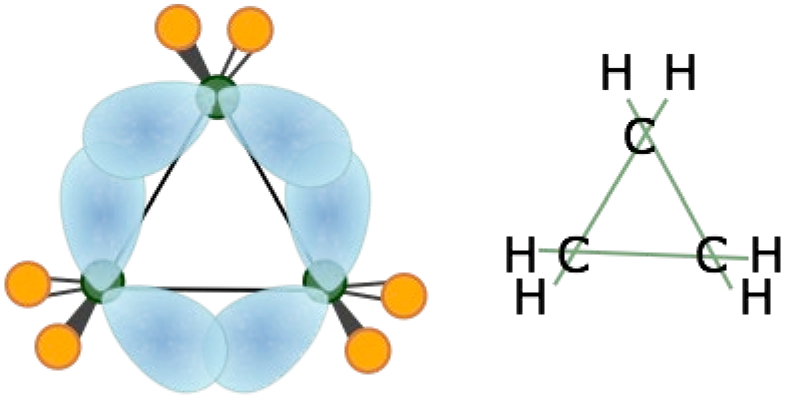


Figure 8.47 Hybrid Orbitals in closed ring molecule

The smallest of the closed-ring hydrocarbons is cyclopropane, a planar molecule in which the C–C bond angles are 120°— quite a departure from the tetrahedral angle of 109.5° associated with sp^3 hybridization! Theoretical studies suggest that the bent-bond model does quite well in predicting its properties.

What you should be able to do

1) Make sure you thoroughly understand the following essential ideas which have been presented above.
2) Sketch out diagrams showing the hybridization and bonding in compounds containing single, double, and triple carbon-carbon bonds.
3) Define *sigma* and *pi* bonds.
4) Describe the hybridization and bonding in the *benzene* molecule.

****

The theory given by Lewis explained the structure of molecules. However, it failed to explain the chemical bond formation. Similarly, VSEPR theory explained the shape of simple molecules. But, it's application was very limited. It also failed to explain the geometry of complex molecules. Hence, scientists had to introduce the theory of valence bonds to answer and overcome these limitations.

The basic principle of VB theory is proposed Heitler & London and by scientist Pauling. The theory states that a covalent bond forms when orbitals of two atoms overlap and the overlap region, which is in between the nuclei, is occupied by a pair of electrons.

HYBRIDIZATION WORKSHEET:

Put your own molecule and fill out the table!

Molecule	Electronic Geormetry	Molecular Geometry	Hybridization	Bond Angle	Polarity

III. ORBITAL OVERLAPS AND TYPES OF BONDS

In this section we will see how these orbitals can be used to account for the bonds in different molecules.

In this lesson, we extend this idea to compounds containing double and triple bonds, and to those in which atomic d electrons are involved (and which do not follow the octet rule.)

1 Hybrid types and multiple bonds

We have already seen how *sp* hybridization in carbon leads to its combining power of four in the methane molecule. Two such tetrahedrally coordinated carbons can link up together to form the molecule ethane C_2H_6. In this molecule, each carbon is bonded in the same way as the other; each is linked to four other atoms, three hydrogens and one carbon. The ability of carbon-to-carbon linkages to extend themselves indefinitely and through all coordination positions accounts for the millions of organic molecules that are known.

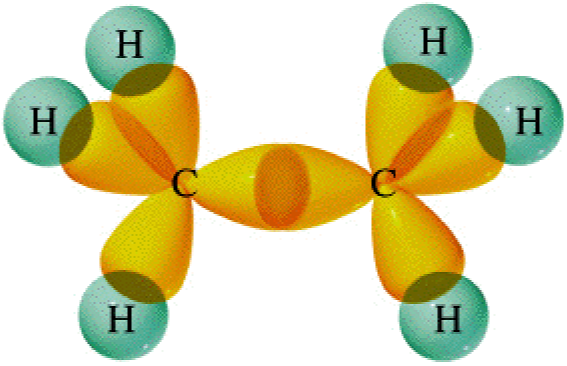


Figure 8.48 Orbitals overlap in C_2H_6

Trigonal hybridization in carbon: the double bond

Carbon and hydrogen can also form a compound ethylene (ethene) in which each carbon atom is linked to only three other atoms. Here, we can regard carbon as being trivalent. We can explain this trivalence by supposing that the orbital hybridization in carbon is in this case not sp^3, but is sp^2 instead; in other words, only two of the three *p* orbitals of carbon mix with the 2*s* orbital to form hybrids; the remaining p-orbital, which we will call the i orbital, remains unhybridized. Each carbon is bonded to three other atoms in the same kind of plane trigonal configuration that we saw in the case of boron trifluoride, where the same kind of hybridization occurs. Notice that the bond angles around each carbon are all 120°.

This alternative hybridization scheme explains how carbon can combine with four atoms in some of its compounds and with three other atoms in other compounds. You may be aware of the conventional way of depicting carbon as being tetravalent in all its compounds; it is often stated that carbon always forms four bonds, but that sometimes, as in the case of ethylene, one of these may be a double bond. This concept of the multiple bond preserves the idea of tetravalent carbon while admitting the existence of molecules in which carbon is clearly combined with fewer than four other atoms.

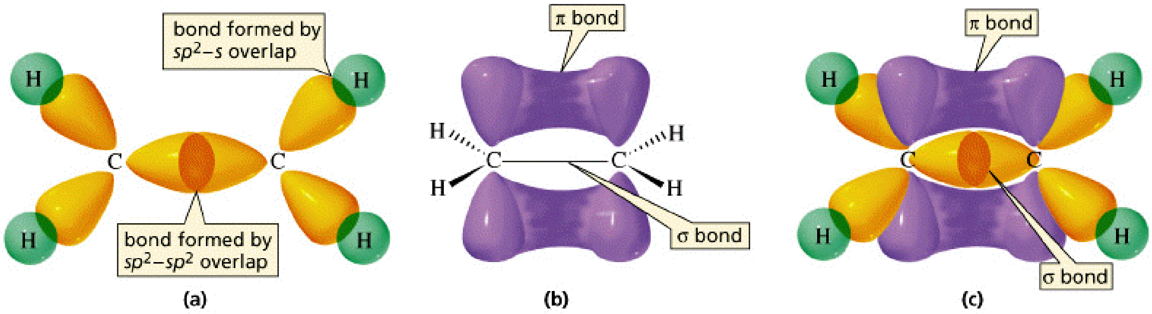


Figure 8.49 Sigma and Pi bonding in C_2H_6, C_2H_4 and C_2H_2

These three views of the ethylene molecule emphasize different aspects of the disposition of shared electron pairs in the various bonding orbitals of ethene (ethylene). (a) The "backbone" structure consisting of σ (*sigma*) bonds formed from the three sp^2-hybridized orbitals on each carbon. (b) The π (*pi*) bonding system formed by overlap of the unhybridized p_z orbital on each carbon. The π orbital has two regions of electron density extending above and below the plane of the molecule. (c) A cutaway view of the combined σ and π system.

As shown above, ethylene can be imagined to form when two -CH_2 fragments link together through overlap of the half-filled sp^2 hybrid orbitals on each. Since sp^2 hybrid orbitals are always in the same plane, the entire ethylene molecule is planar. However, there remains on each carbon atom an electron in an unhybridized atomic p_z orbital that is perpendicular to the molecular plane. These two parallel p_z orbitals will interact with each other; the two orbitals merge, forming a sausage-like charge cloud (the π bond) that extends both above and belowthe plane of the molecule. It is the pair of electrons that occupy this new extended orbital that constitutes the "fourth" bond to each carbon, and thus the "other half" of the double bond in the molecule.

More about *sigma* and *pi* bonds

The σ (*sigma*) bond has its maximum electron density along the line-of-centers joining the two atoms (below left). Viewed end-on, the σ bond is cylindrically symmetrical about the line-of-centers. It is this symmetry, rather than its parentage, that defines the σ bond, which can be formed from the overlap of two *s*-orbitals, from two *p*-orbitals arranged end-to-end, or from an *s*- and a *p*-orbital. They can also form when *sp* hybrid orbitals on two atoms overlap end-to-end.

Pi orbitals, on the other hand, require the presence of two atomic *p* orbitals on adjacent atoms. Most important, the charge density in the π orbital is concentrated above and below the molecular plane; it is almost zero along the line-of-centers between the two atoms. It is this perpendicular orientation with respect to the molecular plane (and the consequent lack of cylindrical symmetry) that defines the π orbital. The combination of a σ bond and a π bond extending between the same pair of atoms constitutes the double bond in molecules such as ethylene.

Carbon-carbon triple bonds: *sp* hybridization in acetylene

We have not yet completed our overview of multiple bonding, however. Carbon and hydrogen can form yet another compound, acetylene (ethyne), in which each carbon is connected to only two other atoms: a carbon and a hydrogen. This can be regarded as an example of divalent carbon, but is usually rationalized by writing a triple bond between the two carbon atoms.

We assume here that since each carbon forms two geometrically equivalent bonds, this atom must be *sp*-hybridized in acetylene. On each carbon, one *sp* hybrid bonds to a hydrogen and the other bonds to the other carbon atom, forming the σ bond skeleton of the molecule.

In addition to the *sp* hybrids, each carbon atom has two half-occupied *p* orbitals oriented at right angles to each other and to the interatomic axis. These two sets of parallel and adjacent *p* orbitals can thus merge into two sets of π orbitals.

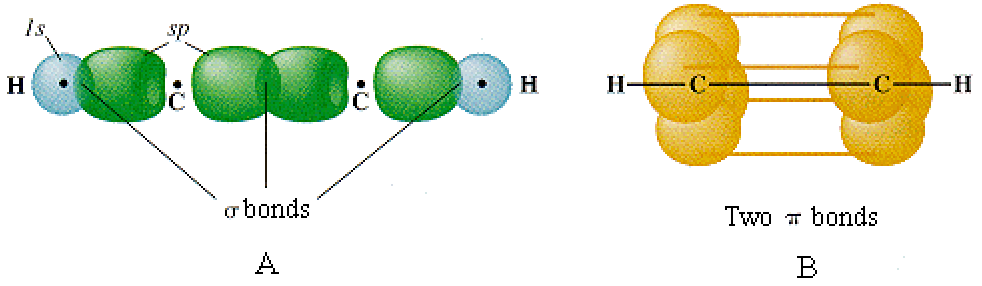


Figure 8.50 Sigma and Pi bonding

The triple bond in acetylene is seen to consist of one σ bond joining the line-of-centers between the two carbon atoms, and two π bonds whose lobes of electron density are in mutually-perpendicular planes. The acetylene molecule is of course linear, since the angle between the two *sp* hybrid orbitals that produce the *s* skeleton of the molecule is 180°.

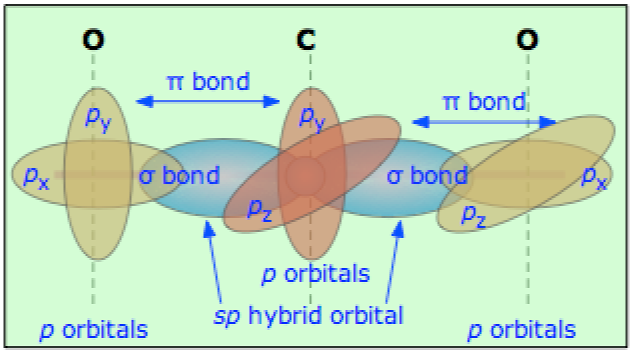


Figure 8.51 Sigma and Pi bonding Formation

Multiple bonds between unlike atoms

Multiple bonds can also occur between dissimilar atoms. For example, in **carbon dioxide** each carbon atom has two unhybridized atomic *p* orbitals, and each oxygen atom still has one *p* orbital available. When the two O-atoms are brought up to opposite sides of the carbon atom, one of the *p* orbitals on each oxygen forms a π bond with one of the carbon *p*-orbitals. In this case, *sp*-hybridization is seen to lead to two double bonds. Notice that the two C–O π bonds are mutually perpendicular.

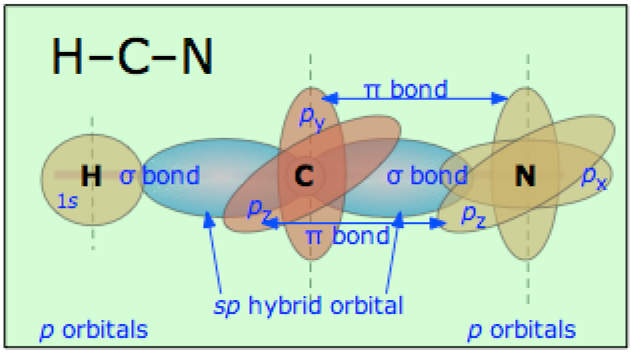


Figure 8.52 Sigma and Pi bonding in HCN

Similarly, in **hydrogen cyanide**, HCN, we assume that the carbon is *sp*-hybridized, since it is joined to only two other atoms, and is hence in a divalent state. One of the *sp*-hybrid orbitals overlaps with the hydrogen 1*s* orbital, while the other overlaps end-to-end with one of the three unhybridized *p* orbitals of the nitrogen atom. This leaves us with two nitrogen *p*-orbitals which form two mutually perpendicular π bonds to the two atomic *p* orbitals on the carbon. Hydrogen cyanide thus contains one single and one triple bond. The latter consists of a σ bond from the overlap of a carbon *sp* hybrid orbital with a nitrogen *p* orbital, plus two mutually perpendicular π bonds deriving from parallel atomic *p* orbitals on the carbon and nitrogen atoms.

The nitrate ion

Pi bond delocalization furnishes a means of expressing the structures of other molecules that require more than one electron-dot or structural formula for their accurate representation. A good example is the nitrate ion, which contains 24 electrons:

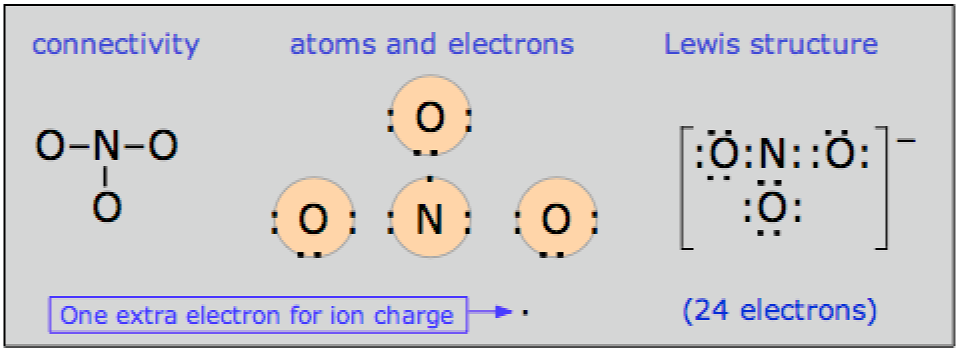


Figure 8.53 Pi delocalization in NO_3^- ion

The electron-dot formula shown above is only one of three equivalent resonamce strutcures that are needed to describe trigonal symmetry of this ion.

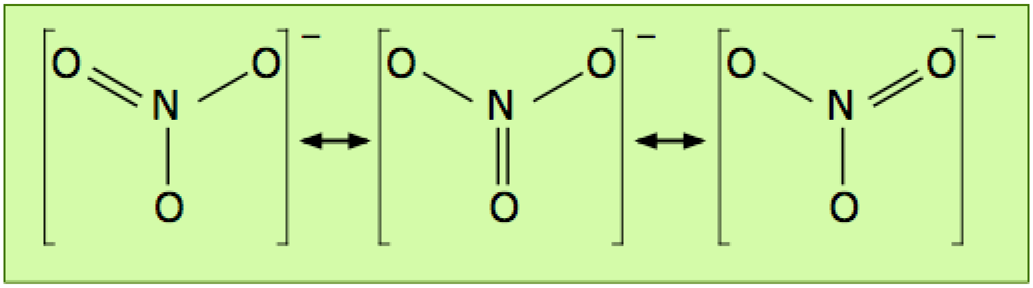


Figure 8.54 Resonating forms in NO_3^- ion

Nitrogen has three half-occupied *p* orbitals available for bonding, all perpendicular to one another. Since the nitrate ion is known to be planar, we are forced to assume that the nitrogen outer electrons are sp^2-hybridized. The addition of an extra electron fills all three hybrid orbitals completely. Each of these filled sp^2 orbitals forms a σ bond by overlap with an empty oxygen $2p_z$ orbital; this, you will recall, is an example of ***coordinate covalent bonding***, in which one of the atoms contributes both of the bonding electrons. The empty oxygen 2*p* orbital is made available when the oxygen electrons themselves become *sp* hybridized; we get three filled *sp* hybrid orbitals, and an empty 2*p* atomic orbital, just as in the case of nitrogen.

The π bonding system arises from the interaction of one of the occupied oxygen *sp* orbitals with the unoccupied $2p_x$ orbital of the nitrogen. Notice that this, again, is a coordinate covalent sharing, except that in this instance it is the oxygen atom that donates both electrons.

Pi bonds can form in this way between the nitrogen atom and any of the three oxygens; there are thus three equivalent π bonds possible, but since nitrogen can only form one complete π bond at a time, the π bonding is divided up three ways, so that each N–O bond has a bond order of 4/3.

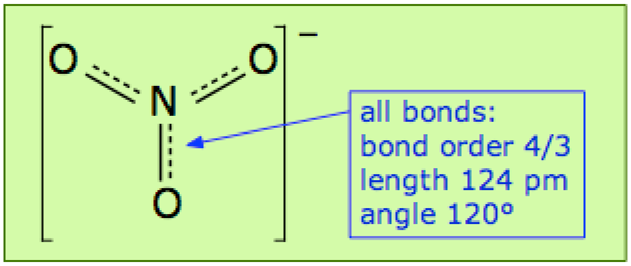
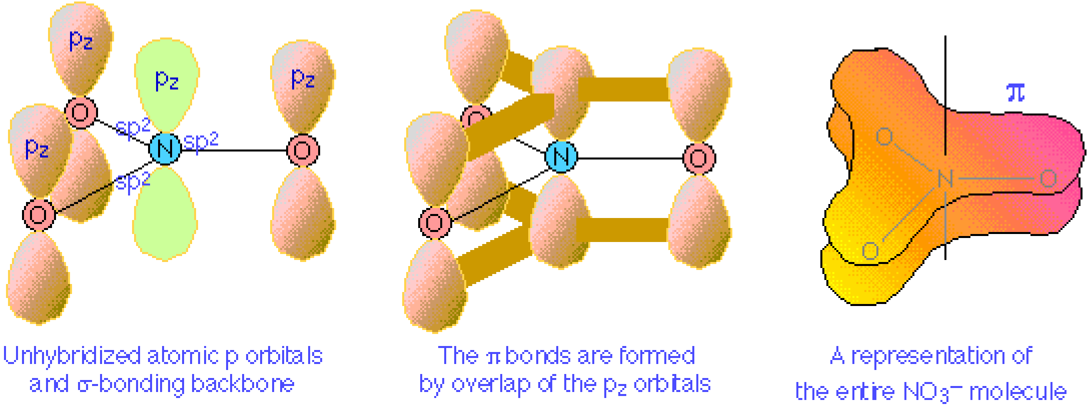


Figure 8.55 NO_3^- ion structure



Unhybridized atomic p orbitals and σ-bonding backbone

The π bonds are formed by overlap of the p_z orbitals

A representation of the entire NO_3^- molecule

Ref: https://www.chem1.com/acad/webtext/chembond/cb06.html

Figure 8.56 Pi bonding overlap in NO_3^- ion

SUPPLEMENTAL

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Conjugated double bonds

We have seen that the π bonding orbital is distinctly different in shape and symmetry from the σ bond. There is another important feature of the π bond that is of far-reaching consequence, particularly in organic and coordination chemistry.

Consider, for example, an extended hydrocarbon molecule in which alternate pairs of carbon atoms are connected by double and single bonds. Each non-terminal carbon atom forms two σ bonds to two other carbons and to a hydrogen (not shown.) This molecule can be viewed as a series of ethylene units joined together end-to-end. Each carbon, being *sp* hybridized, still has a half-filled atomic *p* orbital. Since these *p* orbitals on adjacent carbons are all parallel, we can expect them to interact with each other to form π bonds between alternate pairs of carbon atoms as shown below.

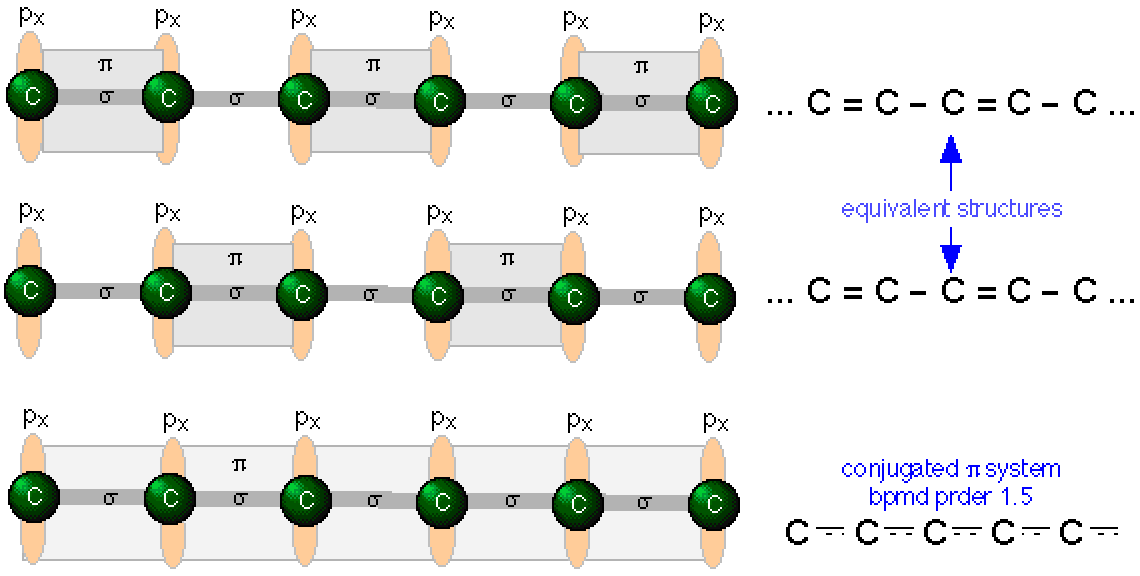

Figure 8.57 Conjugate Double Bonds

But since each carbon atom possesses a half-filled *p* orbital, there is nothing unique about the π bond arrangement; an equally likely arrangement might be one in which the πbonding orbitals are shifted to neighboring pairs of carbons (middle illustration above).

You will recall that when there are two equivalent choices for the arrangements single and double bonds in a molecule, we generally consider the structure to be a ***resonance hybrid***. In keeping with this idea, we would expect the electron density in a π system of this kind to be extended or shared out evenly along the entire molecular framework, as shown in the bottom figure.

A system of alternating single and double bonds, as we have here, is called a ***conjugated system***. Chemists say that the π bonds in a conjugated system are ***delocalized***; they are, in effect, “smeared out” over the entire length of the conjugated part of the molecule. Each pair of adjacent carbon atoms is joined by a σ bond and "half" of a π bond, resulting in an a C-C ***bond order*** of 1.5.

An even higher degree of conjugation exists in compounds containing extended $(C=C)_n$ chains. These compounds, known as **cumulenes**, exhibit interesting electrical properties, and whose derivatives can act as "organic wires".

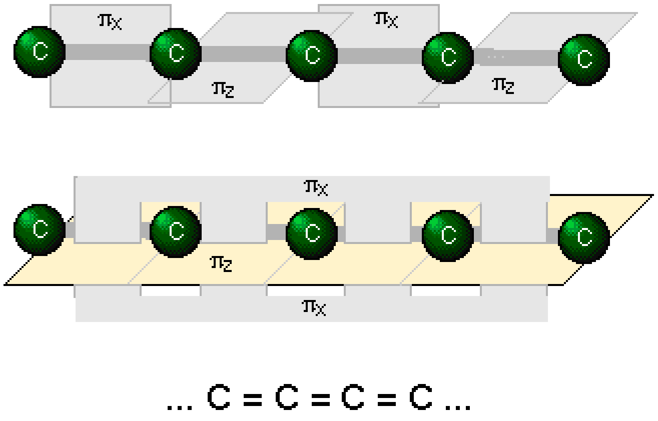

Figure 8.58 Plane of Hybridization in Cumulenes

Hybrid orbitals in benzene

The classic example of π bond delocalization is found in the cyclic molecule ***benzene*** (C_6H_6) which consists of six carbon atoms bound together in a hexagonal ring. Each carbon has a single hydrogen atom attached to it.

The lines in this figure represent the σ bonds in benzene. The basic ring structure is composed of σ bonds formed from overlap of sp^2 hybrid orbitals on adjacent carbon atoms. The unhybridized carbon p_z orbitals project above and below the plane of the ring. They are shown here as they might appear if they did not interact with one another.

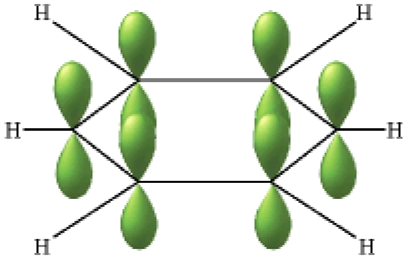

Figure 8.59 Plane of Hybridization in Benzene

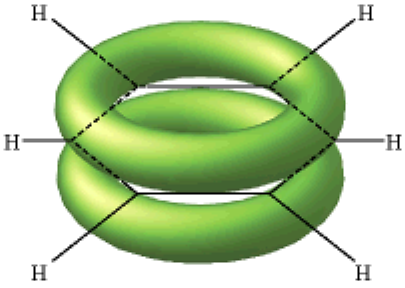

Figure 8.60 Pi Orbitals in Benzene

But what happens, of course, is that the lobes of these atomic orbitals meld together to form circular rings of electron density above and below the plane of the molecule. The two of these together constitute the "second half" of the carbon-carbon double bonds in benzene.

This computer-generated plot of electron density in the benzene molecule is derived from a more rigorous theory that does not involve hybrid orbitals; the highest electron density (blue) appears around the periphery of the ring, while the lowest (red) is in the "doughnut hole" in the center.

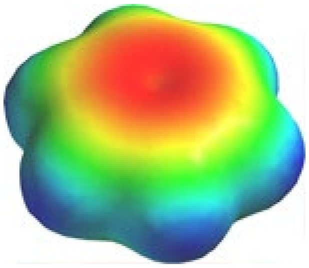

Figure 8.61 Electron Cloud in Benzene

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End to end overlap and sigma (σ) bonding. The bond resulting from such end-to-end overlap is called sigma bond.

1. Side-to-side overlap and pi (π) bonding: A close look at the nature of carbon-carbon double bond in ethylene . Each C atom's four valence electrons half-fill its three sp2 orbitals and its un-hybridized 2p orbitals.

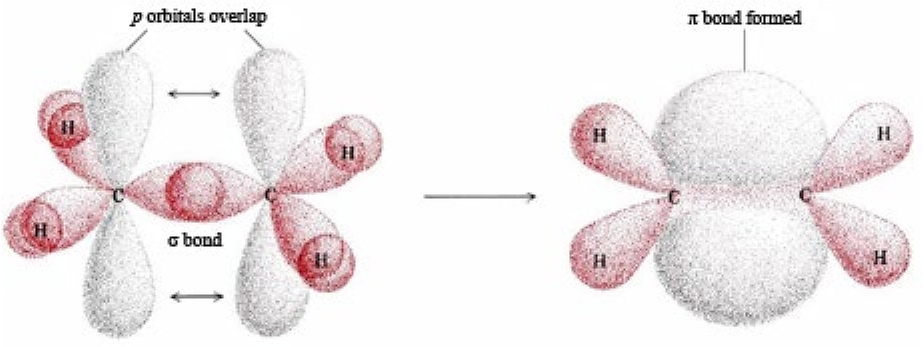


Figure 8.62 Sigma and Pi bond in C_2H_4

Ref: commons.wikimedia.org/

Notice the overlap between the half-filled p orbitals on the carbon and oxygen atoms. When p orbitals overlap this way (side by side), the resulting bond is a pi bond (**π**) bond and the electron density is above and below the internuclear axis. When orbitals overlap end to end as in the case in all of the rest of the bonds in molecule the resulting bond is sigma bond.($\boldsymbol{\sigma}$)

In case of ethane (C_2H_6) in the above figure, both C atoms of ethane are sp3 hybridized. The C-C bond involves the overlap of one sp3 orbital from each C, and each of the six C-H bonds involves overlap of a C sp3 orbital with an H 1s orbital. These bonds are formed as a result of end to end overlap. They are assigned as sigma bond.

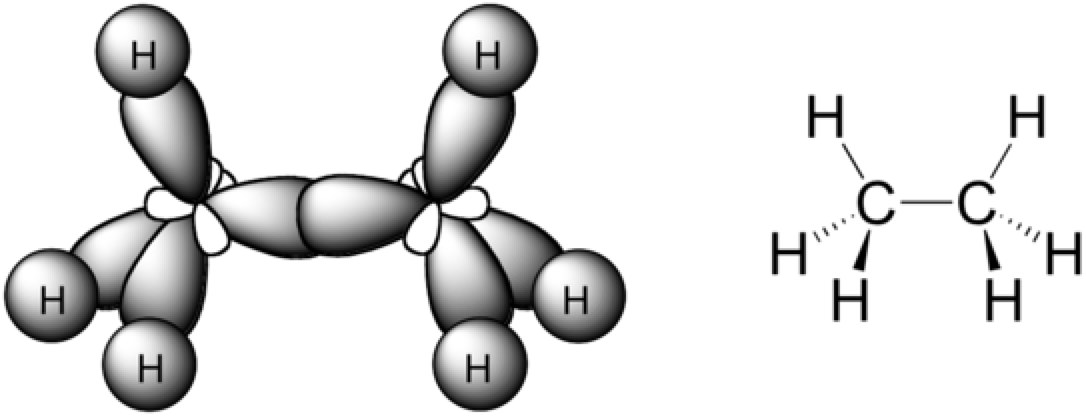


Figure 8.63(a) Sigma and Pi bond in C_2H_4

Figure 8.63(b) 3D shape of C_2H_4

Ref: commons.wikimedia.org/

In case of ethylene, each C atom is sp2hybridized. Each C atom's four valence electrons half-fill its three sp2 orbitals and its unhybridized 2p orbital, which is perpendicular

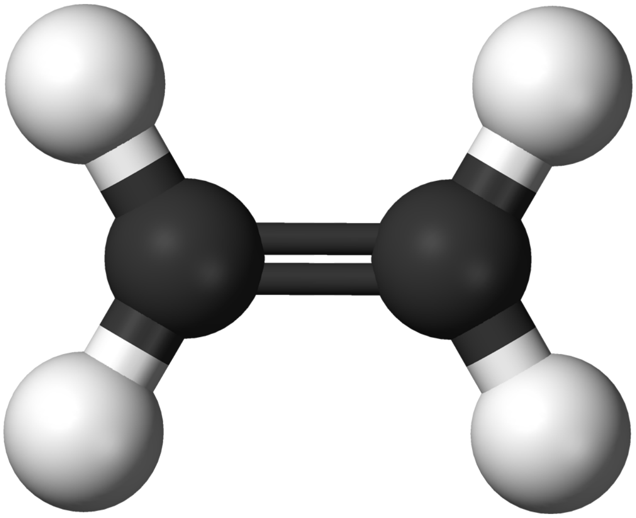


Figure 8.64 3D shape of C_2H_4

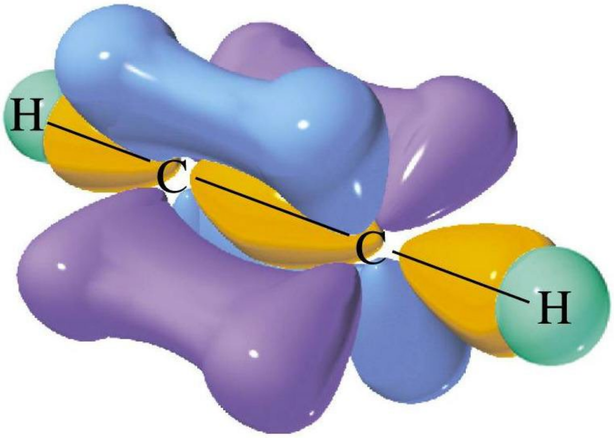
Ref: commons.wikimedia.org/

In case of acetylene, we see a triple bond C≡C consists of one sigma bond and two pi bond are formed. To maximize overlap in a linear shape, one s and one p orbital in each C atom form two sp hybrids, and two 2p orbitals remain unhybridized. Each C uses one of its sp orbitals to form a sigma bond with an H atom and uses the other form the C-C σ bond. Side to side overlap of one pair of 2p orbitals gives one π bond, and the other pair of 2p orbitals gives another π bond. The second pi bond is perpendicular to the first pi bond. The electron density in the front and back of the sigma bond. The result is cylindrically symmetrical H-C≡C-H molecule.

In terms of strength, the double bond is about twice as strong as a single bond and a triple bond is about three times as strong.

Figure 8.65 3D shape of C_2H_2

Ref: commons.wikimedia.org/



The correspondence between valence bond theory and Lewis theory is striking here. In both models, the central carbon atom forms four bonds: two single bonds and one double bond. However, Valence bond theory gives us more insight into the bonds. According to Valence Bond theory, any double bond between two atoms consists of two different kinds of bonds-one sigma and one pi. In Lewis model two bonds within the double bond appear identical.

In general pi bonds are weaker than sigma bonds because side to side orbital overlap tends to be less efficient than end to end overlap. Consequently, the pi bond in a double bond is generally easier to break than sigma bond.

Valence bond theory allows us to see why the rotation about a double bond is severely restricted. Due to side wise overlap of the p-orbitals, the pi bond must essentially break for rotation to occur.

Although rotation about the double bond is highly restricted but rotation around the single bond is possible. For example, 1,2-dichloroenthane and 1,2-dichloroethene.

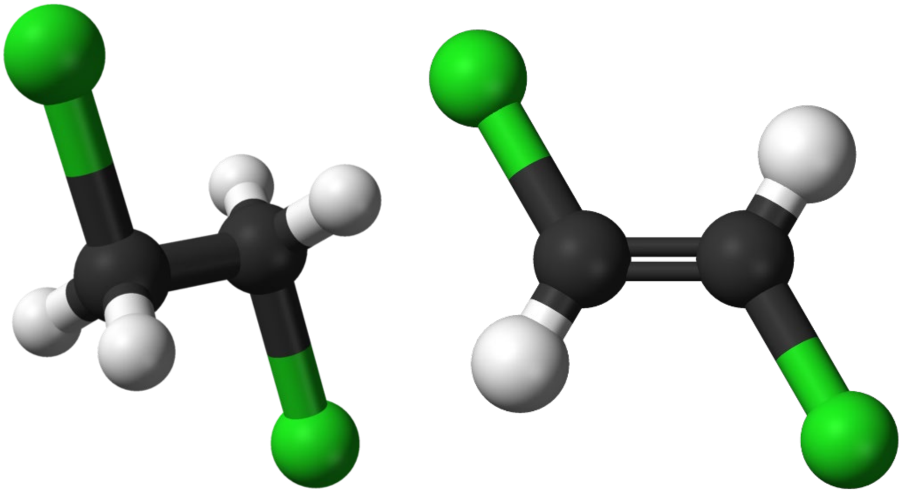
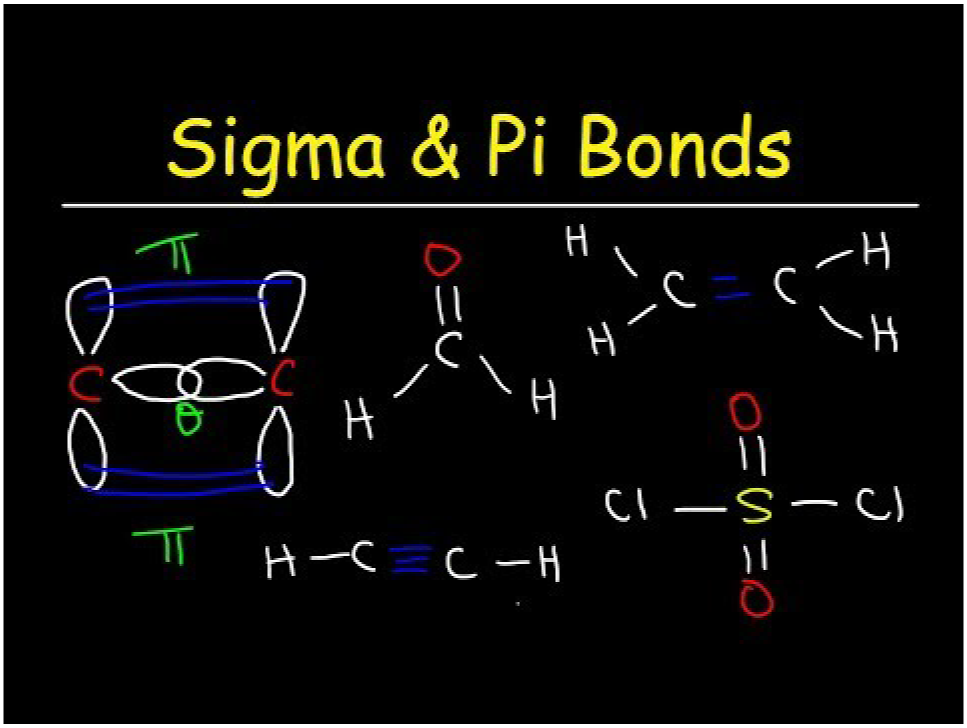


Figure 8.66 1,2-dichloroethane(left, rotation possible) 1,2-dichloroethene(right, rotation restricted)

Watch the following video for more explanation.



What you should be able to do

1) Make sure you thoroughly understand the following essential ideas which have been presented above.
2) Sketch out diagrams showing the hybridization and bonding in compounds containing single, double, and triple carbon-carbon bonds.
3) Define *sigma* and *pi* bonds.
4) Describe the hybridization and bonding in the *benzene* molecule.

Concept Map

Practice Questions:

1. Describe the types of bonds and orbitals in
   a) acetone($(CH_3)_2CO$,
   b) formaldehyde(H_2CO)
   c) HCN
   d) CO_2

Limitation:

The valence bond approach is especially useful in organic chemistry where so many molecules are built of tetrahedral C atoms, sp^3 hybridised. The concept of hybrids is intuitively very satisfying because they fit visually with our perceived picture of the shape of a molecule with its directed bonds between pairs of atoms. Unfortunately, the VB approach is not satisfactory for species like $CO_3^{=}$, NO_3^{-}, and benzene because the VB picture does not reflect the known chemical structure. A new concept of resonance hybrids must be introduced, and $CO_3^{=}$ must now be represented by a combination of three Lewis-octet structures. Worse still, the VB approach cannot easily give a satisfactory bonding picture for either of the important molecules O_2 or CO.

In cases where the VB approach does not work well, the molecular orbital (MO) method is often more successful. The situation is best summarized by using the strengths of the VB approach where they are appropriate, as in CH_4, and using the MO approach where it is best suited, as in O_2 and benzene. After all, each approach is an approximation, incomplete and imperfect.

Read more: http://www.chemistryexplained.com/Te-Va/Valence-Bond-Theory.html#ixzz6VbHDEIOG

IV. MOLECULAR ORBITAL THEORY

Look at the computer-generated model of the nicotine molecule shown at the upper right corner of this window. The colors of the sculpted folds represent different electron densities—probabilities of finding an electron at any given point. The sculpting itself is created by the positive cores that remain after the "atoms" in this molecule have been stripped of their valence electrons, which are now able to range over the entire molecule, occupying orbitals whose spatial extent and properties depend entirely on the charges and geometric distribution of the collection of positive centers.

Welcome to the world of ***molecular orbitals*** !

This is a big departure from the simple ***Lewis*** and ***VSEPR*** models that were based on the one-center orbitals of individual atoms. The more sophisticated ***hybridization*** model recognized that these orbitals will be modified by their interaction with other atoms. But all of these ***valence-bond*** models, as they are generally called, are very limited in their applicability and predictive power, because they fail to recognize that distribution of the pooled valence electrons is governed by the totality of positive centers.

The molecular orbital model is by far the most productive of the various models of chemical bonding, and serves as the basis for most quantiative calculations, including those that lead to many of the computer-generated images that you have seen elsewhere in these units. In its full development, molecular orbital theory involves a lot of complicated mathematics, but the fundamental ideas behind it are quite easily understood, and this is all we will try to accomplish in this lesson.

Chemical bonding occurs when the net attractive forces between an electron and two nuclei exceeds the electrostatic repulsion between the two nuclei. For this to happen, the electron must be in a region of space which we call the *binding region*. Conversely, if the electron is off to one side, in an *anti-binding region*, it actually adds to the repulsion between the two nuclei and helps push them away.

The easiest way of visualizing a molecular orbital is to start by picturing two isolated atoms and the electron orbitals that each would have separately. These are just the orbitals of the separate atoms, by themselves, which we already understand. We will then try to predict the manner in which these atomic orbitals interact as we gradually move the two atoms closer together. Finally, we will reach some point where the internuclear distance corresponds to that of the molecule we are studying. The corresponding orbitals will then be the ***molecular orbitals*** of our new molecule.

The simplest molecule: hydrogen molecule ion

To see how this works, we will consider the simplest possible molecule, H_2^+. This is the **hydrogen molecule ion**, which consists of two nuclei of charge +1, and a single electron shared between them.

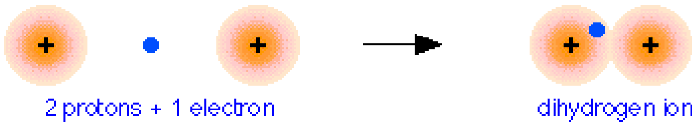


Figure 8.67 Overlap of Atomic Orbitals

As two H nuclei move toward each other, the 1*s* atomic orbitals of the isolated atoms gradually merge into a new molecular orbital in which the greatest electron density falls between the two nuclei. Since this is just the location in which electrons can exert the most attractive force on the two nuclei simultaneously, this arrangement constitutes a ***bonding molecular orbital***. Regarding it as a three-dimensional region of space, we see that it is symmetrical about the line of centers between the nuclei; in accord with our usual nomenclature, we refer to this as a ***σ (sigma) orbital***.

Bonding and antibonding molecular orbitals

Orbitals are conserved

There is one minor difficulty: we started with two orbitals (the 1*s* atomic orbitals), and ended up with only one orbital. Now according to the rules of quantum mechanics, orbitals cannot simply appear and disappear at our convenience. For one thing, this would raise the question of at just what internuclear distance do we suddenly change from having two orbitals, to having only one? It turns out that when orbitals interact, they are free to change their forms, but there must always be the same number. This is just another way of saying that there must always be the same number of possible allowed sets of electron quantum numbers.

In-phase and out-of-phase wave combinations

How can we find the missing orbital? To answer this question, we must go back to the wave-like character of orbitals that we developed in our earlier treatment of the hydrogen atom. You are probably aware that wave phenomena such as sound waves, light waves, or even ocean waves can combine or interact with one another in two ways: they can either reinforce each other, resulting in a stronger wave, or they can interfere with and partially destroy each other. A roughly similar thing occurs when the "matter waves" corresponding to the two separate hydrogen 1*s* orbitals interact; both in-phase and out-of-phase combinations are possible, and both occur. The in-phase, reinforcing interaction yields the ***bonding orbital*** that we just considered. The other, corresponding to out-of-phase combination of the two orbitals, gives rise to a molecular orbital that has its greatest electron probability in what is clearly the antibonding region of space. This second orbital is therefore called an ***antibonding*** orbital.

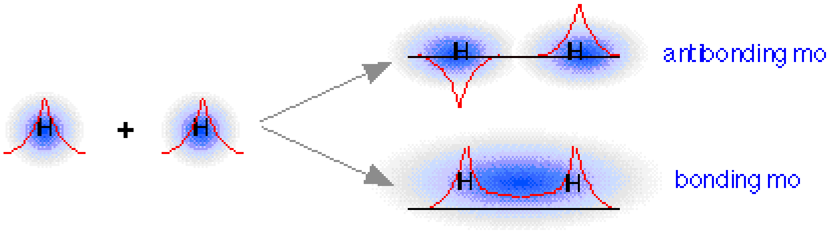


Figure 8.68 formation of Bonding and antibonding MOs through electron cloud

When the two 1*s* wave functions combine out-of-phase, the regions of high electron probability do not merge. In fact, the orbitals act as if they actually repel each other. Notice particularly that there is a region of space exactly equidistant between the nuclei at which the probability of finding the electron is zero. This region is called a *nodal surface*, and is characteristic of antibonding orbitals. It should be clear that any electrons that find themselves in an antibonding orbital cannot possibly contribute to bond formation; in fact, they will actively oppose it.

We see, then, that whenever two orbitals, originally on separate atoms, begin to interact as we push the two nuclei toward each other, these two atomic orbitals will gradually merge into a pair of molecular orbitals, one of which will have bonding character, while the other will be antibonding. In a more advanced treatment, it would be fairly easy to show that this result follows quite naturally from the wave-like nature of the combining orbitals.

What is the difference between these two kinds of orbitals, as far as their potential energies are concerned? More precisely, which kind of orbital would enable an electron to be at a lower potential energy? Clearly, the potential energy decreases as the electron moves into a region that enables it to “see” the maximum amount of positive charge. In a simple diatomic molecule, this will be in the internuclear region— where the electron can be simultaneously close to two nuclei. The bonding orbital will therefore have the lower potential energy.

A molecule is assumed to be a new entity consisting of positively charged nuclei and electrons.

The electrons in the molecule are contained in the molecular orbitals, which is the simplest form of the model are constructed from the atomic orbitals of the constituent atoms.

The model correctly predicts relative bond strength, magnetism and bond polarity.

It correctly portrays electrons as being delocalized in polyatomic molecule. The main disadvantage of the model is that it is difficult to apply qualitatively to polyatomic molecules.

We will discuss more in detail about this theory with an example of H_2 moelcule

When two H nuclei lie near each other as in H_2, their AOs overlap. The two AOS of combining the AOs are as follows:

Adding he wave functions together: This combination forms a bonding MO, which has a region of high electron density between the nuclei. Additive overlap is analogous to light waves reinforcing each other, making the resulting amplitude

Subtracting the wave functions from each other: This combination forms an antibonding MO, which has a region of zero electron density (a node) between the nuclei.

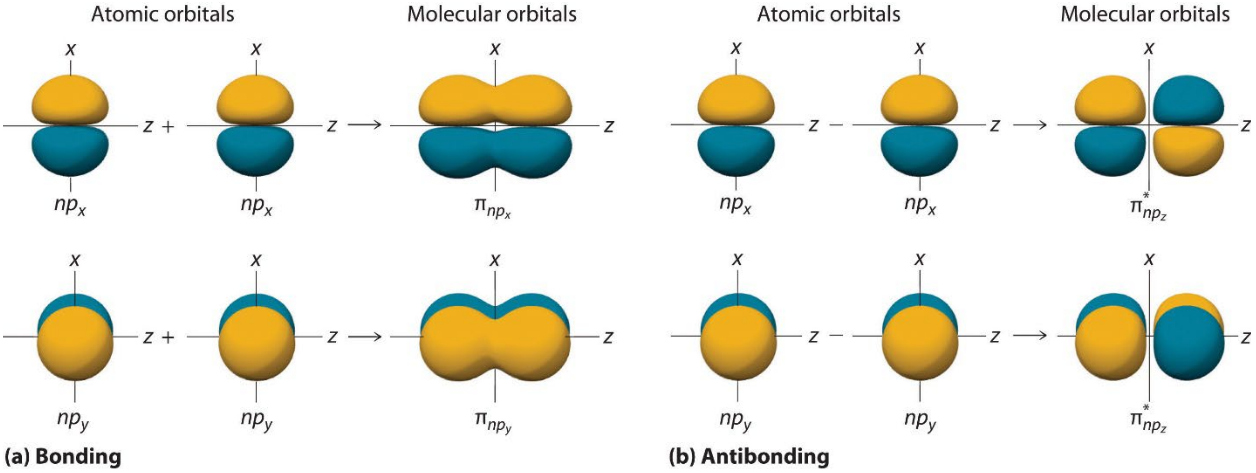


Figure 8.69 fFormation of Bonding and antibonding MOs

Ref: commons.wikimedia.org/

According to MO theory, a bonding MO is lower in energy than the atomic orbitals from which it is constructed. Electrons in this type of MO are lower in energy in the molecule than in the separated atoms and thus favor molecule formation.

An antibonding MO is higher in energy than the atomic orbitals from which it is constructed. Electrons in this type of MO are higher in energy in the molecule than in the separated atoms and thus do not favor molecule formation.

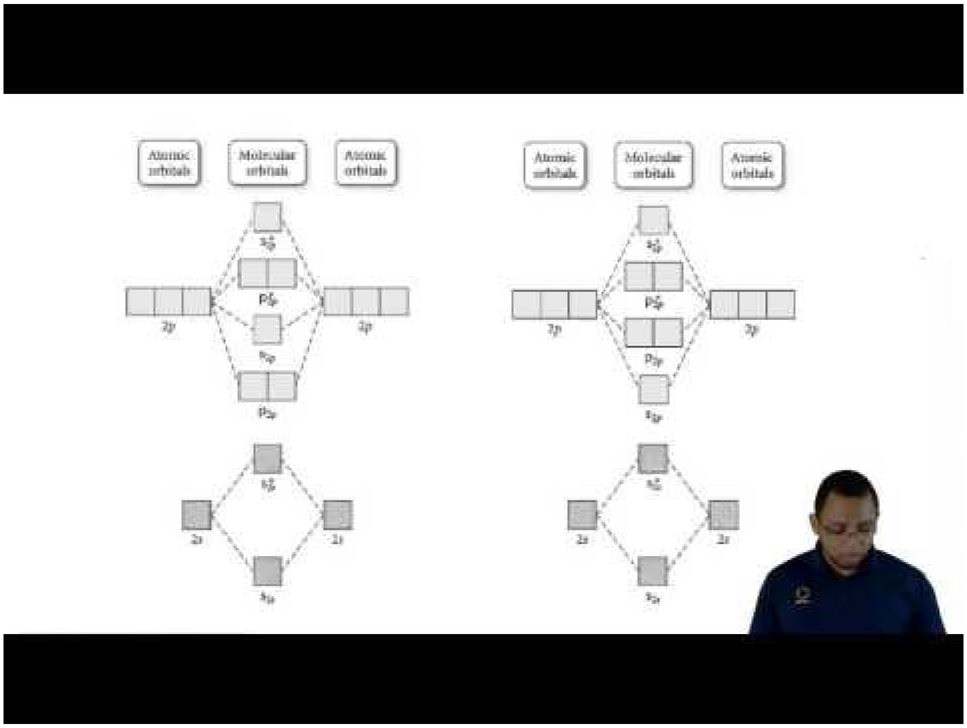
σ MOs have their electron probability centered on a line passing through the nuclei.

Π Mos have their electron probability concentrated above and below the line connecting the atoms.

$$\text{Bond order} = \frac{\text{\# of bonding MOs} - \text{\# of Antibonding MOs}}{2}$$

Bond order is measure of bond strength.

Watch the following video:



Filling Molecular Orbitals with Electrons: Electrons fill MOs just as they fill AOs.

MOs are filled in order of increasing energy (Aufbau Principle)

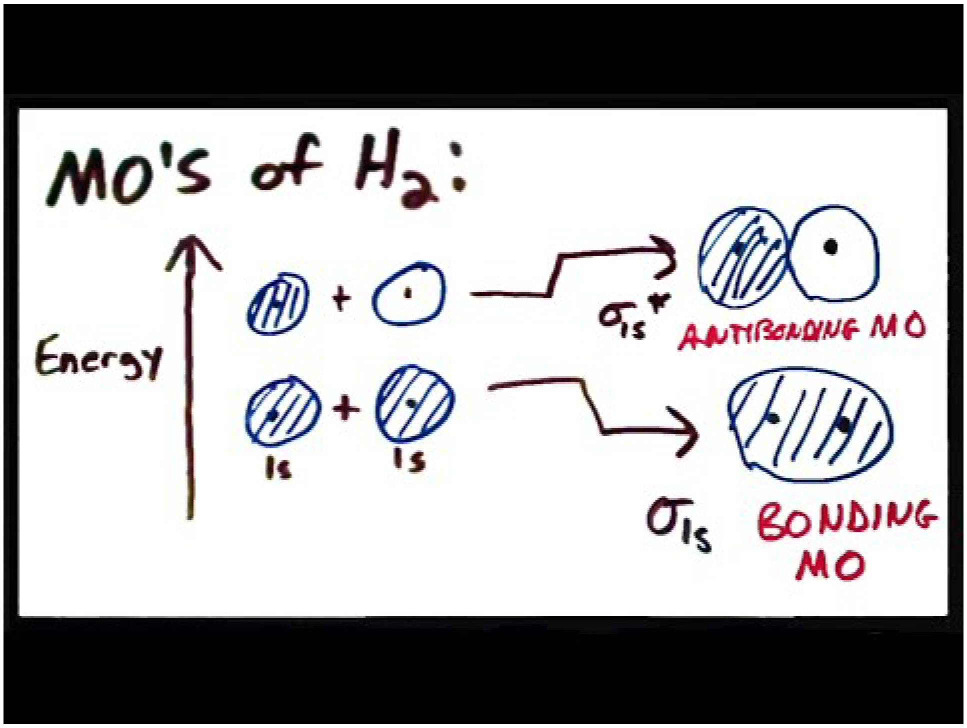
An MO has a maximum capacity of two electrons with opposite spins (exclusion principle)

Orbitals of equal energy are half-filled, with spins parallel, before any of them is completely filled (Hind’s Rule).

Understanding molecular orbital diagrams

Homonuclear Diatomic Molecules of Period 1 elements

The bonding MO in H_2 is spread mostly between the nuclei, with the nuclei attracted to the intervening electrons, An electron in this MO can delocalize its charge over a much larger volume than it is possible. Because the electron density-electron repulsions are reduced, the bonding MO is lower in energy than the isolated AOs. Therefore when electrons occupy this orbital, the molecule is more stable than the separate atoms. In contrast, the antibonding MO has a node between the nuclei



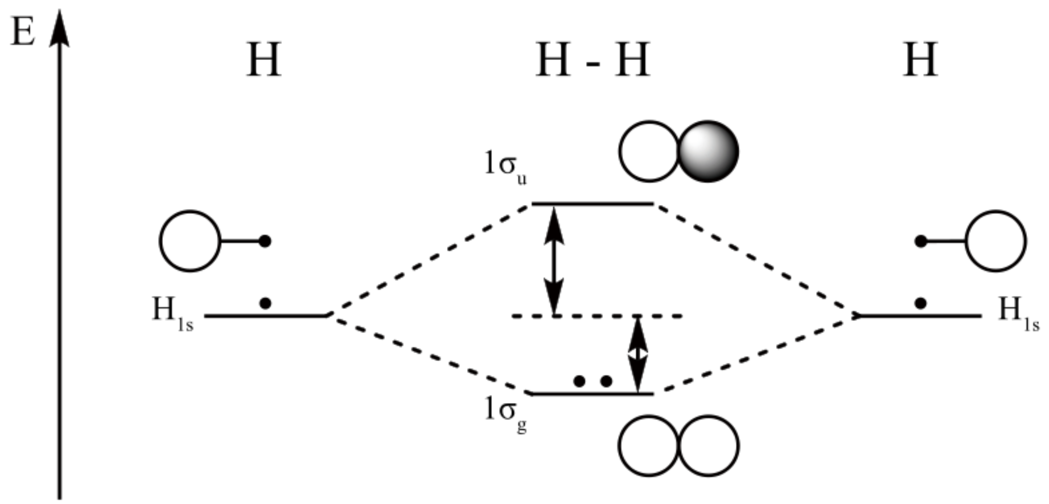


Figure 8.70 MO Diagram of H_2

Ref: commons.wikimedia.org/

The diagram below is for He_2 molecule. Bond order indicates that He_2 doesn't exist.

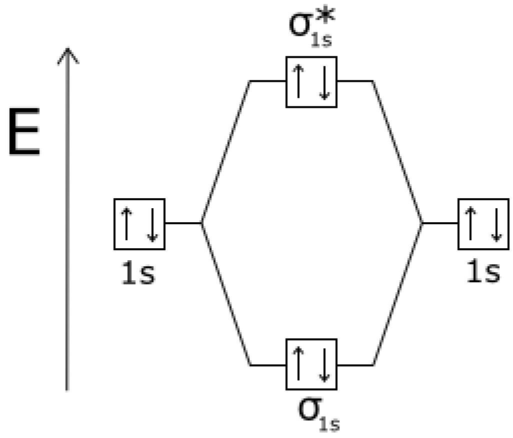


Figure 8.71 MO Diagram of He_2

Ref: commons.wikimedia.org/

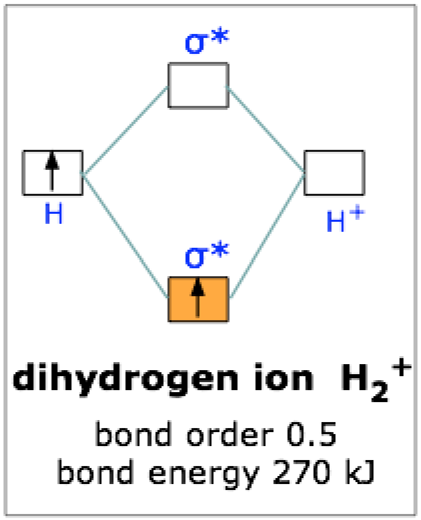


Figure 8.71 MO Diagram of $H_2{}^+$

This scheme of bonding and antibonding orbitals is usually depicted by a molecular orbital diagram such as the one shown here for the **dihydrogen ion H_2^+**. Atomic valence electrons (shown in boxes on the left and right) fill the lower-energy molecular orbitals before the higher ones, just as is the case for atomic orbitals. Thus, the single electron in this simplest of all molecules goes into the bonding orbital, leaving the antibonding orbital empty. Since any orbital can hold a maximum of two electrons, the bonding orbital in H_2^+ is only half-full. This single electron is nevertheless enough to lower the potential energy of one mole of hydrogen nuclei pairs by 270 kJ— quite enough to make them stick together and behave like a distinct molecular species. Although H_2^+ is stable in this energetic sense, it happens to be an extremely reactive molecule— so much so that it even reacts with itself, so these ions are not commonly encountered in everyday chemistry.

Bonding in dihydrogen

If one electron in the bonding orbital is conducive to bond formation, might two electrons be even better? We can arrange this by combining two hydrogen atoms-- two nuclei, and two electrons. Both electrons will enter the bonding orbital, as depicted in the Figure. We recall that one electron lowered the potential energy of the two nuclei by 270 kJ/mole, so we might expect two electrons to produce twice this much stabilization, or 540 kJ/mole.

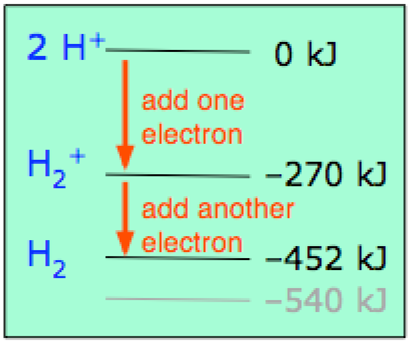


Figure 8.72 Energy correlation in MO Diagram of H_2^+

Bond order is defined as the difference between the number of electron pairs occupying bonding and nonbonding orbitals in the molecule. A bond order of unity corresponds to a conventional "single bond".

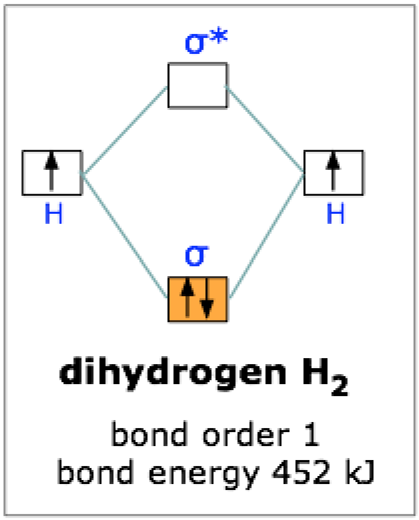


Figure 8.73 MO Diagram of H_2

Experimentally, one finds that it takes only 452 kJ to break apart a mole of hydrogen molecules. The reason the potential energy was not lowered by the full amount is that the presence of two electrons in the same orbital gives rise to a repulsion that acts against the stabilization. This is exactly the same effect we saw in comparing the ionization energies of the hydrogen and helium atoms

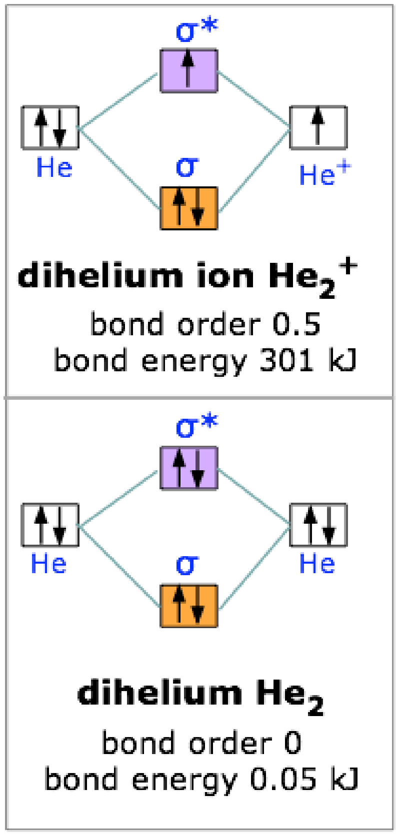


Figure 8.74 MO Diagram of He_2^+

***MO's in dihelium

With two electrons we are still ahead, so let's try for three. The dihelium positive ion is a three-electron molecule. We can think of it as containing two helium nuclei and three electrons. This molecule is stable, but not as stable as dihydrogen; the energy required to break He_2+ is 301 kJ/mole. The reason for this should be obvious; two electrons were accommodated in the bonding orbital, but the third electron must go into the next higher slot— which turns out to be the sigma antibonding orbital. The presence of an electron in this orbital, as we have seen, gives rise to a repulsive component which acts against, and partially cancels out, the attractive effect of the filled bonding orbital.

Taking our building-up process one step further, we can look at the possibilities of combining to helium atoms to form dihelium. You should now be able to predict that He_2 cannot be a stable molecule; the reason, of course, is that we now have four electrons— two in the bonding orbital, and two in the antibonding orbital. The one orbital almost exactly cancels out the effect of the other. Experimentally, the bond energy of dihelium is only .084 kJ/mol; this is not enough to hold the two atoms together in the presence of random thermal motion at ordinary temperatures, so dihelium dissociates as quickly as it is formed, and is therefore not a distinct chemical species.

MO's in diatomic molecules containing second-row atoms

The four simplest molecules we have examined so far involve molecular orbitals that derived from two 1*s* atomic orbitals. If we wish to extend our model to larger atoms, we will have to contend with higher atomic orbitals as well. One greatly simplifying principle here is that only the ***valence-shell*** orbitals need to be considered. Inner atomic orbitals such as 1*s* are deep within the atom and well-shielded from the electric field of a neighboring nucleus, so that these orbitals largely retain their atomic character when bonds are formed.

MO's in dilithium

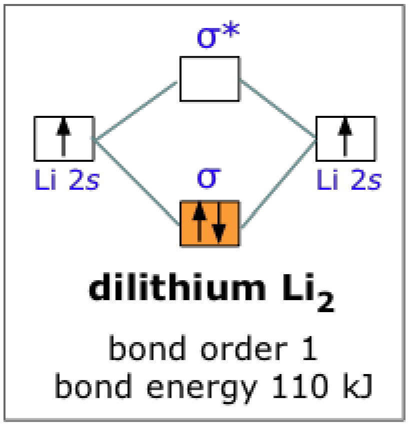


Figure 8.75 MO Diagram of Li_2

For example, when lithium, whose configuration is $1s^22s^1$, bonds with itself to form Li_2, we can forget about the 1*s* atomic orbitals and consider only the σ bonding and antibonding orbitals. Since there are not enough electrons to populate the antibonding orbital, the attractive forces win out and we have a stable molecule. The bond energy of dilithium is 110 kJ/mole; notice that this value is less than half of the 270 kJ bond energy in dihydrogen, which also has two electrons in a bonding orbital. The reason, of course, is that the 2*s* orbital of Li is much farther from its nucleus than is the 1*s* orbital of H, and this is equally true for the corresponding molecular orbitals. It is a general rule, then, that the larger the parent atom, the less stable will be the corresponding diatomic molecule.

Bonding of the Period 2 s-block Diatomic molecule

Both Li and Be occur s metal under normal conditions, but MO theory predict their stability as dilithium and diberyllium.

These molecules have both inner 1s and outer 2s orbitals. Is orbitals are core orbitals. We ignore inner or core 1s orbitals since only valence orbitals interact enough to form molecular orbitals. Like the MOS formed from 1s AOs, those formed from 2s AOs are also σ orbitals, cylindrically symmetrical around the internuclear axis. Bonding σ_{2s} and antibonding σ^*_{2s} MOS form and valence electrons occupy bonding σ2s MO with opposite spins for lithium molecule and σ*2s MO for Be_2 molecule. Bond oder in Li_2= 1/2(2-0)= 1 and bond order for Be_2= ½(2-2)=0. Therefore, ground state of Be_2 molecule doesn't exist.

Molecular orbitals from the atomic p-orbital combination:

As we move from Be to B, atomic 2p orbitals become involved. We will first consider the shapes and energies of the MOs resulting from their combinations. P orbital can overlap in two ways, end to end combination will give a pair of σ MOs, σ2p and σ*2p. Side to side combination will give a pair of п MOs. π_{2p} and π^*_{2p}. Similar to MOs formed from s orbitals, bonding MOs from p-orbital combinations have their greatest electron density between the nuclei whereas antibonding MOs from p-orbital combinations have a node between the nuclei and most of their electron density outside the internuclear region.

- Ms formed from 2s orbitals are lower in energy than MOs formed from 2p orbitals because 2s AOs are lower in energy than 2p AOs.
- Bonding MOs have lower in energy than anti-bonding MOs. Therefore σ2p is lower in energy than σ*2p and п2p is lower in energy than п*2p.
- p-orbitals can interact more extensively end to end than side to side. Thus σ2p is lower in energy than п2p. Similarly, destabilizing effect of σ*2p MO is greater than that of the п*2p MO.

Energy order of MO derived from p orbital:

σ2p< п2p< п*2p< σ*2p

When all six p –orbitals combine to form MOs, two of the six combine end to end to produce sigma and sigma* MOs. Other four p-orbitals produce two pi-bonding MOs and two antibonding MOs.Two pi-bonding MOs are degenerate as well as two pi-antibonding MOs.

But since B, C and N atoms are larger and p orbitals are not completely filled up, atomic orbitals repel each other and energy of 2p orbitals become closer to the energy of the 2s orbital. As a result, some mixing occurs between the 2s orbital of one atom and the end-on 2p orbital of another atom. This orbital mixing lowers the energy of the σ2s and σ*2s MOs and raises the energy of the σ2p and σ*2p MOs. **That creates dengerate π2p MOs lower in energy than σ2p.**

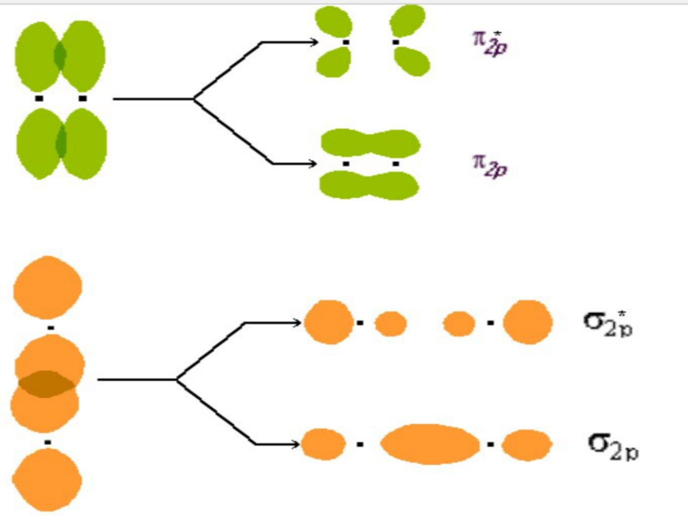


Figure 8.76 Degenerate Pi orbitals

Ref: commons.wikimedia.org/

After Be , porbitals are involved in MO formation. Here is the MO diagram for B_2 molecule including 1 2p electron from each atom. Possible energy levels look like the following diagram.

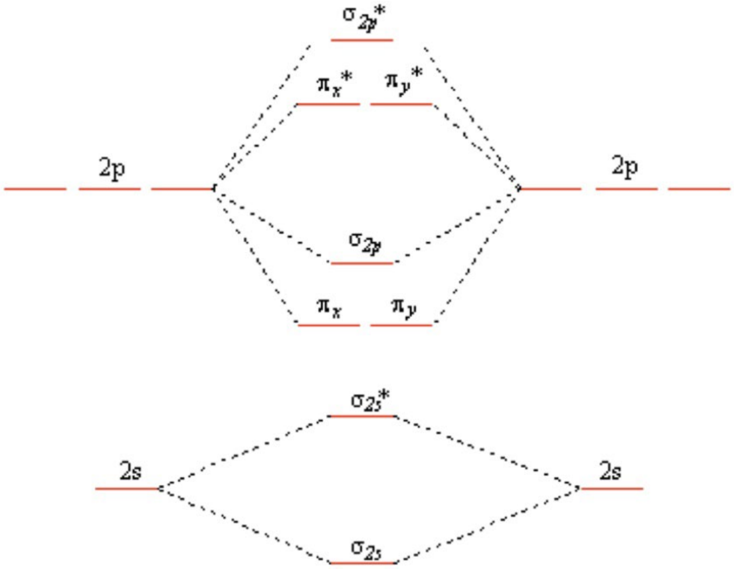


Figure 8.76 MO diagram for Li_2-N_2

Ref: commons.wikimedia.org/

Following the above energy scheme: B_2 molecule

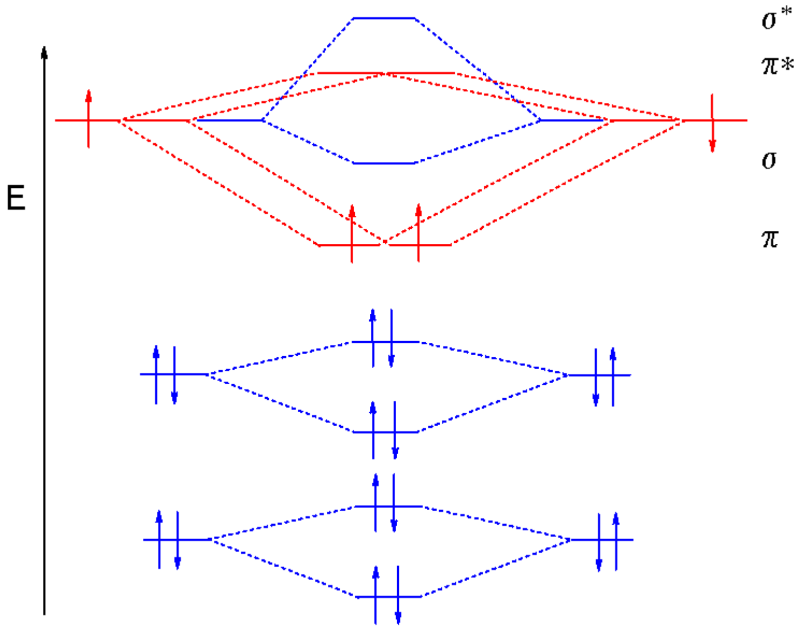


Figure 8.77 MO diagram for B_2

Ref: commons.wikimedia.org/

Following diagram is for N_2 molecule

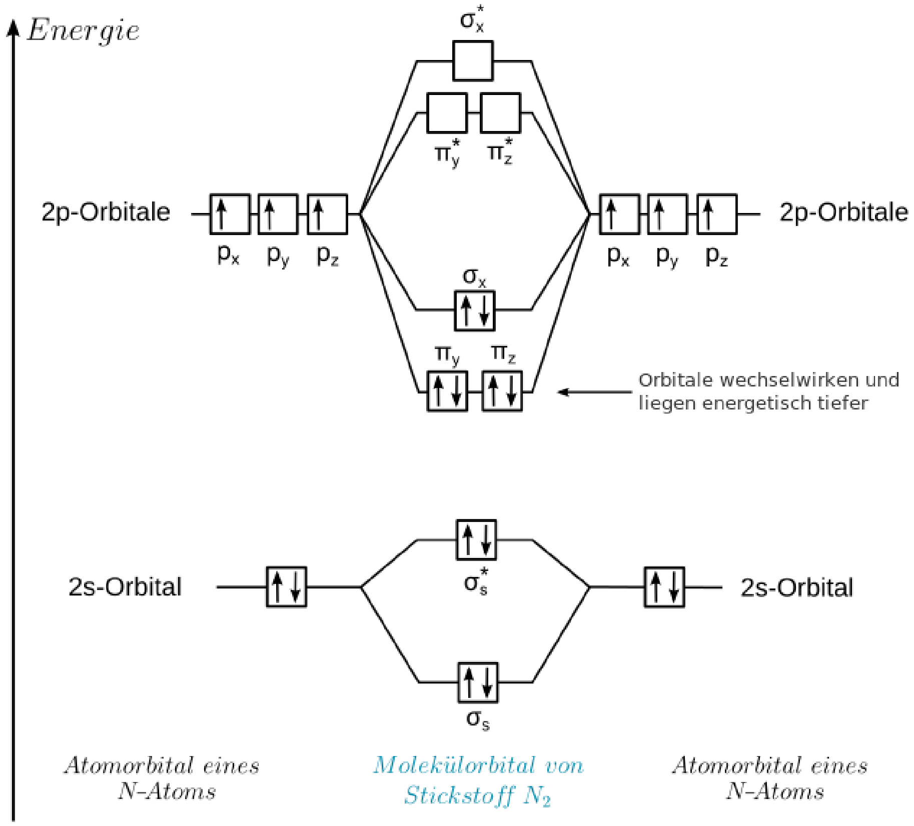


Figure 8.78 MO diagram for N_2

Ref: commons.wikimedia.org/

Bonding in the p-block homonuclear diatomic molecules

The B_2 molecule has six outer electrons to place in its MOs. Four of these fill σ_{2s} and σ^*_{2s} MOs. The remaining two electrons occupy the two π_{2p} MOs, one in each orbital, in keeping with Hund's rule. With four electrons in the bonding MOs and two electrons in the antibonding MOs, the bond order of B_2 is ½(4-2)=1, therefore B_2 is diamagnetic.

The two additional electrons present in C_2 will fill the $\pi_{2p.}$ Since C_2 has two more bonding electrons than B_2, it has bond order of 2, and bond is expected to be stronger, shorter. With all electrons paired, C_2 is diamagnetic.

In N_2, two additional electrons fill the σ2p MO. The resulting bond order is 3. According to theory, bond energy is higher, bond length is shorter and N_2 is diamagnetic.

V. MAGNETISM & MO THEORY

2s-2p interactions in MO theory

An important factor influences MO energy order. We know that AOS of similar energy interact to form MOs. We assume that s and p orbitals are so different in energy that they don't mix. This is true for O, F and Ne. With O_2 we really see the power of MO theory

Now consider the example of O_2. Experimentally, O_2 is known to paramagnetic. According to VBT, O_2 should look like this:

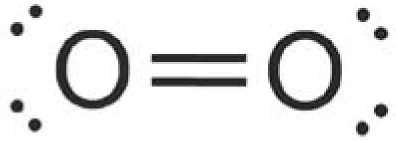


Figure 8.79 O_2 Molecule

Ref: commons.wikimedia.org/

As you can see, all the electrons are paired. Therefore VBT predicts that O_2 should be diamagnetic.

Now let's examine how the electrons are arranged according to MOT. In MOT, unlike VBT, it involves the creation of bonding and anti-bonding MOs. MOs are basically the supposition of the wavefunctions of atomic orbitals. In O_2 the 2s AOs of each oxygen atom constructively and destructively overlap with each other while their 2p AOs also constructively and destructively overlap with each other The resulting MOs for O_2 looks like this:

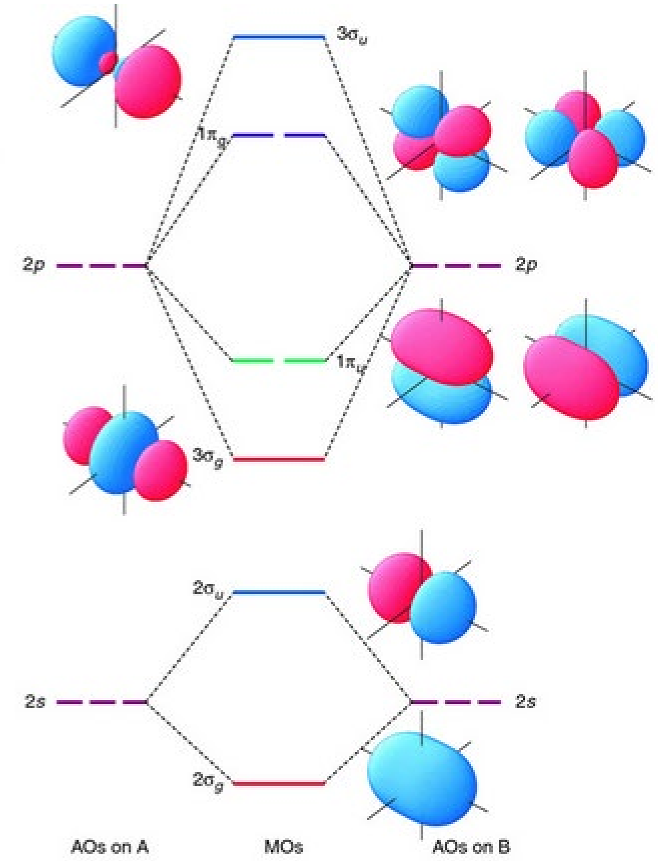


Figure 8.80 MO diagram for O_2 Molecule

Ref: commons.wikimedia.org/

Now that we got the MOs, all we have to do is fill them with electrons using the same method that we use for AOs. By doing that we get 2 unpaired electrons. Therefore MOT correctly predicts that O2 should be paramagnetic, unlike VBT which predicts that O_2 is diamagnetic.

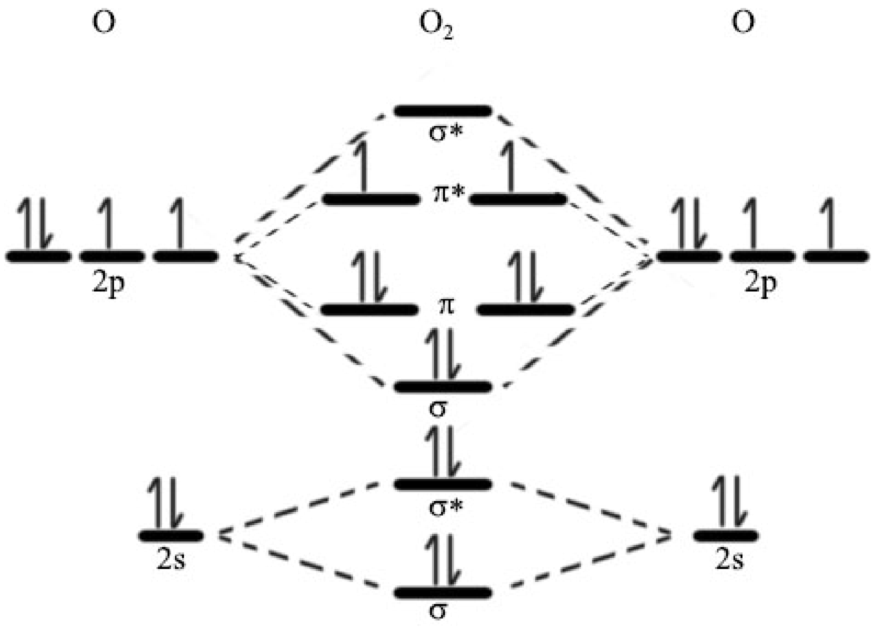


Figure 8.81 Paramagnetic O_2 Molecule

Ref: commons.wikimedia.org/

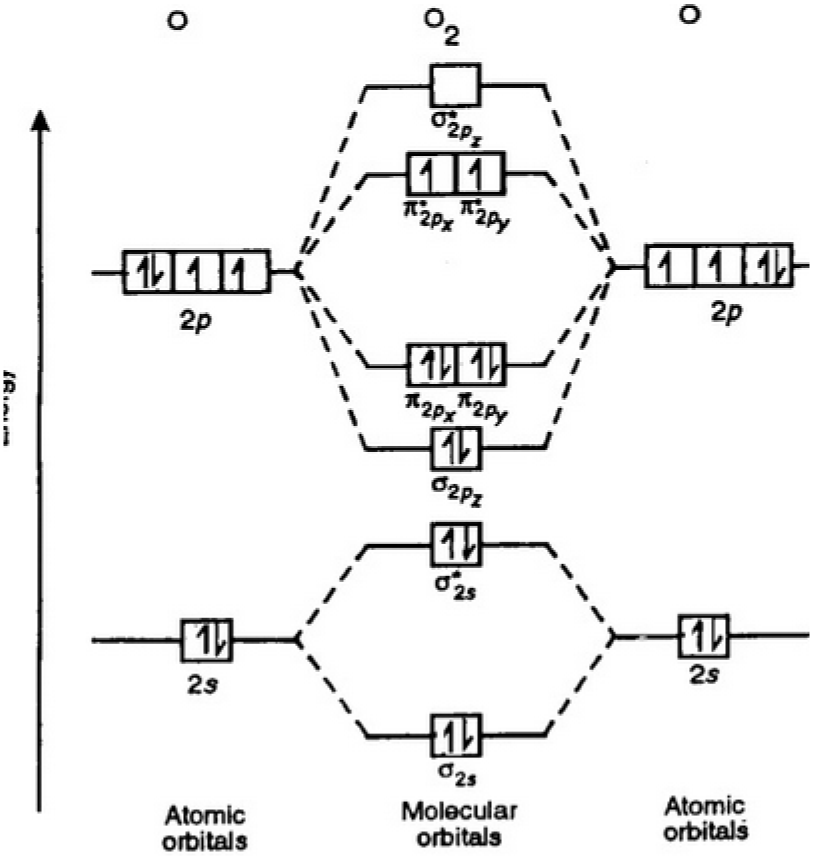


Figure 8.82 MO diagram for Paramagnetic O_2 Molecule

Ref: commons.wikimedia.org/

SUPPLEMENTAL

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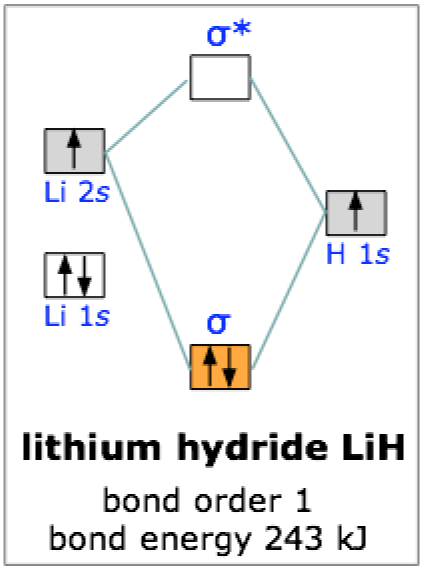
MO's in lithium hydride

Figure 8.83 MO diagram for LiH



Molecule

All the molecules we have considered thus far are ***homonuclear***; they are made up of one kind of atom. As an example of a ***heteronuclear*** molecule, let's take a look at a very simple example— lithium hydride. Lithium hydride is a stable, though highly reactive molecule. The diagram shows how the molecular orbitals in lithium hydride can be related to the atomic orbitals of the parent atoms. One thing that makes this diagram look different from the ones we have seen previously is that the parent atomic orbitals have widely differing energies; the greater nuclear charge of lithium reduces the energy of its 1*s* orbital to a value well below that of the 1*s* hydrogen orbital.

There are two occupied atomic orbitals on the lithium atom, and only one on the hydrogen. With which of the lithium orbitals does the hydrogen 1*s* orbital interact? The lithium 1*s* orbital is the lowest-energy orbital on the diagram. Because this orbital is so small and retains its electrons so tightly, it does not contribute to bonding; we need consider only the 2*s* orbital of lithium which combines with the 1*s* orbital of hydrogen to form the usual pair of sigma bonding and antibonding orbitals. Of the four electrons in lithium and hydrogen, two are retained in the lithium 1*s* orbital, and the two remaining ones reside in the σ orbital that constitutes the Li–H covalent bond.

The resulting molecule is 243 kJ/mole more stable than the parent atoms. As we might expect, the bond energy of the heteronuclear molecule is very close to the average of the energies of the corresponding homonuclear molecules. Actually, it turns out that the correct way to make this comparison is to take the geometric mean, rather than the arithmetic mean, of the two bond energies. The geometric mean is simply the square root of the product of the two energies.

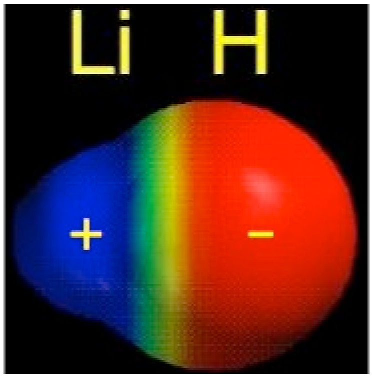


Figure 8.84 Electron Cloud for LiH Molecule

The geometric mean of the H_2 and Li_2 bond energies is 213 kJ/mole, so it appears that the lithium hydride molecule is 30 kJ/mole more stable than it “is supposed” to be. This is attributed to the fact that the electrons in the 2σ bonding orbital are not equally shared between the two nuclei; the orbital is skewed slightly so that the electrons are attracted somewhat more to the hydrogen atom. This *bond polarity*, which we considered in some detail near the beginning of our study of covalent bonding, arises from the greater electron-attracting power of hydrogen— a consequence of the very small size of this atom. The electrons can be at a lower potential energy if they are slightly closer to the hydrogen end of the lithium hydride molecule. It is worth pointing out, however, that the electrons are, on the average, also closer to the lithium nucleus, compared to where they would be in the 2*s* orbital of the isolated lithium atom. So it appears that everyone gains and no one loses here!

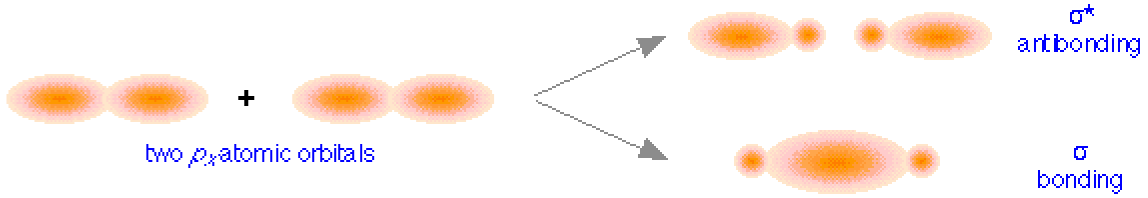
[LiH image source]

3***Sigma*** and ***pi*** orbitals

The molecules we have considered thus far are composed of atoms that have no more than four electrons each; our molecular orbitals have therefore been derived from *s*-type atomic orbitals only. If we wish to apply our model to molecules involving larger atoms, we must take a close look at the way in which *p*-type orbitals interact as well. Although two atomic *p* orbitals will be expected to split into bonding and antibonding orbitals just as before, it turns out that the extent of this splitting, and thus the relative energies of the resulting molecular orbitals, depend very much on the nature of the particular *p* orbital that is involved.

The importance of direction

You will recall that there are three possible *p* orbitals for any value of the principal quantum number. You should also recall that *p* orbitals are not spherical like *s* orbitals, but are elongated, and thus possess definite directional properties. The three *p* orbitals correspond to the three directions of Cartesian space, and are frequently designated p_x, p_y, and p_z, to indicate the axis along which the orbital is aligned. Of course, in the free atom, where no coordinate system is defined, all directions are equivalent, and so are the *p* orbitals. But when the atom is near another atom, the electric field due to that other atom acts as a point of reference that defines a set of directions. The line of centers between the two nuclei is conventionally taken as the *x* axis. If this direction is represented horizontally on a sheet of paper, then the *y* axis is in the vertical direction and the *z* axis would be normal to the page.



These directional differences lead to the formation of two different classes of molecular orbitals. The above figure shows how two p_x atomic orbitals interact. In many ways the resulting molecular orbitals are similar to what we got when *s* atomic orbitals combined; the bonding orbital has a large electron density in the region between the two nuclei, and thus corresponds to the lower potential energy. In the out-of-phase combination, most of the electron density is away from the internuclear region, and as before, there is a surface exactly halfway between the nuclei that corresponds to zero electron density. This is clearly an ***antibonding orbital***— again, in general shape, very much like the kind we saw in hydrogen and similar molecules. Like the ones derived from *s*-atomic orbitals, these molecular orbitals are σ (*sigma*) orbitals.

Sigma orbitals are cylindrically symmetric with respect to the line of centers of the nuclei; this means that if you could look down this line of centers, the electron density would be the same in all directions.

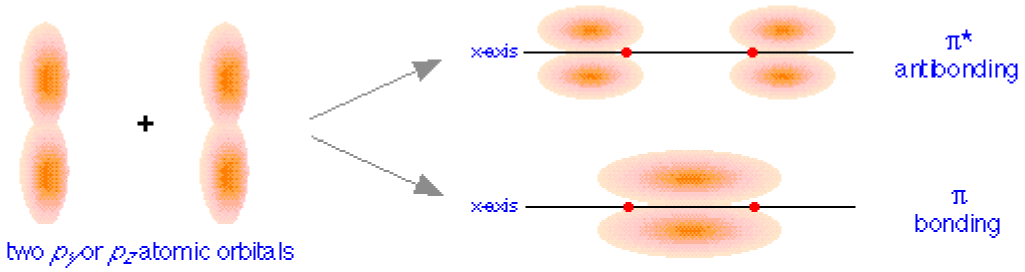


Figure 8.85 Pi bonding and antibonding MOs

When we examine the results of the in- and out-of-phase combination of p_y and p_z orbitals, we get the bonding and antibonding pairs that we would expect, but the resulting molecular orbitals have a different symmetry: rather than being rotationally symmetric about the line of centers, these orbitals extend in both perpendicular directions from this line of centers. Orbitals having this more complicated symmetry are called π (*pi*) orbitals. There are two of them, π_y and π_z differing only in orientation, but otherwise completely equivalent.

The different geometric properties of the π and σ orbitals causes the latter orbitals to split more than the π orbitals, so that the σ* antibonding orbital always has the highest energy. The σ bonding orbital can be either higher or lower than the π bonding orbitals, depending on the particular atom.

****

MO splitting patterns for second-row diatomics

If we combine the splitting schemes for the 2*s* and 2*p* orbitals, we can predict bond order in all of the diatomic molecules and ions composed of elements in the first complete row of the periodic table. Remember that only the ***valence orbitals*** of the atoms need be considered; as we saw in the cases of lithium hydride and dilithium, the inner orbitals remain tightly bound and retain their localized atomic character.

Notice that the relative energies of the 2*p*-derived σ and π bonding molecular orbitals are reversed in O_2 and F_2. This is attributed to interactions between the 2*s* orbital each atom with the $2p_x$ orbital of the other, an effect similar to hybridizaton. However, the order in which these two orbitals are filled has no effect on the predicted bond orders, so there is ordinarily no need to know which molecules follow which scheme.

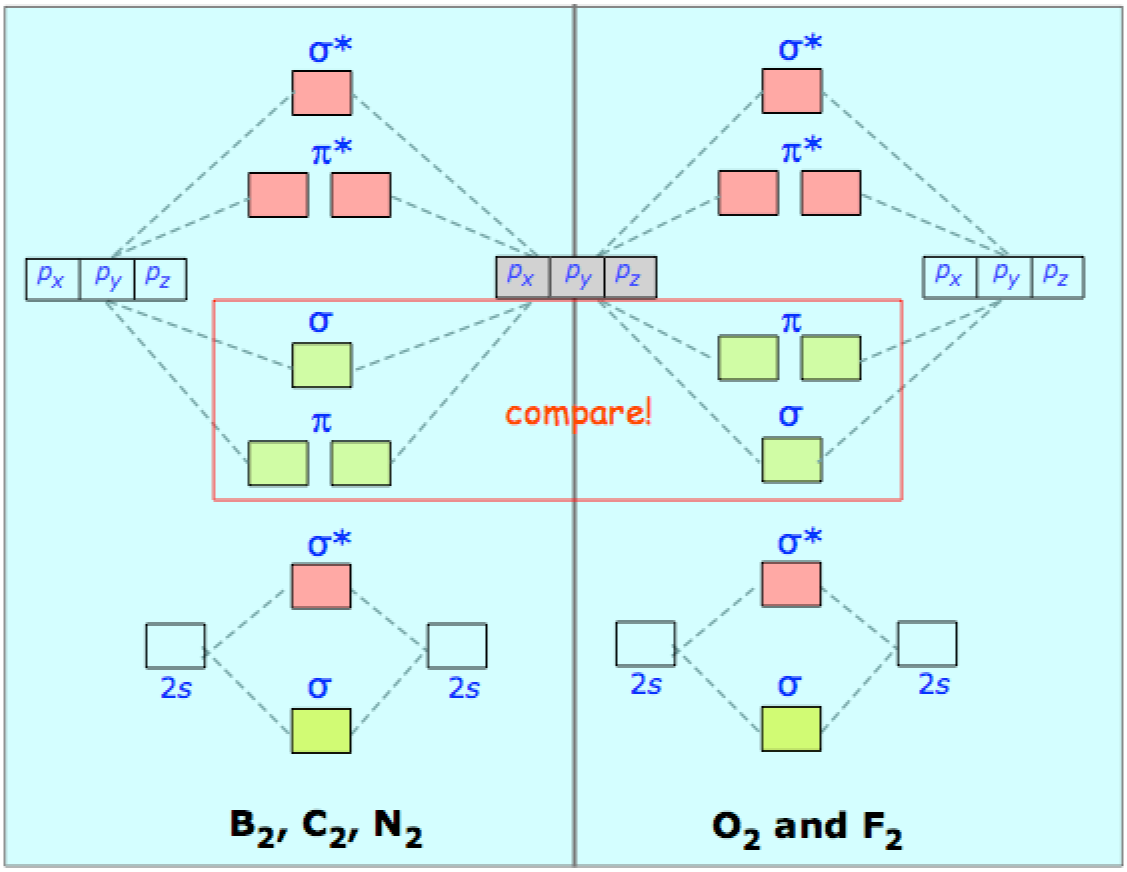


Figure 8.86 Pi –Pi interactions in MOs

MO's in dicarbon: Carbon has four outer-shell electrons, two 2*s* and two 2*p*. For two carbon atoms, we therefore have a total of eight electrons, which can be accommodated in the first four molecular orbitals. The lowest two are the 2*s*-derived bonding and antibonding pair, so the “first” four electrons make no net contribution to bonding. The other four electrons go into the pair of *pi* bonding orbitals, and there are no more electrons for the antibonding orbitals— so we would expect the dicarbon molecule to be stable, and it is. (But being extremely reactive, it is known only in the gas phase.)

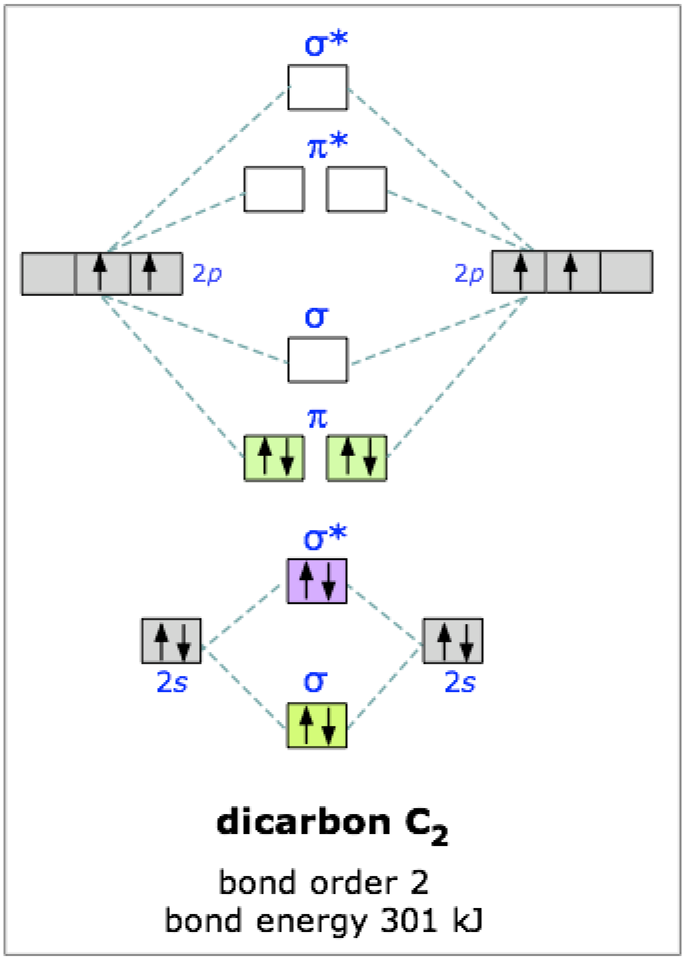


Figure 8.87 MO diagram of C_2

You will recall that one pair of electrons shared between two atoms constitutes a "single" chemical bond; this is Lewis' original definitio>n of the covalent bond. In C_2 there are two paris of electrons in the π bonding orbitals, so we have what amounts to a double bond here; in other words, the bond order in dicarbon is two.

More on dicarbon.

MO's in dioxygen

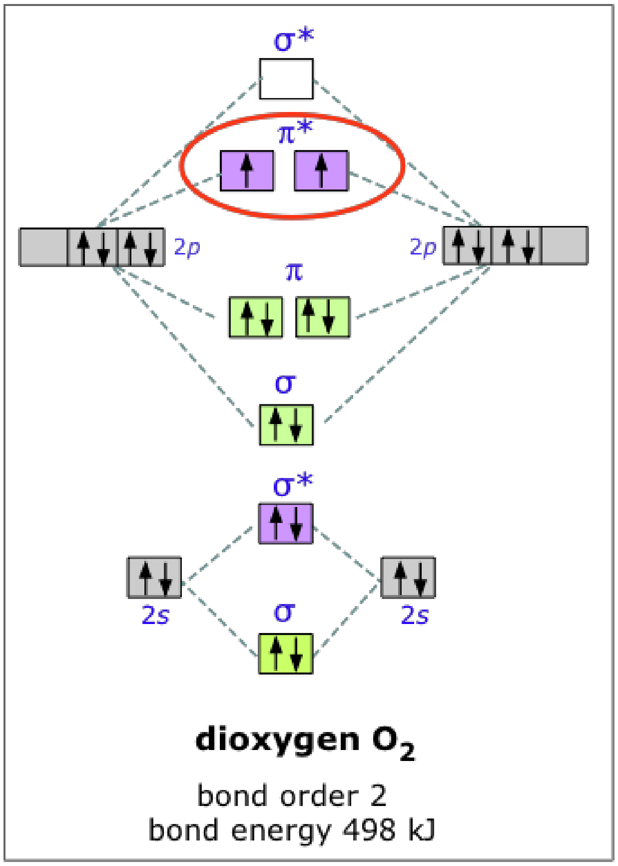


Figure 8.88 MO diagram of O_2

The electron configuration of oxygen is $1s^22s^22p^4$. In O_2, therefore, we need to accommodate twelve valence electrons (six from each oxygen atom) in molecular orbitals. As you can see from the diagram, this places two electrons in antibonding orbitals. Each of these electrons occupies a separate π^* orbital because this leads to less electron-electron repulsion.

The bond energy of molecular oxygen is 498 kJ/mole. This is smaller than the 945 kJ bond energy of N_2— not surprising, considering that oxygen has two electrons in an antibonding orbital, compared to nitrogen's one.

Although this paramagnetic *ground-state* form of O_2 (also known as *triplet* oxygen) is the energetically favored, and therefor is the common form of this element, another variety, in which the two electrons are paired up in a single *pi* antibonding orbital, is also well known. This *singlet oxygen*, as it is called, has a bond energy of only 402 kJ/mole. The lower value reflects the action of electrostatic repulsion between the two electrons in the same orbital.

Singlet oxygen, being less stable, does not exist under normal conditions. It can be formed by the action of light and in certain chemical reactions, and it has an interesting and unique chemistry of its own.

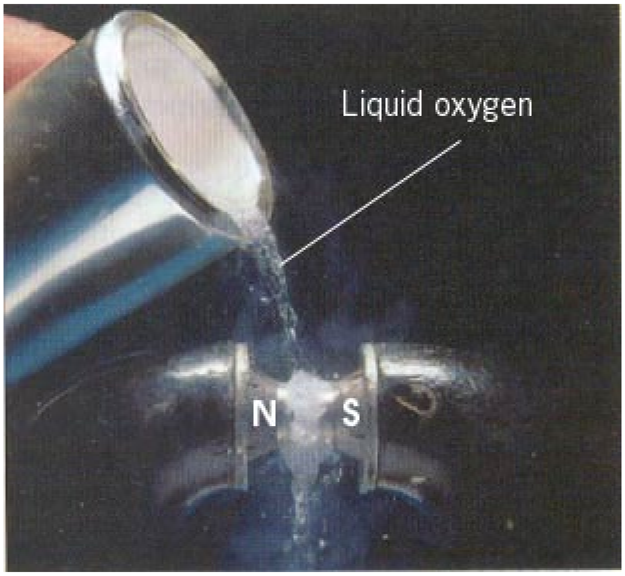
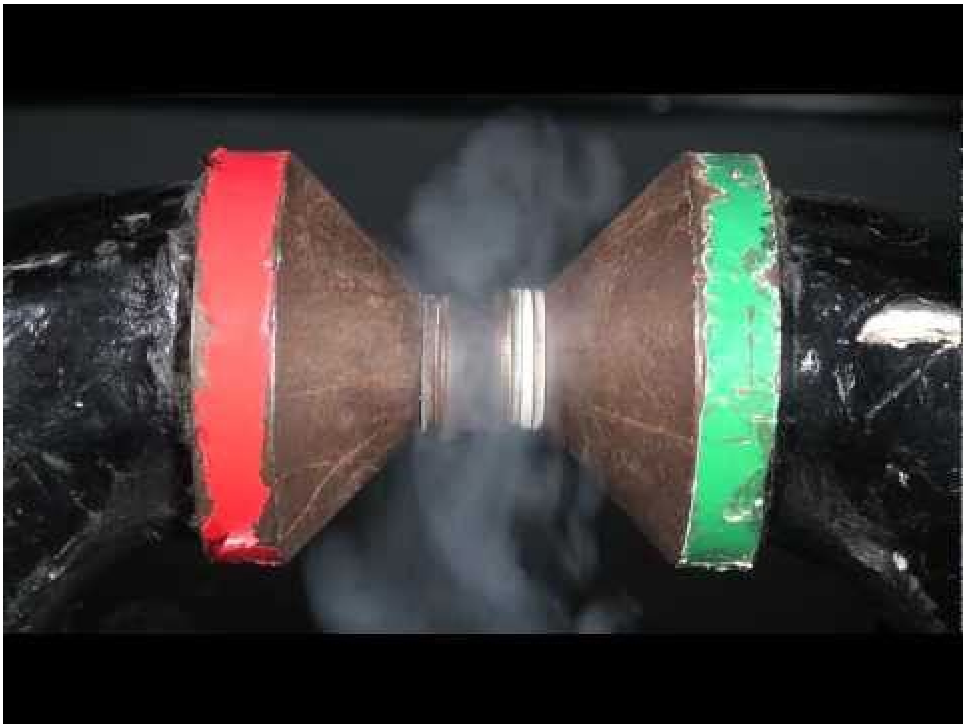


Figure 8.89 Paramagnetic behavior of Liquid Oxygen

The two unpaired electrons of the dioxygen molecule give this substance an unusual and distinctive property: O_2 is ***paramagneti***c. The paramagnetism of oxygen can readily be demonstrated by pouring liquid O_2 between the poles of a strong permanent magnet; the liquid stream is trapped by the field and fills up the space between the poles.

https://www.youtube.com/watch?v=Lt4P6ctf06Q



Since molecular oxygen contains two electrons in an antibonding orbital, it might be possible to make the molecule more stable by removing one of these electrons, thus increasing the ratio of bonding to antibonding electrons in the molecule. Just as we would expect, and in accord with our model, O_2^+ has a bond energy higher than that of neutral dioxygen; removing the one electron actually gives us a more stable molecule. This constitutes a very good test of our model of bonding and antibonding orbitals. In the same way, adding an electron to O_2 results in a weakening of the bond, as evidenced by the lower bond energy of O_2^-. The bond energy in this ion is not known, but the length of the bond is greater, and this is indicative of a lower bond energy. These two dioxygen ions, by the way, are highly reactive and can be observed only in the gas phase.

References

Introductory tutorials from various sources

The Chemogenesis WebBook site has a nice page on MO theory

This page from Imperial College (London) has MO diagrams for molecules such as ethane, ethylene, and water.

Wikipedia article on molecular orbitals

Visualizations

Viewer applet for the MO's of the hydrogen molecule ion

Atom-in-a-box (Mac only) - Orbital viewer (Windows only)

More advanced stuff (probably best avoided by first-year students!)

A more advanced introduction to MO theory (J Harvey, U of Bristol)

This one is even more advanced, and introduces the mathematical methods used to calculate molecular properties

What you should be able to do

1) Make sure you thoroughly understand the following essential ideas which have been presented above.
2) In what fundamental way does the molecular orbital model differ from the other models of chemical bonding that have been described in these lessons?
3) Explain how bonding and antibonding orbitals arise from atomic orbitals, and how they differ physically.
4) Describe the essential difference between a *sigma* and a *pi* molecular orbital.
5) Define *bond order*, and state its significance.
6) Construct a "molecular orbital diagram" of the kind shown in this lesson for a simple diatomic molecule, and indicate whether the molecule or its positive and negative ions should be stable.

***** Adapted from Chem I Virtual textbook**
http://www.chem1.com/acad/webtext/virtualtextbook.html.

PRACTICE QUESTIONS: CHAPTER 8

1. The hybridization of the central atom in I_3^- is:

A) *sp*

B) sp^2

C) sp^3

D) dsp^3

E) d^2sp^3

2. The electron configuration of a particular diatomic species is $(\sigma_{2s})^2(\sigma^*_{2s})^2(\sigma_{2p})^2(\pi_{2p})^4(\pi^*_{2p})^2$. What is the bond order for this species?

A) 3.5

B) 3

C) 2.5

D) 2

E) 1.5

3. A π (pi) bond is the result of the

- A) overlap of two *s* orbitals
- B) overlap of an *s* orbital and a *p* orbital
- C) overlap of two *p* orbitals along their axes
- D) sidewise overlap of two parallel *p* orbitals
- E) sidewise overlap of two *s* orbital

4. The configuration $(\sigma_{2s})^2(\sigma_{2s}^*)^2(\pi_{2py})^1(\pi_{2pz})^1$ is the molecular orbital description for the ground state of

A) Li_2^+

B) Be_2

C) B_2

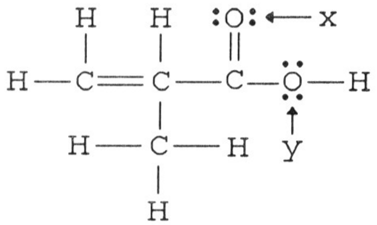
D) B_2^{2-}

E) C_2

5. The sp^2 atomic hybrid orbital set accommodates ________ electron domains.

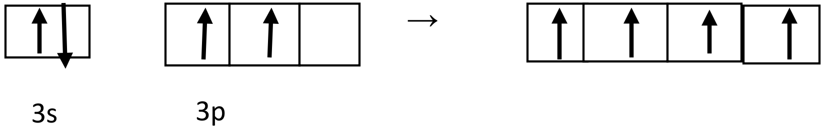
A) 2 B) 3 C) 4 D) 5 E) 6

6. The hybridization of the oxygen atom labeled "x" in the structure below is ________. The C-O-H bond angle at the oxygen atom labeled "y" is ________.



A) sp^3d^2, 90° B) sp, 180° C) sp, 90° D) sp^2, 109.5° E) sp^3, 109.5°

7. The orbital diagram that follows presents the final step in the formation of hybrid orbitals by a silicon atom. Which of the following best describes what took pictured in the diagram:



A) Two 3p electrons became unpaired
B) An electron was promoted from the 2p orbital to 3s orbital
C) sp^3 hybrid orbitals were produced
D) sp^2 hybrid orbitals were produced

8. There are ________ σ bonds and ________ π bonds in

$H_3C\text{-}CH_2\text{-}CH\text{=}CH\text{-}CH\text{=}CH_2$.

A) 10, 3 B) 14, 2 C) 12, 2 D) 15, 2 E) 13, 2

9. Molecular Orbital theory correctly predicts paramagnetism of oxygen gas, O_2. This is because ________.

A) the energy of the π_{2p} MOs is higher than that of the σ_{2p} MO

B) the O=O bond distance is relatively short
C) there are more electrons in the bonding orbitals than in the antibonding orbitals.
D) the bond order in O_2 can be shown to be equal to 2.
E) there are two unpaired electrons in the MO electron configuration of O_2

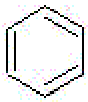
10. The hybridization of the central carbon in the $H_2C{=}C{=}CH_2$ molecule is ________.
A) sp^3d B) sp^3d^2 C) sp^2 D) sp E) sp^3

11. A bonding or antibonding π orbital contains a maximum of ________ electrons.
A) 1 B) 2 C) 4 D) 6 E) 8

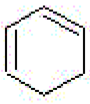
12. Use molecular orbital theory to predict which molecule or ion has the highest bond energy?

C_2
a) C_2^+
b) C_2^-

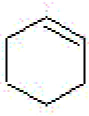
13. Use the molecules below to answer the next three questions.



C_6H_6
(I)



C_6H_8
(II)



C_6H_{10}
(III)

14. Which molecule(s) have *p* orbitals that share an electron pair to create π bonding?

a. I

b. II

c. III

d. all of the above

e. none of the above

ANSWER: d

15. Which molecule(s) have at least one carbon atom that is *sp* hybridized?

a. I

b. II

c. III

d. all of the above

e. none of the above

ANSWER: e

16. Which molecule(s) have equivalent C–C bonds throughout the molecule?

a. I

b. II

c. III

d. all of the above

e. none of the above

ANSWER: a

17. Whenever a set of equivalent tetrahedral atomic orbitals is required, an atom will adopt a set of sp^3 orbitals.

a. True

b. False

ANSWER: True

18. The hybridization of the B in BH_3 is sp^3.

a. True

b. False

ANSWER: False

19. The hybridization of a molecule is measured to determine the shape of the molecule.

a. True

b. False

ANSWER: False

20. Which of the following statements is true?

a. Electrons are never found in an antibonding MO.

b. All antibonding MOs are higher in energy than the atomic orbitals of which they are composed.

c. Antibonding MOs have electron density mainly outside the space between the two nuclei.

d. None of the above is true.

e. Two of the above statements are true.

ANSWER: e

21. Which of the following statements is (are) incorrect?

I. The hybridization of boron in BF_3 is sp^2.

II. The molecule XeF_4 is nonpolar.

III. The bond order of N_2 is three.

IV. The molecule HCN has two pi bonds and two sigma bonds.

a. All four statements are correct.

b. II is incorrect.

c. I and IV are incorrect.

d. II and III are incorrect.

e. II, III, and IV are incorrect.

ANSWER: a

22. Which of the following molecules contains the shortest C–C bond?

a. C_2H_2

b. C_2H_4

c. C_2H_6

d. C_2Cl_4

e. b and d

ANSWER: a

23. The electron configuration of a particular diatomic species is $(\sigma_{2s})^2(\sigma^*_{2s})^2(\sigma_{2p})^2(\pi_{2p})^2(\pi^*_{2p})^4$. What is the bond order for this species?

a. 1.5

b. 1

c. 0.5

d. 0

e. 2

ANSWER: d

24. What is the bond order of He_2^+?

a. 0

b. $\frac{1}{2}$

c. 1

d. $1\frac{1}{2}$

e. 2

ANSWER: b

25. If four orbitals on one atom overlap four orbitals on a second atom, how many molecular orbitals will form?

a. 1

b. 4

c. 8

d. 16

e. none of these

ANSWER: c

26. Larger bond order means greater bond strength.

a. True

b. False

ANSWER: True

27. When an electron pair is shared in the area centered on a line joining the atoms, a σ (sigma) bond is formed.

a. True

b. False

ANSWER: True

28. As the bond order of a bond increases, the bond energy _______ and the bond length _______.

a. increases, increases

b. decreases, decreases

c. increases, decreases

d. decreases, increases

e. More information is needed to answer this question.

ANSWER: c

29. When comparing Be_2 and H_2:

I. Be_2 is more stable because it contains both bonding and antibonding valence electrons.

II. H_2 has a higher bond order than Be_2.

III. H_2 is more stable because it only contains σ_{1s} electrons.

IV. H_2 is more stable because it is diamagnetic, whereas Be_2 is paramagnetic.

a. I, II

b. III only

c. II, III

d. II, III, IV

e. III, IV

ANSWER: c

30. If a molecule demonstrates paramagnetism, then :

I. The substance can have both paired and unpaired electrons.

II. The bond order is not a whole number.

III. It can be determined by drawing a Lewis structure.

IV. It must be an ion.

a. I, II

b. I, II, IV

c. II, III

d. I only

e. All of the above are correct.

ANSWER: d

31. For which of the following diatomic molecules would the bond order become greater if an electron is removed (i.e., if the molecule is converted to the positive ion in its ground state)?

a. B_2

b. C_2

c. P_2

d. F_2

e. Na_2

ANSWER: d

GASES

Key Concepts:

9.1 Atmosphere
9.2 Characteristics of Gases
9.3 Gas laws
9.4 Ideal gas Law
9.5 Gas Stoichiometry
9.6 Kinetic Molecular Theory
9.7 Real Gases

I. Atmosphere

Figure 9.1 Atmosphere

Ref: commons.wikimedia.org/

On earth, we live under a blanket of air that presses down us and everything else surrounding us. According to weather report, the pressure of atmosphere varies day to day. Atmosphere contains several gases like nitrogen, oxygen, argon etc. Their relative percentages in air are given below.

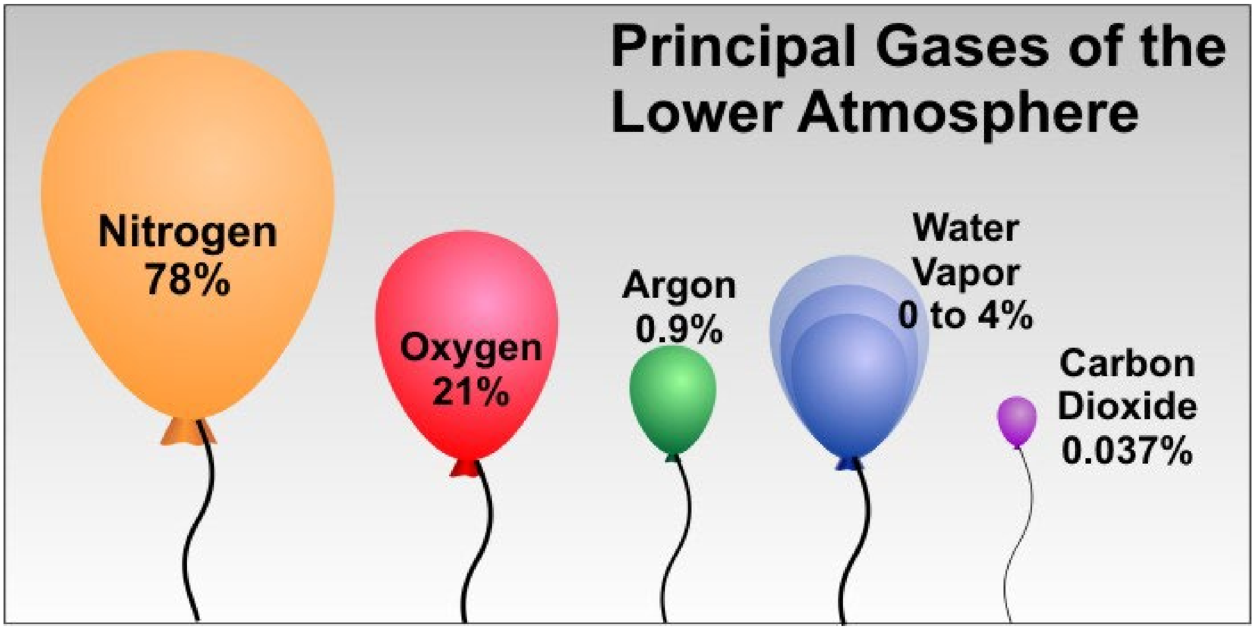


Figure 9.2 Different gases present in atmosphere

Ref: commons.wikimedia.org/

As the height of the air column decreases in higher altitude, the atmospheric pressure decreases. Air pressure is highest at the sea level. Below sea level pressure increases due to water pressure and atmospheric pressure.

Throughout much of human history, “airs” or gases were not believed to be *matter* at all; their apparently weightless nature and their ability to move about freely and fill all available space, while carrying with them definite physical properties such as odor and sometimes color, conferred upon them a somewhat mysterious nature. Even the scientist Robert Boyle wrote about “*The Strange Subtility, Great Efficacy and Determinate Nature of Effluviums*"

It's interesting, however, that around 550 BCE the Greek philosopher Anaximenes maintained that *all* matter consists of air: "*It is from air that all the things that exist, have existed, or will exist come into being.*"

The invention of the sensitive *balance* in the early seventeenth century showed once and for all that gases have weight and are therefore matter. Guericke's invention of the air pump (which led directly to his discovery of the *vacuum*) launched the “pneumatic era" of chemistry long before the existence of atoms and molecules had been accepted. Indeed, the behavior of gases was soon to prove an invaluable tool in the development of the atomic theory of matter.

The study of gases allows us to understand the behavior of matter at its simplest: individual particles, acting independently, almost completely uncomplicated by interactions and interferences between each other. Later on, our knowledge of gases will serve as the pathway to our understanding of the far more complicated *condensed phases* (liquids and solids) in which the theory of gases will no longer give us correct answers, but it will still provide us with a useful *model* that will at least help us to rationalize the behavior of these more complicated states of matter.

II. Characteristics of Gases

1 What's special about gases?

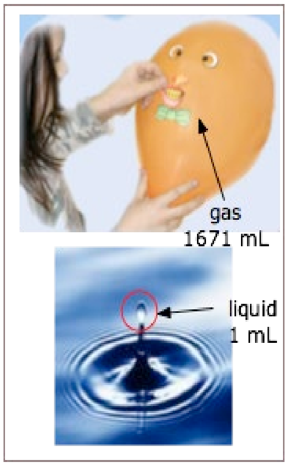


Fig. 9.3 Difference Between Gas & Liquid

First, we know that a gas has **no definite volume or shape**; a gas will fill whatever volume is available to it. Contrast this to the behavior of a liquid, which always has a distinct upper surface when its volume is less than that of the space it occupies.

The other outstanding characteristic of gases is their **low *densities***, compared with those of liquids and solids. One mole of liquid water at 298 K and 1 atm pressure occupies a volume of 18.8 cm^3, whereas the same quantity of water vapor at the same temperature and pressure has a volume of 30200 cm^3, more than 1000 times greater.

The most remarkable property of gases, however, is that to a very good approximation, **they all *behave the same way*** in response to changes in temperature and pressure, expanding or contracting by predictable amounts. This is very different from the behavior of liquids or solids, in which the properties of each particular substance must be determined individually.

We will see later that each of these three ***macroscopic*** characteristics of gases follows directly from the ***microscopic*** view— that is, from the *atomic* nature of matter.

The pressure of a gas

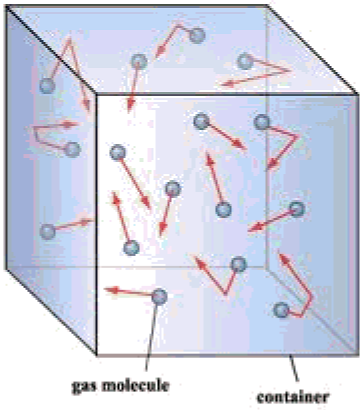


Figure 9.4 Gas Particles in a container

For some deeper insight into the meaning of pressure, see John Denker's page *A Fluid Has Pressure Everywhere*

The molecules of a gas, being in continuous motion, frequently strike the inner walls of their container. As they do so, they immediately bounce off without loss of kinetic energy, but the reversal of direction (*acceleration*) imparts a *force* to the container walls. This force, divided by the total surface area on which it acts, is the ***pressure*** of the gas.

The pressure of a gas is observed by measuring the pressure that must be applied externally in order to keep the gas from expanding or contracting. To visualize this, imagine some gas trapped in a cylinder having one end enclosed by a freely moving piston. In order to keep the gas in the container, a certain amount of weight (more precisely, a *force, f*) must be placed on the piston so as to exactly balance the force exerted by the gas on the bottom of the piston, and tending to push it up. The pressure of the gas is simply the quotient f/A, where A is the cross-section area of the piston.

Pressure units

The unit of pressure in the SI system is the *pascal* (Pa), defined as a force of one newton per square metre ($1\ Nm^{-2} = 1\ kg\ m^{-1}\ s^{-2}$.)

At the Earth's surface, the force of gravity acting on a 1 kg mass is 9.81 N. Thus if, in the illustration above, the weight is 1 kg and the surface area of the piston is 1 M^2, the pressure of the gas would be 9.81 Pa. A 1-gram weight acting on a piston of 1 cm^2 cross-section would exert a pressure of 98.1 pA. (If you wonder why the pressure is higher in the second example, consider the number of cm^2 contained in 1 m^2.)

In chemistry, it is more common to express pressures in units of *atmospheres* or *torr*: 1 atm = 101325 Pa = 760 torr.

Need to convert pressure units? Use this on-line converter.

The older unit *millimetre of mercury* (mm Hg) is almost the same as the torr; it is defined as one mm of level difference in a mercury barometer at 0°C. In meteorology, the pressure unit most commonly used is the *bar*:

1 bar = 10^5 N m^{-2} = 750.06 torr = 0.987 atm.

In engineering work the *pound per square inch* is still widely used; standard atmospheric pressure is 14.7 psi. For the definition of the *standard atmosphere*, see here.

The pressures of gases encountered in nature span an exceptionally wide range, only part of which is ordinarily encountered in chemistry. Note that in the chart below, the pressure scales are logarithmic; thus 0 on the atm scale means 10^0 = 1 atm.

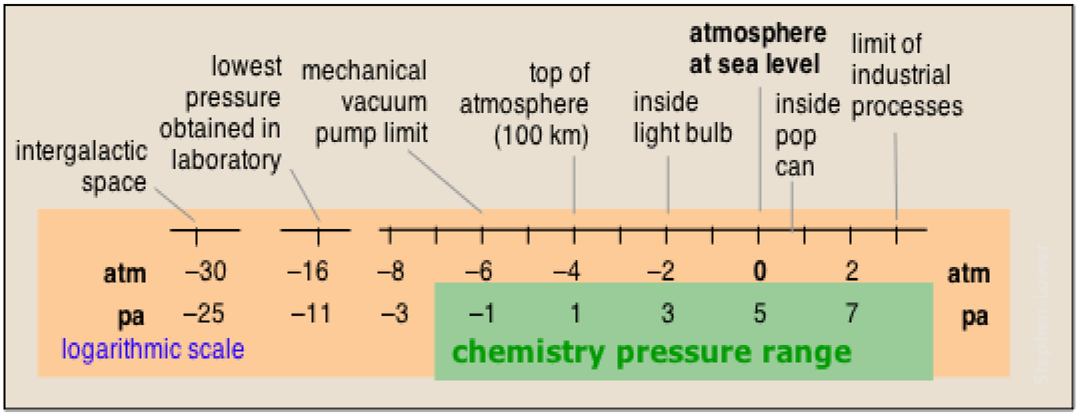


Figure 9.5 Atmospheric Pressure

Atmospheric pressure and the barometer

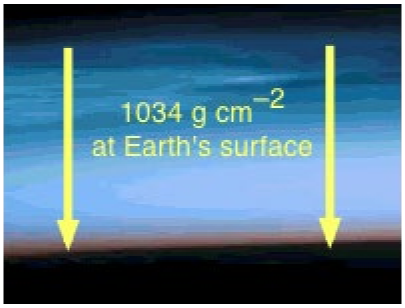


Figure 9.6 Atmospheric Pressure at sea level

The column of air above us exerts a force on each 1-cm^2 of surface equivalent to a weight of about 1034 g. The higher into the air you go, the smaller the mass of air above you, and the lower the pressure (right).

The surface pressure of 1034 g cm^{-2} is obtained by solving Newton's law $f = ma$ for m, using the acceleration of gravity for a:

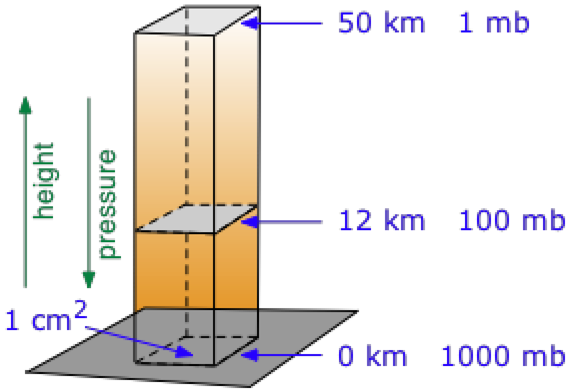


Figure 9.7 Determination of Gas Pressure

$$m = \frac{\overset{\text{standard atmospheric pressure}}{101325 \text{ kg m}^{-1} \text{ s}^{-2}}}{\underset{\text{accelaration of gravity}}{9.8 \text{ m s}^{-2}}} = 10340 \text{ kg m}^{-1} = 1034 \text{ g cm}^{-2}$$

Table of atmospheric pressure by elevation - go here for elevation of your US city

So, if this huge column of air are constantly pressing down on your body, why do you not feel it?

Answer: because every other part of your body (including within your lungs and insides) also experiences the same pressure, so there is no net force (other than gravity) acting on you.

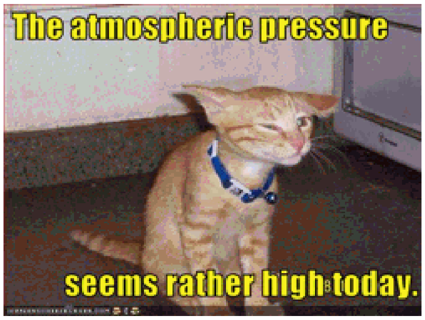


Figure: 9.8

SUPPLEMENTAL

****

***The discovery of atmospheric pressure

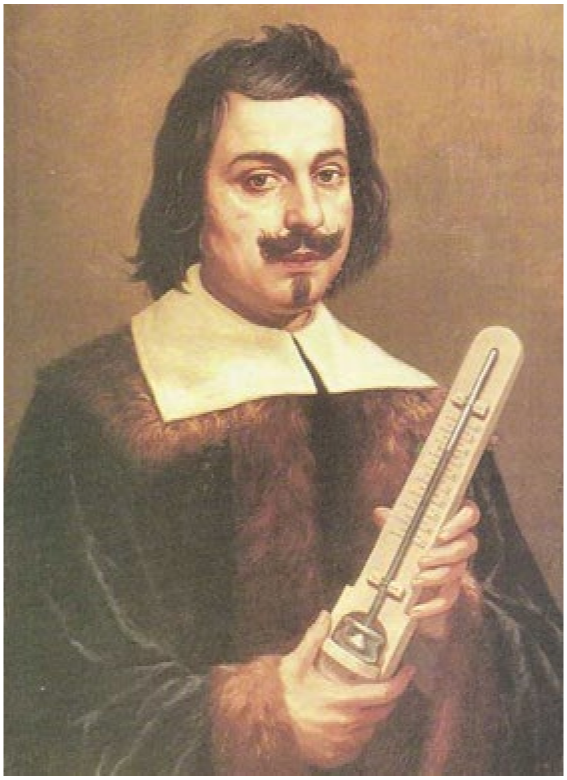


Fig. 9.9 Torricelli

Ref: commons.wikimedia.org/

This was the crucial first step that led eventually to the concept of gases and their essential role in the early development of Chemistry.

In the early 17th century the Italian Evangelista Torricelli invented a device — the ***barometer*** — to measure the pressure of the atmosphere. A few years later, the German scientist and some-time mayor of Magdeburg Otto von Guericke devised a method of pumping the air out of a container, thus creating which might be considered the opposite of air: the ***vacuum***.

As with so many advances in science, idea of a vacuum — a region of nothingness — was not immediately accepted; see here for an interesting account of the controversy.

Torricelli's invention overturned the then-common belief that air (and by extension, all gases) are weightless.


Figure 9.10 Tug of War

Ref: flickr.com/

The fact that we live at the bottom of a sea of air was most spectacularly demonstrated in 1654, when two teams of eight horses were unable to pull apart two 14-inch copper hemispheres (the "Magdeburg hemispheres") which had been joined together and then evacuated with Guericke's newly-invented vacuum pump.

Figure: 9.11 barometer Invention

Measurement of atmospheric pressure: the barometer

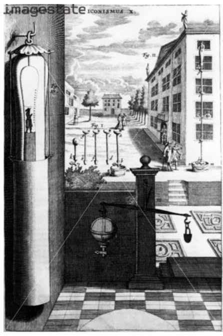
The classical barometer, still used for the most accurate work, measures the height of a column of liquid that can be supported by the atmosphere. As indicated below, this pressure is exerted directly on the liquid in the reservoir, and is transmitted hydrostatically to the liquid in the column.

Metallic mercury, being a liquid of exceptionally high density and low vapor pressure, is the ideal barometric fluid. Its widespread use gave rise to the "millimeter of mercury" (now usually referred to as the "torr") as a measure of pressure.

How is the air pressure of 1034 g cm^{-3} related to the 760-mm height of the mercury column in the barometer? What if water were used in place of mercury?

Answer: The density of Hg is 13.6 g cm^{-3}, so in a column of 1-cm^2 cross-section, the height needed to counter the atmospheric pressure would be (1034 g × 1 cm^2) / (13.6 g cm^{-3}) = 76 cm.

The density of water is only 1/13.6 that of mercury, so standard atmospheric pressure would support a water column whose height is 13.6 x 76 cm = 1034 cm, or 10.3 m. You would have to read a water barometer from a fourth-story window!



left: A water-barometer (set up on the building on the right) by von Guericke in the 17th century.

Below: The Thames Water Barometer is probably the most spectacular one in the world. It was built in 1995 in a London roundabout to conceal a surge standpipe for the local water distribution system.

Figure 9.12 Water Barometer

Figure 9.13 Thames Water Barometer

Ref: https://www.geograph.org.uk/photo/4143789

Water barometers were once employed to measure the height of the ground and the heights of buildings before more modern methods were adopted.

Barometers take many forms!

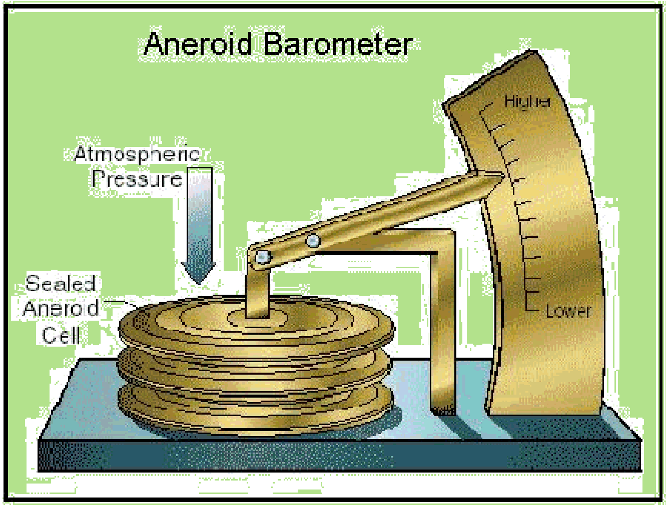
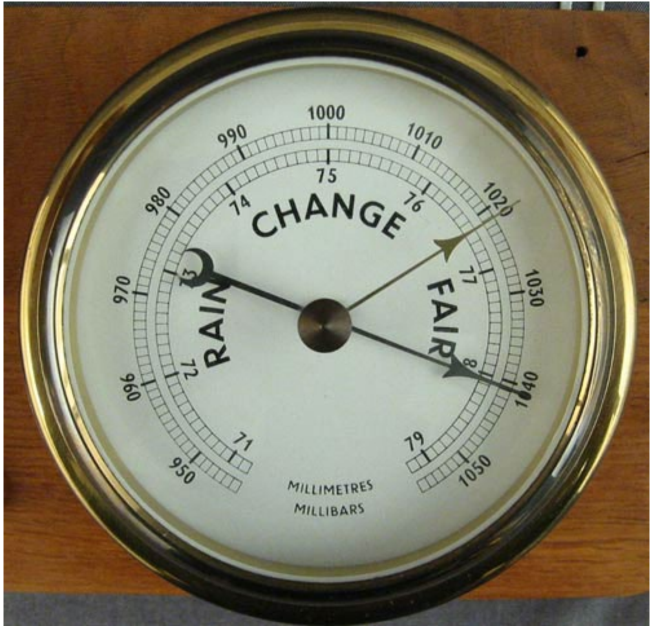


Figure 9.14 Different Types of barometers

Ref: commons.wikimedia.org/



950
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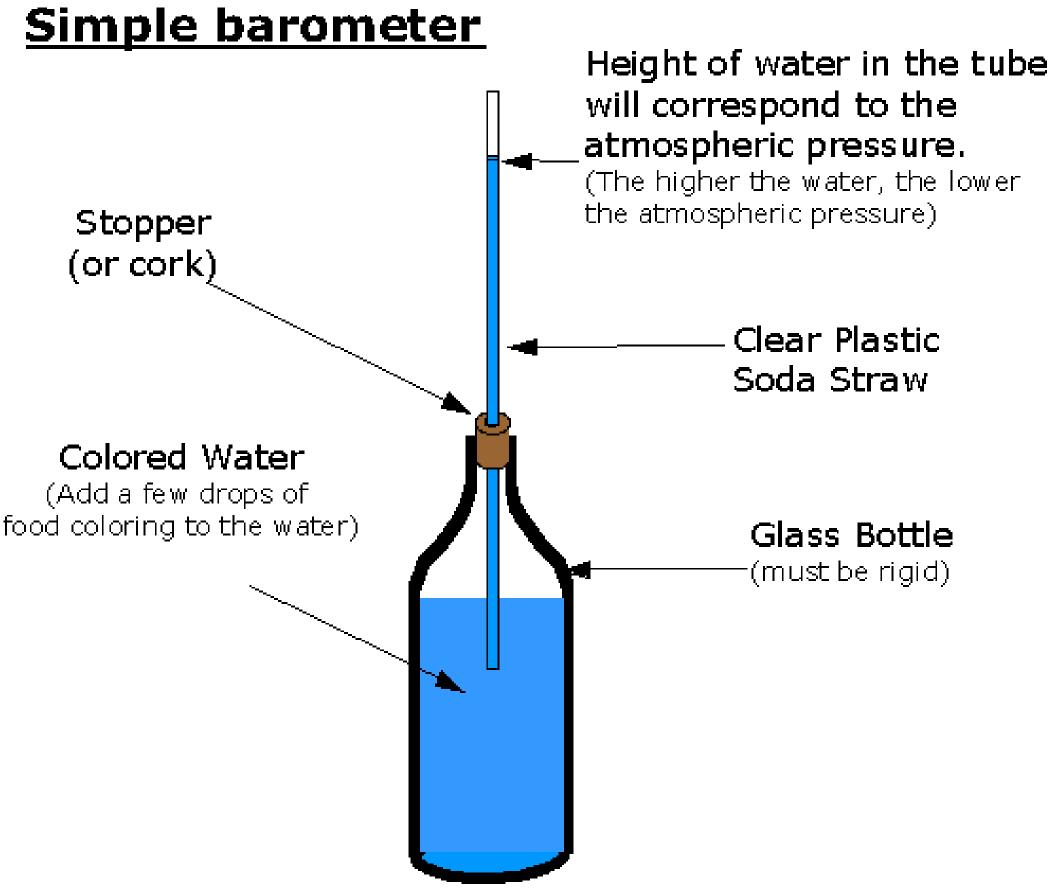
RAIN
CHANGE
FAIR
MILLIMETRES
MILLIBARS



Aneroid barometers employ a sealed bellows which moves a pointer,

Figure 9.15 Barometer diagram

Figure 9.14 When the children retreat inside and the old lady emerges, the Weather Bureau predicts inclement weather.Small water barometers such as this one register only *variations* in the pressure; the swan's body is open to the air.Build-your-own water barometer to follow changes in the barometric pressure.

****

Gas pressure

The pressure of a gas is the force exerted when gas particles strike the surface of the walls of the container. The pressure a gas exerts on a surface, such as the walls of a container, results from the continual bombardment on the walls of the container by the rapidly moving gas molecules. We use an instrument called barometer to measure atmospheric pressure. One type of barometer consists of a long glass tube that is completely filled with mercury and then inverted into a pool of mercury in a dish. Because there is no air at the top of the mercury column inside the tube no gas pressure is exerted on the mercury column. The atmosphere, however, exerts its pressure on the mercury in the open dish. The difference in the heights of the two mercury levels is a measure of the atmospheric pressure. Pressure is measured by barometer and units are:

Atmosphere(atm), millimeter of Hg(mm Hg) , torr.

1atm= 760 torr=760 mm of Hg= 14.7 psi= 101,325 Pa

Other units of pressure are pascal, bar etc. All the units can be interconverted.

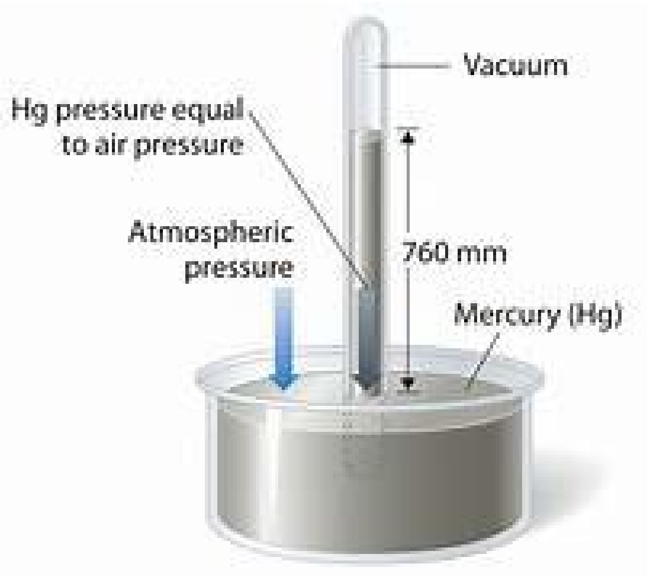
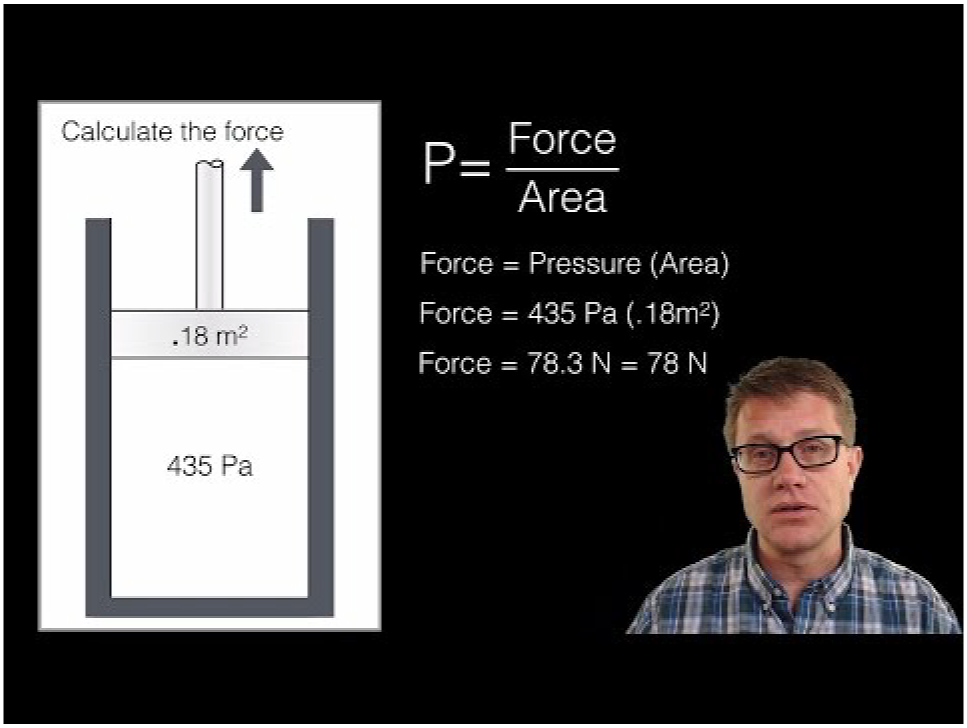


Figure 9.20 Determination of Atmospheric Pressure

Ref: commons.wikimedia.org/

https://www.youtube.com/watch?v=H9VtHkPWNeA



Calculate the force

$$P = \frac{\text{Force}}{\text{Area}}$$

Force = Pressure (Area)

Force = 435 Pa (.18m^2)

Force = 78.3 N = 78 N

Example: On a dry day, atmospheric pressure is 734 torr. What is the pressure in atmospheric unit?

Ans: 734 torr * $\frac{1 \text{ atm}}{760 \text{ torr}}$ = 0.966 atm

The manometer

This Davidson College page has a very good treatment of pressure measurement with a manometer, with simulations. And this manufacturer's site surveys the many kinds of devices used to measure the pressure of gases in practical applications.

A modification of the barometer, the *U-tube manometer*, provides a simple device for measuring the pressure of any gas in a container. The U-tube is partially filled with mercury, one end is connected to container, while the other end can either be opened to the atmosphere. The pressure inside the container is found from the difference in height between the mercury in the two sides of the U-tube. The illustration below shows how the two kinds of manometer work.

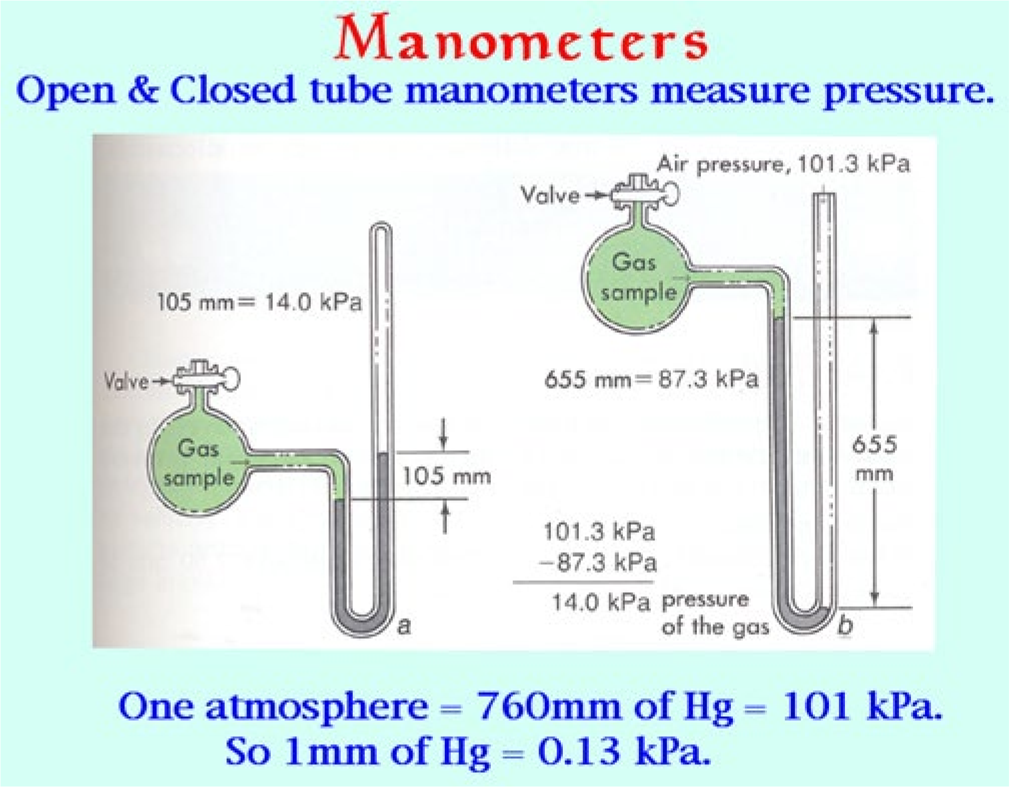
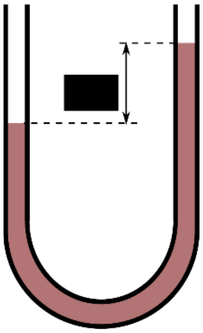


Figure 9.16 Different Types of manometers

Ref: Wikimedia.org/



Ref: http://boomeria.org/physicslectures/atmospheric/atmospheric.html

The manometers ordinarily seen in the laboratory come in two flavors: closed-tube and open-tube. In the closed-tube unit shown at the left, the longer limb of the J-tube is evacuated by filling it with mercury and then inverting it. If the sample container is also evacuated, the mercury level will be the same in both limbs. When gas is let into the container, its pressure pushes the mercury down on one side and up on the other; the difference in levels is the pressure in torr.

In the open-tube manometer on the right, the atmosphere pushes the mercury column down in the open side, and again the pressure in torr is found from the difference in the levels. When using this method, the atmospheric pressure must be determined by means of a barometer.

For practical applications in engineering and industry, especially where higher pressures must be monitored, many types of mechanical and electrical *pressure gauges* are available.

Figure 9.17 gas Pressure gauge

Ref: commons.wikimedia.org/

The temperature of a gas

If two bodies are at different temperatures, heat will flow from the warmer to the cooler one until their temperatures are the same. This is the principle on which *thermometry* is based; the temperature of an object is measured indirectly by placing a calibrated device known as a *thermometer* in contact with it. When thermal equilibrium is obtained, the temperature of the thermometer is the same as the temperature of the object.

Temperature scales

A *thermometer* makes use of some temperature-dependent quantity, such as the density of a liquid, to allow the temperature to be found indirectly through some easily measured quantity such as the length of a mercury column. The resulting scale of temperature is entirely arbitrary; it is defined by locating its zero point, and the size of the *degree* unit.

At one point in the 18th century, 35 different temperature scales were in use!

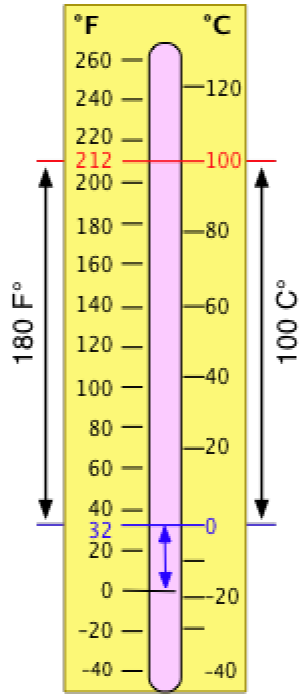


Figure: 9.18 Temperature Scale

The *Celsius* temperature scale locates the zero point at the freezing temperature of water; the Celsius degree is defined as 1/100 of the difference between the freezing and boiling temperatures of water at 1 atm pressure.

The older *Fahrenheit* scale placed the zero point at the coldest temperature it was possible to obtain at the time (by mixing salt and ice.) The 100° point was set with body temperature (later found to be 98.6°F.) On this scale, water freezes at 32°F and boils at 212°F. The Fahrenheit scale is a finer one than the Celsius scale; there are 180 Fahrenheit degrees in the same temperature interval that contains 100 Celsius degrees, so 1F° = 5/9 C°. Since the zero points are also different by 32F°, conversion between temperatures expressed on the two scales requires the addition or subtraction of this offset, as well as multiplication by the ratio of the degree size.

If you take the effort to understand the above paragraph, you will never need to waste your time with *formula*s for converting between Fahrenheit and Celsius!

...and if you live in any country other the U.S. or Belize, you can forget about Fahrenheit altogether.

Notice also that temperature is expressed by placing the degree symbol *in front* of the scale abbreviation (37°C), whereas a temperature interval is written with the degree sign *following* the symbol (2 C°).

Absolute temperature

In 1802 the French mathematician and physicist Joseph Gay-Lussac discovered that for each Celsius degree that the temperature of a gas is lowered, the volume of the gas will diminish by 1/273 of its volume at 0°C. The obvious implication of this is that if the temperature could be reduced to –273°C, the volume of the gas would contract to zero. Of course, all real gases condense to liquids before this happens, but at sufficiently low pressures their volumes are linear functions of the temperature
(*Charles' Law*), and extrapolation of a plot of volume as a function of temperature predicts zero volume at -273°C. This temperature, known as ***absolute zero***, corresponds to the total absence of thermal energy.

The temperature scale on which the zero point is –273.15°C was suggested by Lord Kelvin, and is usually known as the *Kelvin* scale. Since the size of the Kelvin and Celsius degrees are the same, conversion between the two scales is a simple matter of adding or subtracting 273.15; thus room temperature, 20°, is about 293 K.

A rather fine point to note: the degree symbol is not used with the "K", which should always be separated from the preceding number by a space. See here for an explanation.

Because the Kelvin scale is based on an absolute, rather than on an arbitrary zero of temperature, it plays a special significance in scientific calculations; most fundamental physical relations involving temperature are expressed mathematically in terms of absolute temperature. In engineering work, an absolute scale based on the Fahrenheit degree is sometimes used; this is known as the Rankine scale.

About Temperature is a far-ranging but very readable site by Beverly Lynds.

History of the thermometer

How cold can it get?

How ultra low temperatures are achieved and measured

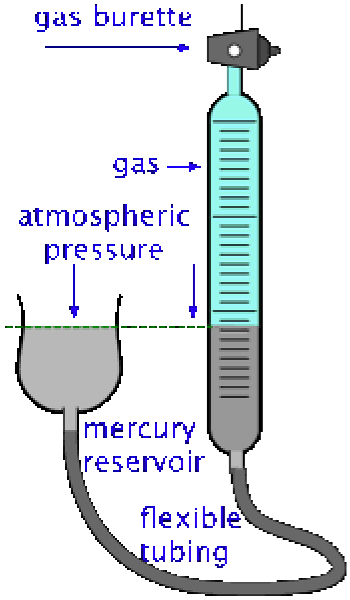
4 The volume occupied by a gas

The *volume* of a gas is simply the space in which the molecules of the gas are free to move. If we have a mixture of gases, such as air, the various gases will coexist within the same volume. In these respects, gases are very different from liquids and solids, the two condensed states of matter.

The volume of a gas can be measured by trapping it above mercury in a calibrated tube known as a *gas burette*. The SI unit of volume is the cubic metre, but in chemistry we more commonly use the *litre* and the *millilitre* (ml). The *cubic centimetre* (cc) is also frequently used; it is very close to 1 milliliter (mL).

It's important to bear in mind, however, that the volume of a gas varies with both the temperature and the pressure, so reporting the volume alone is not very useful. A common practice is to measure the volume of the gas under the ambient temperature and atmospheric pressure, and then to correct the observed volume to what it would be at standard atmospheric pressure and some fixed temperature, usually 0° C or 25°C.

Figure: 9.19 manometer Diagram



What you should be able to do

Make sure you thoroughly understand the following essential ideas which have been presented above. It is especially important that you know the precise meanings of all the green-highlighted terms in the context of this topic.

State the ***three major properties of gases*** that distinguish them from condensed phases of matter.

Define ***pressure***, and explain why a gas exerts pressure on the walls of a container.

Explain the operation of a simple ***barometer***, and why its invention revolutionized our understanding of gases.

Explain why a barometer that uses water as the barometric fluid is usually less practical than one which employs mercury.

How are the Celsius and Fahrenheit ***temperature scales*** defined? How do the magnitudes of the "degree" on each scale related?

Why must the temperature and pressure be specified when reporting the ***volume*** of a gas?

Question:

1. A scuba diver begins diving at 3000 psi. Convert this pressure into 1) atm 2) mm of Hg.

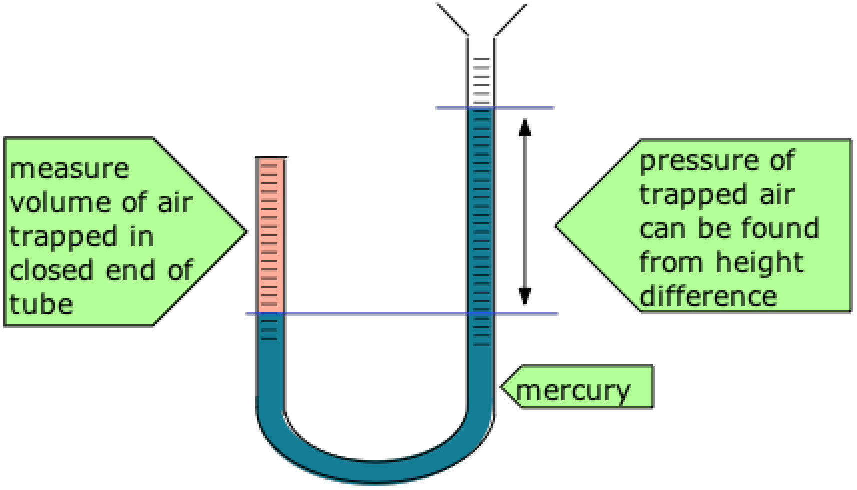
III. Gas Laws

The "pneumatic" era of chemistry began with the discovery of the *vacuum* around 1650 which clearly established that gases are a form of matter. The ease with which gases could be studied soon led to the discovery of numerous empirical (experimentally-discovered) laws that proved fundamental to the later development of chemistry and led indirectly to the atomic view of matter. These laws are so fundamental to all of natural science and engineering that everyone learning these subjects needs to be familiar with them.

1 Pressure-volume relations: Boyle's law

Robert Boyle (1627-91) showed that the volume of air trapped by a liquid in the closed short limb of a J-shaped tube decreased in exact proportion to the pressure produced by the liquid in the long part of the tube. The trapped air acted much like a spring, exerting a force opposing its compression. Boyle called this effect “*the spring of the air*", and published his results in a pamphlet of that title.

volume	**pressure**	$P \times V$
96.0	2.00	192
76.0	2.54	193
46.0	4.20	193
26.0	7.40	193



The difference between the heights of the two mercury columns gives the pressure (76 cm = 1 atm), and the volume of the air is calculated from the length of the air column and the tubing diameter.

Some of Boyle's actual data are shown in the table.

Figure 9.21 Pressure determination using manometer

Boyle's law states that the pressure of a gas, held at a constant temperature, varies inversely with its volume:

It is very important that you understand how these two equations express the green-highlighted statement of the law.

If you feel the need to memorize Eqn 1-2, you probably lack this understanding; please study the paragraph that follows.

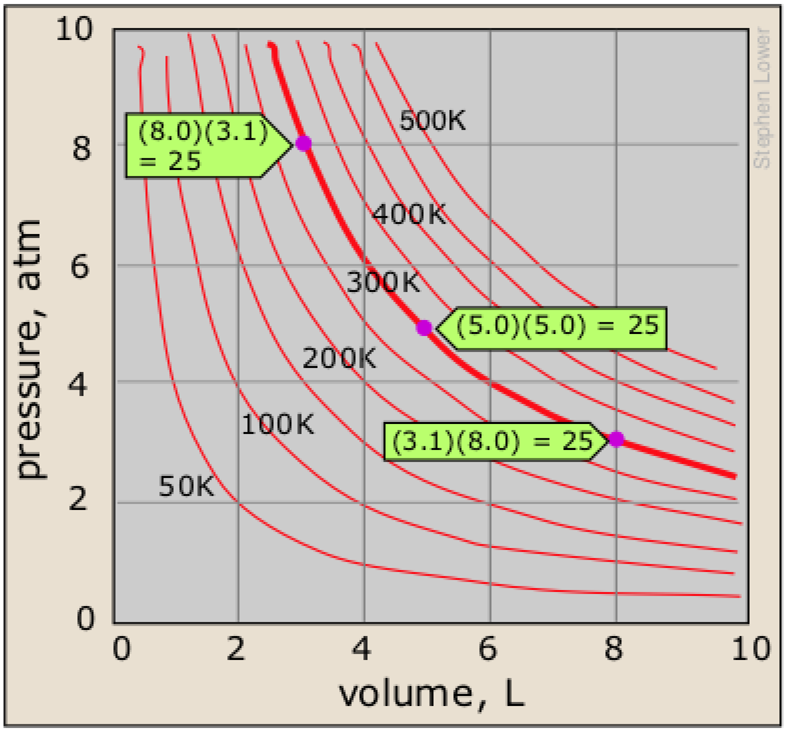
PV = constant (1-1) must know!

or, equivalently,

$P_1V_1 = P_2V_2$ (1-2)

Boyle's law is a relation of *inverse proportionality*; any change in the pressure is exactly compensated by an opposing change in the volume. As the pressure decreases toward zero, the volume will increase without limit. Conversely, as the pressure is increased, the volume decreases, but can never reach zero. There will be a separate P-V plot for each temperature; a single P-V plot is therefore called an ***isotherm***.

Please take the time to understand this kind of plot which governs *any relationship of inverse proportionality, and why the curves never reach the* x- *and* y *axes*. You should be able to sketch out such a plot when given the value of any one (x,y) pair.



Shown here are some isotherms for one mole of an ideal gas at several different temperatures. Each plot has the shape of a *hyperbola*— the locus of all points having the property $x\,y = a$, where a is a constant. You will see later how the value of this constant (PV=25 for the 300K isotherm shown here) is determined.

Figure 9.22 Boyle's Law graph

A related type of plot with which you should be familiar shows the product PV as a function of the pressure. You should understand why this yields a straight line, and how this set of plots relates to the one immediately above.

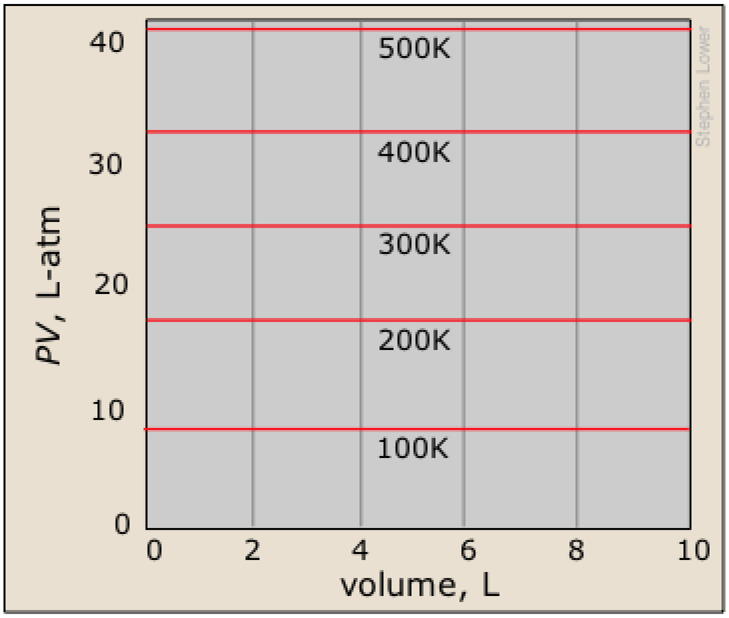


Figure 9.23 Boyle's law graph

Problem Example 1

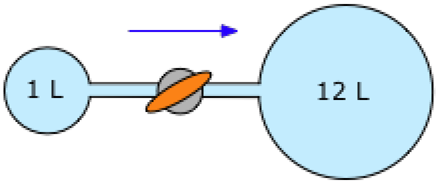


Figure 9.24 Gas expansion

In an industrial process, a gas confined to a volume of 1 L at a pressure of 20 atm is allowed to flow into a 12-L container by opening the valve that connects the two containers. What will be the final pressure of the gas?

Solution: The final volume of the gas is (1 + 12)L = 13 L. The gas expands in inverse proportion two volumes

$P_2 = (20\text{ atm}) \times (1\text{ L} \div 13\text{ L}) = 1.5\text{ atm}$

Note that there is no need to make explicit use of any "formula" in problems of this kind!

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2 How the temperature affects the volume: Charles' law

Figure 9.25 jacques Charles

Figure 9.26 Gay Lussac

All matter expands when heated, but gases are special in that their degree of expansion is independent of their composition. In 1802, the French scientist Joseph Gay-Lussac (right, 1778-1850) found that if the pressure is held constant, the volume of any gas changes by the same fractional amount (1/273 of its value) for each C° change in temperature.

On learning that another scientist, Jacques Charles, had observed the proportionality between the volume and temperature of a gas 15 years earlier but had never published his findings, Gay-Lussac generously acknowledged this fact. Eventually, the "law of Charles and Gay-Lussac" become commonly known simply as "Charles' law".

The volume of a gas confined against a constant pressure is directly proportional to the absolute temperature.

A graphical expression of Charles' law can be seen in these plots of the volume of one mole of an ideal gas as a function of its temperature at various constant pressures.

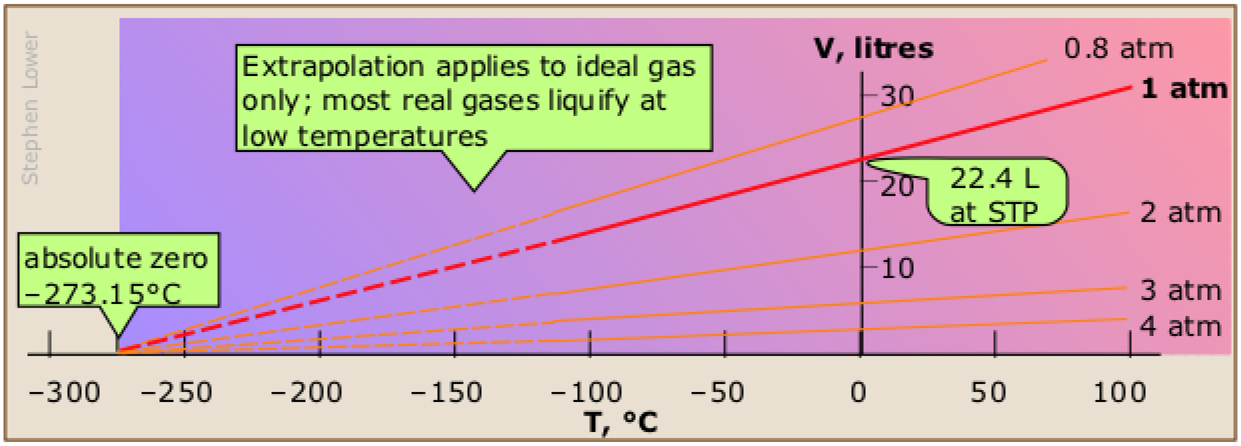


Figure 9.27: Charles's law graph

What do these plots show?

The straight-line plots show that the ratio V/T (and thus dV/dT) is a constant at any given pressure. Thus we can express the law algebraically as

V/T = constant *or* $V_1/T_1 = V_2/T_2$

(be sure you understand why these two equations are equivalent!)

What is the significance of the extrapolation to zero volume?

If a gas contracts by 1/273 of its volume for each degree of cooling, it should contract to zero volume at a temperature of –273°C. This, of course, is the absolute zero of temperature, and this extrapolation of Charles' law is the first evidence of the special significance of this temperature.

Why do the plots for different pressures have different slopes?

The lower the pressure, the greater the volume (Boyle's law), so at low pressures the fraction (V/273) will have a larger value. You might say that the gas must "contract faster" to reach zero volume when its starting volume is larger.

•Try this interactive exploration of the Law of Charles and Gay-Lussac

•Carleton University lecture demonstration video of Charles' Law (YouTube)

Problem Example 2

The air pressure in a car tire is 30 psi (pounds per square inch) at 10°C. What will be pressure be after driving has raised its temperature to 45°C ? (Assume that the volume remains unchanged.)

Solution:The gas expands in direct proportion to the ratio of the absolute temperatures:

$P_2 = (30 \text{ psi}) \times (318\text{K} \div 283\text{K}) = 33.7 \text{ psi}$

Historical notes

The fact that a gas expands when it is heated has long been known. In 1702, Guillaume Amontons (1163-1705), who is better known for his early studies of friction, devised a thermometer that related the temperature to the volume of a gas. Robert Boyle had observed this relationship in 1662, but the lack of any uniform temperature scale at the time prevented them from establishing the relationship as we presently understand it.

Jacques Charles discovered the law that is named for him in the 1780s, but did not publish his work. John Dalton published a form of the law in 1801, but the first thorough published presentation was made by Gay-Lussac in 1802, who acknowledged Charles' earlier studies.

Figure 9.28 Hot-air balloons and Charles' Law

Ref: commons.wikimedia.org/

The buoyancy that lifts a hot-air balloon into the sky depends on the difference between the density (mass ÷ volume) of the air entrapped within the balloon's envelope, compared to that of the air surrounding it. When a balloon on the ground is being prepared for flight, it is first partially inflated by an external fan, and possesses no buoyancy at all. Once the propane burners are started, this air begins to expand according to Charles' law. After the warmed air has completely inflated the balloon, further expansion simply forces excess air out of the balloon, leaving the weight of the diminished mass of air inside the envelope smaller than that of the greater mass of cooler air that the balloon displaces.

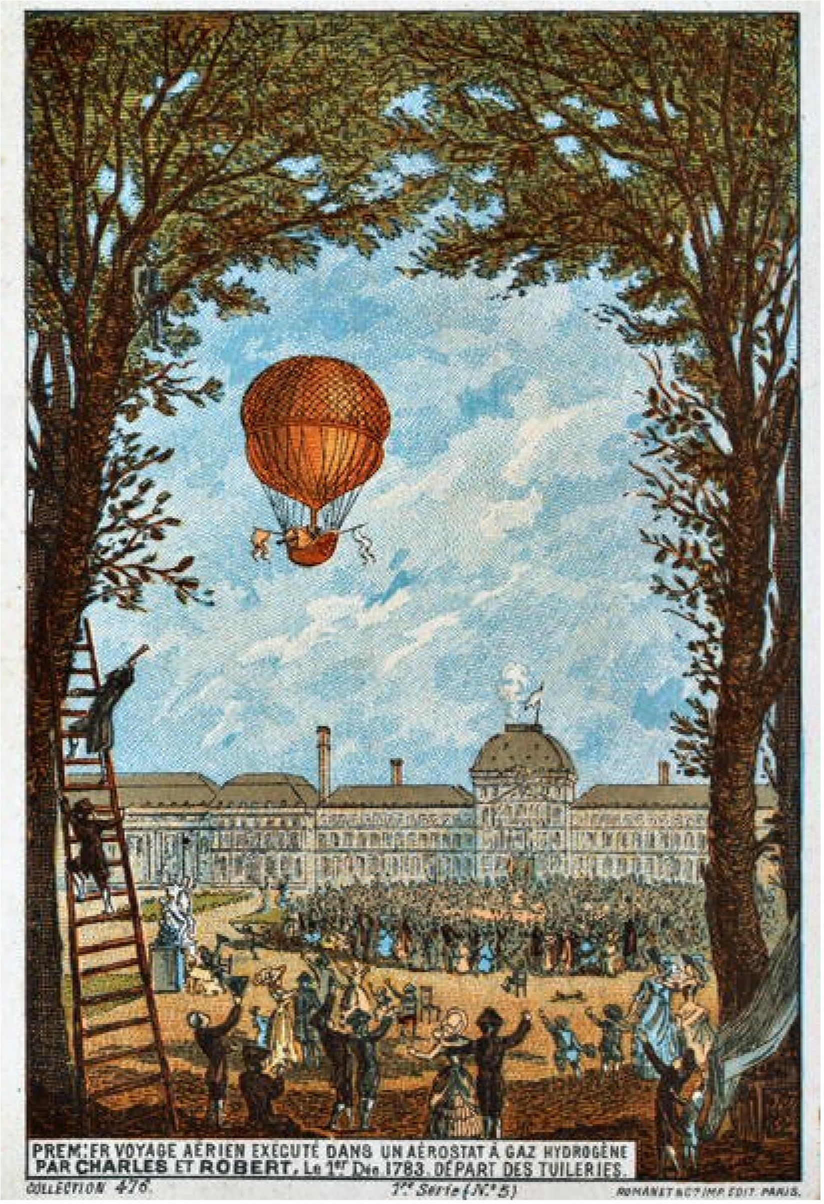
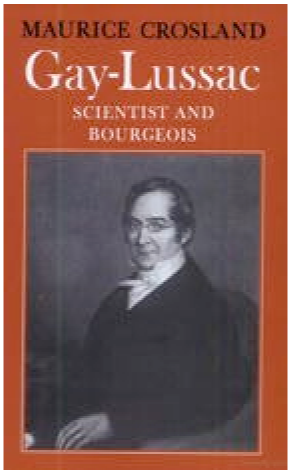


Figure 9.29 Hot air-balloon

Figure 9.30 Hot air balloon

Jacques Charles collaborated with the Montgolfier Brothers whose hot-air balloon made the world's first manned balloon flight in June, 1783 (left). Ten days later, Charles himself co-piloted the first hydrogen-filled balloon. Gay-Lussac (right), who had a special interest in the composition of the atmosphere, also saw the potential of the hot-air balloon, and in 1804 he ascended to a then-record height of 6.4 km. [images: Wikimedia]

Jacques Charles' understanding of buoyancy led to his early interest in balloons and to the use of hydrogen as an inflating gas. His first flight was witnessed by a crowd of 40,000 which included Benjamin Franklin, at that time ambassador to France. On its landing in the countryside, the balloon was reportedly attacked with axes and pitchforks by terrified peasants who believed it to be a monster from the skies. Charles' work was mostly in mathematics, but he managed to invent a number of scientific instruments and confirmed experiments in electricity that had been performed earlier by Benjamin Franklin and others.



Gay-Lussac's balloon flights enabled him to sample the composition of the atmosphere at different altitudes (he found no difference). His Law of Combining Volumes (described below) constituted one of the foundations of modern chemistry. Gay-Lussac's contributions to chemistry are numerous; his work in electrochemistry enabled him to produce large quantities of sodium and potassium; the availability of these highly active metals led to his co-discovery of the element boron. He was also the the first to recognize iodine as an element. In an entirely different area, he developed a practical method of measuring the alcohol content of beverages, and coined the names "pipette" and "burette" that are known to all chemistry students. A good biography can be viewed at Google Books.

If you ever visit Paris, look for a street and a hotel near the Sorbonne that bear Gay-Lussac's name.

Figure 9.31 Gay-Lussac

3 Volume and the number of molecules: Avogadro's law

Gay-Lussac's Law of Combining Volumes

For a good tutorial overview of the Law of Combining Volumes, see this ChemPaths page.

In the same 1808 article in which Gay-Lussac published his observations on the thermal expansion of gases, he pointed out that when two gases react, they do so in volume ratios that can always be expressed as small whole numbers. This came to be known as the ***Law of combining volumes***.

These "small whole numbers" are of course the same ones that describe the "combining weights" of elements to form simple compounds, as described in the lesson dealing with simplest formulas from experimental data.

Figure 9.32 Amadeo Avogadro

Ref: commons.wikimedia.org/

The Italian scientist Amedeo Avogadro (1776-1856) drew the crucial conclusion: these volume ratios must be related to the relative numbers of molecules that react, and thus the famous "E.V.E.N principle":

Equal **v**olumes of gases, measured at the same temperature and pressure,

contain **e**qual **n**umbers of molecules

Avogadro's law thus predicts a *directly proportional* relation between the number of moles of a gas and its volume.

This relationship, originally known as *Avogadro's Hypothesis*, was crucial in establishing the formulas of simple molecules at a time (around 1811) when the distinction between atoms and molecules was not clearly understood. In particular, the existence of diatomic molecules of elements such as H_2, O_2, and Cl_2 was not recognized until the results of combining-volume experiments such as those depicted below could be interpreted in terms of the E.V.E.N. principle.

How the E.V.E.N. principle led to the correct formula of water

Early chemists made the mistake of assuming that the formula of water is HO. This led them to miscalculate the molecular weight of oxygen as 8 (instead of 16). If this were true, the reaction $H + O \rightarrow HO$ would correspond to the following combining volumes results according to the E.V.E.N principle:

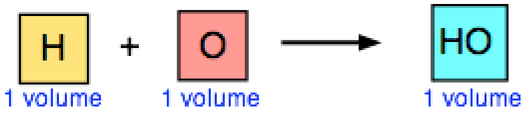


Figure 9.33

But a similar experiment on the formation of hydrogen chloride from hydrogen and chlorine yielded twice the volume of HCl that was predicted by the the assumed reaction H + Cl → HCl. This could be explained only if hydrogen and chlorine were diatomic molecules:

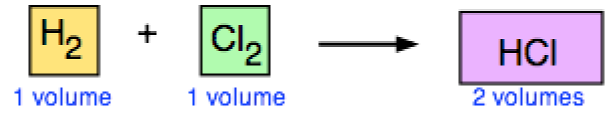


Figure 9.34

This made it necessary to re-visit the question of the formula of water. The experiment immediately confirmed that the correct formula of water is H_2O:

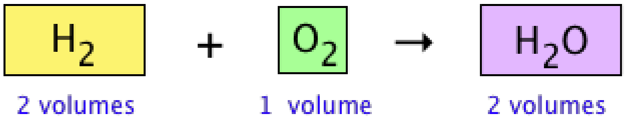


Figure 9.35

This conclusion was also seen to be consistent with the observation, made a few years earlier by the English chemists Nicholson and Carlisle that the reverse of the above reaction, brought about by the electrolytic decomposition of water, yields hydrogen and oxygen in a 2:1 volume ratio.

A nice overview of these developments can be seen at David Dice's Chemistry page, from which this illustration is taken.

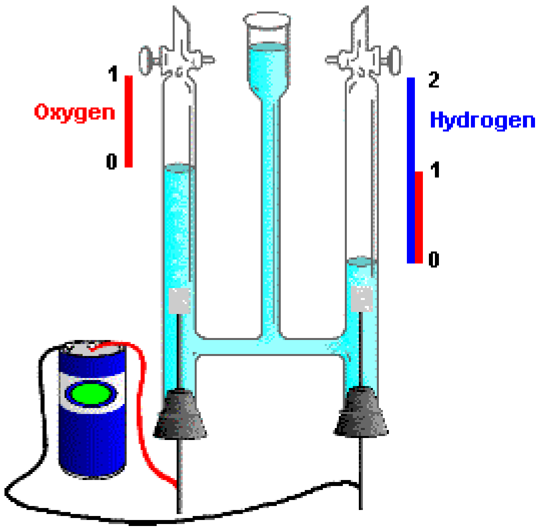


Figure 9.36 electrolysis of water

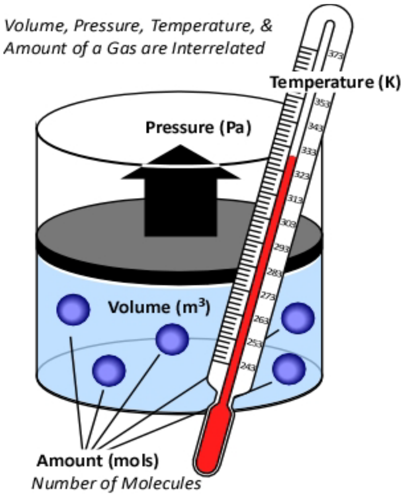
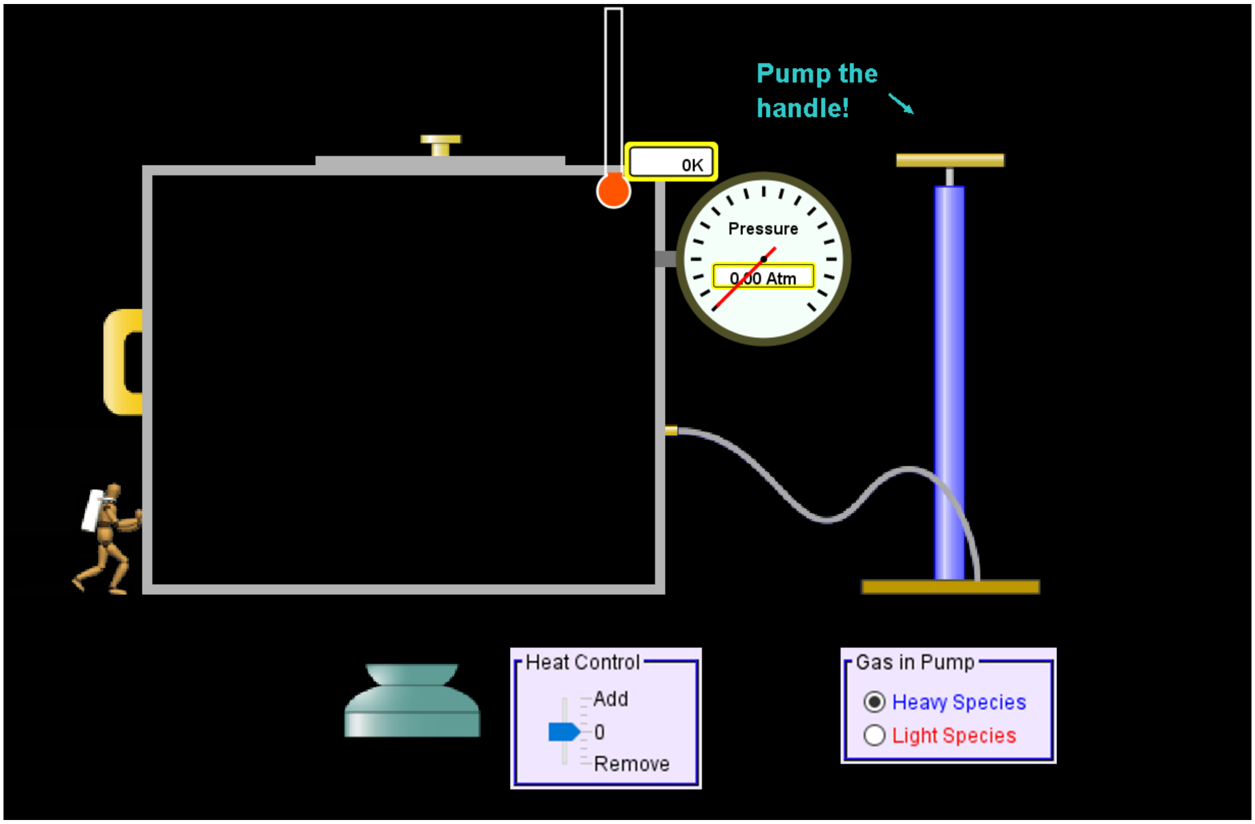


Figure 9.37 System of gas

https://phet.colorado.edu/en/simulation/legacy/gas-properties

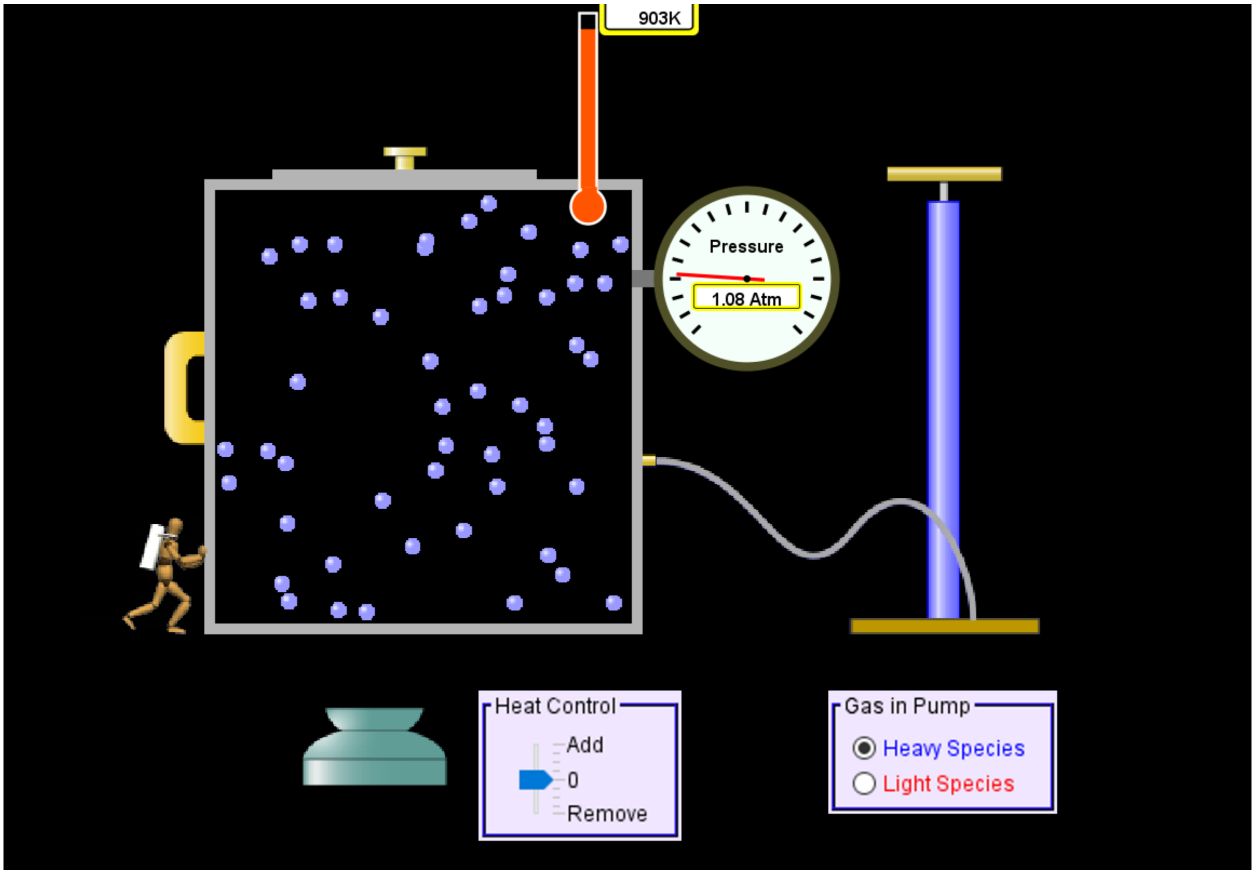
Click on the above simulation and observe the properties of Gas.



Now introduce 50 molecules into the chamber using the handle pump. Slowly decrease the volume of the container using the man symbol. Notice that the pressure monitoring system is giving higher and higher values. This is called Boyle’s law.

Boyle's law: Volume of a fixed amount of gas is inversely proportional to the pressure applied to the gas if the Temp is kept constant.

Boyle’s law has wide application in various fields like scuba diving, human breahing technique.



Heat Control
Add
0
Remove

Gas in Pump
● Heavy Species
○ Light Species

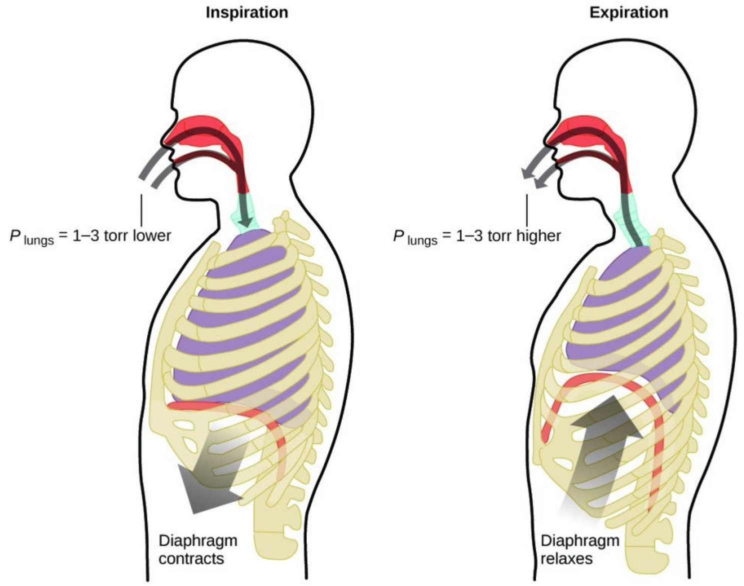


Figure 9.38 Application of Boyle’s law

Ref: common.wikimedia.org/

When a person breathe in, the diaphragm contracts and volume of the lungs get bigger and pressure is low inside the body than outside pressure. Since outside pressure is high, air goes inside the body. When we breathe out, the diaphragm relaxes, volume decreases, high pressure gas comes out of the body.

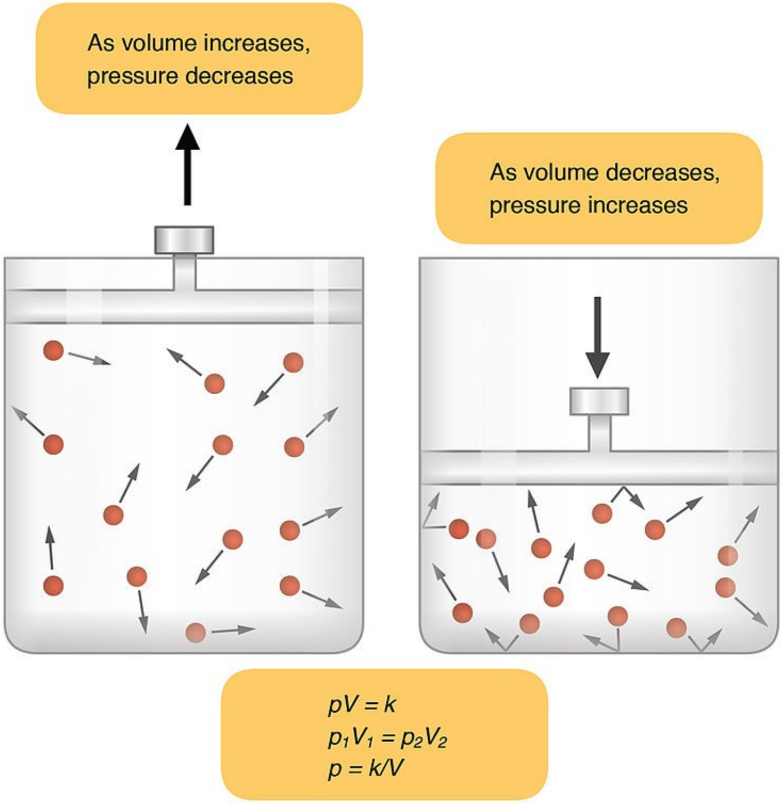


Figure 9.39 Boyle's law

Ref: common.wikimedia.org/

Mathematically we can write,

at constant T

$$P_1 V_1 = P_2 V_2$$

P1= initial pressure, P2= final pressure, T1= initial temp in Kelvin, T2= final temp in Kelvin

If we plot different Pressure vs. Volume for a gaseous system at a constant temperature, the curve will be parabolic in nature.

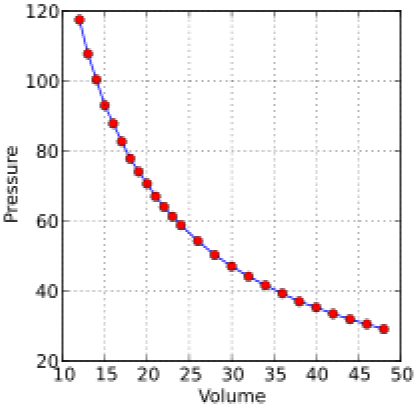


Figure 9.40 Boyle's law graph

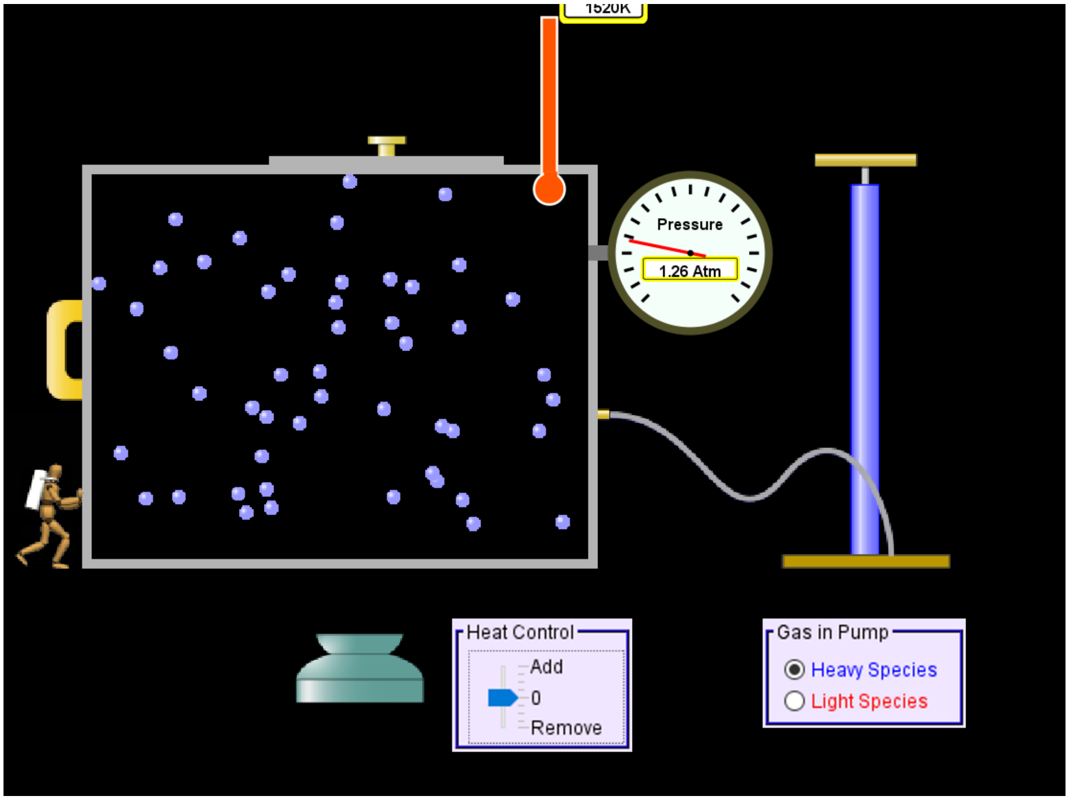
Ref: common.wikimedia.org/

Example: A 4.0 L container of Helium gas has a pressure of 15.0 atm. What pressure does the gas exert if the volume is increased to 8.0 L?

Ans: since the volume is doubled, pressure must be half of the initial pressure.

New pressure= 15.0/2= 7.50 atm

Now introduce heat to the activity: Increase the temp from 400K to 1500K by adding heat keeping the pressure at 1:00atm. On the right top corner of the screen, keep pressure as constant parameter. You will notice that volume of the chamber is increasing. This is called Charles's law.



Heat Control
Add
0
Remove

Gas in Pump
● Heavy Species
○ Light Species

Charles's law: Volume of a fixed amount of gas is directly proportional to the kelvin temp if the pressure is kept constant.

This concept is applied in hot air balloon, where the volume of the gas is expanded by applying heat and once it becomes less dense than air, it can float in air.

Mathematically we can write:

$$\frac{V_1}{T_1} = \frac{V_2}{T_2}$$

V1= initial pressure, V2= final pressure, T1= initial temp in Kelvin, T2= final temp in Kelvin

We can understand the absolute zero temperature from Charles's law. For a sample of gas, when temperature is decreases, volume of the gas molecules decrease. According to the kinetic Molecular theory, the energy of the gas molecules is directly proportional to the kelvin temp. So gas molecules will move slowly as the temperature decreases. Therefore, hypothetically if the absolute temperature of a gaseous system reaches zero i.e. -273^{0}C, all the gas molecules motion will be ceased and the volume of the gas molecule would be zero. In reality, experiments done at lower temp that show the volume decreases steadily but so far, zero volume hasn't reached.

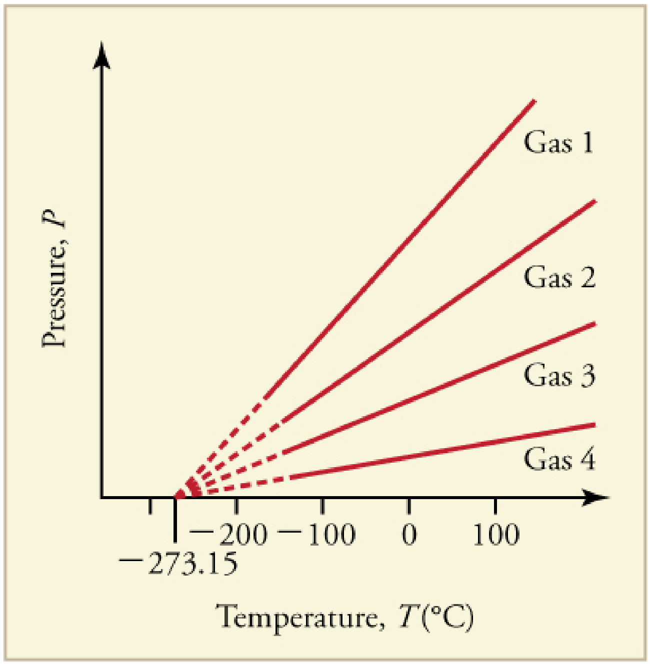
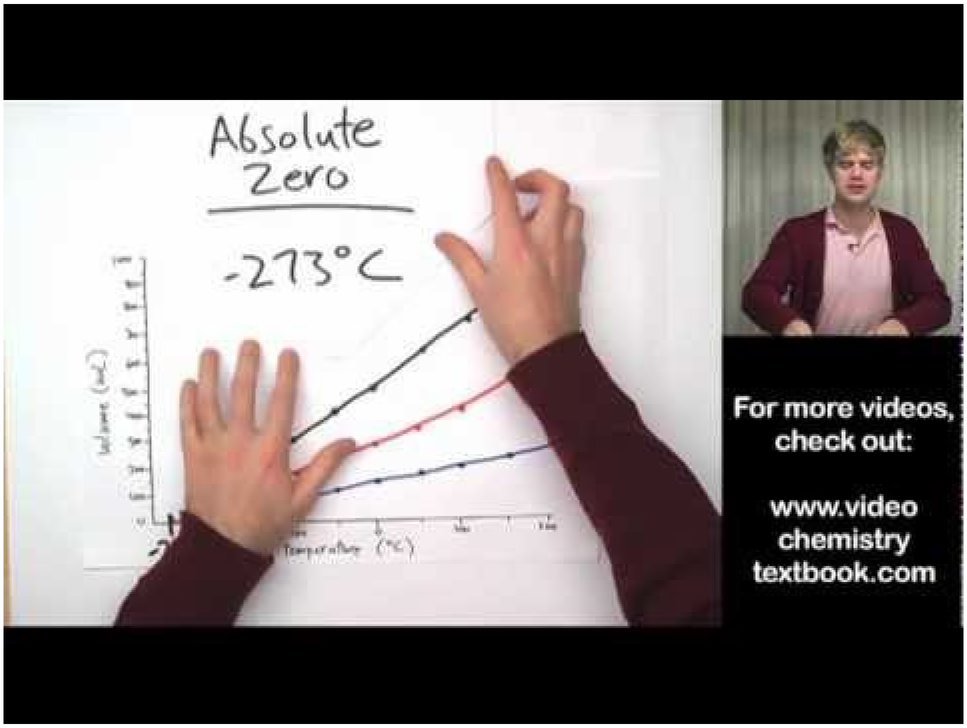


Figure 9.41 Charle's Law graph

Ref: common.wikimedia.org/

https://www.youtube.com/watch?v=JHXxPnmyDbk

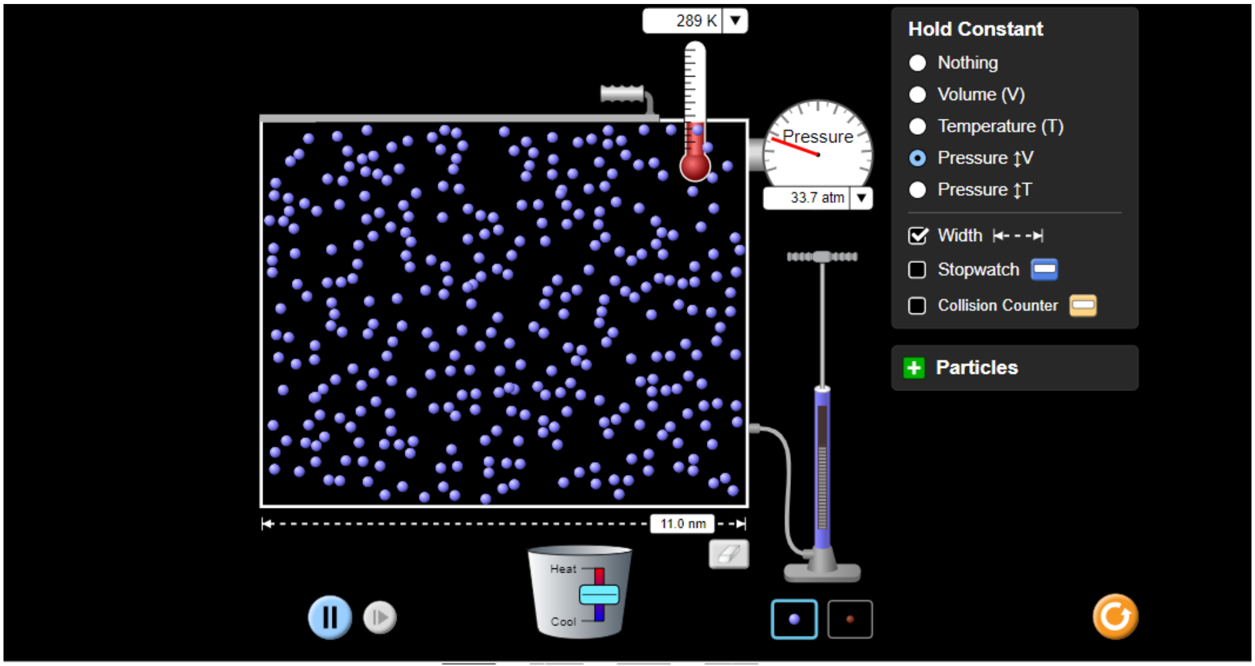


Example: A volume of 1.00L of gas at 37^0C is expelled from the lungs to cold outside at temperature -5^0C. What is the volume of the air at that temperature?

Ans: V2 is unknown.

1.00/(37+ 273) = V2/(-5+ 273) , 1/310=V2/268 or V2= 0.865 L

Avogadro's law: Increase the number of molecules from 50 to 100 in the simulation system keeping the pressure and Temperature constant. You may notice that volume of the container is increasing. This is Avogadro’s law.



Hold Constant
○ Nothing
○ Volume (V)
○ Temperature (T)
● Pressure ↕V
○ Pressure ↕T

☑ Width
☐ Stopwatch
☐ Collision Counter

Avogadro’s law: Volume of a of gas is directly proportional to the number of moles of gas if the pressure and Temp are kept constant.

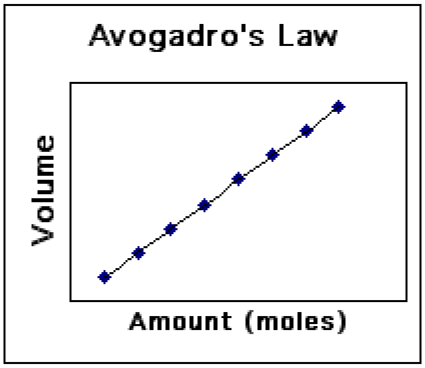


Figure 9.42 Avogadro’s law graph

Ref: common.wikimedia.org/

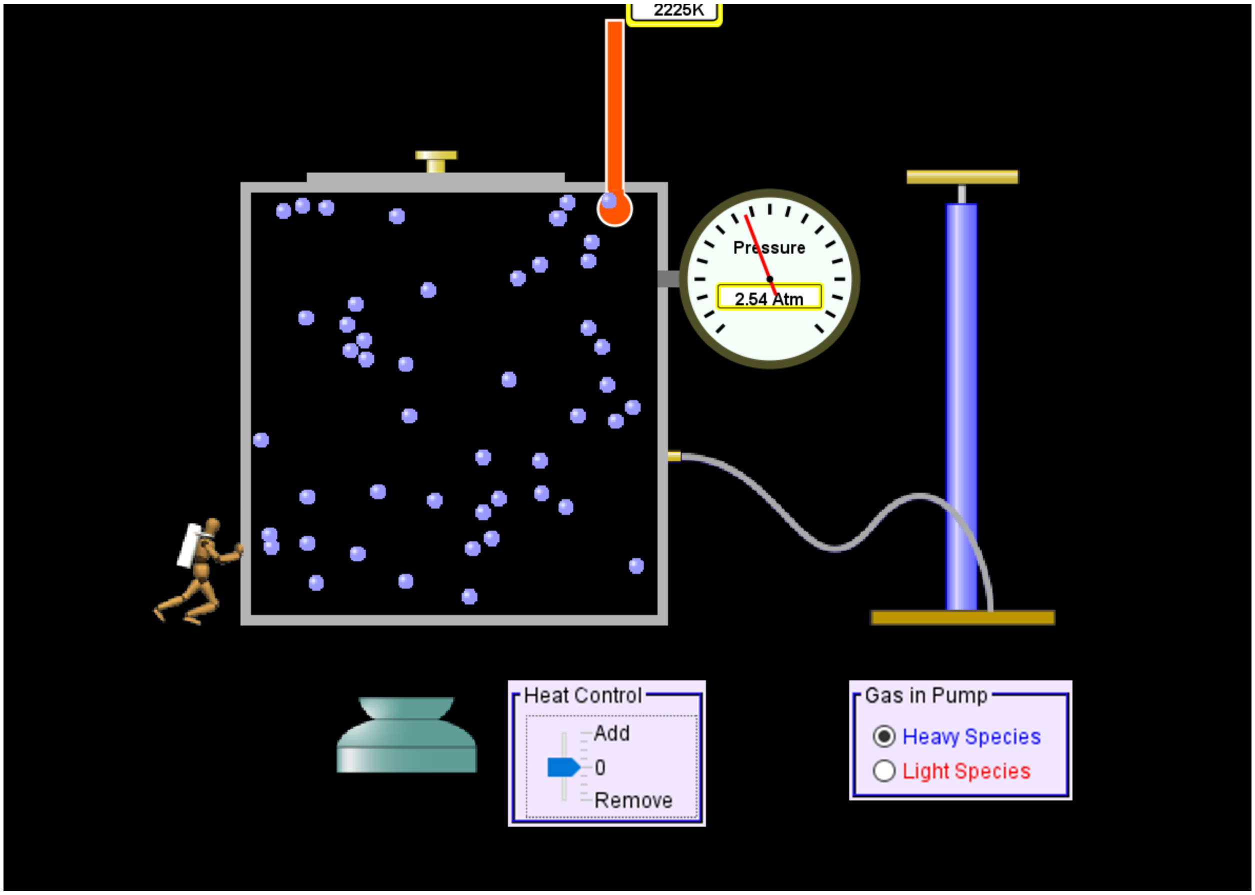
$$\frac{V_1}{n_1} = \frac{V_2}{n_2} \quad \text{at constant } P \text{ and } T$$

$V1$= initial volume $P2$= final volume, $n1$= initial moles $n2$= final moles

Example: The lungs of an average male holds 0.25 mol of air in a volume of 5.5 L. How many mole sof air do the lungs of an average female hold if the volume is 4.5 L?

Ans: $n2$ is unknown.

$5.5/0.25 = 4.5/n2$, $22 = 4.5/n2$ or $n2 = 0.205$ mol or 0.20 mols



Gas in Pump
● Heavy Species
○ Light Species

$$\frac{P_1}{T_1} = \frac{P_2}{T_2} \quad \text{at constant } V \text{ and } n$$

P1= initial pressure, P2= final pressure, T1= initial temp, T2= final temp

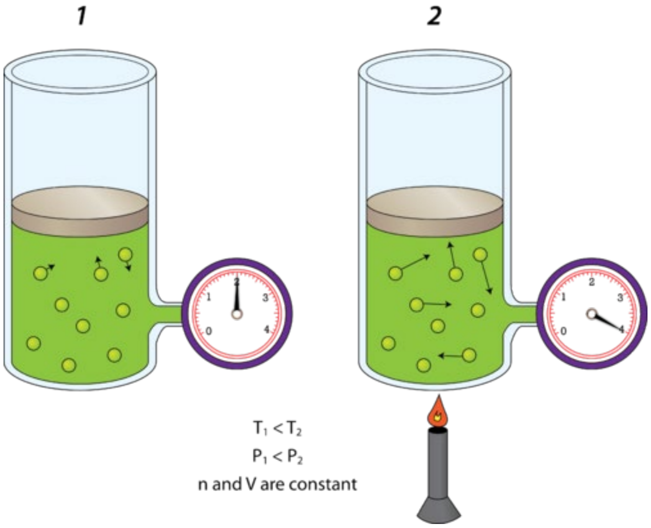


Figure 9.42 Gay-Lusaac's law

Ref: common.wikimedia.org/

Gay Lusaac's law can also be observed the above diagram, where application of heat to a gaseous system increases the pressure of the gas.

Example: The tire on a bicycle in a cool garage is stored at 20^0C and 80. Psi. What is the pressure inside the tire after riding the bike at 43^0C?

Ans: P2 is unknown, 80/(20+273)= P2/(43+ 273)

0.273= P2/316 or P2= 0.273*316= 86.3 psi or 86 psi.

The following activity has been taken from AACT (American association of chemical teachers) https://teachchemistry.org/periodical/issues/november-2015/gas-laws

In this investigation you will examine three gas laws including Boyle's Law, Charles' Law and Gay-Lussac's Law. You will explore how manipulating the variables of volume (L), pressure (atm) and temperature (K) can affect a sample of gas. The formula for each of the gas laws are:

Boyle's Law:

$P_1V_1 = P_2V_2$

Charles' Law:

$\underline{V_1} = \underline{V_2}$

Gay-Lussac's Law:

$\underline{P_1} = \underline{P_2}$

Checking Comprehension

Please create a list of the variable given in each problem and show all your work required to complete the calculation.

1. Calculate the temperature of a gas when it is expanded to 5.25L. The gas originally occupies 3.45L of space at 282K.

2. The temperature of a gas is increased from 125ºC to 182ºC inside of a rigid container. The original pressure of the gas was 1.22atm, what will the pressure of the gas be after the temperature change?

3. The volume of gas in a container was originally 3.24L, while at standard pressure, 1.00atm. What will the volume be if the pressure is increased to 1.20atm?

Combined Gas Law

A: The combined gas law is an expression obtained mathematically combining Boyle's and Charle's laws. A change in pressure, temperature or volume that is brought about by changes in the other two variables can be calculated by using this law.

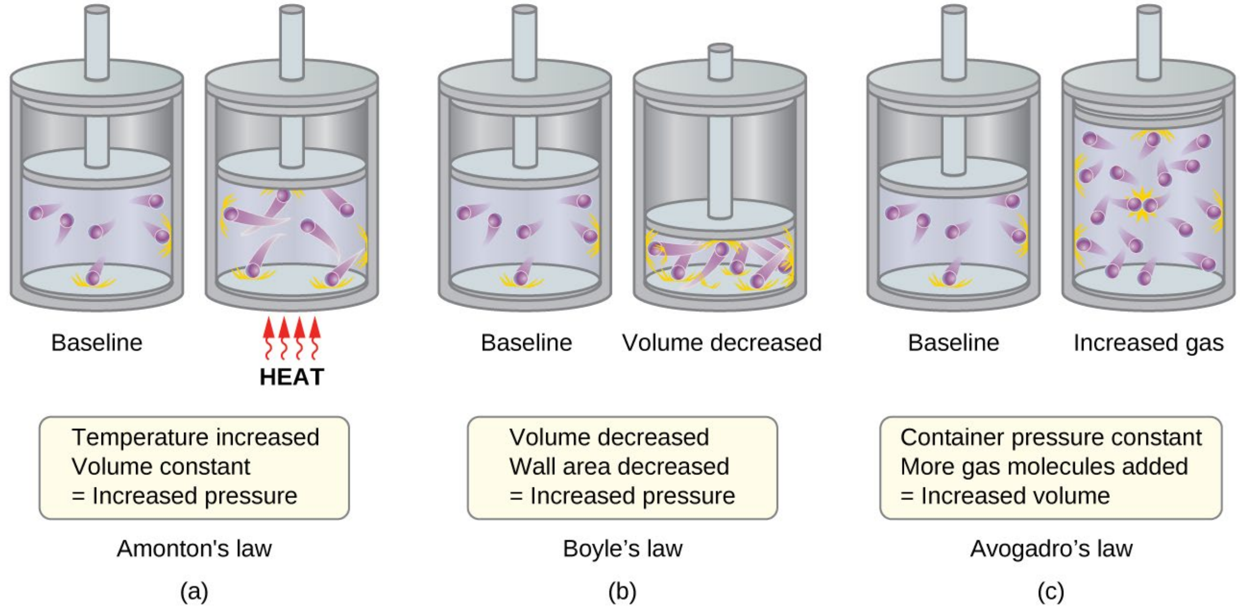


Figure 9.43 Combined Gas law

Ref: common.wikimedia.org/

Mathematically we can write, when amount of gas (n) is constant,

$$\frac{P_1V_1}{T_1} = \frac{P_2V_2}{T_2}$$

Here is the graphical relationship between pressure, volume and temperature of a gaseous system.

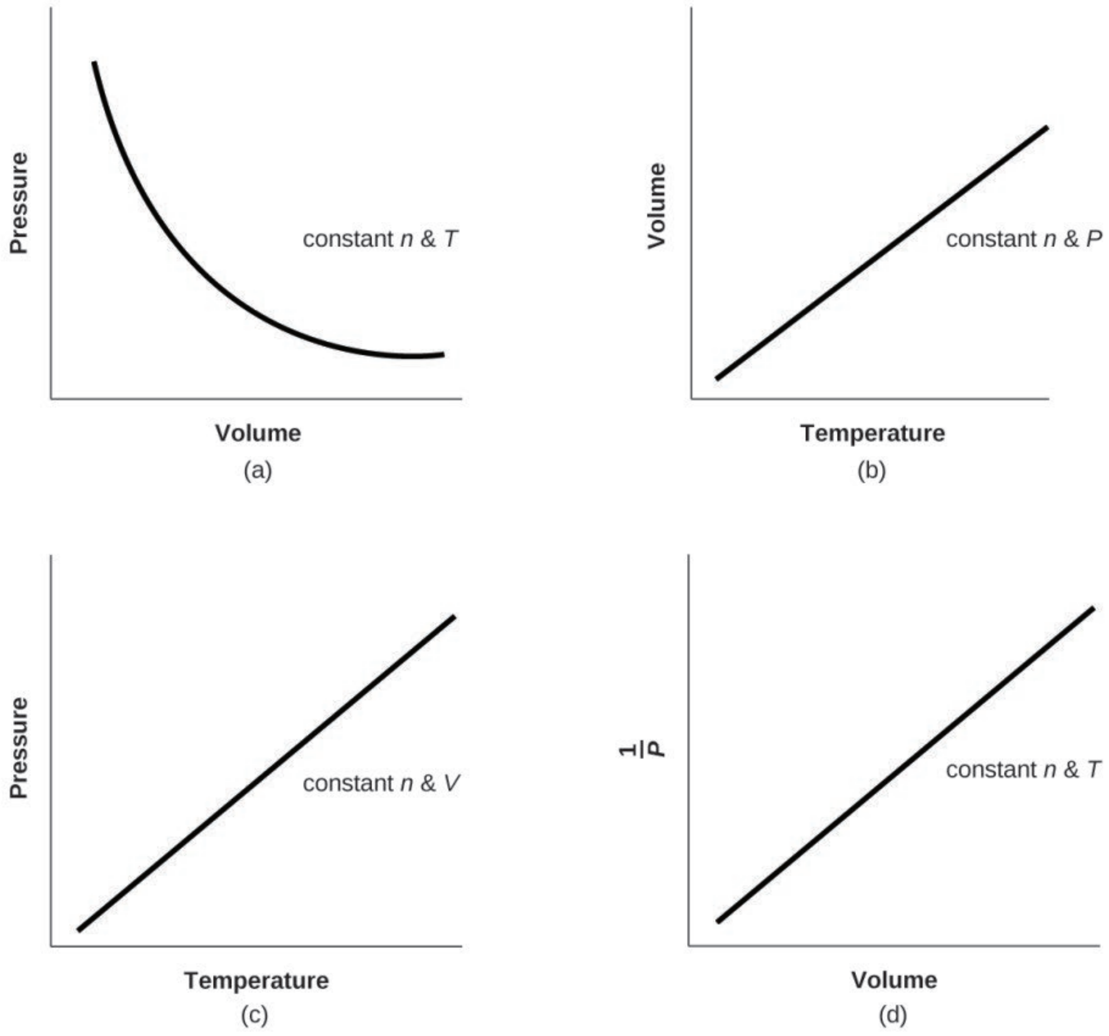


Figure 9.44 Gas Laws Graphical representation

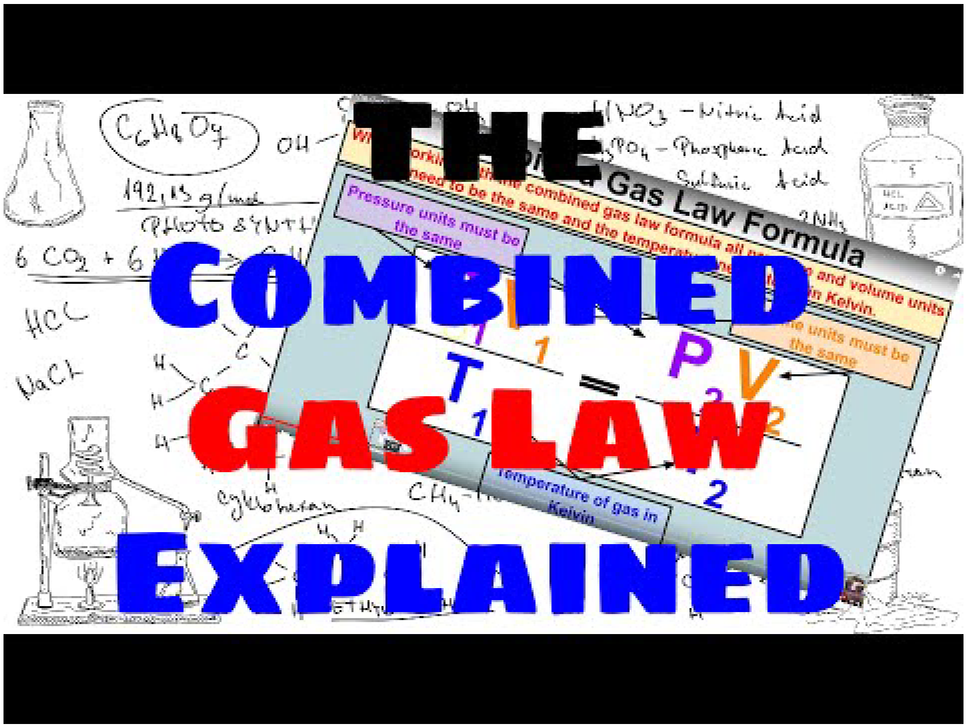
Ref: common.wikimedia.org/

Example: A balloon contains 222 L of Helium at 25.^{0}C and 760 mm of Hg. What is the volume of the balloon when it reaches to an altitude where the temperature is -40^{0}C and the pressure is 540 mm of Hg?

Ans: V2 is unknown.

222* 760/(25+ 273)= 566.17= V2*540/(-40+ 273) , V2= 244.3 L or 244 L.

https://www.youtube.com/watch?v=FSdU6MIjPlo



Questions:

1. The pressure inside a 1.0 L balloon at 25^{0}C was 750 mm of Hg. What is the pressure inside the balloon when it is cooled to -40^{0}C and expands to 5.0 L volume?

IV. Ideal gas law

The ideal gas law holds for all ideal gases at any temperature, pressure, and volume. But the only gases we have around us in the real world are real gases. Real gases behave most like ideal gases at low pressures (atm or less) and high temperatures (K or higher). It combines all the gas laws variable into one condition form.

Based on Boyle's law: P/V = constant

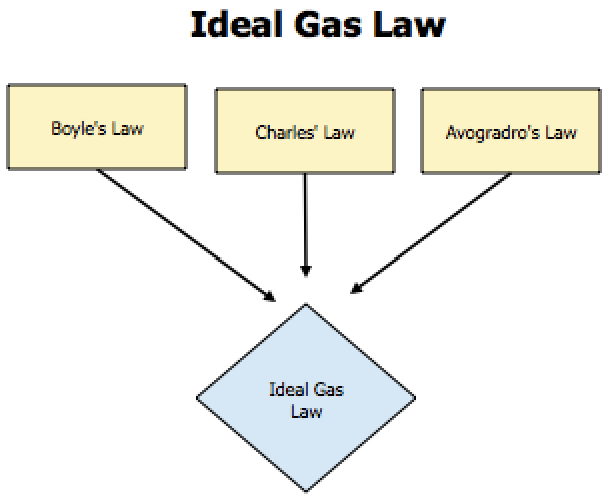
Based on Charles's law: V/T = constant

Based on Avogadro's law: V/n= constant

Combining all, PV/n= constant. This constant is symbolized as R and called universal gas constant.

Figure 9.45 Ideal gas Law

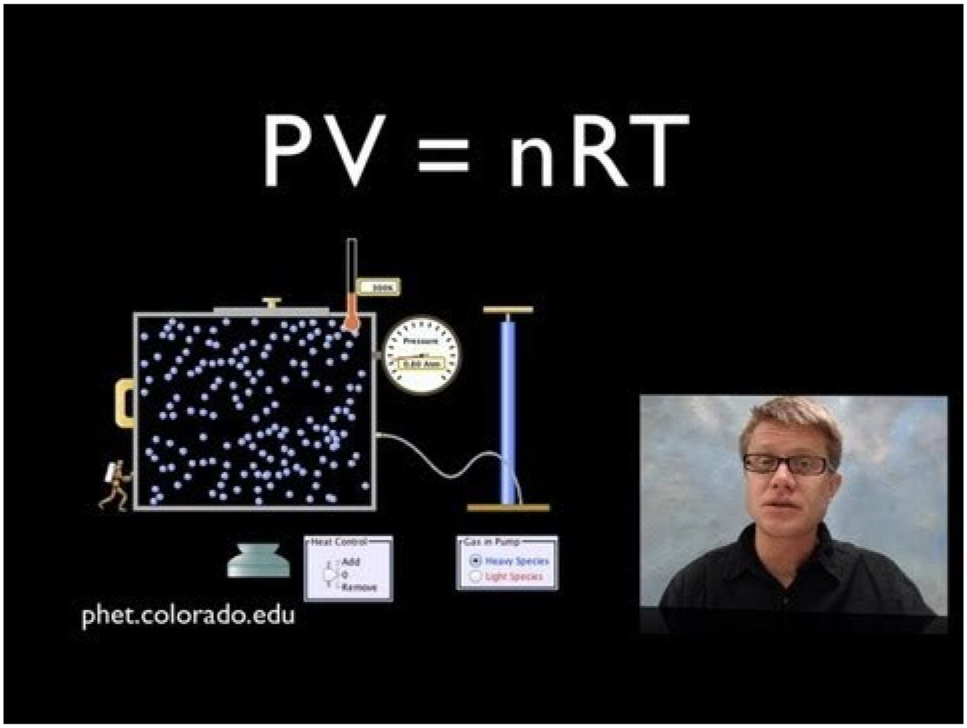
Ref: common.wikimedia.org/



The ideal gas law has the form PV=nRT, where R= Ideal gas Constant (0.08206 L-atm/mol-K). With this equation, any one of the characteristics gas properties (P, V, T or n) can be calculated given the other three.

$$R = 8.314\frac{J}{mol \cdot K} = 8.314\frac{L \cdot kPa}{mol \cdot K} = 0.082057\frac{L \cdot atm}{mol \cdot K} = 62.364\frac{L \cdot mmHg}{mol \cdot K}$$

$$\frac{PV}{nT} = R$$



https://www.youtube.com/watch?v=TqLlfHBFY08&t=2s

Ideal gas law follows al the assumptions of kinetic molecular theory. That is why it is called ideal gas law. In real world gas molecules behave differently. Below is the graph that shows how real molecules deviate from ideal gas law. Ideal gas law indicates that plot and PV vs. P should be a constant because PV= constant when temperature is a constant. Real molecules only behave ideally at low pressure and high temperature.

The ideal gas equation of state

If the variables *P, V, T* and *n* (the number of moles) have known values, then a gas is said to be in a definite ***state***, meaning that all other physical properties of the gas are also defined. The relation between these *state variables* is known as an ***equation of state***. By combining the expressions of Boyle's, Charles', and Avogadro's laws (you should be able to do this!) we can write the very important ***ideal gas*** equation of state

$$\boxed{PV = nRT}$$

Must know this!

where the proportionality constant R is known as the ***gas constant***. This is one of the few equations you *must* commit to memory in this course; you should also know the common value and units of R.

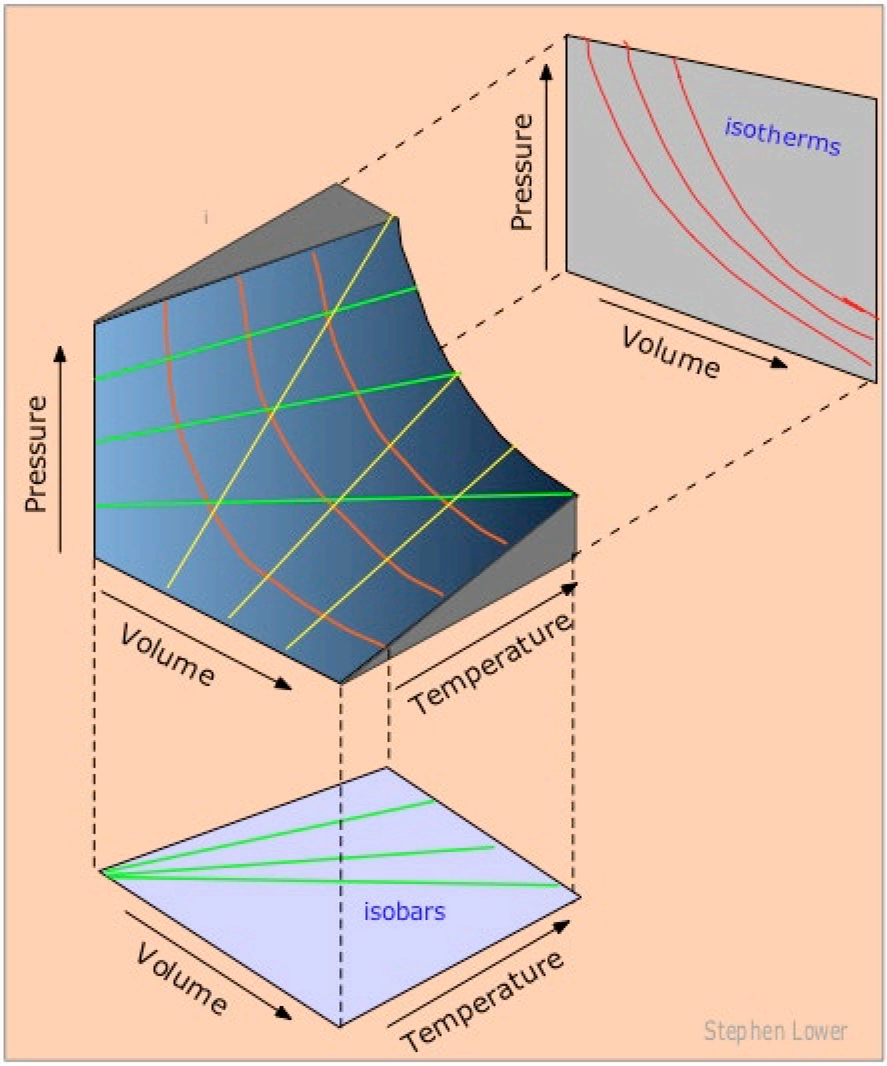
An *ideal gas* is defined as a hypothetical substance that obeys the ideal gas equation of state.

Take note of the word "hypothetical" here. No real gas (whose molecules occupy space and interact with each other) can behave in a truly ideal manner. But we will see in the last lesson of this series that all *gases* behave more and more like an ideal gas as the pressure approaches zero. A pressure of only 1 atm is sufficiently close to zero to make this relation useful for most gases at this pressure.

Many textbooks show formulas, such as $P_1V_1 = P_2V_2$ for Boyle's law. *Don't bother memorizing them*; if you really understand the meanings of these laws as stated above, you can easily derive them on the rare occasions when they are needed. ***The ideal gas equation is the only one you need to know.***

PVT surface for an ideal gas

In order to depict the relations between the three variables P, V and T we need a three-dimensional graph.



Each point on the curved surface represents a possible combination of (*P, V, T*) for an arbitrary quantity of an ideal gas. The three sets of lines inscribed on the surface correspond to states in which one of these three variables is held constant.

The red curved lines, being lines of constant temperature, or *isotherms*, are plots of Boyle's law. These isotherms are also seen projected onto the *P-V* plane at the top right.

The yellow lines are *isochors* and represent changes of the pressure with temperature at constant volume.

Figure 9.46 PVT Surface for Ideal gas

The green lines, known as *isobars*, and projected onto the *V-T* plane at the bottom, show how the volumes contract to zero as the absolute temperature approaches zero, in accordance with the law of Charles and Gay-Lussac.

Problem Example 1

A biscuit made with baking powder has a volume of 20 mL, of which one-fourth consists of empty space created by gas bubbles produced when the baking powder decomposed to CO_2. What weight of $NaHCO_3$ was present in the baking powder in the biscuit? Assume that the gas reached its final volume during the baking process when the temperature was 400°C.

(Baking powder consists of sodium bicarbonate mixed with some other solid that produces an acidic solution on addition of water, initiating the reaction
$NaHCO_3(s) + H^+ \rightarrow Na^+ + H_2O + CO_2$

Solution: Use the ideal gas equation to find the number of moles of CO_2 gas; this will be the same as the number of moles of $NaHCO_3$ (84 g mol^{-1}) consumed :

$$n = \frac{(1\text{ atm})\,(0.005\text{ L})}{(.082\text{ L atm mol}^{-1}\text{ K}^{-1})(673\text{K})} = 9.1\text{E}{-6}\text{ mol}$$

9.1E–6 mol × 84 g mol^{-1} = 0.0076 g

Here is another video to solve problems using ideal gas laws:

https://www.youtube.com/watch?v=oL9XzBcDfF0&t=29s

Example: How many moles of gas are in a typical human breath that takes in 0.50L of air at 1.0 atm pressure and 35^0C?

Number of moles n is unknown. T= 35+ 273= 308K

n= PV/RT i.e. 1.0 * 0.50/(0.0821* 308) n= 0.0198 mol or 0.020 mol

We can determine the mass of a gas from moles if the identity or molar mass of the gas is known. Moles= mass/molar mass.

What you should be able to do

Make sure you thoroughly understand the following essential ideas which have been presented above, and be able to state them in your own words. It is especially important that you know the precise meanings of all the green-highlighted terms in the context of this topic.

Boyle's Law - The *PV* product for any gas at a fixed temperature has a constant value. Understand how this implies an *inverse* relationship between the pressure and the volume.

Charles' Law - The volume of a gas confined by a fixed pressure varies *directly* with the absolute temperature. The same is true of the pressure of a gas confined to a fixed volume.

Avogadro's Law - This is quite intuitive: the volume of a gas confined by a fixed pressure varies directly with the quantity of gas.

The E.V.E.N. principle - this is just another way of expressing Avogadro's Law.

Gay-Lussac's Law of Combining Volumes - you should be able to explain how this principle, that follows from the E.V.E.N. principle and the Law of Combining Weights,

The ideal gas equation of state - this is one of the very few mathematical relations you *must* know. Not only does it define the properties of the hypothetical substance known as an ***ideal gas***, but it's importance extends quite beyond the subject of gases

Volume, temperature, pressure and number of moles are interrelated in gaseous system.

Molar Volume of a Gas

Further application of Ideal Gas Law: Density and Molar mass:

1 The molar volume of a gas

You will recall that the ***molar mass*** of a pure substance is the mass of 6.02 x 10^{23} (***Avogadro's number***) of particles or molecular units of that substance. Molar masses are commonly expressed in units of grams per mole (g mol^{-1}) and are often referred to as ***molecular weight***s.

As was explained in the preceding lesson, equal volumes of gases, measured at the same temperature and pressure, contain equal numbers of molecules (this is the *"EVEN" principle*, more formally known as ***Avogadro's law***.)

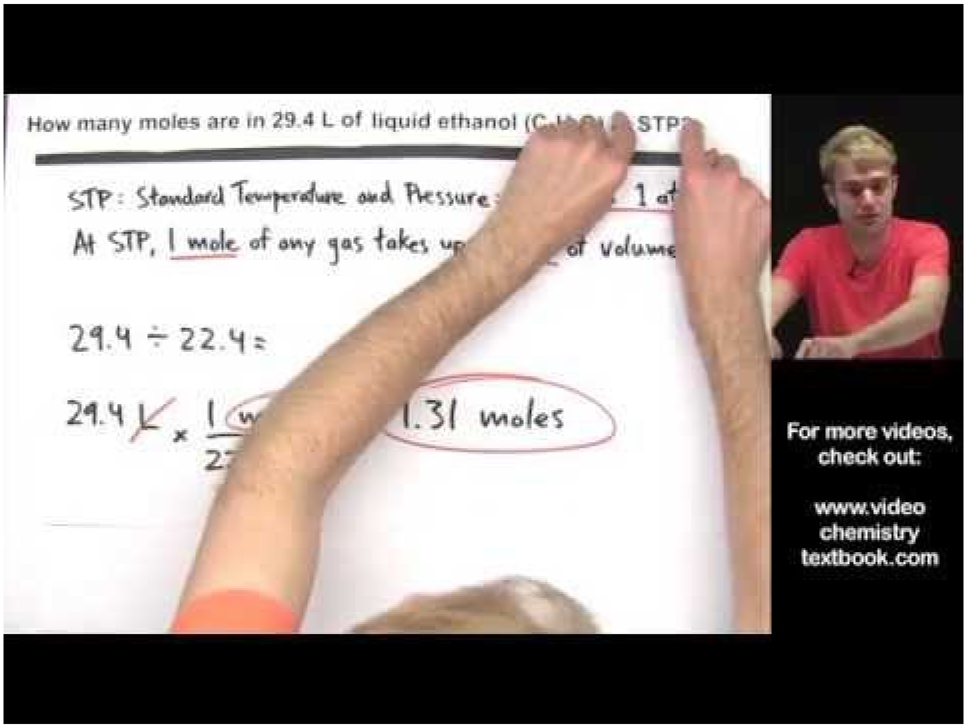
STP

Avogadro’s law allows us to compare the amount of any two gases by comparing their volumes. Often amounts of gas are compared at a set of standard conditins of temperature and pressure called STP.

STP conditions are: 1 atm (760 mm of Pr) and 273 K ((0^0C)

At STP, one mole of any gas has the same volume 22.4 L called the standard molar volume.

https://www.youtube.com/watch?v=Y8e7T09SKZ0&t=14s



Example:

1mol= 22.4 L

Q: How many mols are present Moles of 5.00 L of O_2 at STP?

$\frac{1\text{mol}}{22.4\text{ L}} = \frac{x\text{ mol}}{5.00\text{L}}$ x= 0.223 mols

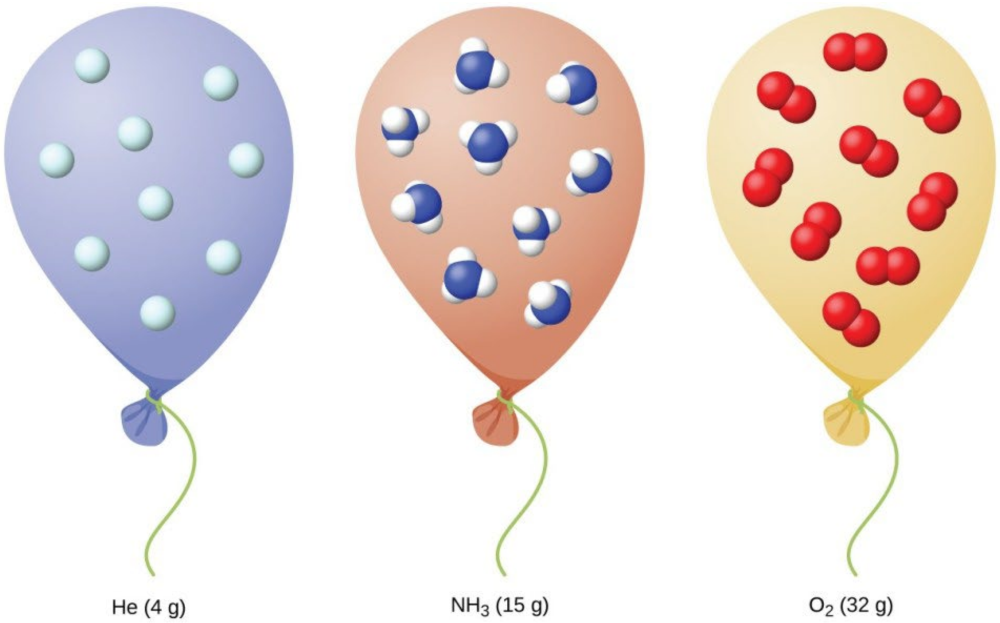


Figure 9.47 STP Condition and molar volume

Ref: common.wikimedia.org/

At STP all different gases occupy same volume.

Questions:

1. Burning 1mol of propane in a gas grill occupies 150. grams of CO_2. What volume of CO_2 does it occupy at STP?

Standard temperature and pressure: 273K, 1 atm

The magnitude of this volume will of course depend on the temperature and pressure, so as a means of convenient comparison it is customary to define a set of conditions T = 273K and P = 1 atm as ***standard temperature and pressure***, usually denoted as ***STP***. Substituting these values into the ideal gas equation of state and solving for *V* yields a volume of 22.414 litres for 1 mole.

Figure 9.48 Muana Kea Hawaii

Ref: commons.wikimedia.org/

Problem Example 1

Estimate the volume of one mole of air at 20°C on top of Muana Kea, Haw'aii (altitude 4.2 km) where the air pressure is typically around 60 kPa.

Click on image to enlarge it →

Solution: Apply Boyle's and Charles' laws as successive correction factors to the STP molar volume. (Recall that
1 atm =101.3 kPa)

$$V_2 = \underset{\substack{\uparrow \\ V_M\text{ at STP}}}{22.4\text{ L}} \times \underset{\substack{\text{Charles'} \\ \text{law}}}{\left(\frac{293\text{K}}{273\text{K}}\right)} \times \underset{\substack{\text{Boyle's} \\ \text{law}}}{\left(\frac{101.3\text{ kPa}}{60\text{ kPa}}\right)} = 41\text{ L}$$

The ***standard molar volume 22.4 L mol^{-1}*** is a value worth memorizing, but remember that it is valid only at STP. The molar volume at other temperatures and pressures can easily be found by simple proportion.

The molar volume of a substance can tell us something about how much space each molecule occupies, as the following example shows.

Problem Example 2

Estimate the average distance between the molecules in a gas at 1 atm pressure and 0°C.

Solution: Consider a 1-cm^3 volume of the gas, which will contain

$(6.02E23 \text{ mol}^{-1})/(22400 \text{ cm}^3 \text{ mol}^{-1}) = 2.69E19 \text{ cm}^{-3}$.

The volume per molecule (not the same as the volume *of* a molecule, which for an ideal gas is zero!) is just the reciprocal of this, or 3.72E–20 cm^3. Assume that the molecules are evenly distributed so that each occupies an imaginary box having this volume. The average distance between the centers of the molecules will be defined by the length of this box, which is the cube root of the volume per molecule:

$(3.72 \times 10^{-20})^{1/3} = 3.38 \times 10^{-7} \text{ cm} = 3.4 \text{ nm}$

Pure gases or mixtures: it makes no difference

Under conditions at which the ideal gas model is applicable (that is, almost always unless you are a chemical engineer dealing with high pressures), "a molecule is a molecule", so the volume of Avogadro's number of molecules will be independent of the composition of the gas. The reason, of course, is that the volume of the gas is mostly empty space; the volumes of the molecules themselves are negligible.

2 Molar mass and density of a gas

The molecular weight (molar mass) of any gas is the mass, expressed in grams, of Avogadro's number of its molecules. This is true regardless of whether the gas is composed of one molecular species or is a mixture.

For a mixture of gases, the molar mass will depend on the molar masses of its components, and on the fractional abundance of each kind of molecule in the mixture. The term "average molecular weight" is often used to describe the molar mass of a gas mixture.

Average molecular weight of a gas

$$\overline{m}$$

110-component gas mixture enters Guinness Book of Records in 2010. The U.S. branch of the Linde Corporation, which supplies specialty gases to industry, concocted this one to calibrate instruments that measure atmospheric pollution.

$$\bar{m} = \sum_i x_i m_i$$

Problem Example 3

Find the average molar mass of dry air whose volume-composition is O_2 (21%), N_2 (78%) and Ar (1%).

Solution: The average molecular weight is the mole-fraction-weighted sum of the molecular weights of its components. The mole fractions, of course, are the same as the volume-fractions (E.V.E.N. principle.)

$m = (.21 \text{ x } 32) + (.78 \text{ x } 28) + (.01 \text{ x } 40) = \mathbf{29}$

Density of a pure gas

The molar volumes of all gases are the same when measured at the same temperature and pressure. But the molar *masses* of different gases will vary. This means that different gases will have different *densities* (different masses per unit volume). If we know the molecular weight of a gas, we can calculate its density.

Problem Example 4

Uranium hexafluoride UF_6 gas is used in the isotopic enrichment of natural uranium. Calculate its density at STP.

Solution: The molecular weight of UF_6 is 352.

(352 g mol^{-1}) ÷ (22.4 L mol^{-1}) = **15.7 g L^{-1}**

Note: there is no need to look up a "formula" for this calculation; simply combine the molar mass and molar volume in such a way as to make the units come out correctly.

More importantly, if we can measure the density of an unknown gas, we have a convenient means of estimating its molecular weight. This is one of many important examples of how a ***macroscopic*** measurement (one made on bulk matter) can yield ***microscopic*** information (that is, about molecular-scale objects.)

Gas densities are now measured in industry by electro-mechanical devices such as vibrating reeds which can provide continuous, on-line records at specific locations, as within pipelines.

Determination of the molecular weight of a gas from its density is known as the *Dumas method*, after the French chemist Jean Dumas (1800-1840) who developed it. One simply measures the weight of a known volume of gas and converts this volume to its STP equivalent, using Boyle's and Charles' laws. The weight of the gas divided by its STP volume yields the density of the gas, and the density multiplied by 22.4 mol^{-1} gives the molecular weight. Pay careful attention to the examples of gas density calculations shown here and in your textbook. You will be expected to carry out calculations of this kind, converting between molecular weight and gas density.

Problem Example 5

The approximate molar mass of a gas whose measured density is 3.33 g/L at 30°C and 780 torr.

Solution: Find the volume that would be occupied by 1 L of the gas at STP; note that correcting to 273 K will reduce the volume, while correcting to 1 atm (760 torr) will increase it:

$$V = (1.00 \text{ L})\left(\frac{273}{303}\right)\left(\frac{780}{760}\right) = 0.924 \text{ L}$$

The number of moles of gas is $n = (.924 \text{ L}) \div (22.4 \text{ L mol}^{-1}) = 0.0412$ mol

The molecular weight is therefore $(3.3 \text{ g L}^{-1}) \div (.0412 \text{ mol L}^{-1}) =$ **80 g mol^{-1}**

Density of a gas mixture

Gas density measurements can be a useful means of estimating the composition of a mixture of two different gases; this is widely done in industrial chemistry operations in which the compositions of gas streams must be monitored continuously.

Problem Example 6

Find the composition of a mixture of CO_2 (44 g/mol) and methane CH_4 (16 g/mol) that has a STP density of 1.214 g/L.

Solution: The density of a mixture of these two gases will be directly proportional to its composition, varying between that of pure methane and pure CO_2. We begin by finding these two densities:

For CO_2: (44 g/mol) ÷ (22.4 L/mol) = 1.964 g/L

For CH_4: (16 g/mol) ÷ (22.4 L/mol) = 0.714 g/L

If x is the mole fraction of CO_2 and $(1–x)$ is the mole fraction of CH_4, we can write

$1.964\ x + 0.714\ (1–x) = 1.214$

(Does this make sense? Notice that if $x = 0$, the density would be that of pure CH_4, while if it were 1, it would be that of pure CO_2.)

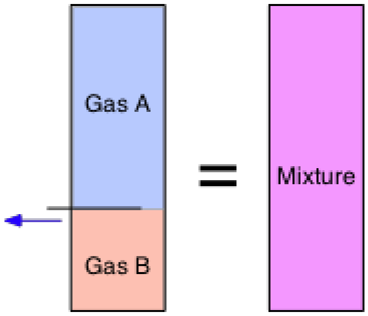
Expanding the above equation and solving for x yields the mole fractions of 0.40 for CO_2 and 0.60 for CH_4.

3 Expressing the composition of a gas mixture

Because most of the volume occupied by a gas consists of empty space, there is nothing to prevent two or more kinds of gases from occupying the same volume. ***Homogeneous mixtures*** of this kind are generally known as ***solutions***, but it is customary to refer to them simply as *gaseous mixtures*.

We can specify the composition of gaseous mixtures in many different ways, but the most common ones are by *volumes* and by *mole fractions*.

Volume fractions in gas mixtures



From Avogadro's Law we know that "equal volumes contain equal numbers of molecules". This means that the volumes of gases, unlike those of solids and liquids, are strictly additive. So if a partitioned container has two volumes of gas A in one section and one volume of gas B in the other (both at the same temperature and pressure), and we remove the partition, the volume remains unchanged.

Figure 9.49 Mixture of Gases

We can specify the composition of this mixture by saying that the ***volume fraction*** of A is 2/3 and that of B is 1/3.

Volume fractions are often called ***partial volumes***:

$$V_i = \frac{v_i}{\sum_i v_i}$$

Don't let this type of notation put you off! The summation sign Σ (Greek Sigma) simply means to add up the v's (volumes) of every gas. Thus if Gas A is the "i-th" substance as in the expression immediately above, the summation runs from i=1 through i=2.

Note that we can employ partial volumes to specify the composition of a mixture even if it had never actually been made by combining the pure gases.

When we say that air, for example, is 21 percent oxygen and 78 percent nitrogen by volume, this is the same as saying that these same percentages of the molecules in air consist of O_2 and N_2. Similarly, in 1.0 mole of air, there is 0.21 mol of O_2 and 0.78 mol of N_2 (the other 0.1 mole consists of various trace gases, but is mostly neon.)

Note that you could never assume a similar equivalence with mixtures of liquids or solids, to which the E.V.E.N. principle does not apply.

Mole fractions in gas mixtures

These last two numbers (.21 and .78) also express the mole fractions of oxygen and nitrogen in air. ***Mole fraction*** means exactly what it says: the fraction of the molecules that consist of a specific substance. This is expressed algebraically by

$$X_i = \frac{n_i}{\sum_i n_i}$$

so in the case of oxygen in the air, its mole fraction is

$$X_{O_2} = \frac{n_{O_2}}{n_{O_2} + n_{N_2} + n_{Ar}} = \frac{.21}{1} = .21$$

Problem Example 7

A mixture of O_2 and nitrous oxide, N_2O, is sometimes used as a mild anesthetic in dental surgery. A certain mixture of these gases has a density of 1.482 g L^{-1} at 25 and 0.980 atm. What was the mole-percent of N_2O in this mixture?

Solution: First, find the density the gas would have at STP:

$$(1.482\text{ g L}^{-1}) \times \left(\frac{298}{273}\right)\left(\frac{1}{.980}\right) = 1.65\text{ g L}^{-1}$$

The molar mass of the mixture is (1.65 g L^{-1})(22.4 L mol^{-1}) = 37.0 g mol^{-1}. The molecular weights of O_2 and N_2 are 32 and 44, respectively. 37.0 is 5/12 of the difference between the molar masses of the two pure gases. Since the density of a gas mixture is directly proportional to its average molar mass, the mole fraction of the heavier gas in the mixture is also 5/12:

$$\frac{37-32}{44-32} = \frac{5}{12} = .42$$

Problem Example 8

What is the mole fraction of carbon dioxide in a mixture consisting of equal masses of CO_2 (MW=44) and neon (MW=20.2)?

Solution: Assume any arbitrary mass, such as 100 g, find the equivalent numbers of moles of each gas, and then substitute into the definition of mole fraction:

n_{CO2} = (100 g) ÷ (44 g mol^{-1}) = 2.3 mol

n_{Ne}= (100 g) ÷ (20.2 g mol^{-1}) = 4.9 mol

X_{Ne} = (2.3 mol) ÷ (2.3 mol + 4.9 mol) = 0.32

The mathematical form of the Ideal Gas Law is:

PV = nRT and n = m/MW and d = m/V

Where:

- P - pressure
- V - volume
- n - number of moles
- T - temperature
- m - mass
- d - dendity
- MW - Molecular Weight
- R - ideal gas constant. If the units of P, V, n and T are atm, L, mol and K, respectively, the value of R is 0.0821 L x atm/K x mol or 8.314 J/K x mol.

The density (d) of a gas is defined as

d = m / V

and the moles of a gas is:

n = m / MW

Where m is the mass of the gas, and

M is the molecular weight.

Substituting the definitions to the original Ideal Gas equation, it becomes:

d = P x M / (R x T)

When any three of the four quantities in the equation are known, the forth can be calculated. For example, we've known d, P and T, M can be:

M = d x R x T / P

Question: What is the density of an ideal gas with a molecular mass of 50 g/mol at 2 atm and 27 °C?

Figure 9.50 Density determination of Gases

Ref: commons.wikimedia.org/

Solution:

Let's start with the ideal gas law:

PV = nRT

where
P = pressure
V = volume
n = number of moles of gas
R = gas constant = 0.0821 L·atm/mol·K
T = absolute temperature

We know density (d) is mass (m) per unit volume. While the equation has a volume variable, there is no obvious mass variable. The mass can be found in the number of moles of the ideal gas.

The molecular mass (*M*) of the gas is the mass of one mole of the gas. This means n moles of the gas has a mass of n*M* grams.

$m = nM$

If we solve this for n we get

$n = m/M$

Now we have enough to find the density of the gas. First, solve the ideal gas equation for V.

$$V = \frac{nRT}{P}$$

Substitute n for what we found earlier

$$V = \frac{mRT}{MP}$$

Divide both sides by m

$$\frac{V}{m} = \frac{RT}{MP}$$

Invert the equation

$$\frac{m}{V} = \frac{MP}{RT}$$

density (d) = m/V, so

$$d = \frac{M*P}{R*T}$$

From our question:
M = 50 g/mol
P = 2 atm
T = 27 °C

The first thing we need to do is convert the temperature to absolute temperature. The conversion between Kelvin and Celsius is:

$T_K = T_C + 273$

$T_K = 27 + 273$

$T_K = 300$ K

Another tricky part of ideal gas problems is matching the units on the ideal gas constant R. We're using liters, atm, and Kelvin so we can use the value

R = 0.0821 L·atm/mol·K

Plug all these values into our equation

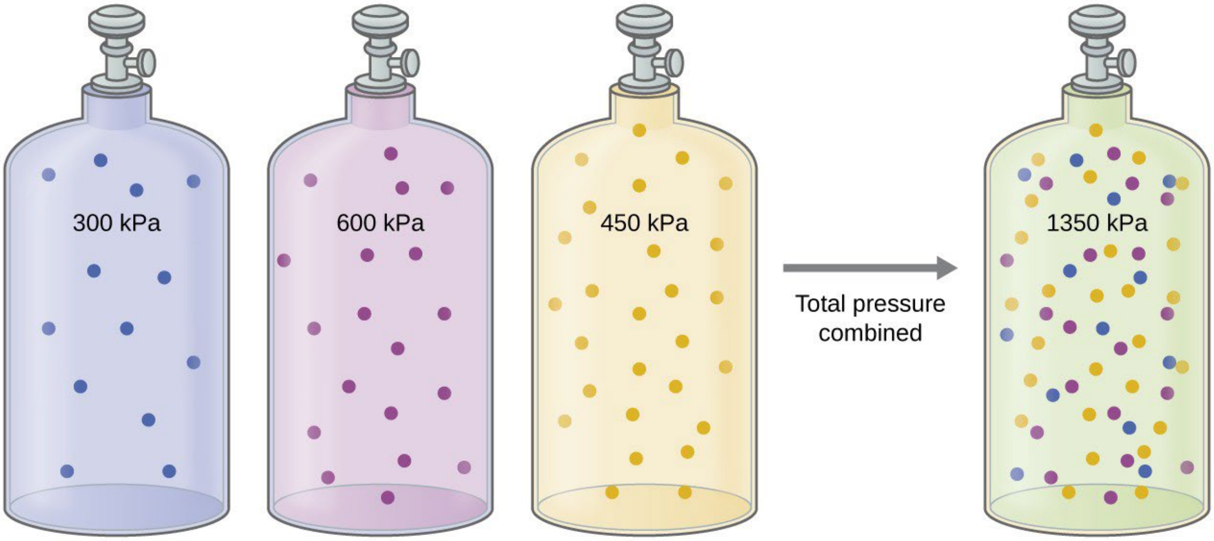
$$d = \frac{50\ g/mol * 2\ atm}{0.0821L\,\frac{atm}{molK} * 300K}$$

d= 4.06 g/L

Answer: The density of an ideal gas of 50 g/mol at 2 atmospheres and 27 °C is 4.06 g/L

Dalton's Law

In a mixture of gases, each molecule acts independently of all the others, provided that the gases behave as ideal gases and do not interact with each other in any way.



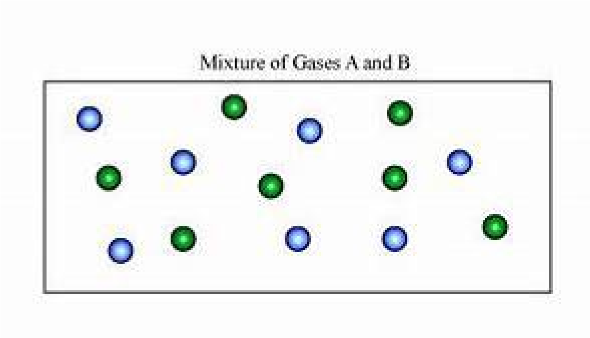
Mathematically we can write,

$$P_{total} = P_1 + P_2 + P_3 + ... + P_n \equiv \sum_{i=1}^{n} P_i$$

Partial pressure of a gas can be calculated using mol fraction of a gas in a gas mixture and total pressure.

Figure 9.51 Mixture of Gases

Ref: commons.wikimedia.org/



Total pressure = 1 atm

For example: in the above diagram, total number of gas molecules =14. Number of A (blue) gas molecules= 7, number of B (green) gas molecule= 7.

Mole fraction gas A= 7/14= 0.5

Mole fraction of B= 7/14= 0.5

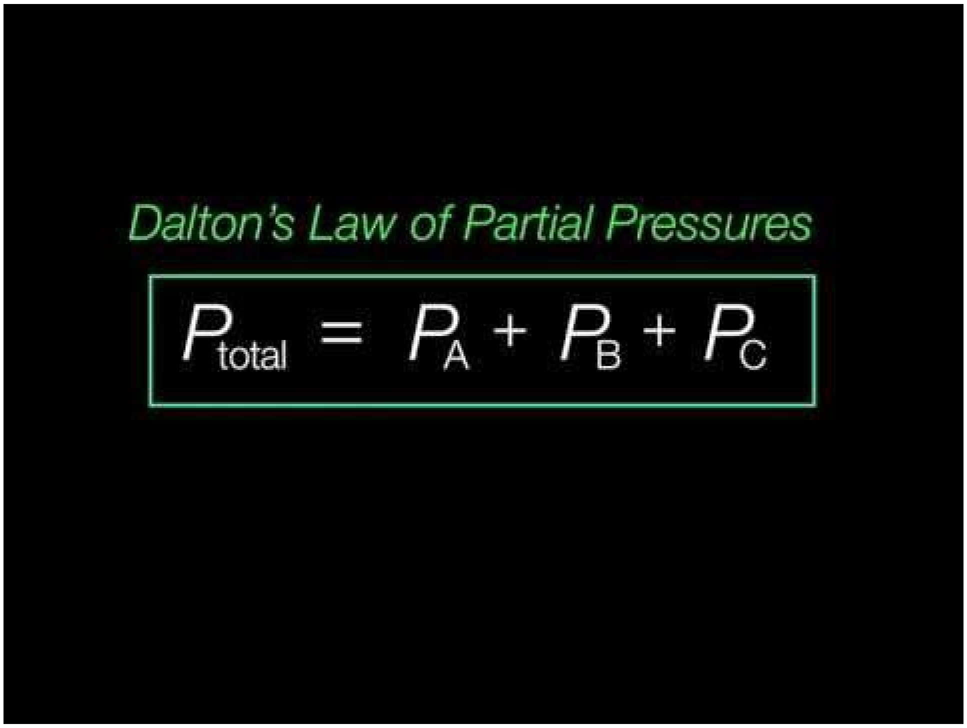
If the total pressure of the gas molecule= 1 aim.

Partial pressure of A= 0.5*1= 0.5 atm

Partial pressure of B= 0.5*1= 0.5 atm

The following videdo might help you to understand the concept.

https://www.youtube.com/watch?v=RqffPYOoxd8



Dalton's Law of Partial Pressures

$$P_{\text{total}} = P_A + P_B + P_C$$

Mole Fractions of Gas Mixtures

The composition of a gas mixture can be described by the mole fractions of the gases present. The mole fraction (X) of any component of a mixture is the ratio of the number of moles of that component to the total number of moles of all the species present in the mixture (n_t):

The mole fraction is a dimensionless quantity between 0 and 1. If $X_A = 1.0$, then the sample is pure A, not a mixture. If $X_A = 0$, then no A is present in the mixture. The sum of the mole fractions of all the components present must equal 1.

To see how mole fractions can help us understand the properties of gas mixtures, let's evaluate the ratio of the pressure of a gas A to the total pressure of a gas mixture that contains A. We can use the ideal gas law to describe the pressures of both gas A and the mixture: $P_A = n_ART/V$ and $P_t = n_tRT/V$. The ratio of the two is thus

Rearranging this equation gives

$P_A = X_A P_t$

That is, the partial pressure of any gas in a mixture is the total pressure multiplied by the mole fraction of that gas. This conclusion is a direct result of the ideal gas law, which assumes that all gas particles behave ideally. Consequently, the pressure of a gas in a mixture depends on only the percentage of particles in the mixture that are of that type, not their specific physical or chemical properties. Please note that earth's atmosphere is about 78% N_2, 21% O_2, and 0.9% Ar, with trace amounts of gases such as CO_2, H_2O, and others. This means that 78% of the particles present in the atmosphere are N_2; hence the mole fraction of N_2 is 78%/100% = 0.78. Similarly, the mole fractions of O_2 and Ar are 0.21 and 0.009, respectively. Using Equation 10.30, we therefore know that the partial pressure of N_2 is 0.78 atm (assuming an atmospheric pressure of exactly 760 mmHg) and, similarly, the partial pressures of O_2 and Ar are 0.21 and 0.009 atm, respectively.

Question: A chemical engineer places a mixture of noble gases consisting of 5.50 g of He, 15.0 g of Ne and 35.0 g of Kr in a chamber at STP. Calculate the partial pressure of Kr gas.

Total pressure = 1 atm (STP)

Mols of He= 5.50/4.023= 1.367

Mols of Ne= 15.5/20.18= 0.7681

Mols of Kr= 35.5/83.798= 0.4237

Total mols= 1.367+0.7681+0.4237= 2.5588

Mol fraction of Kr= 0.4237/2.5588= 0.1656

Partial pressure of Kr= 0.1656*1= 0.166 atm.

*****Dalton's law of partial pressures**

Figure 9.52 Dalton

The ideal gas equation of state applies to mixtures just as to pure gases. It was in fact with a gas mixture, ordinary air, that Boyle, Gay-Lussac and Charles did their early experiments. The only new concept we need in order to deal with gas mixtures is the ***partial pressure***, a concept invented by the famous English chemist John Dalton (1766-1844). Dalton reasoned that the low density and high compressibility of gases indicates that they consist mostly of empty space; from this it follows that when two or more different gases occupy the same volume, they behave entirely independently.

The contribution that each component of a gaseous mixture makes to the total pressure of the gas is known as the *partial pressure* of that gas. Dalton himself stated this law in the simple and vivid way shown at the left.

The usual way of stating ***Dalton's Law of Partial Pressures*** is

The total pressure of a gas is the sum
of the partial pressures of its components

We can express this algebraically as

$$P_{total} = P_1 + P_2 + \cdots = \sum_i P_i$$

or, equivalently

$$P_{total} = \frac{RT}{V} \sum_i n_i$$

(If you feel a need to memorize these formulas, you probably don't really understand Dalton's Law!)

There is also a similar relationship based on *volume fractions*, known as *Amagat's law of partial volumes*. It is exactly analogous to Dalton's law, in that it states that the total volume of a mixture is just the sum of the partial volumes of its components. But there are two important differences:

Amagat's law holds only for ideal gases which must all be at the same temperature and pressure. Dalton's law has neither of these restrictions.

Although Amagat's law seems intuitively obvious, it sometimes proves useful in chemical engineering applications. We will make no use of it in this course.

Problem Example 1

Calculate the mass of each component present in a mixture of fluorine (MW and xenon (MW 131.3) contained in a 2.0-L flask. The partial pressure of Xe is 350 torr and the total pressure is 724 torr at 25°C.

Solution: From Dalton's law, the partial pressure of F_2 is (724 – 350) = 374 torr:

The mole fractions are X_{Xe} = 350/724 = .48 and X_{F2} = 374/724 = .52 . The total number of moles of gas is

$$n = \frac{PV}{RT} = \frac{(724/760)(2)}{(.082)(298)} = .078 \text{ mol}$$

The mass of Xe is (131.3 g mol^{-1}) × (.48 × .078 mol) = 4.9 g

Problem Example 2

Three flasks having different volumes and containing different gases at various pressures are connected by stopcocks as shown. When the stopcocks are opened,

a) What will be the pressure in the system?
b) Which gas will be most abundant in the mixture?

Assume that the temperature is uniform and that the volume of the connecting tubes is negligible.

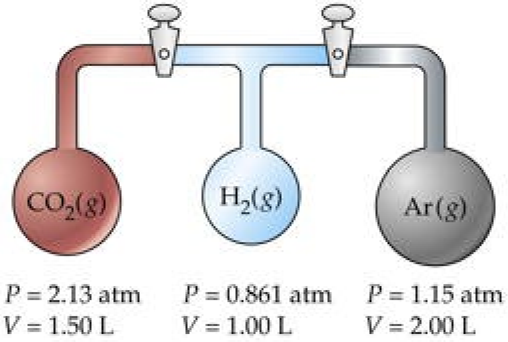


Figure 9.53 Mixture of Gases

Solution: The trick here is to note that the total number of moles n_T and the temperature remain unchanged, so we can make use of Boyle's law PV = constant. We will work out the details for CO_2 only, denoted by subscripts a.

For CO_2, P_aV_a = (2.13 atm)(1.50 L) = 3.19 L-atm.

Adding the PV products for each separate container, we obtain
$\Sigma P_i V_i = 6.36$ L-atm $= n_T RT$. We will call this sum $P_1 V_1$.
After the stopcocks have been opened and the gases mix, the new conditions are denoted by $P_2 V_2$.

From Boyle's law, $P_1 V_1 = P_2 V_2 = 6.36$ L-atm. $V_2 = \Sigma V_i = 4.50$ L.
Solving for the final pressure P_2 we obtain (6.36 L-atm)/(4.50 L) = **1.41 atm**.

For part *(b)*, note that the number of moles of each gas is $n = PV/RT$. The mole fraction if any one gas is $X_i = n_i / n_T$. For CO_2, this works out to
$(3.19/RT) / (6.36/RT) = 0.501$. Because this exceeds 0.5, we know that this is the most abundant gas in the final mixture.

5 Some applications of Dalton's law

Collecting gases over water

A common laboratory method of collecting the gaseous product of a chemical reaction is to conduct it into an inverted tube or bottle filled with water, the opening of which is immersed in a larger container of water. This arrangement is called a *pneumatic trough*, and was widely used in the early days of chemistry. As the gas enters the bottle it displaces the water and becomes trapped in the upper part.

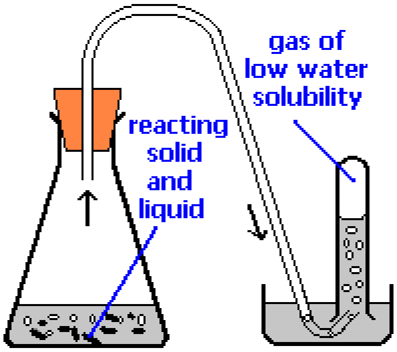


Figure 9.54 Collection of Gas over water

The volume of the gas can be observed by means of a calibrated scale on the bottle, but what about its pressure? The total pressure confining the gas is just that of the atmosphere transmitting its force through the water. (An exact calculation would also have to take into account the height of the water column in the inverted tube.) But liquid water itself is always in equilibrium with its vapor, so the space in the top of the tube is a mixture of two gases: the gas being collected, and gaseous H_2O. The partial pressure of H_2O is known as the vapor pressure of water and it depends on the temperature. In order to determine the quantity of gas we have collected, we must use Dalton's Law to find the partial pressure of that gas.

Problem Example 11

Oxygen gas was collected over water as shown above. The atmospheric pressure was 754 torr, the temperature was 22°C, and the volume of the gas was 155 mL. The vapor pressure of water at 22°C is 19.8 torr. Use this information to estimate the number of moles of O_2 produced.

Solution:

From Dalton's law, $P_{O2} = P_{total} - P_{H2O} = 754 - 19.8 = 734$ torr = .966 atm.

$$n = \frac{PV}{RT} = \frac{0.966 \text{ atm} \times (0.155 \text{ L})}{(.082 \text{ L atm mol}^{-1}\text{K}^{-1})(295\text{K})} = .00619 \text{ mol}$$

Scuba diving and Dalton's law:

Figure 9.55 Scuba diving

Ref: commons.wikimedia.org/

Our respiratory systems are designed to maintain the proper oxygen concentration in the blood when the partial pressure of O_2 is 0.21 atm, its normal sea-level value. Below the water surface, the pressure increases by 1 atm for each 10.3 m increase in depth; thus a scuba diver at 10.3 m experiences a total of 2 atm pressure pressing on the body. In order to prevent the lungs from collapsing, the air the diver breathes should also be at about the same pressure.

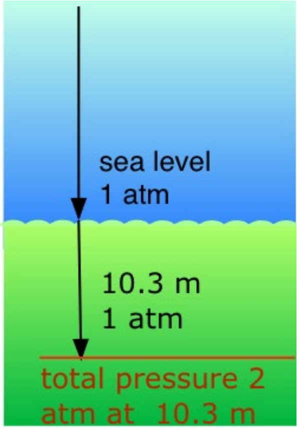


Figure 9.56 Atmospheric Pressure below sea level

But at a total pressure of 2 atm, the partial pressure of O_2 in ordinary air would be 0.42 atm; at a depth of 100 ft (about 30 m), the O_2 pressure of

.8 atm would be sufficiently high to induce *oxygen toxicity*. For this reason, the air mixture in the pressurized tanks that scuba divers wear must contain a smaller fraction of O_2. This can be achieved most simply by raising the nitrogen content, but high partial pressures of N_2 can also be dangerous, resulting in a condition known as nitrogen narcosis. The preferred diluting agent for sustained deep diving is helium, which has very little tendency to dissolve in the blood even at high pressures.

The Chemistry of Scuba Diving

Diving physics and "fizzyology"

Scuba diving and hyperbaric medicine

What you should be able to do

Make sure you thoroughly understand the following essential ideas which have been presented above. It is especially important that you know the precise meanings of all the highlighted terms in the context of this topic.

One mole of a gas occupies a volume of 22.4 L at ***STP*** (standard temperature and pressure, 273K, 1 atm = 103 kPa.)

The above fact allows us to relate the measurable property of the **density of a gas** to its **molar mass**.

The composition of a **mixture of gases** is commonly expressed in terms ***mole fractions***; be sure you know how to calculate them.

Dalton's Law of partial pressures says that every gas in a mixture acts independently, so the total pressure a gas exerts against the walls of a container is just the sum of the partial pressures of the individual components.

Practice Questions:

1. CO_2 is added to a container containing 2.5 atm of O_2 to give total pressure 4.0 atm of the gas. What is the partial pressure of CO_2 in the final mixture?
2. Blast furnaces give off many unpleasant and unhealthy gases. If the total air pressure is 0.99 atm, the partial pressure of carbon dioxide is 0.05 atm, and the partial pressure of hydrogen sulfide is 0.02 atm, what is the partial pressure of the remaining air?
3. Oxygen and chlorine gas are mixed in a container with partial pressures of 401 mmHg and 0.639 atm, respectively. What is the total pressure inside the container (in atm)?

4. If I place 3 moles of N2 and 4 moles of O2 in a 35 L container at a temperature of 250 C, what will the pressure (in atm) of the resulting mixture of gases be?

5. What's the partial pressure of carbon dioxide in a container that holds 5 moles of carbon dioxide, 3 moles of nitrogen, and 1 mole of hydrogen and has a total pressure of 1.05 atm?

6. A container with two gases, helium and argon, is 30.0% by volume helium. Calculate the partial pressure of helium and argon if the total pressure inside the container is 4.00 atm.

7. Two flasks at the same temperature are joined by a glass tube with a stopcock. Flask A is a 4.0 L flask containing N2(g) at 2.0 atm, while flask B is a 10.0 L flask containing CO(g) at 1.4 atm. What is the final pressure in the flasks after the stopcock is opened? Hints: • Determine the final volume for the gases (easy!). • Find the final partial pressure for both N2 and CO individually. (P1V1 = P2V2) • Finally, use Dalton's law to find the total final pressure.

8. Two flasks are connected with a stopcock. The first flask has a volume of 5 liters and contains nitrogen gas at a pressure of 0.75 atm. The second flask has a volume of 8 L and contains oxygen gas at a pressure of 1.25 atm. When the stopcock between the flasks is opened and the gases are free to mix, what will the pressure be in the resulting mixture? 8. Container A (with volume 1.23 L) contains a gas under 3.24 atm of pressure. Container B (with volume 0.93 L) contains a gas under 2.82 atm of pressure. Container C (with volume 1.42 L) contains a gas under 1.21 atm of pressure. If all of these gases are put into Container D (with volume 1.51 L), what is the pressure in Container D?

V. GAS STOICHIOMETRY

Although all gases closely follow the ideal gas law $PV = nRT$ under appropriate conditions, each gas is also a unique chemical substance consisting of molecular units that have definite masses. In this lesson we will see how these molecular masses affect the properties of gases that conform to the ideal gas law.

Following this, we will look at gases that contain more than one kind of molecule— in other words, *mixtures* of gases.

We begin with a review of molar volume and the E.V.E.N. principle, which is central to our understanding of gas mixtures.

In Reactions involving gaseous reactants and products we often report quantities in volumes at specific pressures and temperatures. We can convert this quantities to amounts (in moles) using the ideal gas law. Then we can use the stoichiometric coefficients from the balanced equation to determine the stoichiometric amounts of other reactants and products.

The general form of these types of calculation s is

Volume A → amount of A(in mols) →amount of B(in moles) →molarity of B (in desired units)

In case the reaction is accrued out at STP, we can use the molar volume at STP 22.4 L= 1mol. To convert between volume in liters and amount in moles.

Ideal Gas Law and Reaction Stoichiometry

Question:

In laboratory 25.0 g Barium peroxide, BaO_2 was heated to produce gaseous oxygen. Oxygen gas was collected over water. Reaction produced an unknown gas that was collected at pressure 738 mm of Hg and 23^0C. Vapor pressure of water is 21 torr at 23^0C. How many Liters of oxygen was produced?

Molar mass of BaO_2= 169.3 g/mol

$$2\ BaO_2 \rightarrow 2BaO + 2O_2$$

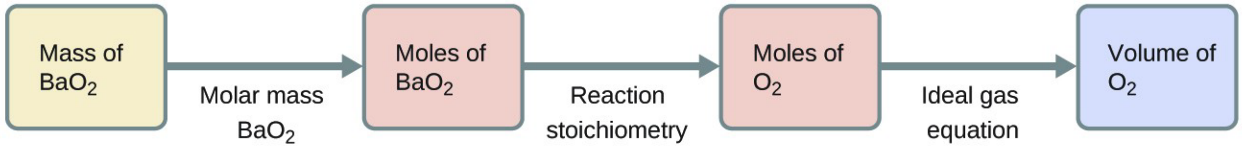


Figure 9.57 gas Stoichiometry

Ref: commons.wikimedia.org/

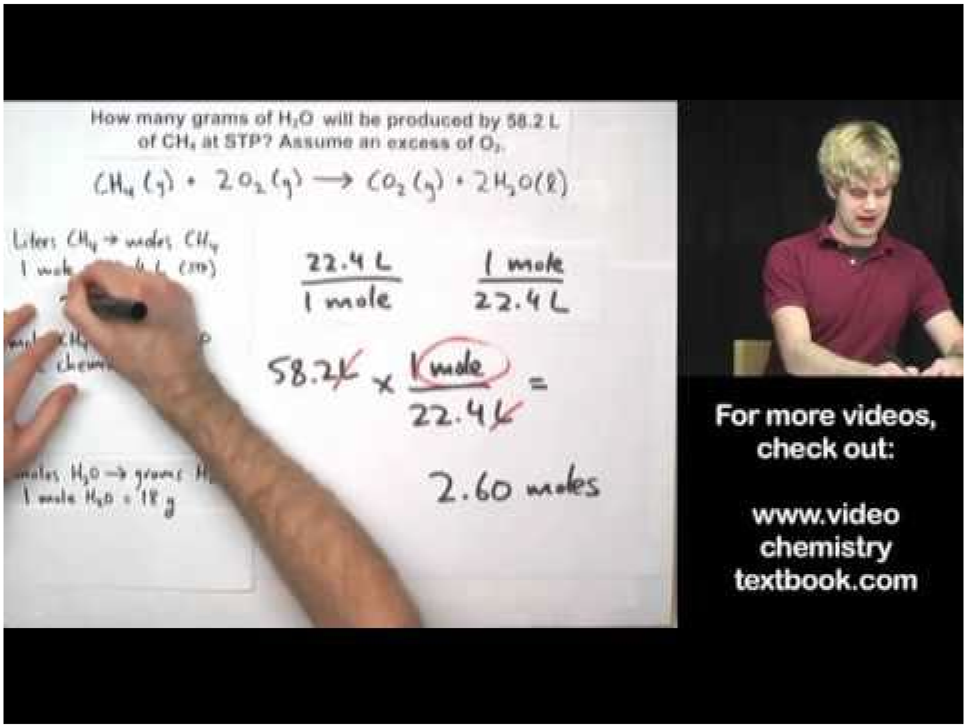
Mols of BaO_2= 25.0g/169.3 g/mol= 0.1477 mol

Mols of O2= 0.1477 mol * $\frac{2 \text{ mols of } O_2}{2 \text{ mols of } BaO_2}$ = 0.1477 mol

Pressure of O_2= 738-21= 717 torr= 717* $\frac{1 \text{ atm}}{760}$ = 0.943 atm

Temperature= 23+273= 296 K

Applying ideal gas law: V= nRT/P= $\frac{0.1477\text{mol} * 0.0821\text{L-atm/mol-K} * 296\text{K}}{0.943 \text{ atm}}$ = 3.81 L



How many grams of H_2O will be produced by 58.2 L of CH_4 at STP? Assume an excess of O_2.

$$CH_4(g) + 2O_2(g) \rightarrow CO_2(g) + 2H_2O(l)$$

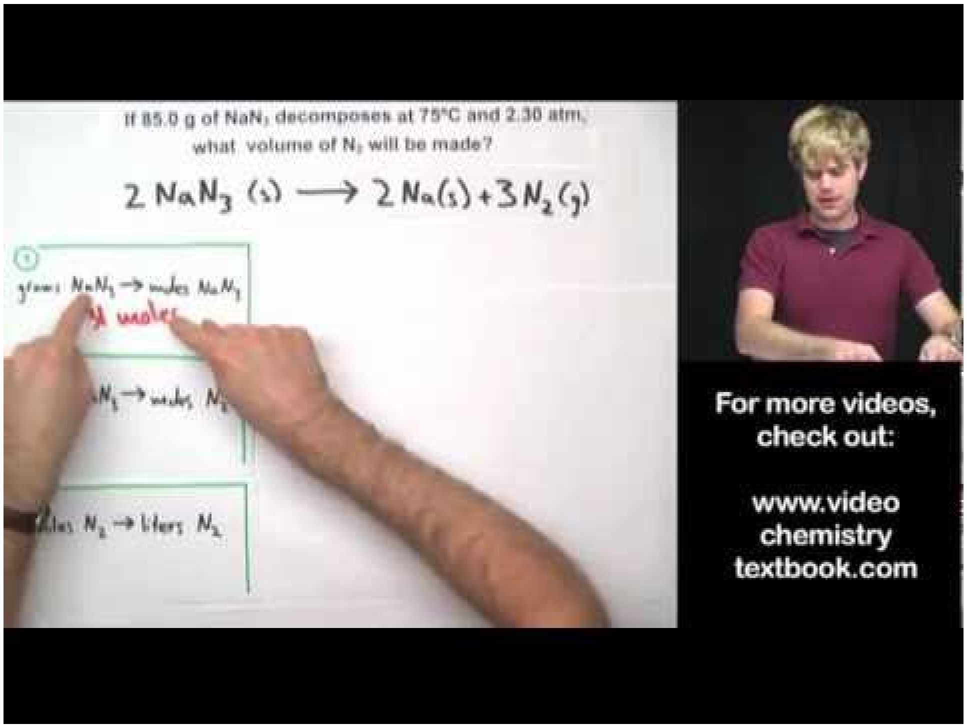
$$\frac{22.4 \text{ L}}{1 \text{ mole}} \qquad \frac{1 \text{ mole}}{22.4 \text{ L}}$$

$$58.2\cancel{L} \times \frac{1 \text{ mole}}{22.4\cancel{L}} =$$

2.60 moles

For more videos, check out:

www.video chemistry textbook.com



Gas Collected Over Water

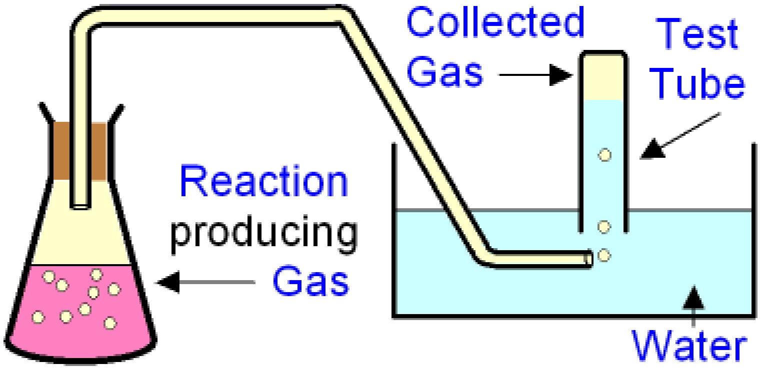


Figure 9.58 Gas collected over water

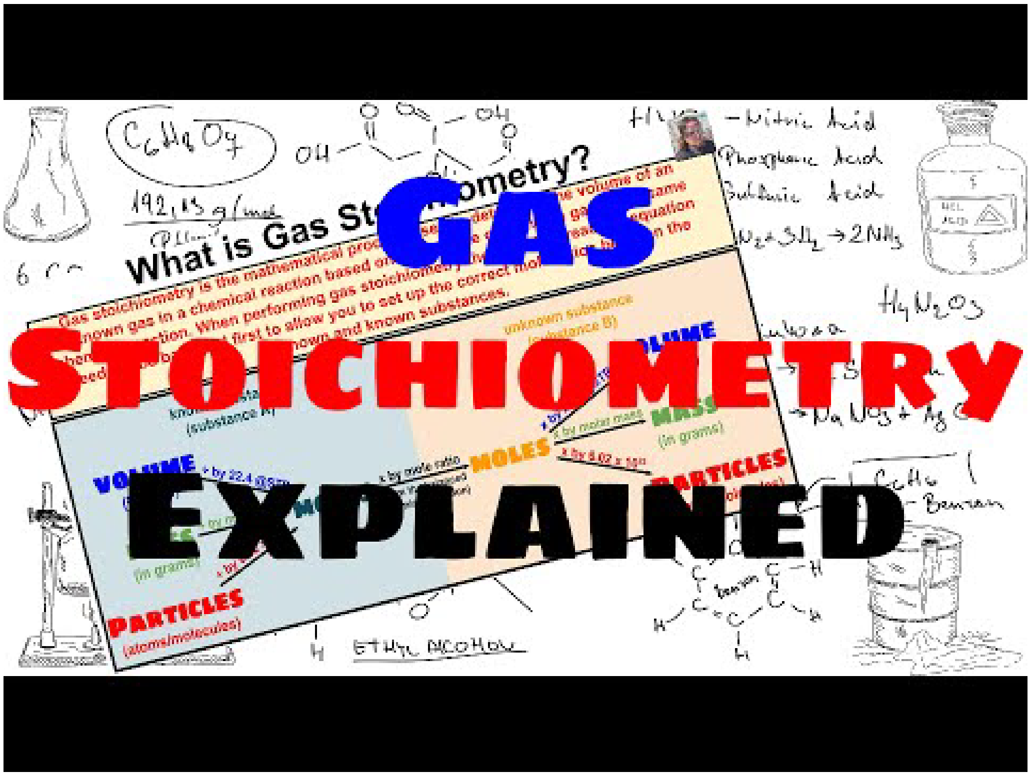
Ref: commons.wikimedia.org/

The law of partial pressure is frequently used to determine the yield of a water-insoluble gas formed in a reaction. The gaseous product bubble through the water and is collected into an inverted container. The water vapor that mixes with the gas contributes a portion of the total pressure, called the vapor pressure, which depends only on the water temperature.

Ptotal- P_{H2O}= Pgas

Apply PV/RT to find the moles

Knowing the molar mass, find the mass of the gas



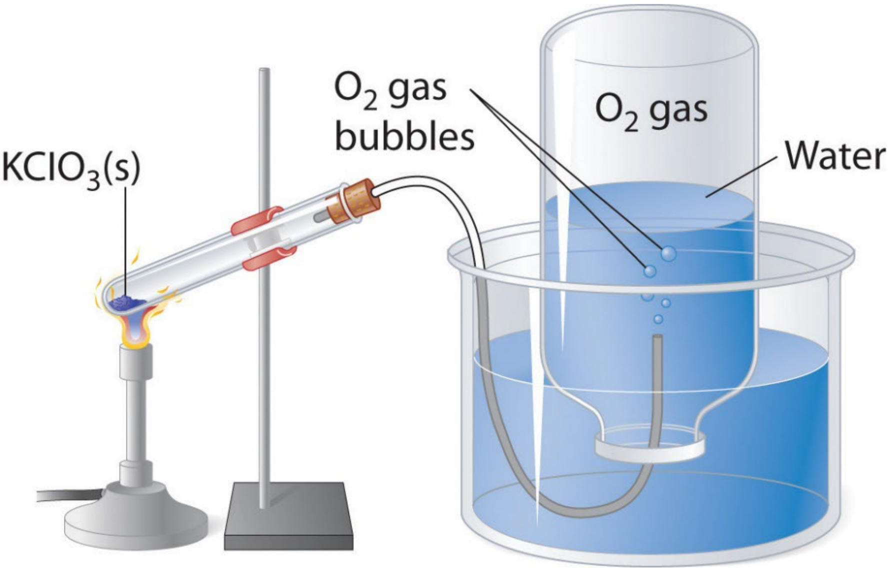


Figure 9.59 An apparatus for collecting Gases by the displacement of water

Ref: commons.wikimedia.org/

When $KClO_3(s)$ is heated, O_2 is produced according to the equation . The oxygen gas travels through the tube, bubbles up through the water, and is collected in a bottle as shown.

The only gases that cannot be collected using this technique are those that readily dissolve in water (e.g., NH_3, H_2S, and CO_2) and those that react rapidly with water (such as F_2 and NO_2). Remember, however, when calculating the amount of gas formed in the reaction, the gas collected inside the bottle is *not* pure. Instead, it is a mixture of the product gas and water vapor. As we know all liquids (including water) have a measurable amount of vapor in equilibrium with the liquid because molecules of the liquid are continuously escaping from the liquid's surface, while other molecules from the vapor phase collide with the surface and return to the liquid. The vapor thus exerts a pressure above the liquid, which is called the liquid's *vapor pressure*. In the case shown above, the bottle is therefore actually filled with a mixture of O_2 and water vapor, and the total pressure is, by Dalton's law of partial pressures, the sum of the pressures of the two components:

If we want to know the pressure of the gas generated in the reaction to calculate the amount of gas formed, we must first subtract the pressure due to water vapor from the total pressure. This is done by referring to tabulated values of the vapor pressure of water as a function of temperature. As shown in figure below, the vapor pressure of water increases rapidly with increasing temperature, and at the normal boiling point (100°C), the vapor pressure is exactly 1 atm. The methodology is illustrated in Example 14.

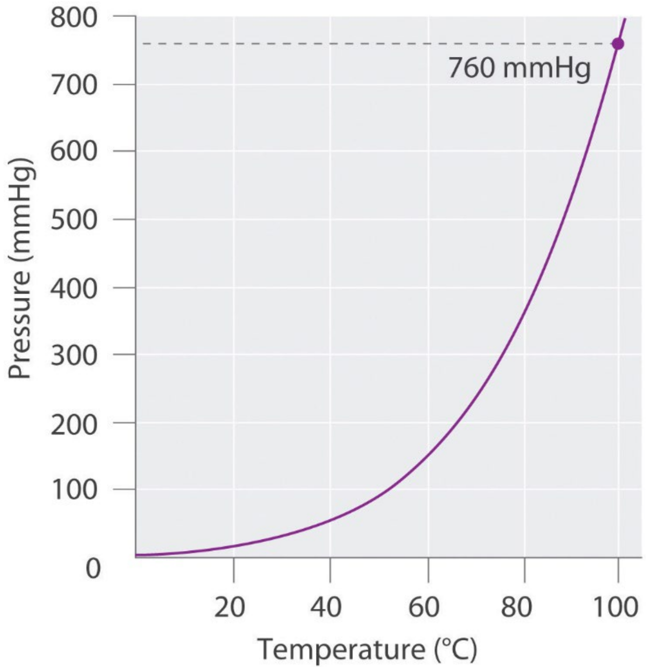
Table 10.4 Vapor Pressure of Water at Various Temperatures

***T* (°C)**	***P* (in mmHg)**	***T***	***P***	***T***	***P***	***T***	***P***
0	4.58	21	18.66	35	42.2	92	567.2
5	6.54	22	19.84	40	55.4	94	611.0
10	9.21	23	21.08	45	71.9	96	657.7
12	10.52	24	22.39	50	92.6	98	707.3
14	11.99	25	23.77	55	118.1	100	760.0
16	13.64	26	25.22	60	149.5	102	815.8
17	14.54	27	26.75	65	187.7	104	875.1

T **(°C)**	***P*** **(in mmHg)**	***T***	***P***	***T***	***P***	***T***	***P***
18	15.48	28	28.37	70	233.8	106	937.8
19	16.48	29	30.06	80	355.3	108	1004.2
20	17.54	30	31.84	90	525.9	110	1074.4

Figure 9.60 A Plot of the Vapor Pressure of Water versus Temperature

Ref: commons.wikimedia.org/



The vapor pressure is very low (but not zero) at 0°C and reaches 1 atm = 760 mmHg at the normal boiling point, 100°C.

Practice Problems

1. What is the density of laughing gas, dinitrogen monoxide, N_2O, at a temperature of 325 K and a pressure of 113.0 kPa?
2. Calculate the density of Freon 12, CF_2Cl_2, at 30.0°C and 0.954 atm.
3. Which is denser at the same temperature and pressure, dry air or air saturated with water vapor? Explain.

4. A cylinder of $O_2(g)$ used in breathing by emphysema patients has a volume of 3.00 L at a pressure of 10.0 atm. If the temperature of the cylinder is 28.0 °C, what mass of oxygen is in the cylinder?
5. What is the molar mass of a gas if 0.0494 g of the gas occupies a volume of 0.100 L at a temperature 26 °C and a pressure of 307 torr?
6. What is the molar mass of a gas if 0.281 g of the gas occupies a volume of 125 mL at a temperature 126 °C and a pressure of 777 torr?
7. How could you show experimentally that the molecular formula of propene is C_3H_6, not CH_2?
8. The density of a certain gaseous fluoride of phosphorus is 3.93 g/L at STP. Calculate the molar mass of this fluoride and determine its molecular formula.
9. Consider this question: What is the molecular formula of a compound that contains 39% C, 45% N, and 16% H if 0.157 g of the compound occupies 125 mL with a pressure of 99.5 kPa at 22 °C?

VI. Kinetic Molecular Theory

The properties such as temperature, pressure, and volume, together with others dependent on them (density, thermal conductivity, etc.) are known as *macroscopic* properties of matter; these are properties that can be observed in bulk matter, without reference to its underlying structure or molecular nature.

By the late 19th century the atomic theory of matter was sufficiently well accepted that scientists began to relate these macroscopic properties to the behavior of the individual molecules, which are described by the *microscopic* properties of matter. The outcome of this effort was the *kinetic* *molecular theory* of gases. This theory applies strictly only to a hypothetical substance known as an *ideal gas*; we will see, however, that under many conditions it describes the behavior of real gases at ordinary temperatures and pressures quite accurately, and serves as the starting point for dealing with more complicated states of matter.

1 The basic ideas of kinetic-molecular theory

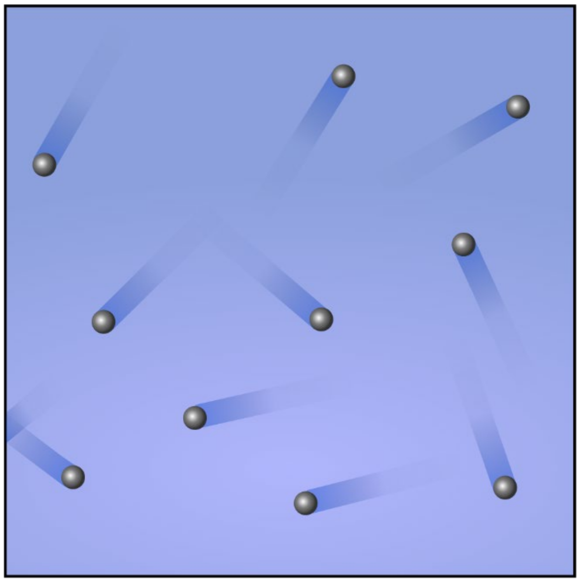
The "kinetic-molecular theory of gases" may sound rather imposing, but it is based on a series of easily-understood assumptions that, taken together, constitute a model that greatly simplifies our understanding of the gaseous state of matter.

The basic tenets of the kinetic-molecular theory are as follows: It is important that you know them!

A) A gas is composed of molecules that are separated by average distances that are much greater than the sizes of the molecules themselves. ***The volume occupied by the molecules of the gas is negligible compared to the volume of the gas itself.***

Figure 9.61 Collection of gas molecules

Ref: commons.wikimedia.org/



B) The molecules of an ideal gas exert **no attractive forces** on each other, or on the walls of the container.

C) The molecules are in **constant random motion**, and as material bodies, they obey Newton's laws of motion. This means that the molecules move in **straight lines** (see demo illustration at the left) until they collide with each other or with the walls of the container.

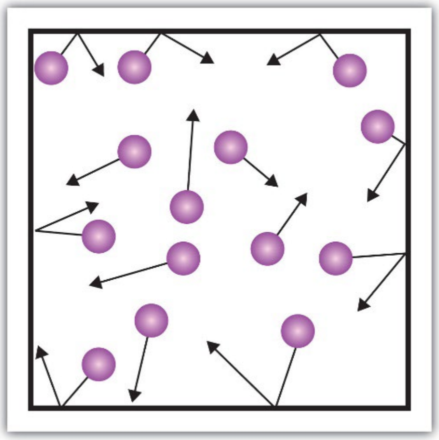
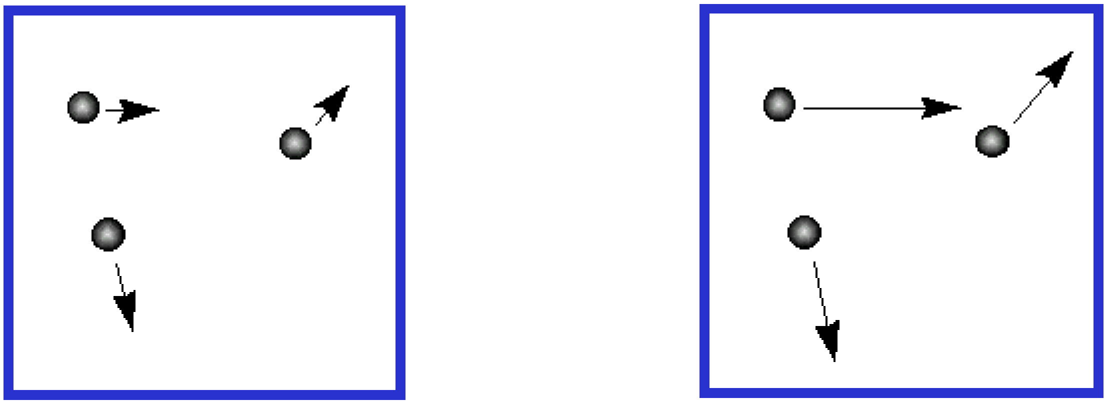


Figure 9.62 Brownian Motion of gas molecules

Ref: commons.wikimedia.org/

D) Collisions are perfectly *elastic*; when two molecules collide, they change their directions and kinetic energies, but the total **kinetic energy is conserved**. *Collisions are not "sticky".*

E) **The average kinetic energy of the gas molecules is directly proportional to the absolute temperature**. (Notice that the term "average" is very important here; the velocities and kinetic energies of individual molecules will span a wide range of values, and some will even have zero velocity at a given instant.) This implies that all molecular motion would cease if the temperature were reduced to absolute zero.



Lower average kinetic energy
Lower absolute temperature

Higher average kinetic energy
Higher absolute temperature

Figure 9.63 Collision of gas molecules

Ref: commons.wikimedia.org/

According to this model, most of the volume occupied by a gas is *empty space*; this is the main feature that distinguishes gases from *condensed* states of matter (liquids and solids) in which neighboring molecules are constantly in contact. Gas molecules are in rapid and continuous motion; at ordinary temperatures and pressures their velocities are of the order of 0.1-1 km/sec and each molecule experiences approximately 10^{10} collisions with other molecules every second.

Here is the particulate view of all states of matter including plasma.

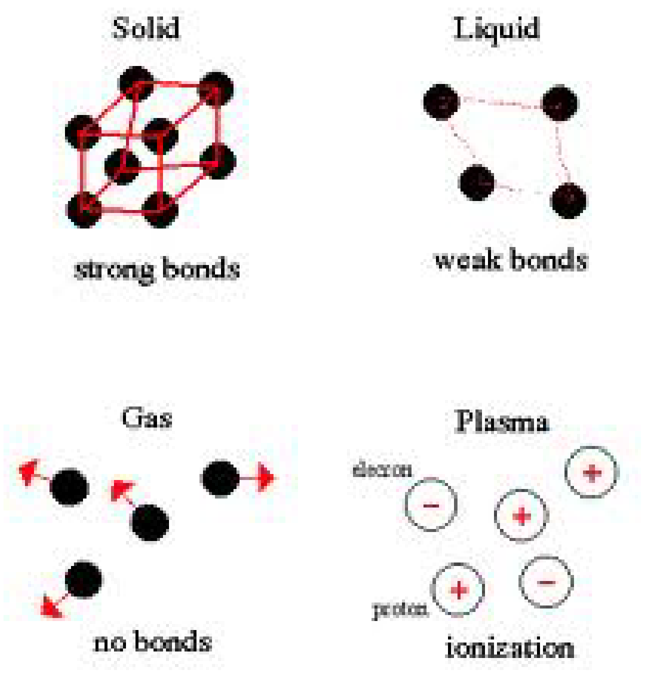


Figure 9.64 state of matter

Ref: commons.wikimedia.org/

2 How kinetic-molecular theory explains the gas laws

If gases do in fact consist of widely-separated particles, then the observable properties of gases must be explainable in terms of the simple mechanics that govern the motions of the individual molecules. This nicely illustrates how a *single theory* (KMT) can explain *all* of the laws of gas behavior.

Kinetic interpretation of gas pressure

The kinetic molecular theory makes it easy to see why a gas should exert a pressure on the walls of a container. Any surface in contact with the gas is constantly bombarded by the molecules. At each collision, a molecule moving with momentum mv strikes the surface. Since the collisions are elastic, the molecule bounces back with the same velocity in the opposite direction. This change in velocity ΔV is equivalent to an *acceleration* a; according to Newton's second law, a *force* $f = ma$ is thus exerted on the surface of area A exerting a pressure $P = f/A$.

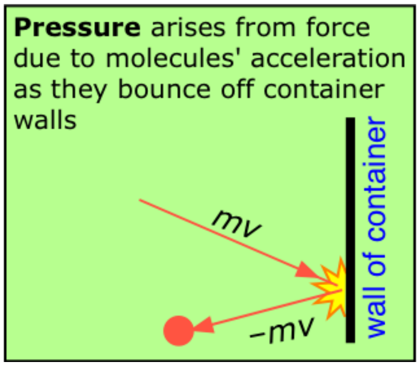


Figure 9.65 Gas Pressure

Kinetic interpretation of gas temperature

According to the kinetic molecular theory, the average kinetic energy of an ideal gas is directly proportional to the absolute temperature. Kinetic energy is the energy a body has by virtue of its motion:

$$\mathrm{ke} = \frac{mv^2}{2}$$

As the temperature of a gas rises, the average velocity of the molecules will increase; a doubling of the temperature will increase this velocity by a factor of four. Collisions with the walls of the container will transfer more momentum, and thus more kinetic energy, to the walls. If the walls are cooler than the gas, they will get warmer, returning less kinetic energy to the gas, and causing it to cool until thermal equilibrium is reached. Because temperature depends on the *average* kinetic energy, the concept of temperature only applies to a statistically meaningful sample of molecules. We will have more to say about molecular velocities and kinetic energies farther on.

Kinetic explanation of Boyle's law

Boyle's law is easily explained by the kinetic molecular theory. The pressure of a gas depends on the number of times per second that the molecules strike the surface of the container. If we compress the gas to a smaller volume, the same number of molecules are now acting against a smaller surface area, so the number striking per unit of area, and thus the pressure, is now greater.

Kinetic explanation of Charles' law

Kinetic molecular theory states that an increase in temperature raises the average kinetic energy of the molecules. If the molecules are moving more rapidly but the pressure remains the same, then the molecules must stay farther apart, so that the increase in the rate at which molecules collide with the surface of the container is compensated for by a corresponding increase in the area of this surface as the gas expands.

Kinetic explanation of Avogadro's law

If we increase the number of gas molecules in a closed container, more of them will collide with the walls per unit time. If the pressure is to remain constant, the volume must increase in proportion, so that the molecules strike the walls less frequently, and over a larger surface area.

Kinetic explanation of Dalton's law

"Every gas is a vacuum to every other gas". This is the way Dalton stated what we now know as his law of partial pressures. It simply means that each gas present in a mixture of gases acts independently of the others. This makes sense because of one of the fundamental tenets of KMT theory that gas molecules have negligible volumes. So Gas A in mixture of A and B acts as if Gas B were not there at all. Each contributes its own pressure to the total pressure within the container, in proportion to the fraction of the molecules it represents.

3 Some important practical applications of KMT

The molecules of a gas are in a state of perpetual motion in which the velocity (that is, the speed and direction) of each molecule is completely random and independent of that of the other molecules. This fundamental assumption of the kinetic-molecular model helps us understand a wide range of commonly-observed phenomena.

Diffusion & Effusion

The process by which gas molecules spread out in response to a concentration gradient is diffusion. Heavier molecules diffuse slowly than lighter molecules.

The process by which a gas escapes from its container through a tiny hole into an evacuated space. In 1846 Thomas Graham examined this process and concluded that the effusion rate is the number of moles (or molecules) of gas effusing per unit time. Since density is directly proportional to molar mass, we state Graham’s law of effusion:

Figure 9.66 Scientist Graham

Ref: commons.wikimedia.org/

Ref: commons.wikimedia.org/

Diffusion: random motion with direction

Diffusion refers to the transport of matter through a ***concentration gradient***; the rule is that substances move (or tend to move) from regions of higher concentration to those of lower concentration. The diffusion of tea out of a teabag into water, or of perfume from a person, are common examples; we would not expect to see either process happening in reverse!

Figure 9.67 Diffusion of Gas

https://www.flickr.com/photos/goalfinder/6968888253

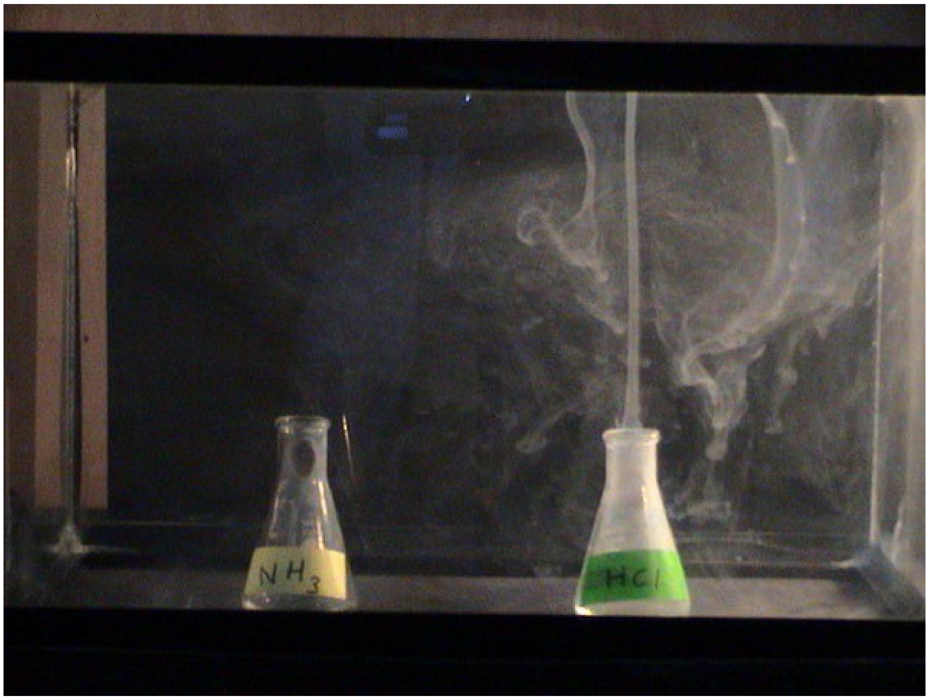


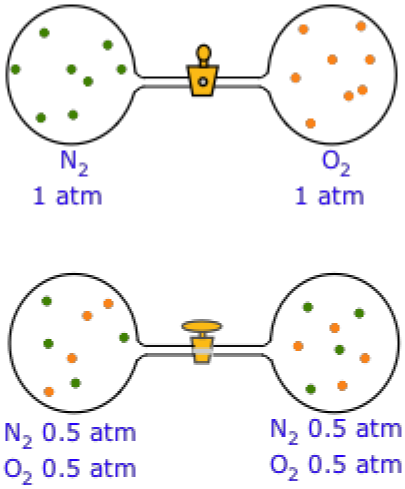
Figure 9.68 Diffusion of Gas

https://www.quora.com/What-chemical-equations-is-the-formation-reaction-of-NH4Cl-s

The white "smoke" consists of tiny particles of solid ammonium chloride, formed when hydrogen chloride and ammonia gas diffuse into the air from their concentrated aqueous solutions in the reagent bottles.

$HCl + NH_3 \rightarrow NH_4Cl(s)$

Figure 9.69 Diffusion of Gases



When the stopcock is opened, random motions cause each gas to diffuse into the other container.

After diffusion is complete (bottom), individual molecules of both kinds continue to pass between the flasks in both directions.

It might at first seem strange that the *random* motions of molecules can lead to a completely predictable (i.e., non-random) drift in their ultimate distribution. The key to this apparent paradox is the distinction between an *individual* and the *population*. Although we can say nothing about the fate of an individual molecule, the behavior of a large collection ("population") of molecules is subject to the laws of statistics. This is exactly analogous to the manner in which insurance actuarial tables can accurately predict the average longevity of people at a given age, but provide no information on the fate of any single person.

Understanding effusion and Graham's law

If a tiny hole is made in the wall of a vessel containing a gas, then the rate at which gas molecules leak out of the container will be proportional to the number of molecules that collide with unit area of the wall per second, and thus with the rms-average velocity of the gas molecules. This process, when carried out under idealized conditions, is known as ***effusion***.

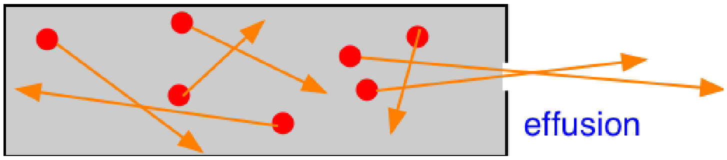


Figure 9.70 Effusion of Gas

Around 1830, the English chemist Thomas Graham (1805-1869) discovered that the relative rates at which two different gases, at the same temperature and pressure, will effuse through identical openings is inversely proportional to the square root of its molar mass.

$$v \propto \frac{1}{\sqrt{M}}$$

Graham's law, as this relation is known, is a simple consequence of the square-root relation between the velocity of a body and its kinetic energy.

According to the kinetic molecular theory, the molecules of two gases at the same temperature will possess the same average kinetic energy. If v_1 and v_2 are the average velocities of the two kinds of molecules, then at any given temperature $ke_1 = ke_2$ and

$$\frac{m_1 v_1^2}{2} = \frac{m_2 v_2^2}{2}$$

or, in terms of molar masses M,

$$\frac{v_1}{v_2} = \sqrt{\frac{M_2}{M_1}}$$

Thus the average velocity of the lighter molecules must be greater than those of the heavier molecules, and the ratio of these velocities will be given by the inverse ratio of square roots of the molecular weights.

Although Graham's law applies exactly only when a gas diffuses into a vacuum, the law gives useful estimates of relative diffusion rates under more practical conditions, and it provides insight into a wide range of phenomena that depend on the relative average velocities of molecules of different masses.

The effusion of a gas is inversely proportional to the square of its molar mass. Graham’s law can be used to determine the molar mass of an unknown gas.

$$\frac{R_1}{R_2} = \sqrt{\frac{M_2}{M_1}}$$

Because of the presence of many other gas molecules, diffusion rates are much lower than effusion rate.

Diffusion can also occur in liquids. However, liquid molecules are very close to each other and attractive force is stronger, therefore collisions are more frequent. Diffusion is much slower in liquid than diffusion in gases.

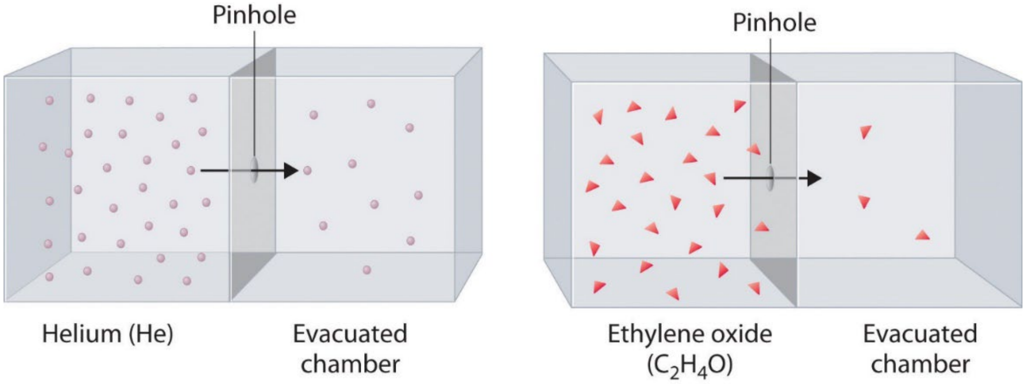


Figure 9.71 Effusion of Gases

Ref: commons.wikimedia.org/

The kinetic molecular theory explains that at a given temperature and pressure, the gas with the lower molar mass effuse faster because the most probable speed of its molecules is higher, therefore more molecules escape per unit time.

Problem Example

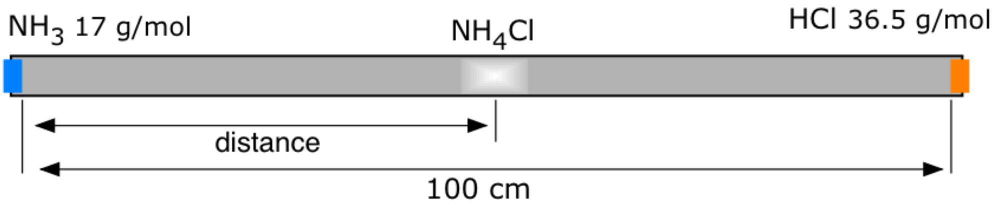


Figure 9.72 Effusion of Gases

Ref: commons.wikimedia.org/

The glass tube shown above has cotton plugs inserted at either end. The plug on the left is moistened with a few drops of aqueous ammonia, from which NH_3 gas slowly escapes. The plug on the right is similarly moisted with a strong solution of hydrochloric acid, from which gaseous HCl escapes. The gases diffuse in opposite directions within the tube; at the point where they meet, they combine to form solid ammonium chloride, which appears first as a white fog and then begins to coat the inside of the tube.

$NH_3(g) + HCl(g) \rightarrow NH_4Cl(s)$

a) In what part of the tube (left, right, center) will the NH_4Cl first be observed?

b) If the distance between the two ends of the tube is 100 cm, how many cm from the left end of the tube will the NH_4Cl first form?

Solution:

a) The lighter ammonia molecules will diffuse more rapidly, so the point where the two gases meet will be somewhere in the right half of the tube.

b) The ratio of the diffusion velocities of ammonia (v_1)and hydrogen chloride (v_2) can be estimated from Graham's law:

$$\frac{v_1}{v_2} = \frac{\sqrt{36.5}}{\sqrt{17}} = 1.46$$

We can therefore assign relative velocities of the two gases as $v_1 = 1.46$ and $v_2 = 1$. Clearly, the meeting point will be directly proportional to v_1. It will, in fact, be proportional to the ratio $v_1/(v_1+v_2)$*:

$$\frac{v_1}{v_1 + v_2} \times 100\text{cm} = \frac{1.46}{1.46 + 1.00} \times 100\text{cm} = 59 \text{ cm}$$

*In order to see how this ratio was deduced, consider what would happen in the three special cases in which v_1=0, v_2=0, and v_1=v_2, for which the distances (from the left end) would be 0, 50, and 100 cm, respectively. It should be clear that the simpler ratio v_1/v_2 would lead to absurd results.

Note that the above calculation is only an estimate. Graham's law is strictly valid only under special conditions, the most important one being that no other gases are present. Contrary to what is written in some textbooks and is often taught, Graham's law does not accurately predict the relative rates of escape of the different components of a gaseous mixture into the outside air, nor does it give the rates at which two gases will diffuse through another gas such as air.
See *Misuse of Graham's Laws* by Stephen J. Hawkes, *J. Chem. Education* 1993 70(10) 836-837

Here is the video on Graham’s law experiment:

Practice problem:

1. A mixture of He and CH_4 are placed in an effusion apparatus. Calculate the ratio of their effusion rates.

2. If it takes 1.25 min for 0.010 mol of He to effuse, how long will it take for the same amount of ethane CH_4 to effuse?

Ans: 1. 2:1

2. 2.50 min

SUPPLEMENTAL

****
*

RESEARCH BASED INFORMATION

***Uranium enrichment

One application of this principle that was originally suggested by Graham himself but was not realized on a practical basis until a century later is the separation of isotopes. The most important example is the enrichment of uranium

Figure 9.73 K-25 diffusion process Building

https://www.energy.gov/management/k-25-gaseous-diffusion-process-building

The K-25 Gaseous Diffusion Plant was one of the major sources of enriched uranium during World War II. It was completed in 1945 and employed 12,000 workers. Owing to the secrecy of the Manhatten Project, the women who operated the system were unaware of the purpose of the plant; they were trained to simply watch the gauges and turn the dials for what they were told was a "government project".

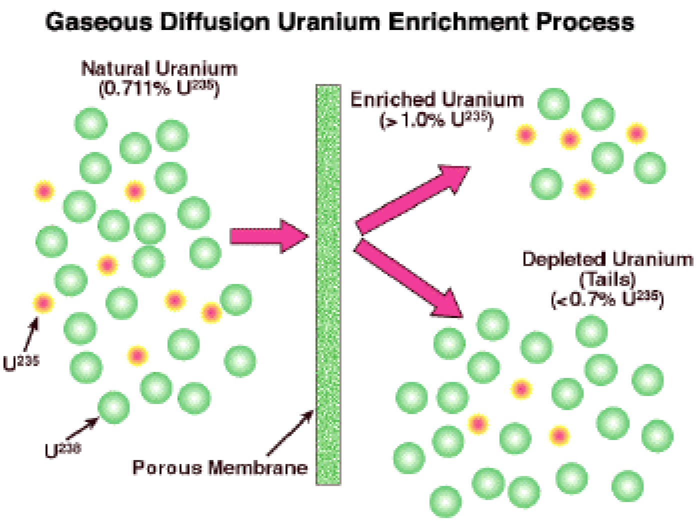


Figure 9.74 effusion of gases

Uranium consists mostly of U^{238}, with only 0.7% of the fissionable isotope U^{235}. Uranium is of course a metal, but it reacts with fluorine to form a gaseous hexafluoride, UF_6. In the very successful *gaseous diffusion process* the UF_6 diffuses repeatedly through a porous wall. Each time, the lighter isotope passes through a bit more rapidly then the heavier one, yielding a mixture that is minutely richer in U^{235}. The process must be ovr a thousand times to achieve the desired degree of enrichment. The development of a large-scale gaseous diffusion plant was a key part of the U.S. development of the first atomic bomb in 1945. This process is now obsolete, having been raplaced by other methods.

Density fluctuations: Why is the sky blue?

Diffusion ensures that molecules will quickly distribute themselves throughout the volume occupied by the gas in a thoroughly uniform manner. The chances are virtually zero that sufficiently more molecules might momentarily find themselves near one side of a container than the other to result in an observable temporary density or pressure difference. This is a result of simple statistics. But statistical predictions are only valid when the sample population is large.


quite likely

not very likely!

Figure 9.75 effusion of Gases

Consider what would happen if we consider extremely small volumes of space: cubes that are about 10^{-7} cm on each side, for example. Such a cell would contain only a few molecules, and at any one instant we would expect to find some containing more or less than others, although in time they would average out to the same value. The effect of this statistical behavior is to give rise to random fluctuations in the density of a gas over distances comparable to the dimensions of visible light waves. When light passes through a medium whose density is non-uniform, some of the light is *scattered*. The kind of scattering due to random density fluctuations is called *Rayleigh scattering*, and it has the property of affecting (scattering) shorter wavelengths more effectively than longer wavelengths. The clear sky appears blue in color because the blue (shorter wavelength) component of sunlight is scattered more. The longer wavelengths remain in the path of the sunlight, available to delight us at sunrise or sunset.

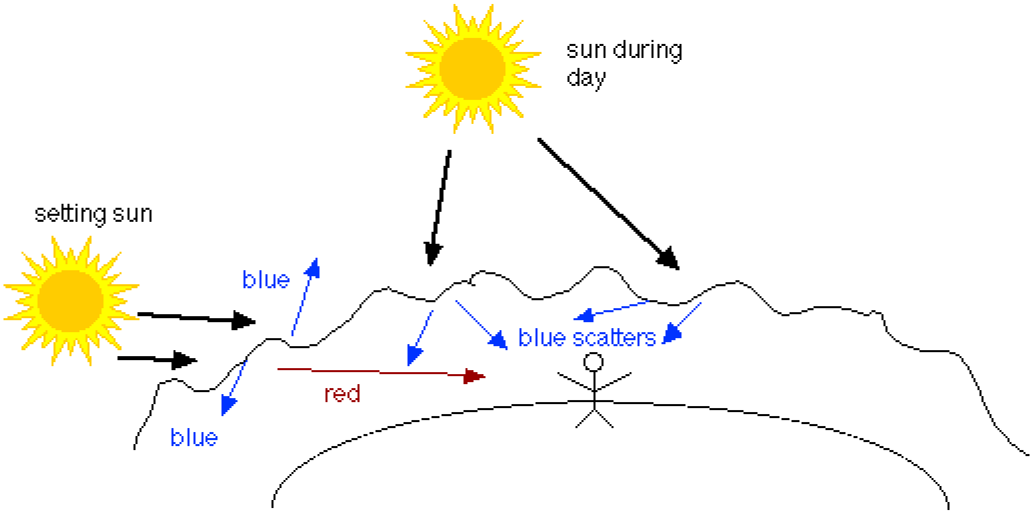
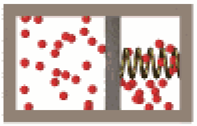


Figure 9.76 scattering of Gases

[source]



What we have been discussing is a form of what is known as *fluctuation phenomena*. As the animation shows, the random fluctuations in pressure of a gas on either side do not always completely cancel when the density of molecules (i.e., *pressures*) are quite small. See here for a more detailed discussion.span.

How Incandescent light bulbs work

Figure 9.77 Incandescent Light

https://pxhere.com/en/photo/964215

An interesting application involving several aspects of the kinetic molecular behavior of gases is the use of a gas, usually argon, to extend the lifetime of incandescent lamp bulbs. As a light bulb is used, tungsten atoms evaporate from the filament and condense on the cooler inner wall of the bulb, blackening it and reducing light output. As the filament gets thinner in certain spots, the increased electrical resistance results in a higher local power dissipation, more rapid evaporation, and eventually the filament breaks.

[Jeff Wall, Tate Museum]

The pressure inside a lamp bulb must be sufficiently low for the *mean free path* of the gas molecules to be fairly long; otherwise heat would be conducted from the filament too rapidly, and the bulb would melt. (Thermal conduction depends on intermolecular collisions, and a longer mean free path means a lower collision frequency). A complete vacuum would minimize heat conduction, but this would result in such a long mean free path that the tungsten atoms would rapidly migrate to the walls, resulting in a very short filament life and extensive bulb blackening.

Figure 9.78 Bulb Filament

Figure 9.79 Irvine Langmuir

Around 1910, the General Electric Company hired Irving Langmuir as one of the first chemists to be employed as an industrial scientist in North America. Langmuir quickly saw that bulb blackening was a consequence of the long mean free path of vaporized tungsten atoms, and he showed that the addition of a small amount of argon will reduce the mean free path, increasing the probability that an outward-moving tungsten atom will collide with an argon atom. A certain proportion of these will eventually find their way back to the filament, partially reconstituting it.

Krypton would be a better choice of gas than argon, since its greater mass would be more effective in changing the direction of the rather heavy tungsten atom. Unfortunately, krypton, being a rarer gas, is around 50 times as expensive as argon, so it is used only in “premium” light bulbs. The more recently-developed *halogen-cycle lamp* is an interesting chemistry-based method of prolonging the life of a tungsten-filament lamp.

Some interesting light-bulb links:

The Great Internet Light Bulb Book (all about incandescent lamps)

Langmuir and the gas-filled incandescent lamp

History of the halogen cycle lamp

Viscosity of gases

Gases, like all fluids, exhibit a resistance to flow, a property known as ***viscosity***. The basic cause of viscosity is the random nature of thermally-induced molecular motion. In order to force a fluid through a pipe or tube, an additional non-random translational motion must be superimposed on the thermal motion.

There is a slight problem, however. Molecules flowing near the center of the pipe collide mostly with molecules moving in the same direction at about the same velocity, but those that happen to find themselves near the wall will experience frequent collisions with the wall. Since the molecules in the wall of the pipe are not moving in the direction of the flow, they will tend to absorb more kinetic energy than they return, with the result that the gas molecules closest to the wall of the pipe lose some of their forward momentum. Their random thermal motion will eventually take them deeper into the stream, where they will collide with other flowing molecules and slow them down. This gives rise to a resistance to flow known as ***viscosity***; this is the reason why long gas transmission pipelines need to have pumping stations every 100 km or so.

Origin of gas viscosity. The illustration shows the boundary region where random movements of molecules in directions other than the one of the flow (**1**) move toward the confining surface and temporarily adsorb to it (**2**). After a short time, thermal energy causes the molecule to be released (**4**) with most of its velocity not in the flow direction. A rapidly-flowing molecule (**3**) collides with it (**5**) and loses some of its flow velocity.

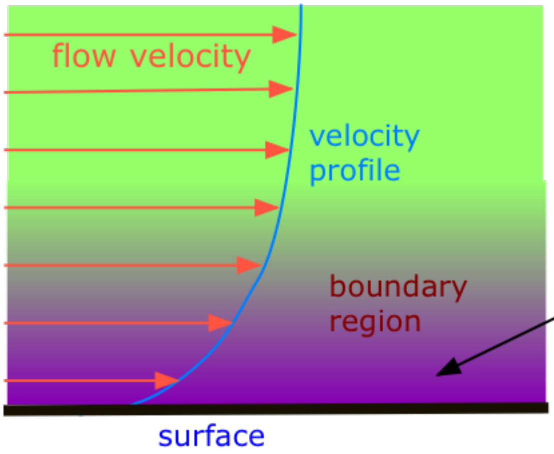


Figure 9.80 Origin of Gas viscosity

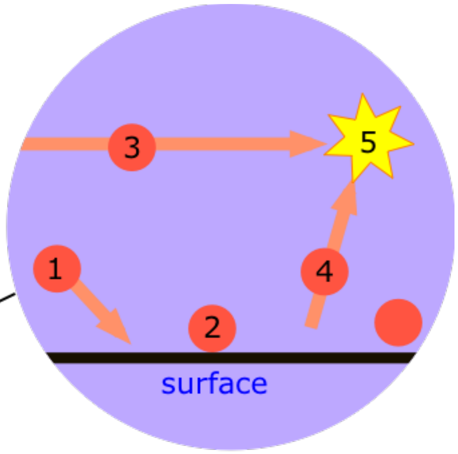


Figure 9.81 Gas Viscosity

As you know, liquids such as syrup or honey exhibit smaller viscosities at higher temperatures as the increased thermal energy reduces the influence of intermolecular attractions, thus allowing the molecules to slip around each other more easily. Gases, however, behave in just the opposite way; gas viscosity arises from collisiion-induced transfer of momentum from rapidly-moving molecules to slow ones that have been released from the boundary layer. The higher the temperature, the more rapidly the molecules move and collide with each other, so the higher the viscosity.

An important practical consequence of this is the need, in the long-distance natural gas pipeline industry, to place pumping stations at intervals along pipelines.

Distribution of gas molecules in a gravitational field

Everyone knows that the air pressure decreases with altitude. This effect is easily understood qualitatively through the kinetic molecular theory.

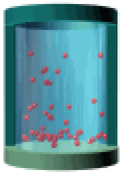


Figure 9.82 Natural gas Pipeline

Random thermal motion tends to move gas molecules in all directions equally. In the presence of a gravitational field, however, motions in a downward direction are slightly favored. This causes the concentration, and thus the pressure of a gas to be greater at lower elevations and to decrease without limit at higher elevations.

The pressure at any elevation in a vertical column of a fluid is due to the weight of the fluid above it. This causes the pressure to decrease exponentially with height.

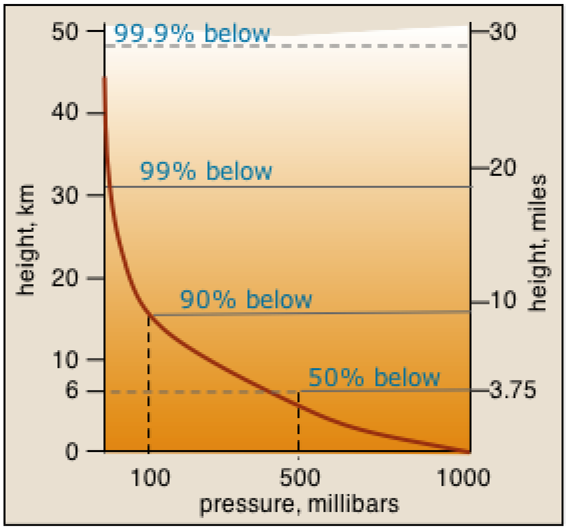


Figure 9.83 Fluid column vs. altitude

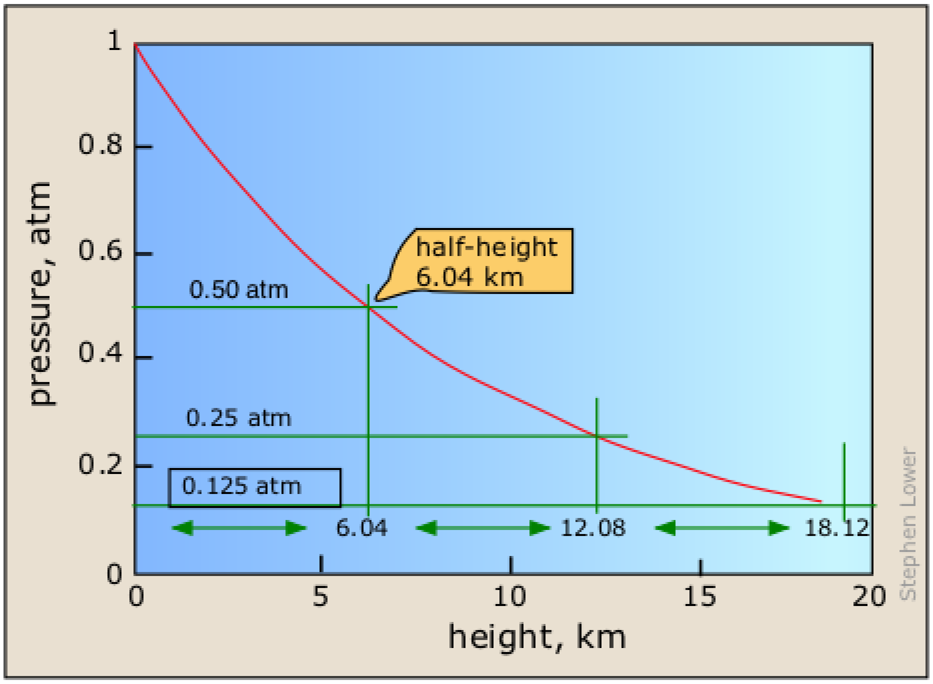


Figure 9.84 Fluid column vs. height

This plot shows how the pressure of air at 25° C decreases with altitude.

Note the constant increment of altitude (6.04 km, the "half height") required to reduce the pressure by half its value. This reflects the special property of an exponential function $a = e^y$, namely that the derivitave da/dy is just e^y itself.

The exact functional relationship between pressure and altitude is known as the ***barometric distribution law***. It is easily derived using first-year calculus. For air at 25°C the pressure P_h at any altitude is given by $P_h = P_o e^{-.11h}$ in which P_o is the pressure at sea level.

This is a form of the very common *exponential decay law* which we will encounter in several different contexts in this course. An exponential decay (or growth) law describes any quantity whose rate of change is directly proportional to its current value, such as the amount of money in a compound-interest savings account or the density of a column of gas at any altitude. The most important feature of any quantity described by this law is that the fractional rate of change of the quantity in question (in this case, $\Delta P/P$ or in calculus, dP/P) is a constant. This means that the increase in altitude required to reduce the pressure by half is also a constant, about 6 km in the Earth's case.

Because heavier molecules will be more strongly affected by gravity, their concentrations will fall off more rapidly with elevation. For this reason the partial pressures of the various components of the atmosphere will tend to vary with altitude. The difference in pressure is also affected by the temperature; at higher temperatures there is more thermal motion, and hence a less rapid fall-off of pressure with altitude. Owing to atmospheric convection and turbulence, these effects are not observed in the lower part of the atmosphere, but in the uppermost parts of the atmosphere the heavier molecules do tend to drift downward.

The ionosphere and radio communication

At very low pressures, mean free paths are sufficiently great that collisions between molecules become rather infrequent. Under these conditions, highly reactive species such as ions, atoms, and molecular fragments that would ordinarily be destroyed on every collision can persist for appreciable periods of time.

The most important example of this occurs at the top of the Earth's atmosphere, at an altitude of 200 km, where the pressure is about 10^{-7} atm. Here the mean free path will be 10^7 times its value at 1 atm, or about 1 m. In this part of the atmosphere, known as the *thermosphere*, the chemistry is dominated by species such as O, O_2^+ and HO which are formed by the action of intense solar ultraviolet light on the normal atmospheric gases near the top of the stratosphere. The high concentrations of electrically charged species in these regions (sometimes also called the *ionosphere*) reflect radio waves and are responsible for around-the-world transmission of mid-frequency radio signals.

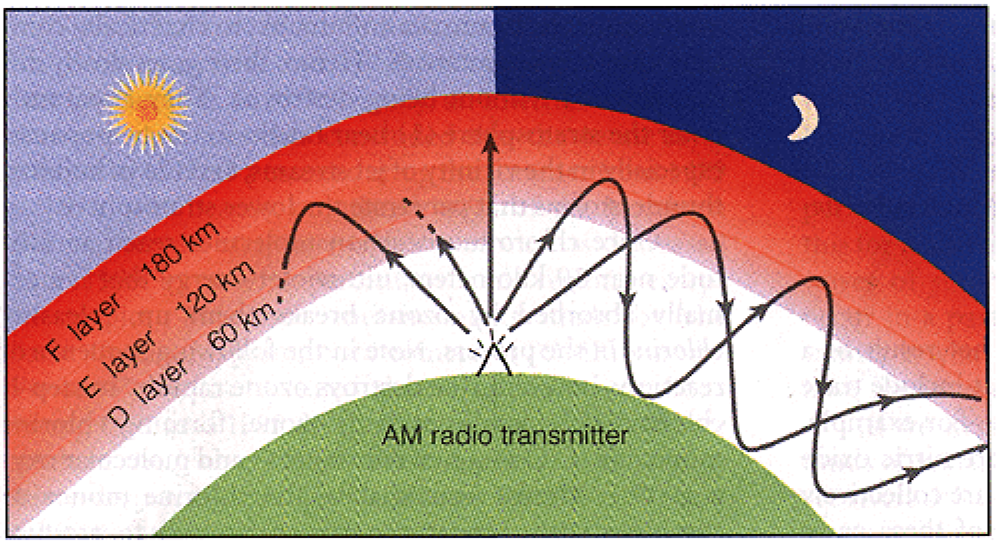


Figure 9.85 Ionosphere & radio communication

https://apollo.nvu.vsc.edu/classes/met130/notes/chapter1/ion2.html

The ion density in the lower part of the ionosphere (about 80 km altitude) is so great that the radiation from broadcast-band radio stations is absorbed in this region before these waves can reach the reflective high-altitude layers. However, the pressure in this region (known as the *D-layer*) is great enough that the ions recombine soon after local sunset, causing the D-layer to disappear and allowing the waves to reflect off of the upper (F-layer) part of the ionosphere. This is the reason that distant broadcast stations can only be heard at night.

References and simulations

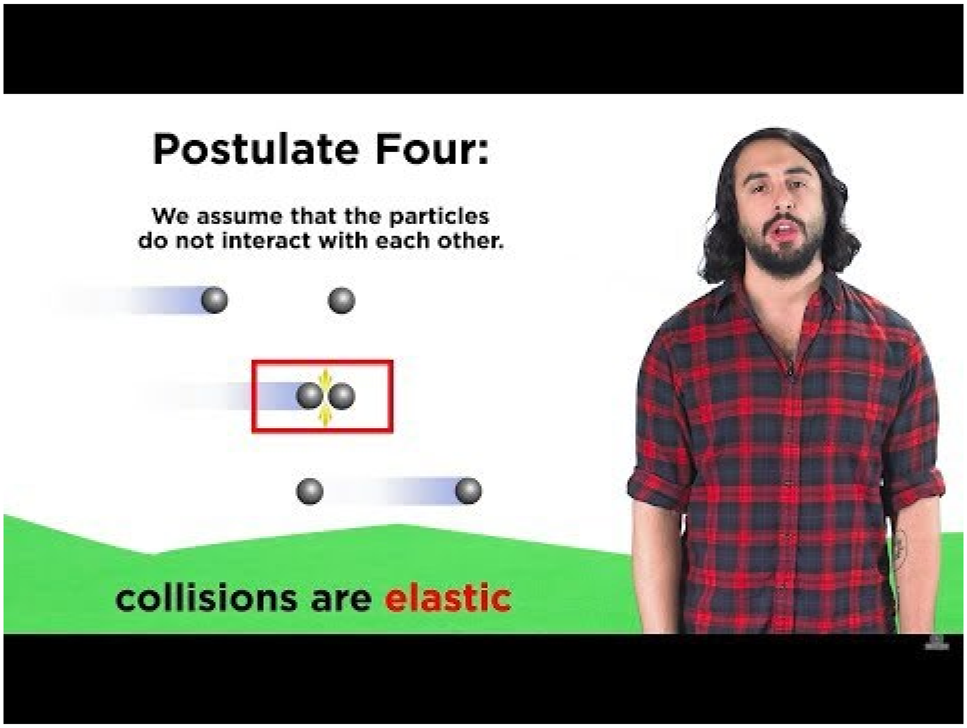
One excellent gas simulations you can play with:

This online program (a Java applet) allows you to explore the effects of changing the number of molecules, the temperature, and the gravitational field. An especially nice feature shows fluctuations in the distribution of molecular velocities.

This video may help to get a overview of the properties of gases.

****

https://www.youtube.com/watch?v=o3f_VJ87Df0

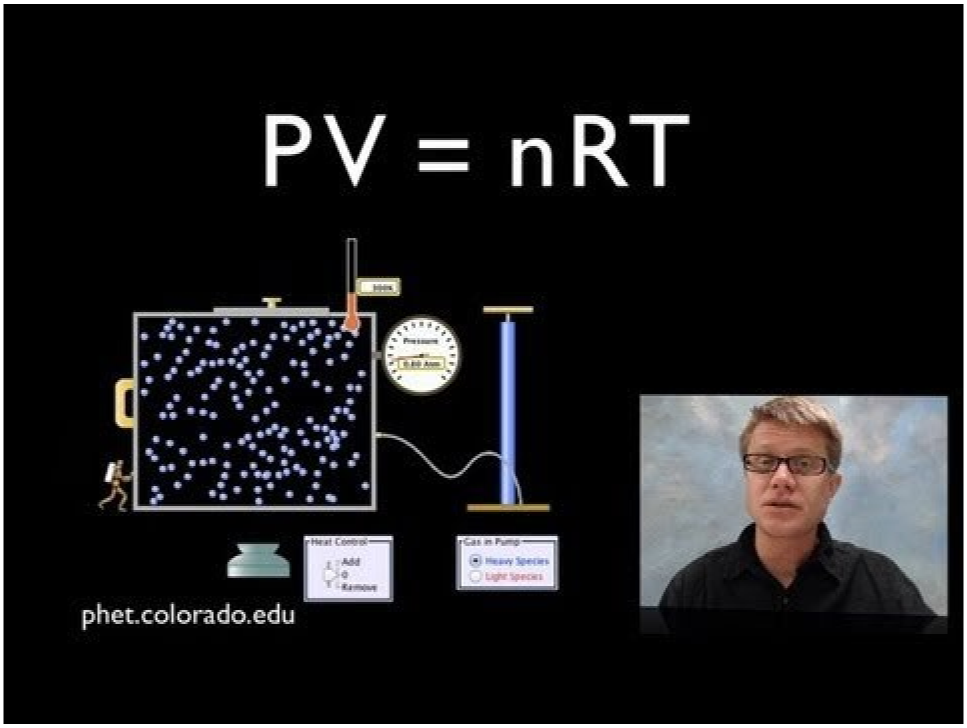


Postulate Four:

We assume that the particles do not interact with each other.

collisions are elastic

https://www.youtube.com/watch?v=gmN2fRlQFp4



$$PV = nRT$$

phet.colorado.edu

All the gas laws Boyles's law, Charles's law, Dalton's law of partial pressure can be explained in terms of kinetic molecular theory. The most important relation is the the relationship between kinetic energy and temperature:

The kinetic energy of an object is the energy associated with its motion. It is related to object's mass and speed according to the formula:

This equation shows that a heavy object and a light object have the same kinetic energy, heavy object must be moving more slowly. Different gases at the same temperature have same kinetic energy. For this to be true, molecules with higher mass have lower speed.

We can use the kinetic molecular theory to derive the expression for Root Mean Square Velocity (rms) for the gas particles. This velocity of any gas particle is inversely proportional to the molar mass of the gas. Therefore, at particular temp, smaller the gas particles, higher the speed.

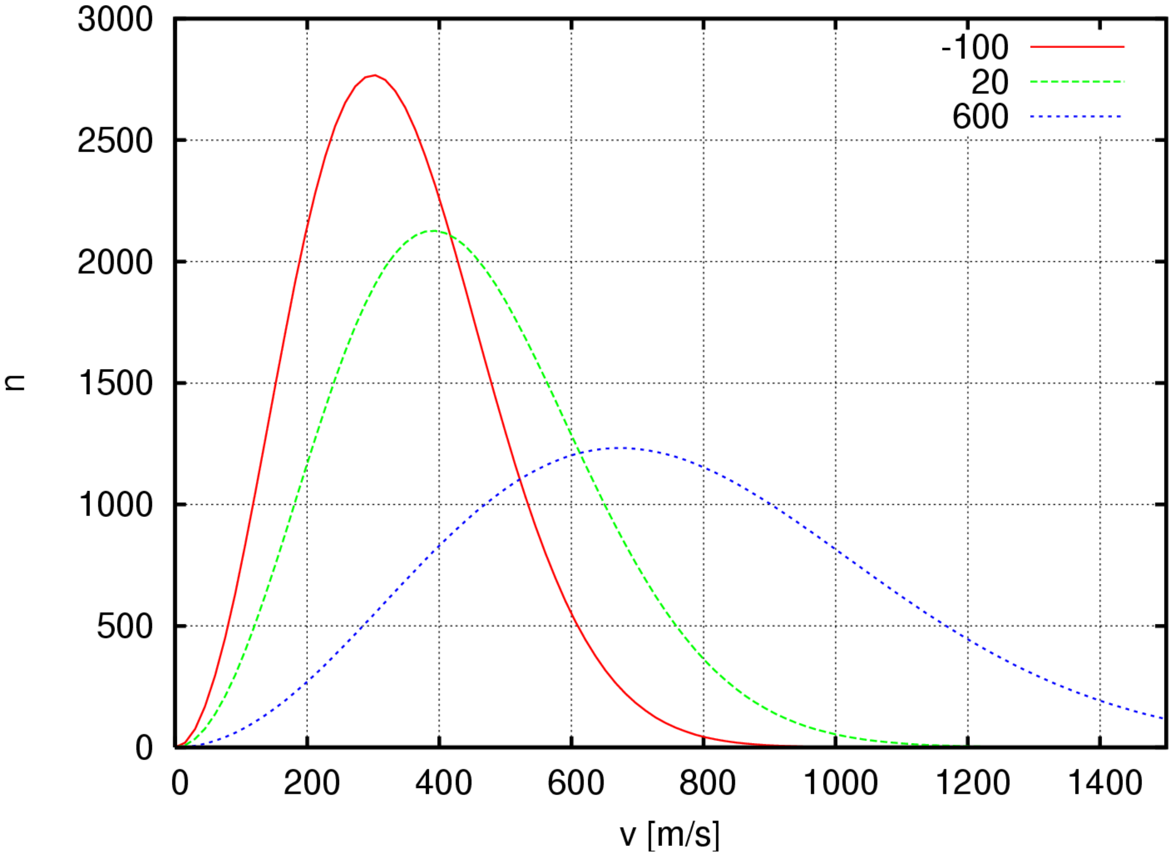


Figure 9.86 Energy Distribution with Temperature

Ref: commons.wikimedia.org/

$$u = \sqrt{\frac{3RT}{M}}$$

Distribution of Molecular speed: Refinement of the basic kinetic molecular theory provide us with a view into the world of gas molecules. In a sample of gas, several different molecules are moving at different speed.

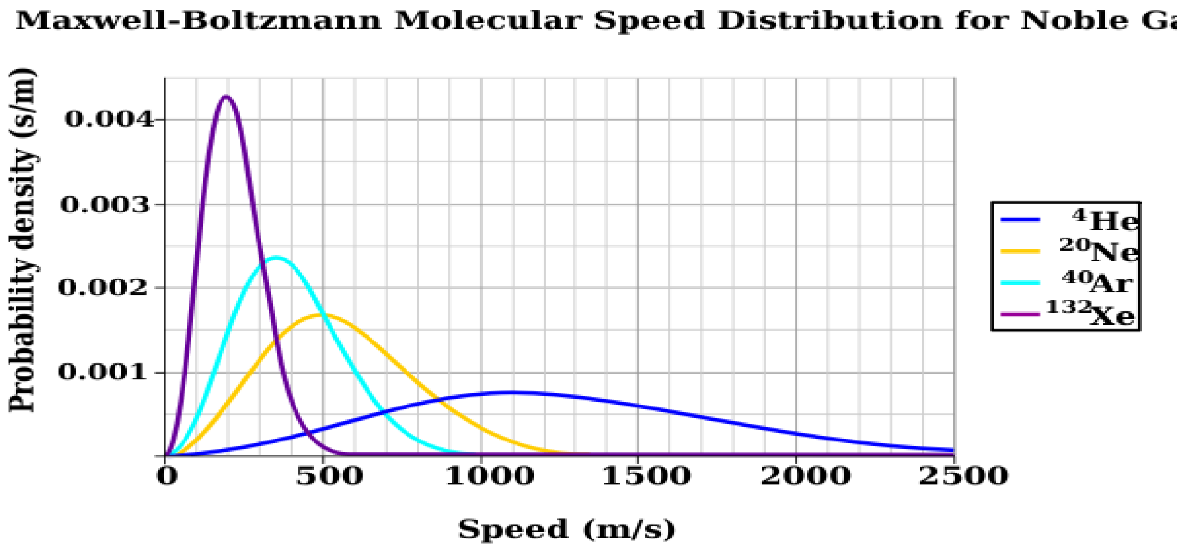


Figure 9.87 Molecular speed Distribution

Ref: commons.wikimedia.org/

Q: What is the root-mean-square speed for a sample of oxygen gas at 298 K?

Molar mass of O_2= M= 16.00*2= 32.00 g/mol= 0.032 kg/mol

R= 8.3145 J/mol-K

Ans: $u=((3*8.3145 * 298)/0.032)^{1/2}=$ meter/sec

Mean free path (distance travelled between two collisions) of gas particles and the rate of effusion and diffusion.

What you should be able to do

Make sure you thoroughly understand the following essential ideas which have been presented above. It is especially important that you know the principal assumptions of the kinetic-molecular theory. These can be divided into those that refer to the nature of the molecules themselves, and those that describe the nature of their motions:

The molecules - Negligible volume, absence of inermolecular attractions (think of them as very hard, "non-sticky" objects.)

Their motions - Completely random in direction, in straight lines only (this is a consequence of their lack of attractions), average velocities proportional to the absolute temperature..

The idea that random motions of individual molecules can result in non-random (directed) movement of the gas as a whole is one of the most important concepts of chemistry, exemplified here as the principle of ***diffusion***.

In most courses you will be expected to know and be able to use (or misuse!) ***Graham's law***.

VII. Behavior of Real Gases:

Real Gases differ from the ideal gases to the extent that do not always fit the assumption of kinetic molecular theory.

The assumptions tends to break at high pressure where the volume is higher than predicted for an ideal gas. Because the partial pressures are no longer negligibly small compared to the space between them.

The assumptions also break at low temp where the pressure is lowered than predicted because the attraction between molecules combined with low kinetic energy causes partially elastic collisions. Several experiments show the deviation of real gases from ideal behavior.

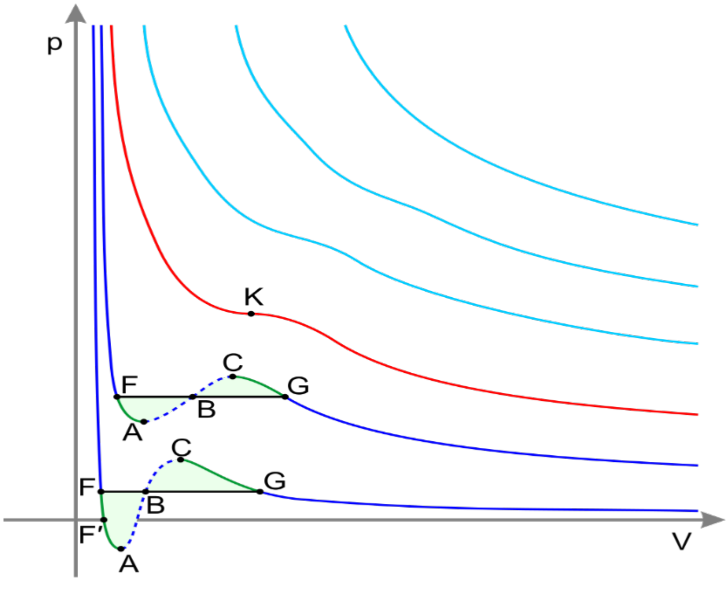


Figure 9.88 real Gas Behavior

Ref: commons.wikimedia.org/

.The above diagram shows how real gases tend to behave ideally when volume is very high.

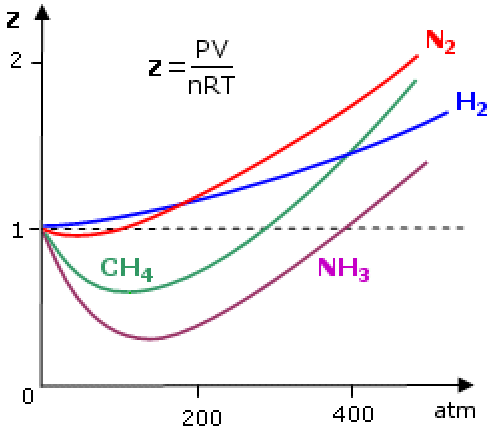


Figure 9.89 PV/nRT vs. P Graph for Real Gases

Ref: commons.wikimedia.org/

Above diagram shows the plot of PV/RT (Z) versus P for 1 mol of different gases. For ideal gases, the value of PV/RT is equal to 1 at any pressure. The values on the horizontal axis are the external pressures at which the PV/RT ratios are calculated. The pressure ranges from normal to very high (~600 atm) and PV/RT>1.

For example, in case of methane gas, it deceases below the ideal value at moderately high pressure and then rises above it as the pressure increases.

This observation can be summarizes as mentioned:

1. At moderately high pressure, values of PV/RT lower than ideal (less than 1) are mainly due to intermolecular attractions.
2. At very high pressure, values of PV/RT greater than ideal (more than 1) are mainly due to molecular volume.

Intermolecular attraction: Attractive forces between molecules are much weaker than covalent bonding. Most intermolecular attractions occur within a very short distance between the molecules. At lower temperature, molecules have less kinetic energy and they are relatively closer to each other. Attractive force between the molecules lower the number of collisions between the molecules and pressure decreases, Therefore a smaller numerator in PV/RT ratio. At low enough temperature, the attraction among molecules become overwhelming and gas may condense to a liquid.

Molecular volume: At normal pressures, the space between molecule of a real gas (free volume) is large enough to consider container volume. As the applied pressure increases, free volume decreases, the molecular volume makes up the greater portion of the container volume. Therefore at high pressure free volume is less than container volume and the ratio PV/RT is high compared to the ideal volume "V". Molecular volume effect becomes very significant as pressure increase and eventually PV/RT rises above the ideal value.

Vander Waal equation: The Ideal Gas Law redesigned:

Figure 9.90 Van der Waals

Ref: commons.wikimedia.org/

To describe the real gas more accurately, we need to redesign the ideal gas equation to do two things:

1. Adjust the measured pressure up by adding a factor that accounts for intermolecular attractions, and
2. Adjust the measured volume down by subtracting a factor that accounts from the entire container volume that accounts for the molecular volume.

$$\left[P + \frac{an^2}{v^2}\right](V - nb) = nRT$$

P= observed pressure

V= observed volume

T, n = Temp and moles respectively

“a” and “b” are called Van der Waal’s constant. The constant “a” relates to the number of electrons which in turn relates to the complexity of the molecules and strength of its intermolecular attractions. The constant “b” relates to the molecular volume.

According to kinetic molecular theory, the constants a, b are zero for an ideal gas because the particles do not attract each other and have no volume. Even for a real gas at ordinary pressures, the molecules are very far apart. Thus observed pressure and volume become ideal pressure and volume. At ordinary condition, Vander Waals equation becomes the ideal gas equation.

***** Adapted from Chem I Virtual textbook**
http://www.chem1.com/acad/webtext/virtualtextbook.html.

Practice Questions: Chapter 9

Indicate the answer choice that best completes the statement or answers the question.

5. What temperature scale should be used if we wish to express Charles's Law as a simple direct proportionality?

a. Fahrenheit b. Celsius
c. Kelvin d. It makes no difference.

6. Which law relates the volume and pressure of a gas under conditions of constant temperature?

a. Avogadro's law b. Boyle's law
c. Charles's law d. Dalton's law

12. Which of the following is a mathematical statement of the combined gas law?

a. $P_1V_2T_1 = P_2V_1T_2$ b. $P_1V_2T_2 = P_2V_1T_1$
c. $P_1V_1T_2 = P_2V_2T_1$ d. $P_1V_1T_1 = P_2V_2T_2$

13. Which law relates the volume and number of molecules of a gas under conditions of constant temperature and pressure?

a. Avogadro's law b. Boyle's law
c. Charles's law d. Dalton's law

15. A certain quantity of neon gas is under 1.05 atm pressure at 303 K in a 10.0 L vessel. How many moles of neon are present?

a. 0.222 mol b. 0.402 mol
c. 0.422 mol d. 2.37 mol

16. Which of the following will occur if the temperature of a gas is increased from 20°C to 40°C at constant pressure?

a. The volume will double.
b. The volume will be halved.
c. The volume will decrease slightly.
d. The volume will increase slightly.

17. Which of the following will occur if the temperature of a gas is decreased from 60°C to 30°C at constant pressure?
a. The volume will double.
b. The volume will be halved.
c. The volume will decrease slightly.
d. The volume will increase slightly.

18. Which of the following increases as temperature increases?
a. kinetic energy b. nuclear forces
c. potential energy d. none of these

19. At constant temperature the pressure on a 10.0 L sample of gas is changed from 1140 torr to 1.00 atm. What is the new volume of the gas sample?
a. 0.00877 L b. 6.67 L
c. 15.0 L d. 114 L

20. What is the volume occupied by an 8.00 gram sample of molecular oxygen at STP?
a. 5.60 L b. 11.2 L
c. 22.4 L d. 44.8 L

21. Which of the following instruments is used to measure atmospheric pressure?
a. an altimeter b. a barometer
c. a manometer d. an odometer

22. A sample of carbon dioxide occupies 22.4 L at STP. Which of the following statements apply to the sample?
a. The sample contains 6.02×10^{23} carbon atoms.
b. The sample contains 6.02×10^{23} molecules.
c. Both a and b are correct.
d. Neither a nor b is correct.

23. Chloroform has a normal boiling point of 61.7°C. Which of the following is true?
a. At any temperature the vapor pressure of chloroform is less than that of water.
b. Chloroform is more volatile than water.
c. Both a and b are correct.
d. Neither a nor b is correct.

24. Which of the following is true of London dispersion forces?
  a. They increase as the number of electrons in a molecule increases.
  b. They are only present in some molecules.
  c. Both a and b are correct.
  d. Neither a nor b is correct.

25. Which of the following pairs do not engage in hydrogen bonding?
  a. H_2O with NH_3
  b. H_2O with H_2O
  c. NH_3 with NH_3
  d. None, they all engage in hydrogen bonding.

26. Which of the following is a mathematical statement of the ideal gas law?
  a. $PV = n/RT$ b. $PV = nRT$
  c. $V = nP/RT$ d. $PV = RT/n$

27. Which of the following molecules can engage in hydrogen bonding?
  a. HF b. HCl
  c. HBr d. HI

28. Which of the following is a mathematical statement of the ideal gas law?
  a. $PVRT = n$ b. $PV/RT = n$
  c. $VRT/P = n$ d. $n = RT/PV$

29. Which of the following is a mathematical statement of Boyle's Law?
  a. $P_1V_2 = P_2V_1$ b. $P_1\mathrm{V}_1 = P_2V_2$
  c. $P_1/T_2 = P_2/T_1$ d. $P_1/T_1 = P_2/T_2$

30. Suppose a balloon is filled so that its volume is 2.00 L when the pressure is 1.10 atm and the temperature is 300 K. What volume will it occupy if it rises to an elevation where the pressure is 418 mm Hg and the temperature is 200 K?
  a. 3.30 L b. 2.67 L
  c. 0.375 L d. 0.303 L

31. According to the kinetic molecular theory, which of the following is not true?
  a. Gas molecules are assumed to have no volume.
  b. Gas pressure is caused by collisions between gas molecules and the container walls.
  c. When gas molecules collide they stick together.
  d. None, all of the above are true.

32. Which of the following phase changes does not involve a liquid?
a. evaporation b. melting
c. sublimation d. None, they all involve a liquid.

33. Dry air is 78.08% nitrogen, 20.95% oxygen and 0.93% argon with the 0.04% being other gases. If the atmospheric pressure is 760.0 torr, what is the partial pressure of nitrogen in dry air?
a. 78.08 torr b. 166.6 torr
c. 593.4 torr d. 760.0 torr

34. Which law applies only to mixtures of gases?
a. Avogadro's law b. Boyle's law
c. Charles's law d. Dalton's law

Answer Key

1. d

2. c

3. a

4. d

5. c

6. b

7. b

8. d

9. d

10. d

11. a

12. c

13. a

14. c

15. c

16. d

17. c

18. a

19. c

20. a

21. b

22. c

23. b

24. a

25. d

26. b

27. a

28. b

29. b

30. b

31. c

32. c

33. c

34. d