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

Section 1.1. 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.

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).

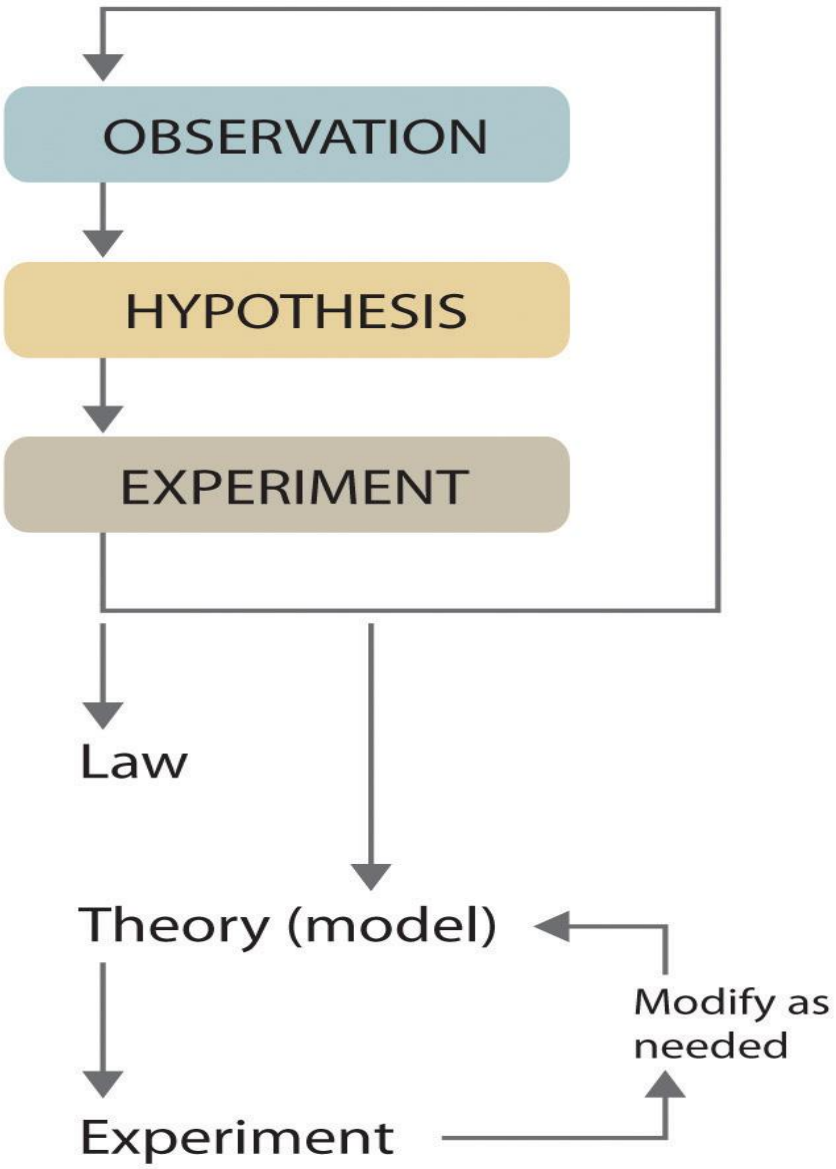


Figure 1.2 The Scientific metho_

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 collecting many observations, a scientist may devise 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.

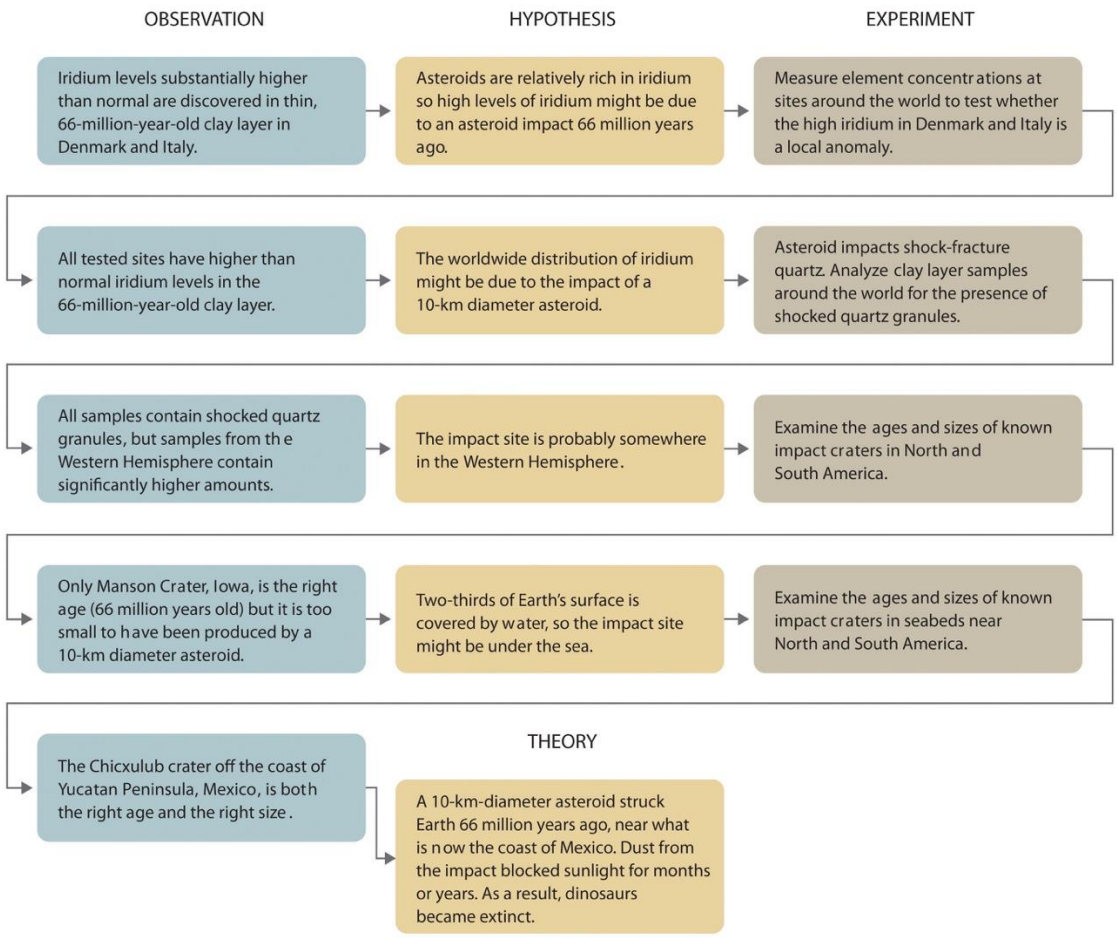


Figure 1.3 The scientific method.

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 "+2" on one side of the equation, we will solve for "x". Everything that is

Visit the followingwebsites 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

2. X/A= B

X=?

X= A.B

3. F/X= G

X=?

X= F/G

A/B =?? Ans: AS/BR

R/S

12 = Ans is 9 not 1

4/3

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} = 1/10^3 = 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. $(10^a)^b = 10^{a \times b}$

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

2. $(10^{-3})^2 = 10^{-3 \times 2} = 10^{-6}$ = 0.000001

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

4. $(2 + 102)^2 = (2 + 100)^2 = 102^2 = 10404$ $(2 + 102^2)$ is NOT $(22 + 104^2)$ which would give you the wrong answer of 10004! The distributive property 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: $4 + 9 \div 3 - 2 \times 3 + (3 + 1) \times 4$ First think about which operation must be done FIRST. First you do $9 \div 3 = 3$ and $2 \times 3 = 6$ and $(3+1) = 4$ and so $(3+1) \times 4$ becomes $4 \times 4 = 16$. Then you do $4 + 3 - 6 + 16 = 17$ So $4 + 9 \div 3 - 2 \times 3 + (3 + 1) \times 4 = 4 + 3 - 6 + 16 = 17$ (The correct answer is 17.)

Now try it with your calculator. Try entering in exactly the same order as written: $4 + 9 \div 3 - 2 \times 3 + (3+1) \times 4$ 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..

Practise with this problem, using your calculator: $\frac{? 3.2 \times 10^{3} \times 5.1 \times 10^{-12}}{7.4 \times 10^{12}}$

answer 2.205405×10^{9} ?

Units can be handled just like algebraic terms.

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

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

** **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.

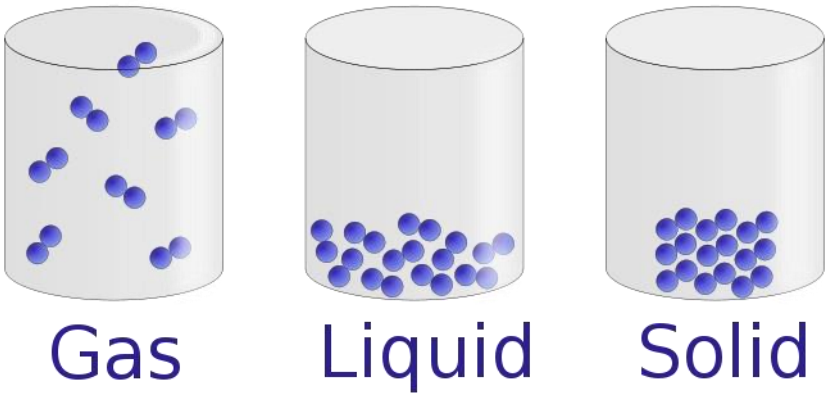


Figure 1.4: Three States of Matter

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 1.4 The States of Matter Example

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

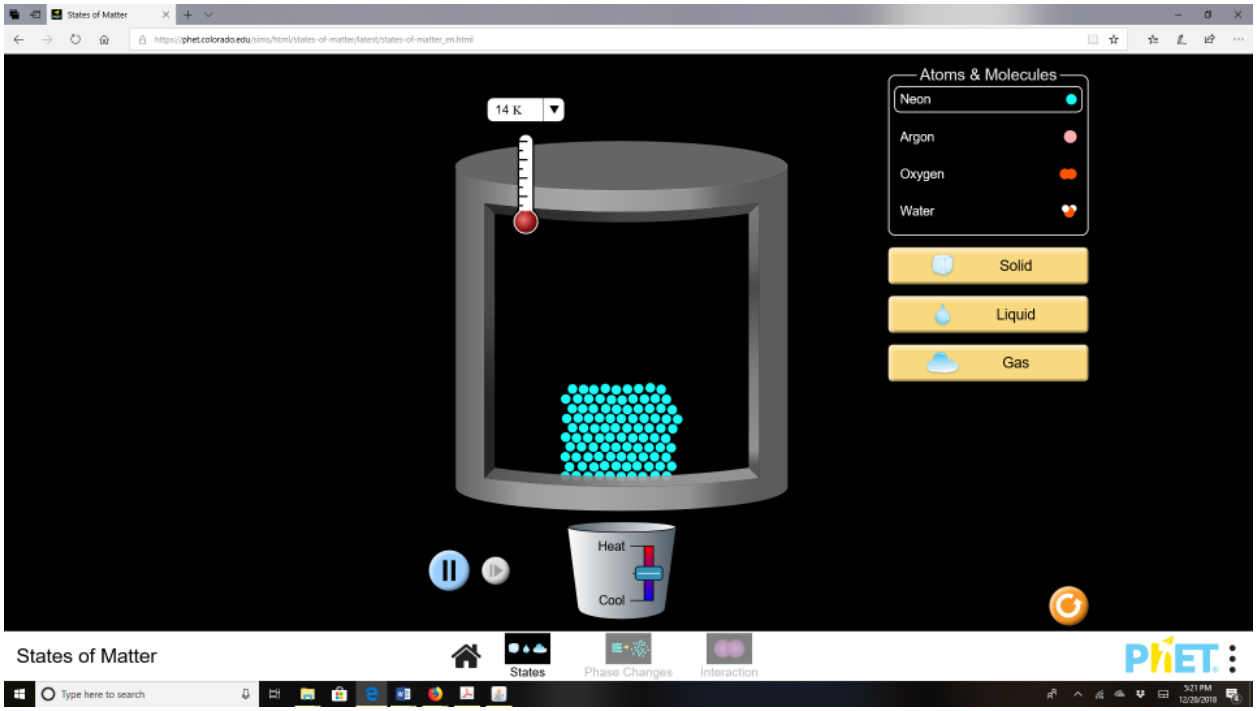


Figure 1.5A: Phet Simulation of States of

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?

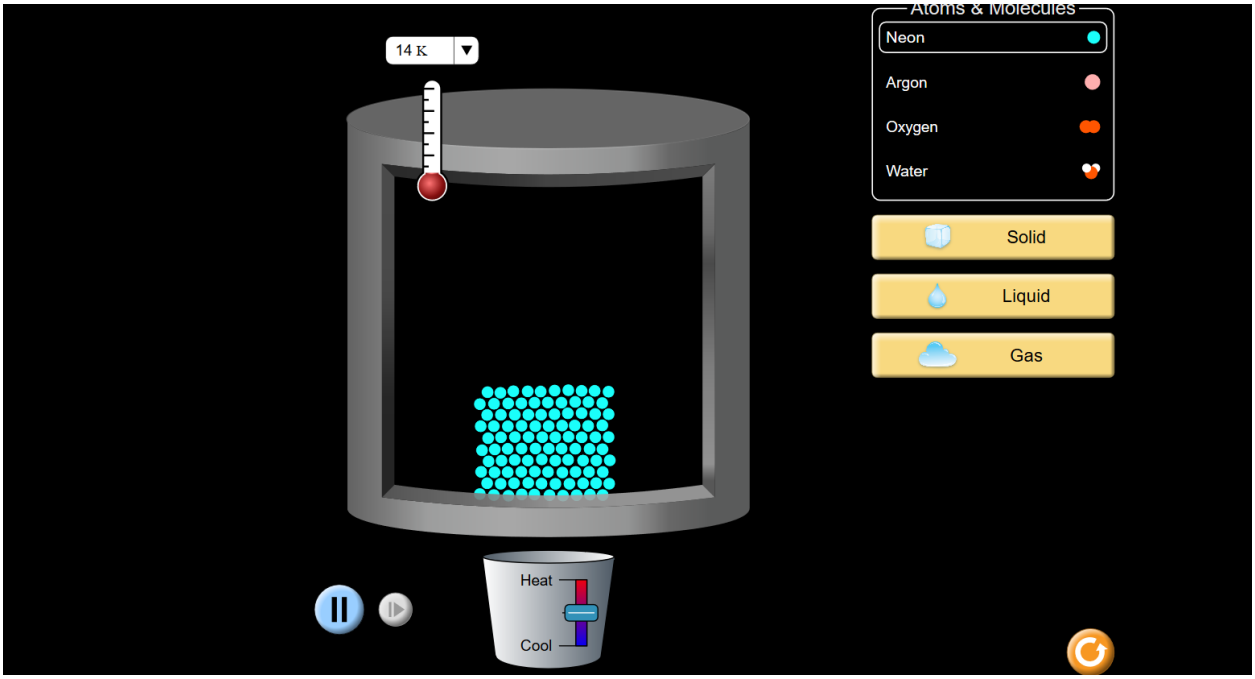


Figure 1.5B: Phet Simulation of States of

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?

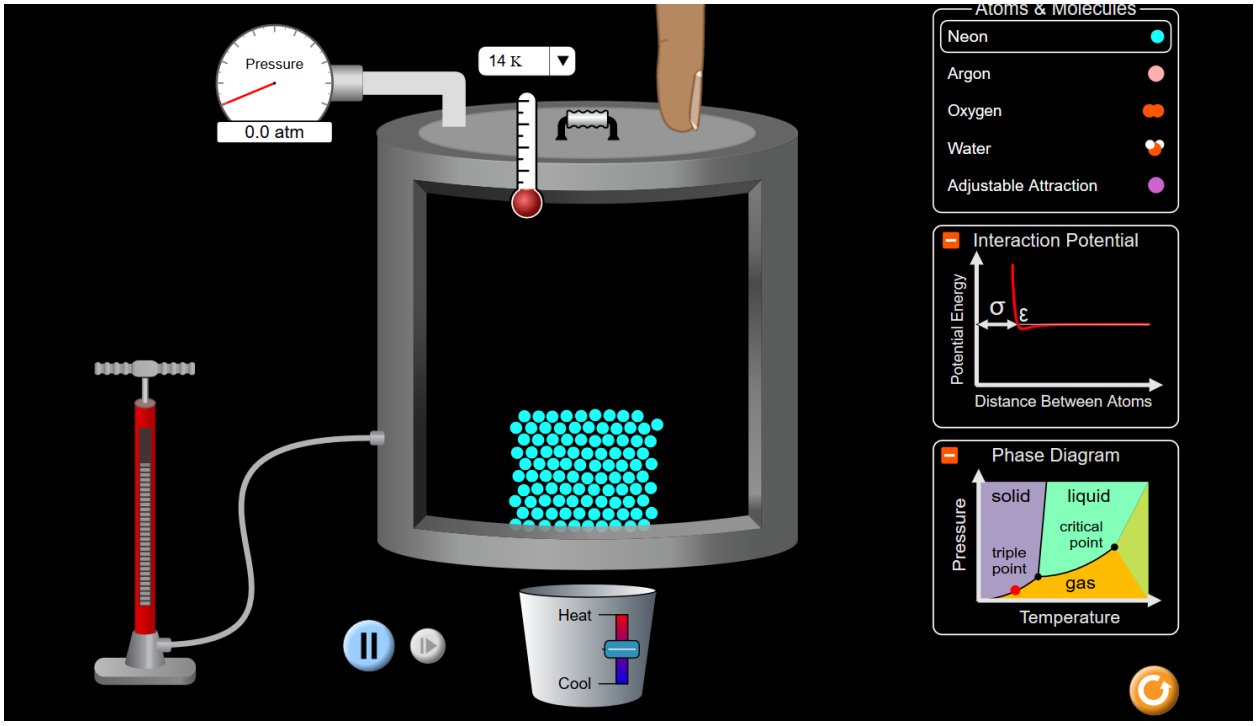


Figure 1.5C: Phet Simulation of States of

Ans: 1) Solid particles are rigid with little vibrating, 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

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 substance, because all samples of oxygen consist of the same molecules, which do not change at 25° C. Two or more pure substances, instead of one, make a mixture, which does not have a fixed composition.

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 liquids, 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).

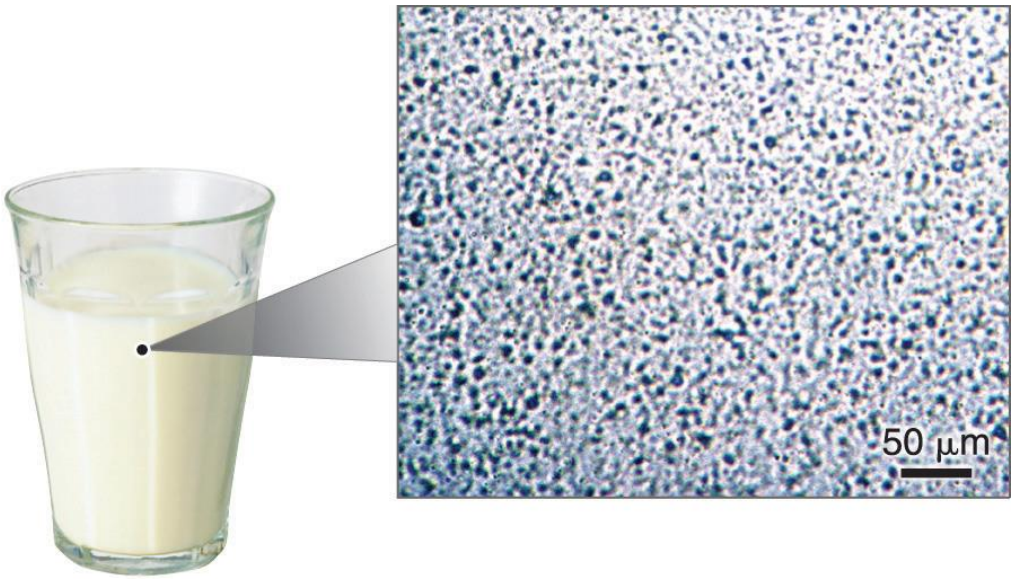


Figure 1.5 Milk, a heterogenous mixture. Under a microscope, whole milk is actually a heterogeneous mixture composed of globules of fat and protein dispersed in water.

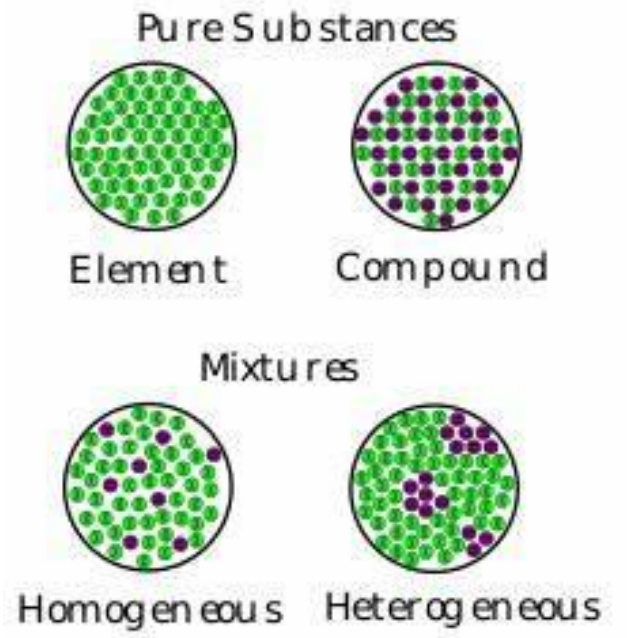
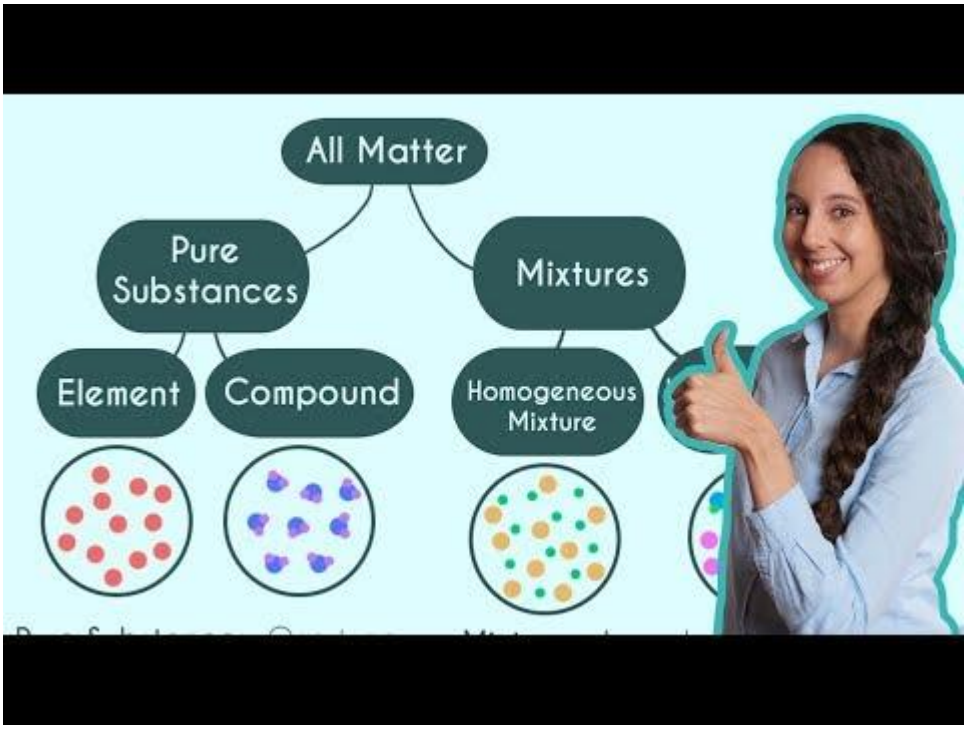


Figure 1.6: Pure Substance vs



https://www.youtube.com/watch?v=pWZlICXw3N

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

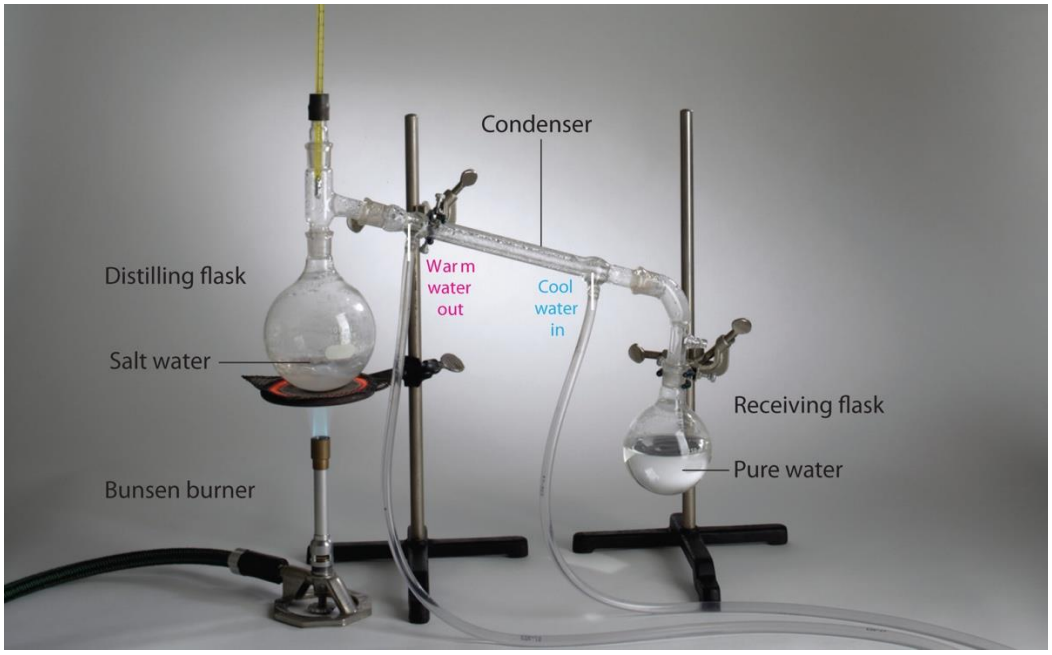
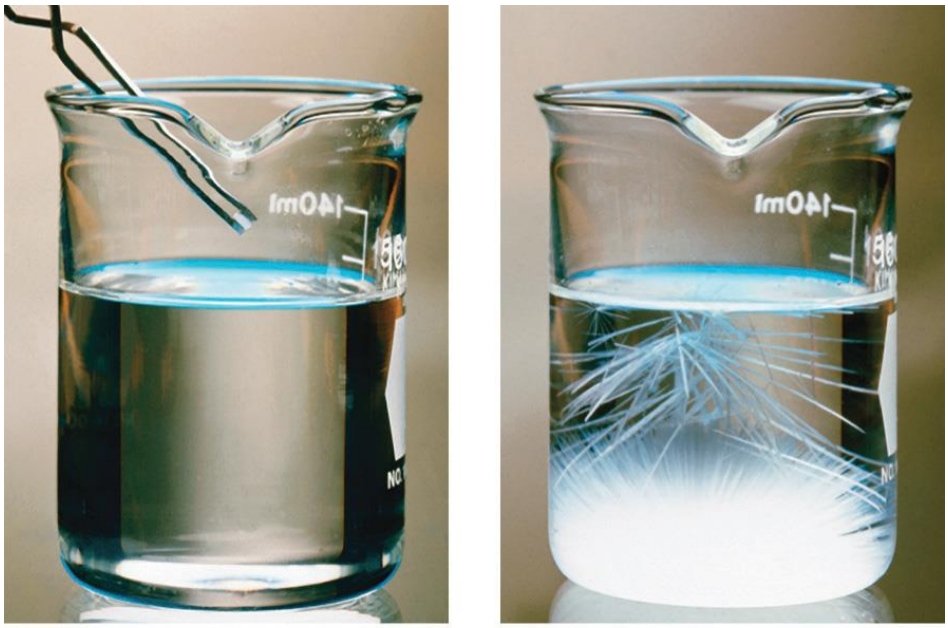


Figure 1.6. The distillation of a solution of table salt in water.

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).



(a) (b)

Figure 1.7. 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.

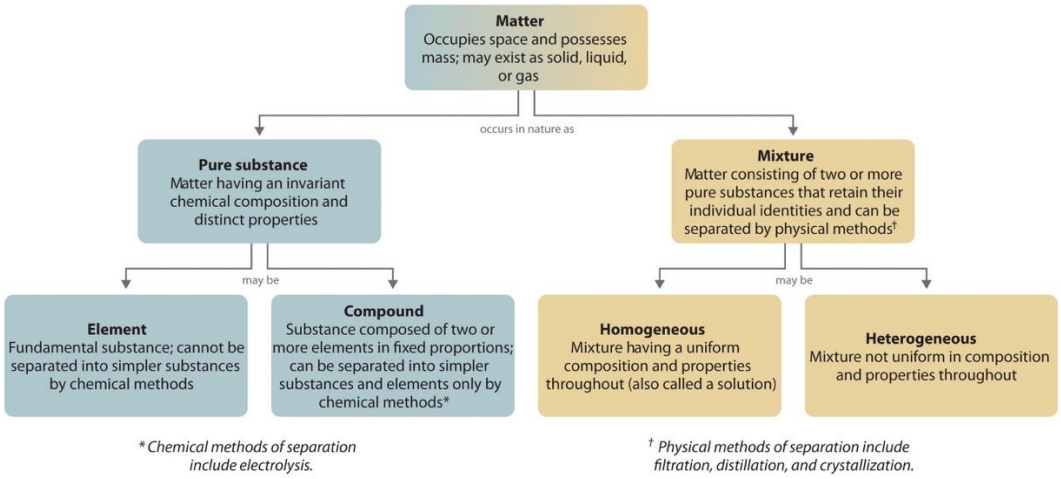


Figure 1.8 Classification of matter.

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.

IBa 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:

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 liquids, 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 composition 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.

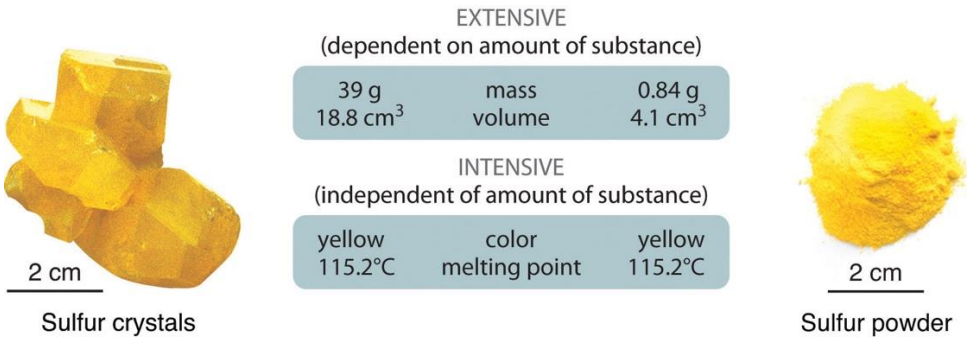


Figure 1.9 The difference between extensive and intensive properties of matter.

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 denser than gas. Water is an exception. Ice is less dense than liquid water. A less dense substance floats on a

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.

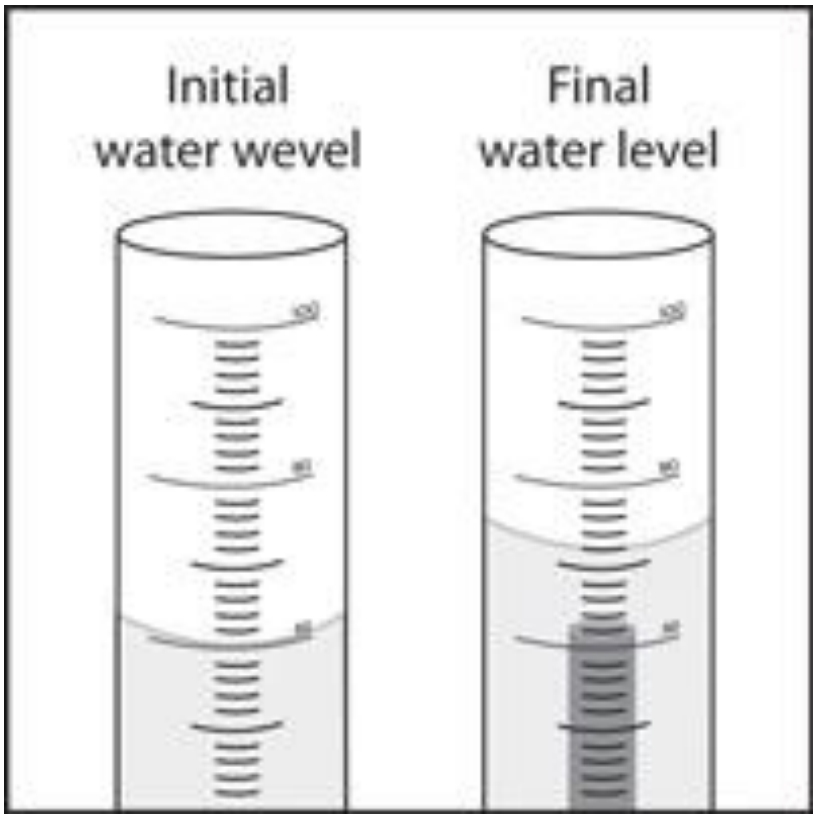
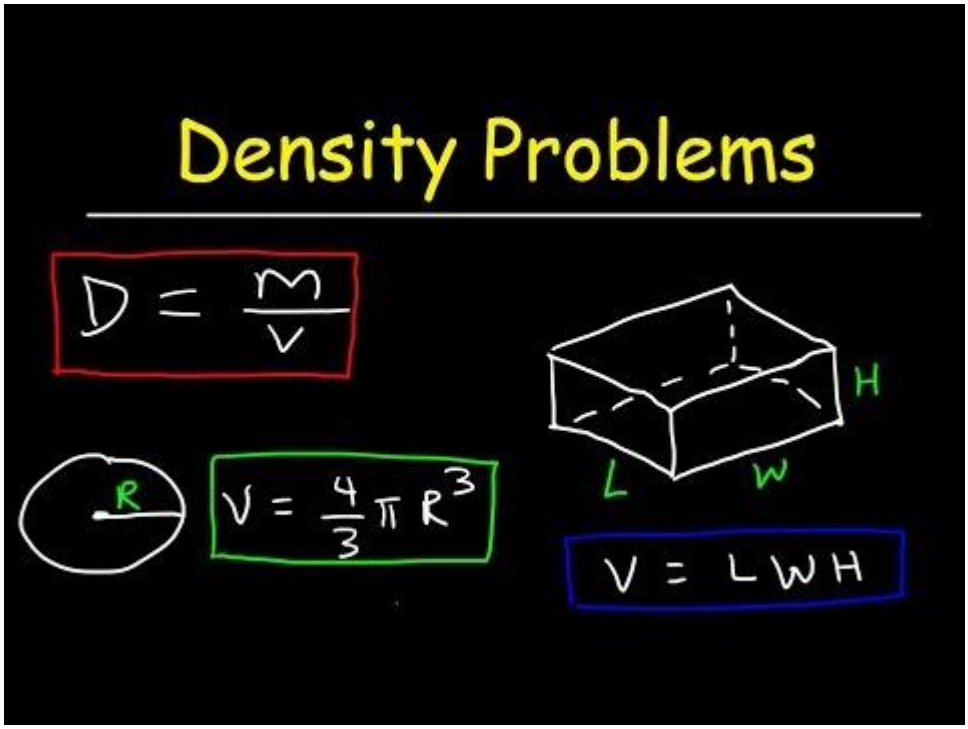


Figure 1.10 A: Finding Volume of a Solid Using the Water Displacement Method

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.



https://www.youtube.com/watch?v=9CKDQE35qX

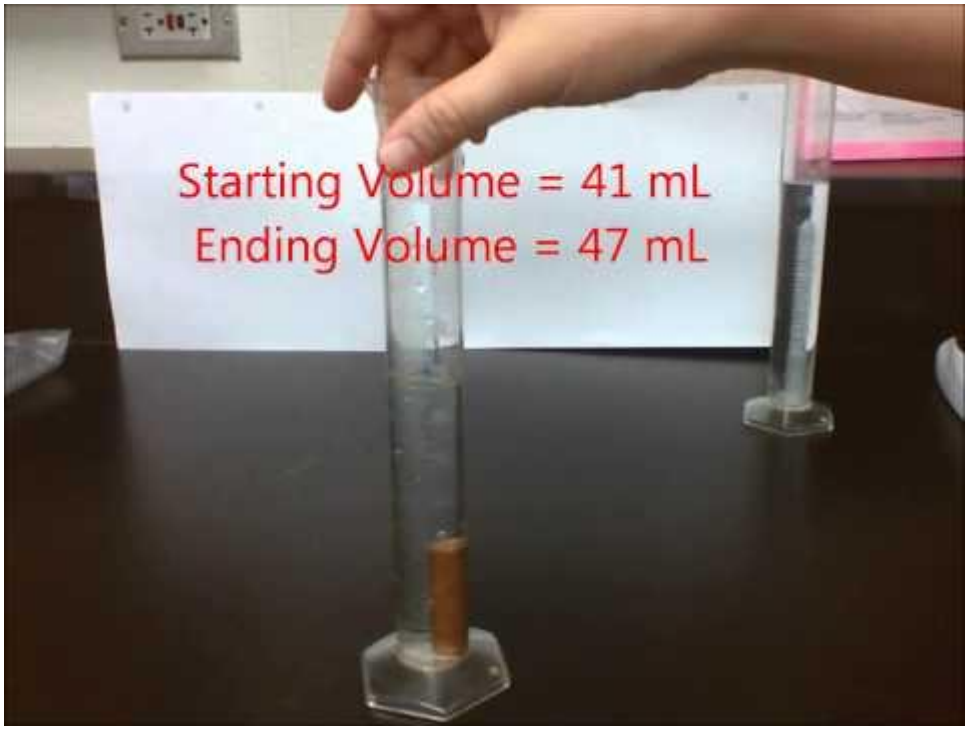


Figure 1.10 B: Finding Volume of a Solid Using the Water Displacement

Go to the following site and check out the simulation

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

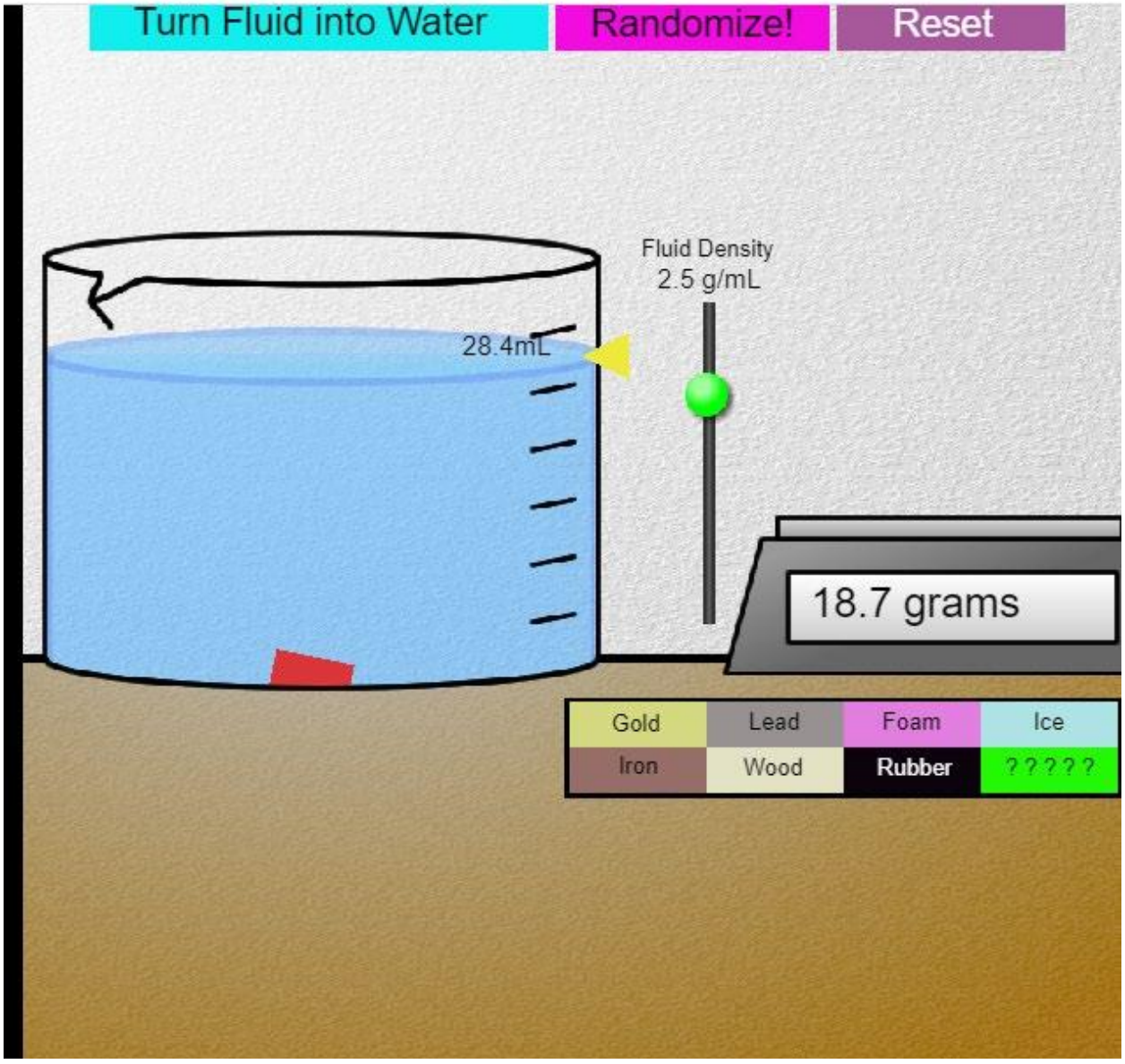


Figure 1.11: Phet Simulation for Finding the Density of an Object

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 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 water molecules containing two hydrogen atoms and one oxygen atom covalently bonded together. When you have a container of pure water or a mixture of pure water and sugar

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 1.10. 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.

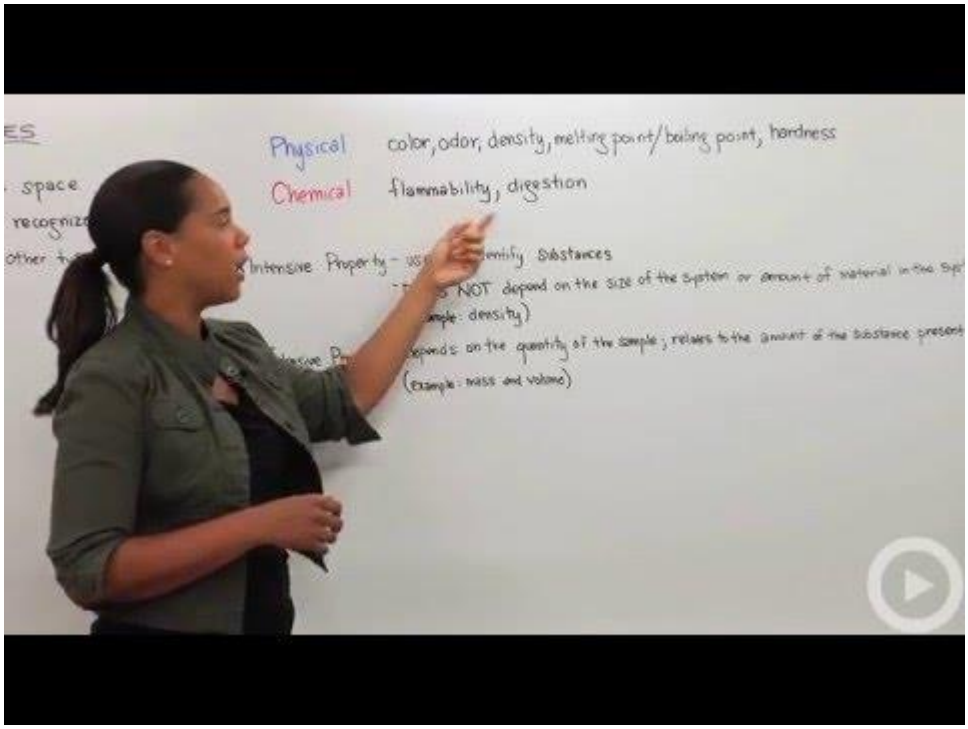
Figure 1.11 Burning of a candle is a type of chemical change.

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.



https://www.youtube.com/watch?v=k7l1d22lFc

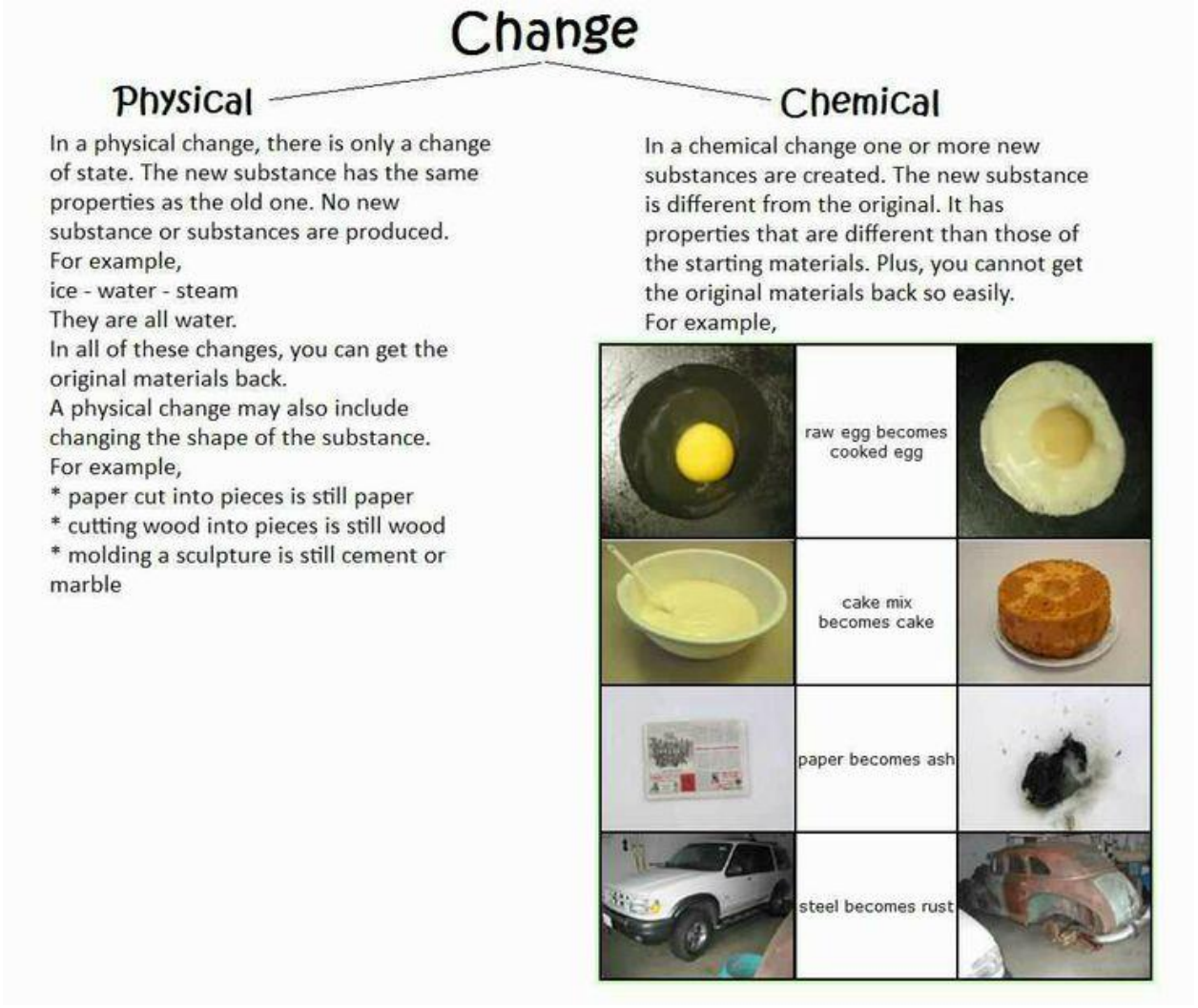
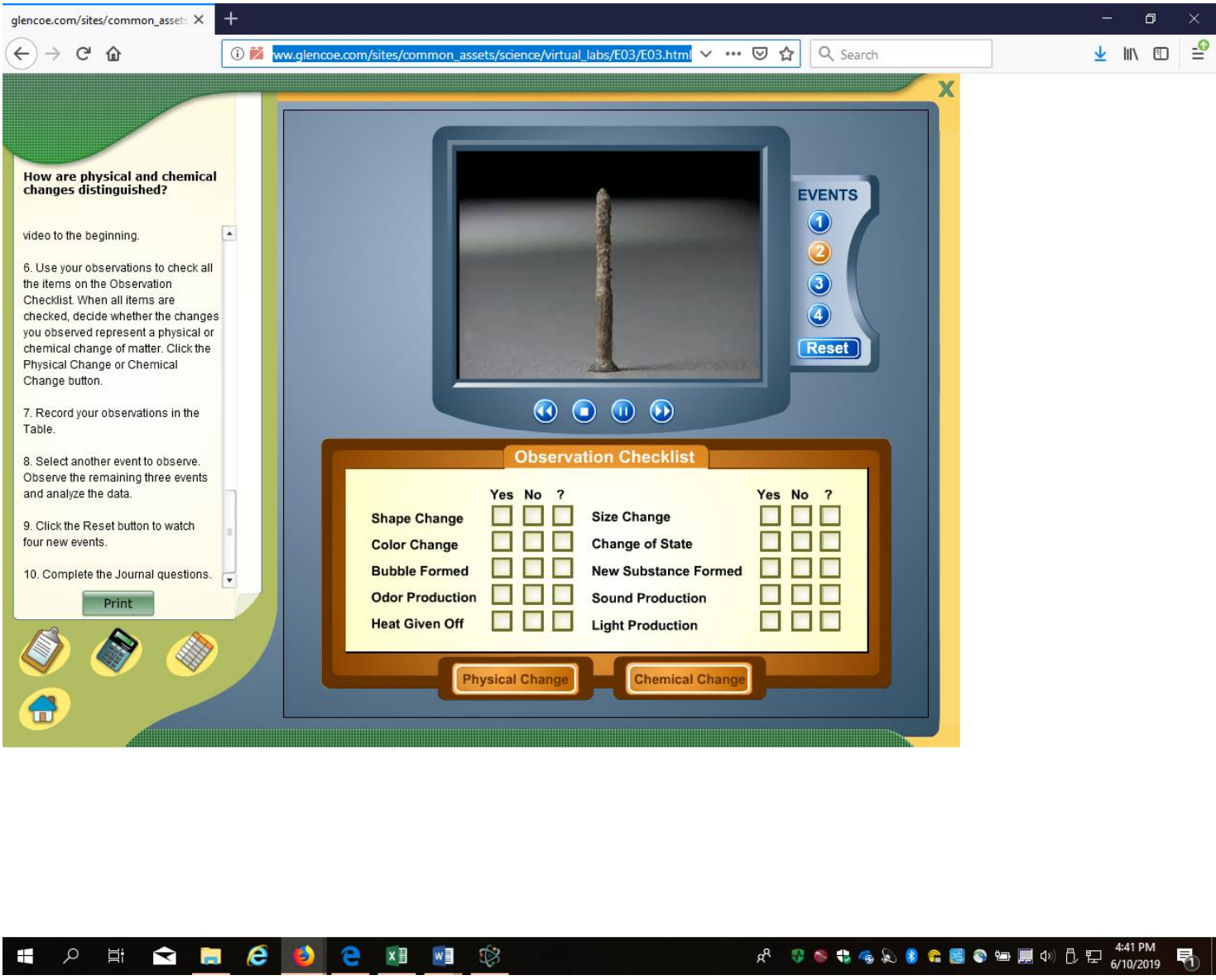


Figure 1.13: Physical and Chemical

Go to the following activity and complete the activity:

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



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

cA 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: $H_2O(l) \rightarrow H_2O(g)$

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: $Fe + O_2 \rightarrow Fe_2O_3$

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

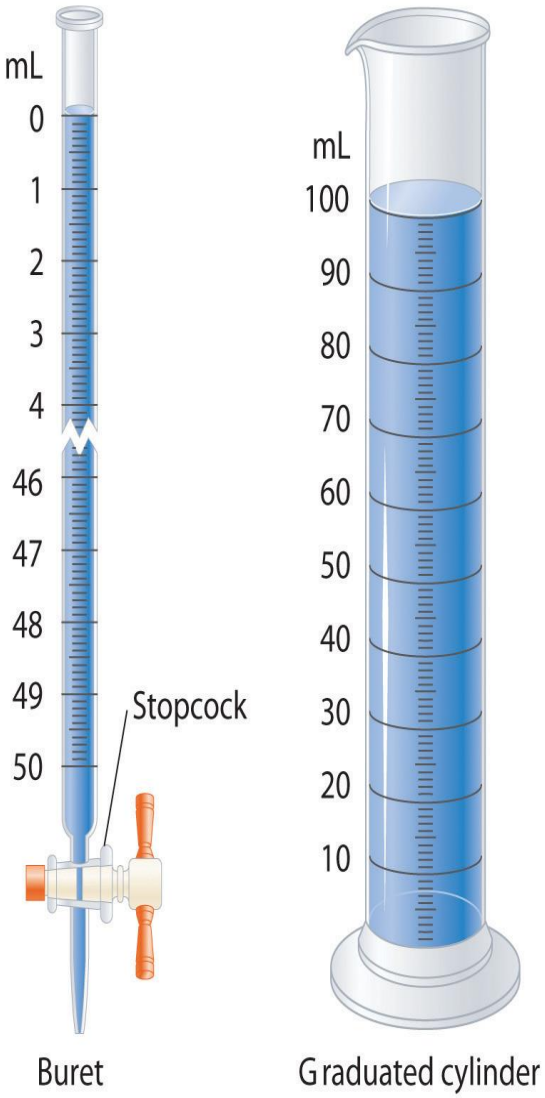


Figure 1.12 Graduated glassware is used to deliver variable volumes of liquid.

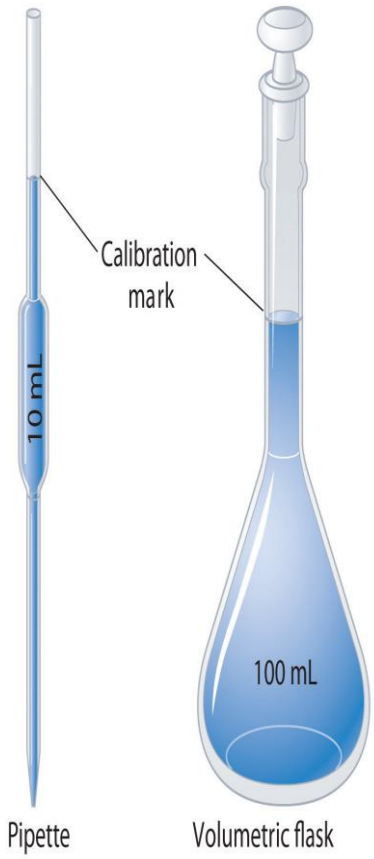


Figure 1.13. Volumetric glassware is used to deliver (pipette) or contain (volumetric flask) a single volume accurately when filled to the calibration mark.

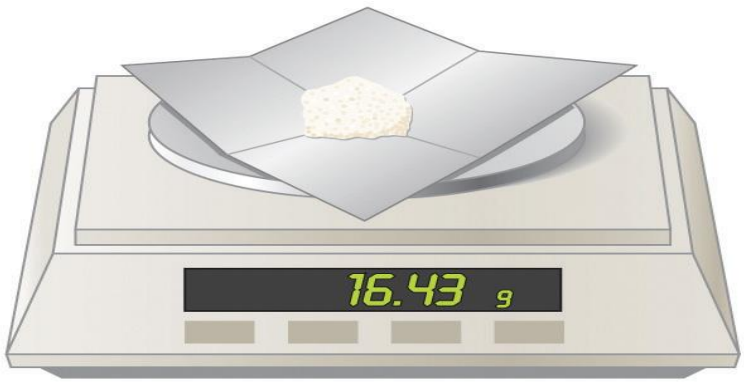


Figure 1.14. A balance is used to measure mass.

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.

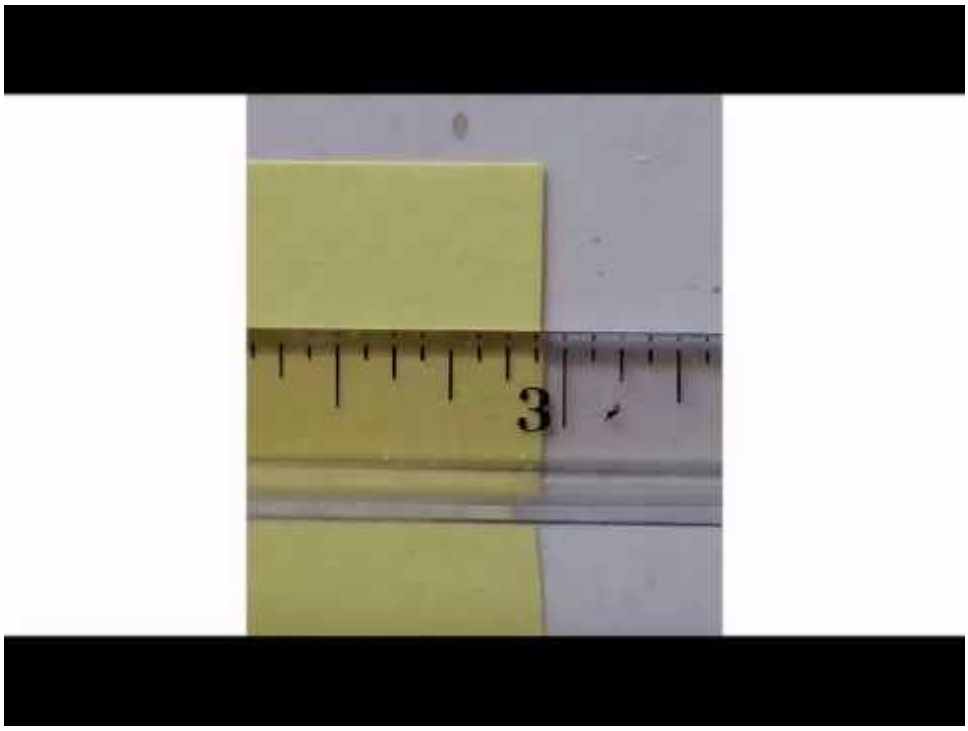
Example of exact number: 30 students in class, 12 oranges. Example of measured number: the child weights 30.5 lbs, The height of Mount Everest is 8,848 meters.

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



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

Following tutorial may help you to understand the concept.

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

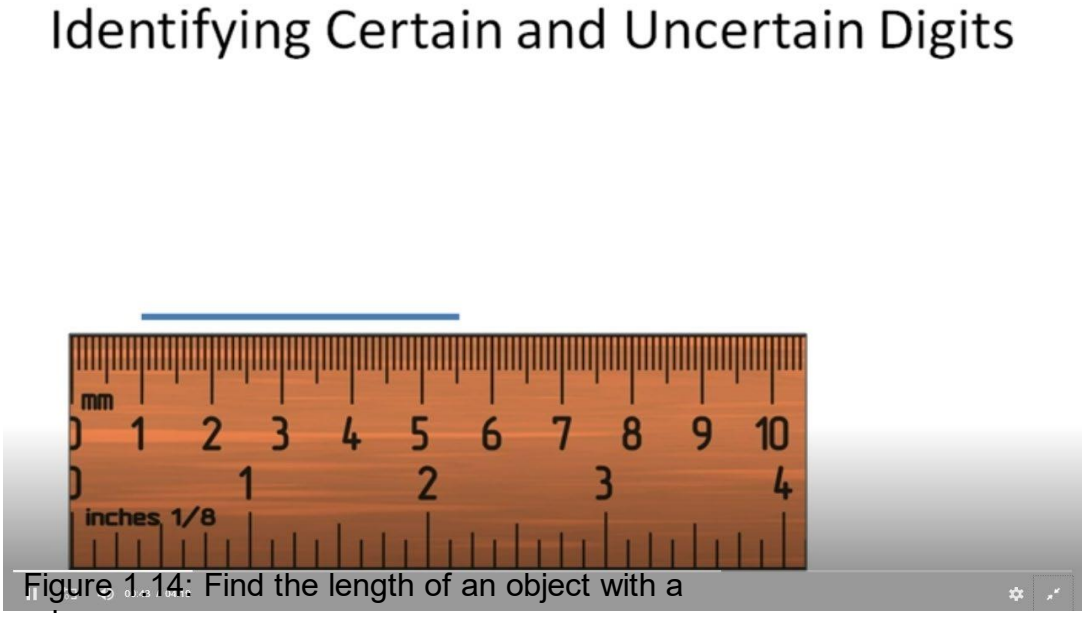


Figure 1.14: Find the length of an object with a

Questions:

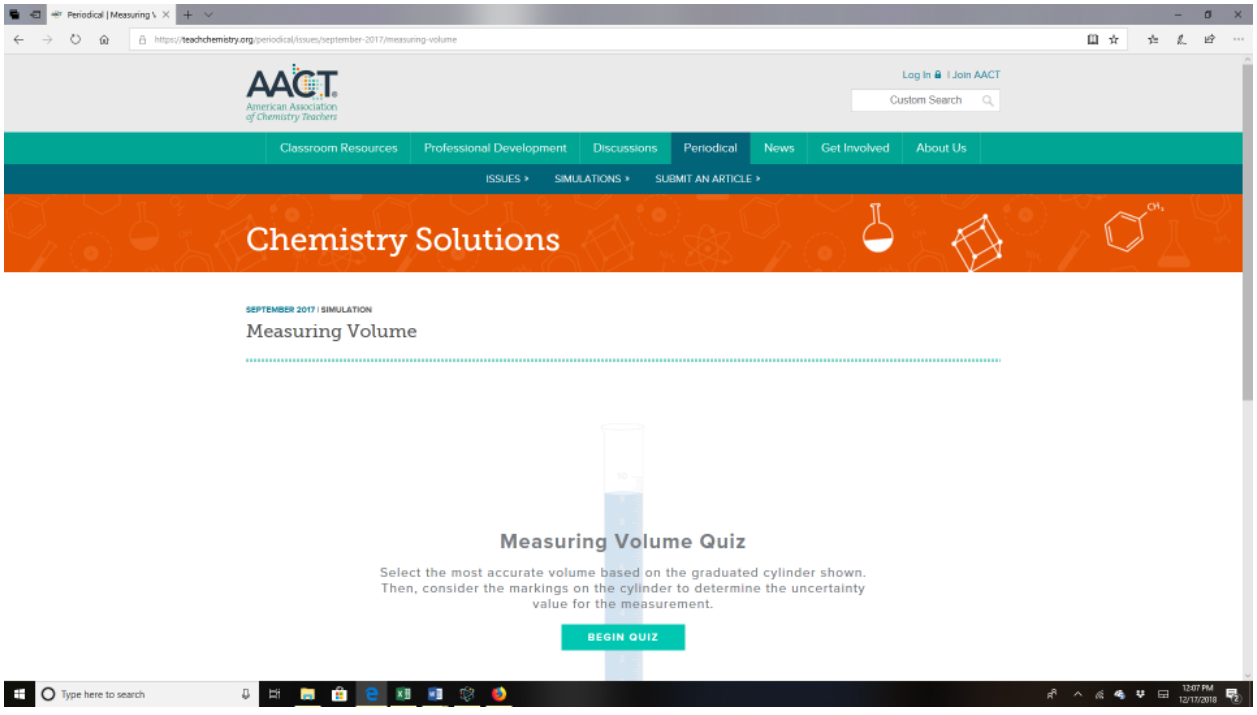
1. Indicate whether the following numbers are exact or inexact?

   a) The length of a river

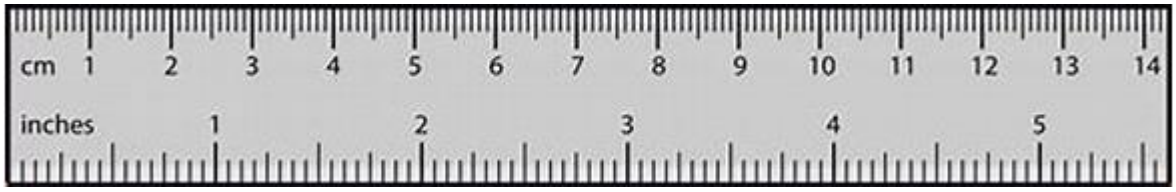
   b) Conference attendees

2. Go to the following link Take the quiz:

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



3. What measurement can be shown with followingruler?



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.

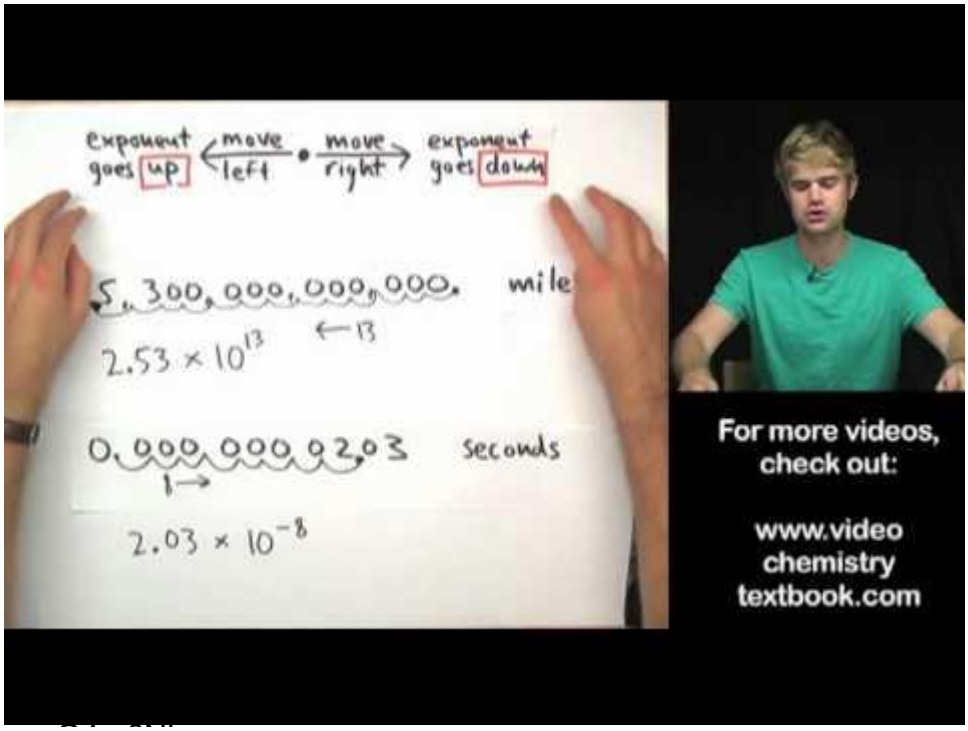
A simple way to convert numbers to scientific notation is to move the decimal point as many places to the left or right as needed to give a number from 1 to 10 (N). The magnitude of n is then determined as follows:

- 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



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 $10^{0} = 1$.)

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 division on a graduated cylinder) and (2) the imperfection of measurements. Although errors in measurements cannot be eliminated, they can be minimized.

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:

$$1\ \text{ft} = 12\ \text{in}$$

An effective method for determining the number of significant figures in a measured or calculated value is to express the number in scientific notation. When a number is written in scientific notation, only significant figures are included in the coefficient. For example, the number 0.0800 has three significant figures, and it may be expressed in scientific notation as 8.00×10^{-2}.

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?

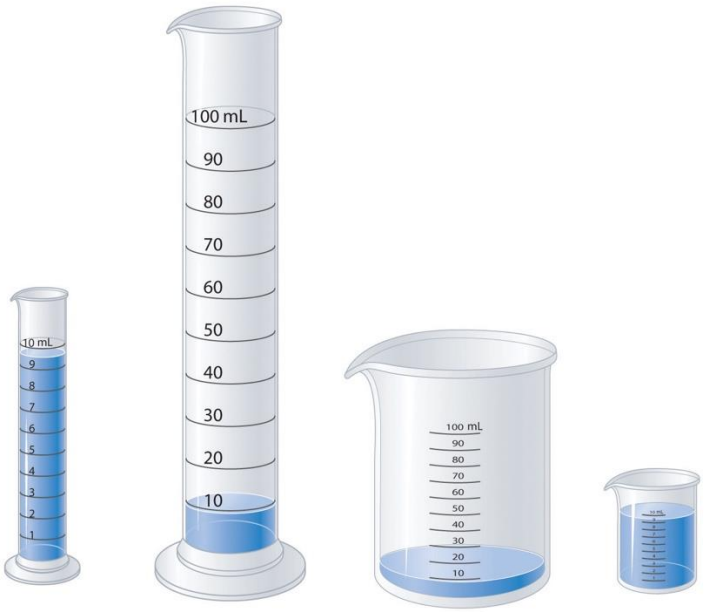


Figure 1.16: Apparatus showing different volumes of liquids

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:

$$3240.7 + 21.236 = 3261.\underline{9}36$$

The last digits for the three digits in all other numbers 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 1.66666667 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

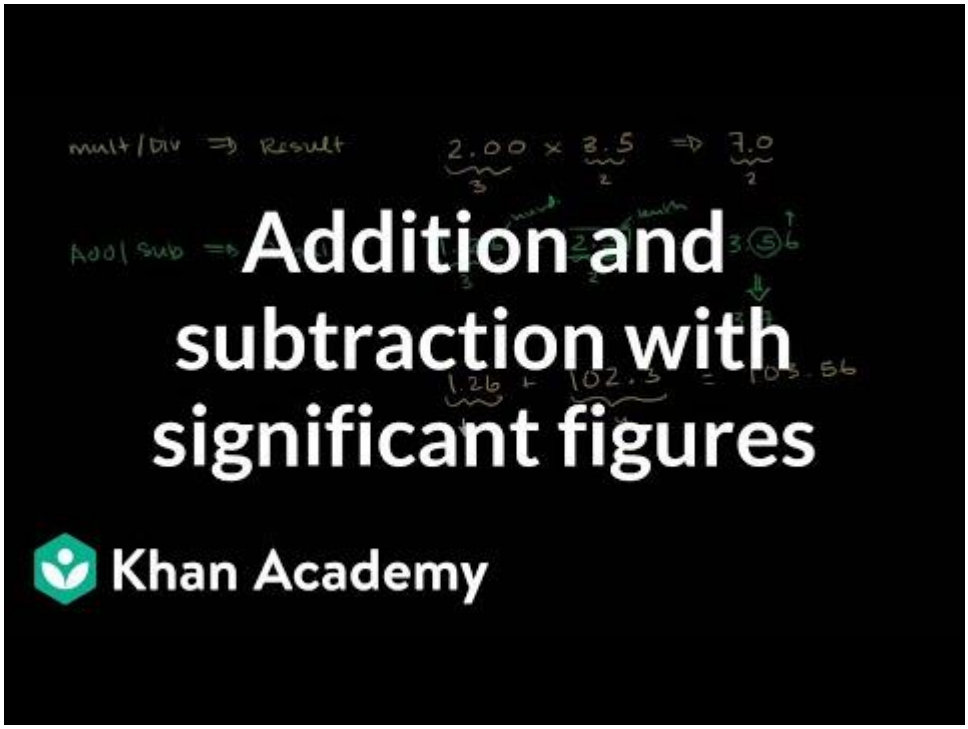
a. Both exponents must have the same value, so these numbers are converted to either $(1.36 \times 10^{2}) + (47.3 \times 10^{2})$ or $(0.136 \times 10^{3}) + (4.73 \times 10^{3})$. Choosing either alternative gives the same answer, reported to two decimal places:

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

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=xHgPtFUbAe

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:

$1.67\times10^{-24}/9.12\times10^{-28} = 1.67/9.12\times10^{[-24 - (-28)]} = 0.183\times10^{4} = 1.83\times10^{3}$

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

$$1.125\ \text{g} + 1.158 + 1.067\ \text{g} 3 = 1.117\ \text{g}$$

The deviations are $1.125\ \text{g} - 1.117\ \text{g} = 0.008\ \text{g}$, $1.158\ \text{g} - 1.117\ \text{g} = 0.041\ \text{g}$, and $|1.067\ \text{g} - 1.117\ \text{g}| = 0.050\ \text{g}$. So, the average deviation is

$$0.008\ \text{g} + 0.041\ \text{g} + 0.050\ \text{g} = 0.033\ \text{g}$$

The precision of this set of measurements is therefore

$$0.033\text{g} 1.117\text{g} \times 100 = 3.0\%$$

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?

Figure 1.16: Dart boards showing examples of Precision and Accuracy

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 $\frac{4.9 \text{ mg}}{457.3 \text{ mg}} \times 100 = 1.1\%$. 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

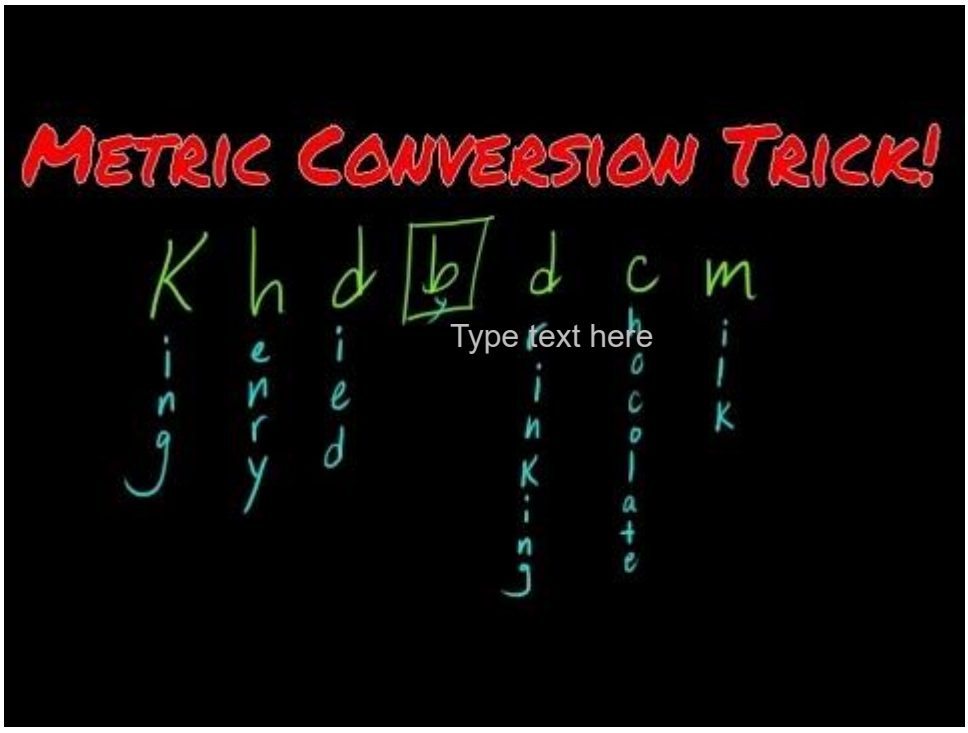
The average values of the measurements are 93.2% zinc and 2.8% copper versus the true values of 97.6% zinc and 2.4% copper. Thus, these measurements are not very accurate, with errors of −4.5% and + 17% for zinc and copper, respectively. The sum of the measured zinc and copper contents is only 96.0% 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



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

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:

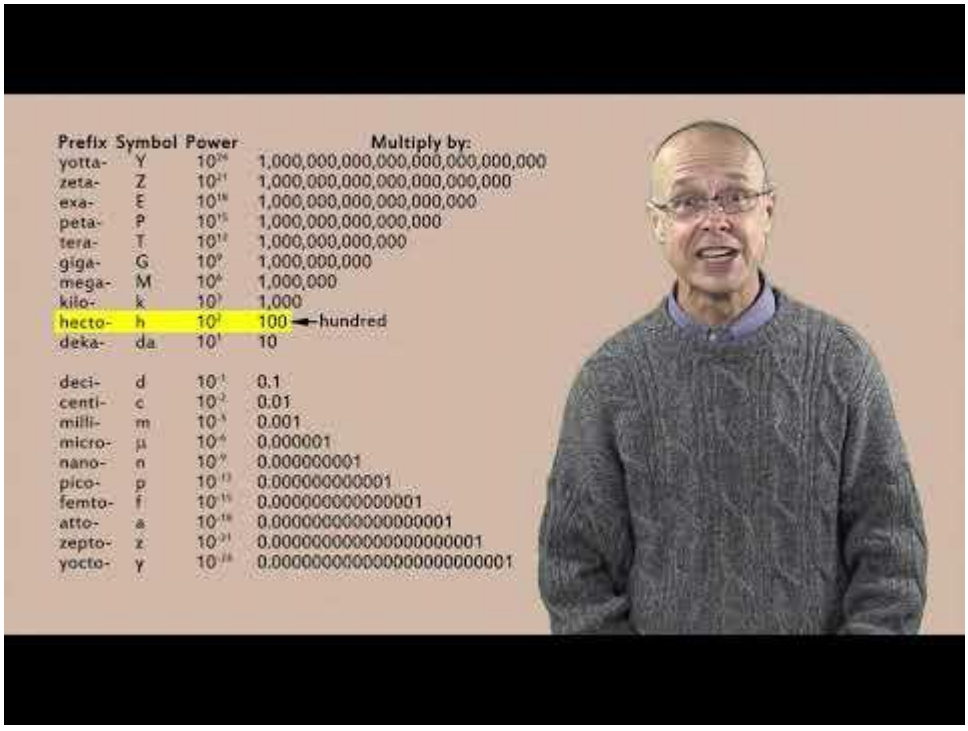
Unit of Measurement	Name of Unit	Abbreviation
Length	Meter	m or cm
Mass	Gram	g
Volume	Liter	L

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

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



https://www.youtube.com/watch?v=xTgRCJQ6w4

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, scientists (mostly) use the International System of Units (abbreviated SI) developed by the General Conference on Weights and Measures and called the **International System**

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.

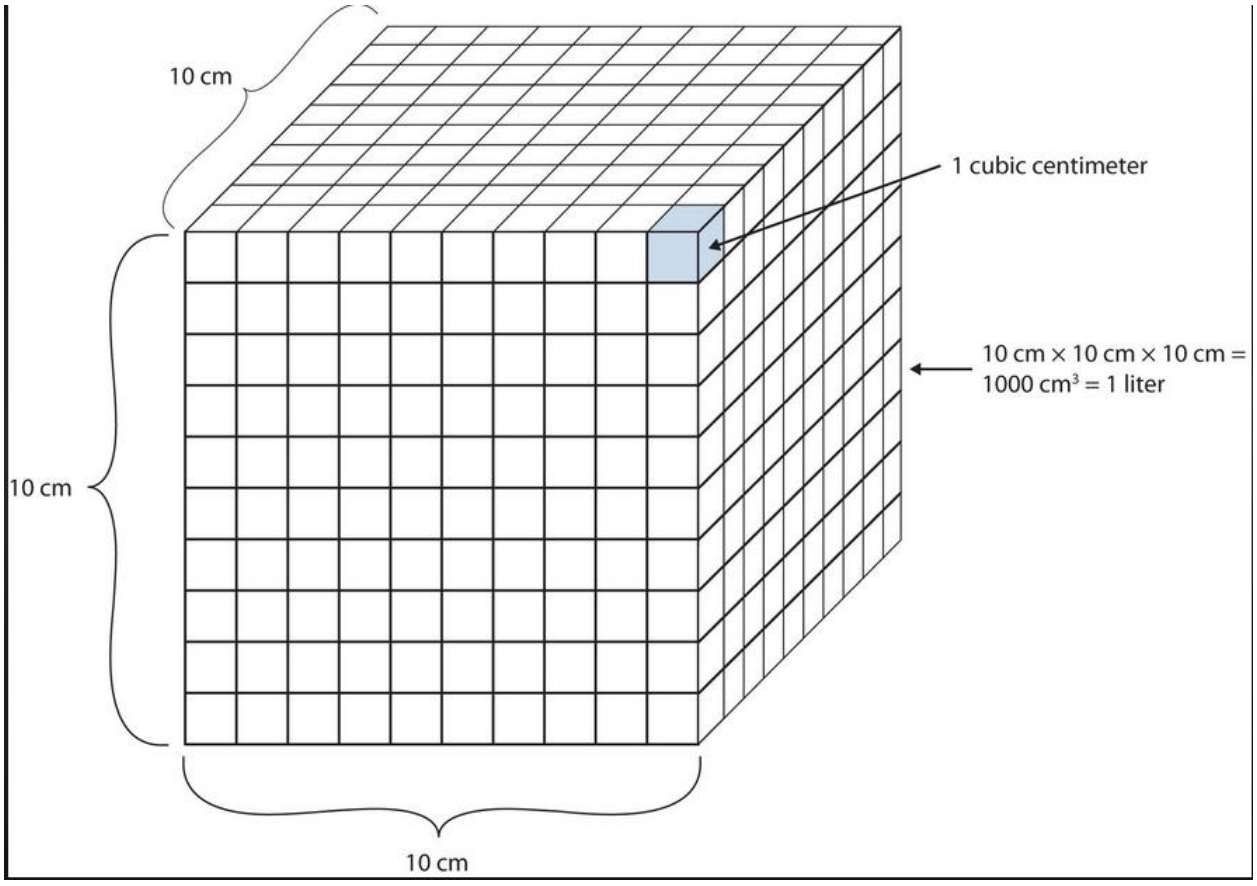


Figure 1.17: Showing the volume of a

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

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 relationshipsas 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 combinationwith other conversion factors in a dimensionalanalysis 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)

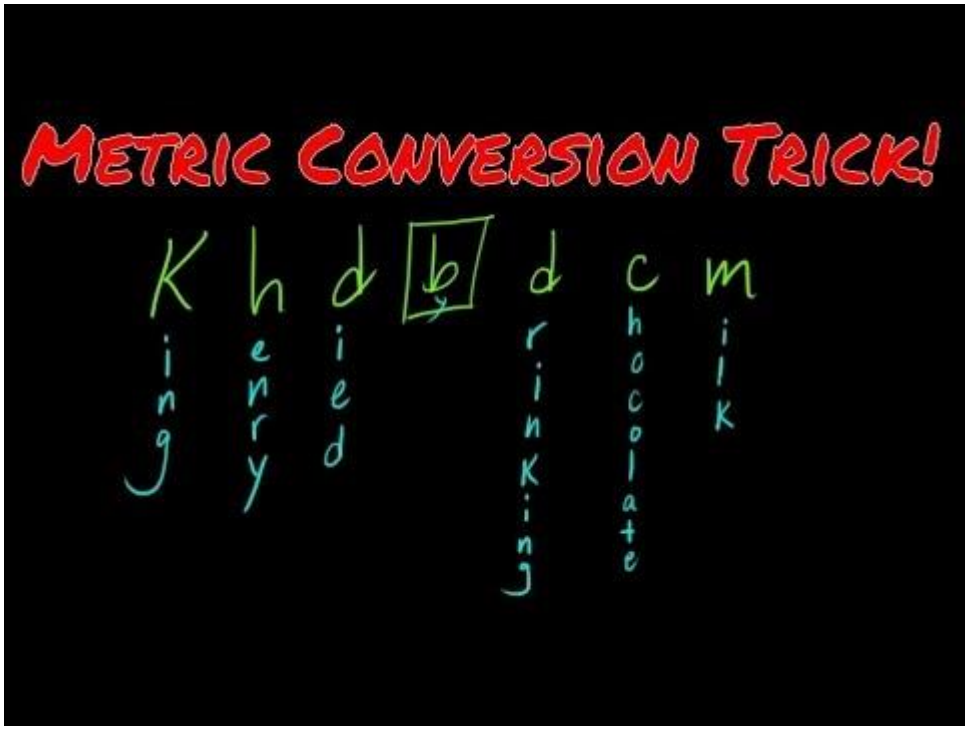
Example problem: A lab test showed an individual's cholesterol level to be 186 mg/dL. Convert this quantity into g/dL

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.

<u>For more information watch</u>:



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

Metric conversion: ladder method

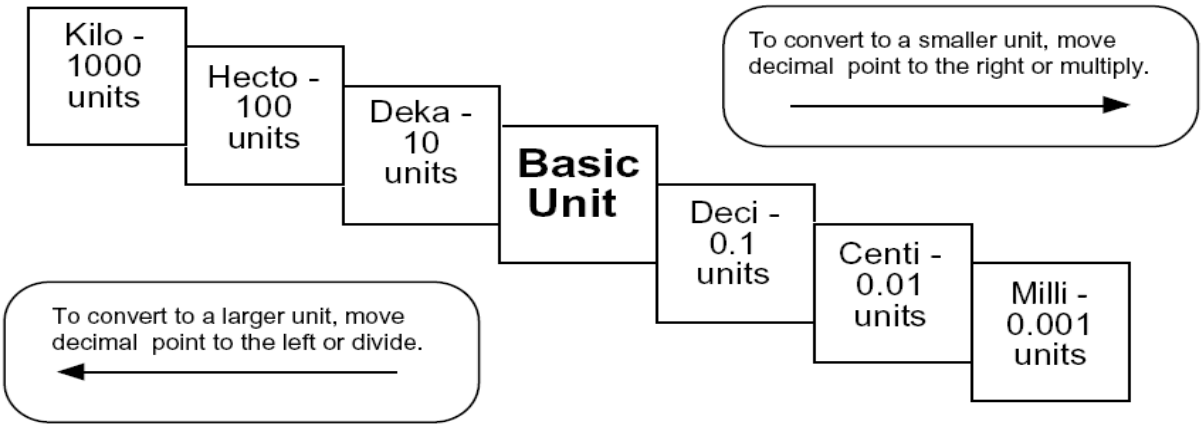


Figure 1.18: Metric system

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 _____ 4) Milliliter _____ 7) Kilometer _____

2) Meter _____ 5) Millimeter _____ 8) Centimeter _____

3) Gram _____ 6) Liter _____ 9) Milligram _____

Try these conversions, using the ladder method.

10) 2000 mg = _____ g 15) 5 L = _____ mL 20) 16 cm = _____ mm

11) 104 km = _____ m 16) 198 g = _____ kg 21) 2500 m = _____ km

12) 480 cm = _____ m 17) 75 mL = _____ L 22) 65 g = _____ mg

13) 5.6 kg = _____ g

18) 50 cm = _____ m

23) 6.3 cm = _____ mm

14) 8 mm = _____ cm

19) 5.6 m = _____ cm

24) 120 mg = _____ g

Compare using <, >, or =.

56 cm 6 m

7 g 698 mg

5 g 508 mg

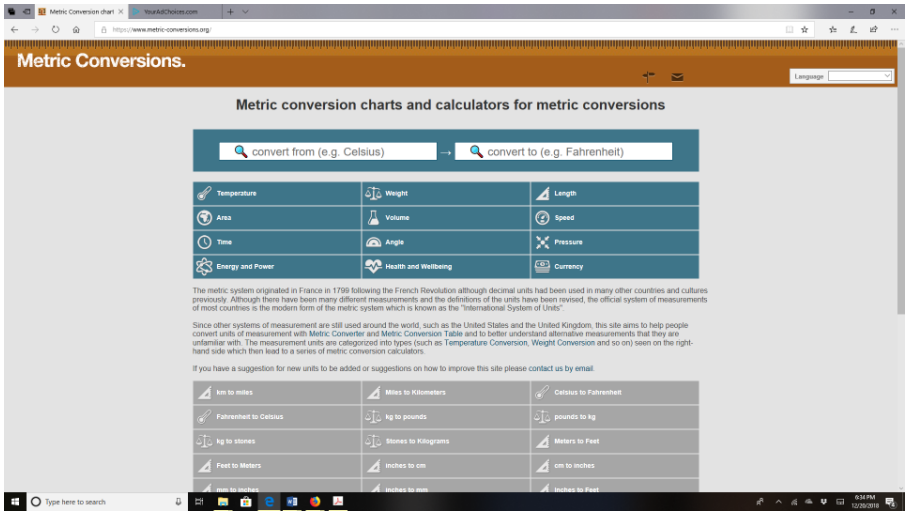
1,500 mL 1.5 L

536 cm 53.6 dm

43 mg 5 g

3.6 m 36 cm

<u>For more information visit</u>:



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

$0.1\ cm \times \frac{1\ inch}{2.54\ cm} = 0.0393\ in = 0.04\ in$ (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

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

Now plug in the numbers in tis problem:

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

Example#3: Convert 58.8 lbs to kg.

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

pathway: lbs * 1kg

1.205 lbs

now use the values given in the problem,

58.8 lbs * 1 kg = 26.7 kg

2.205

Below is the table with common English to metric equalities.

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 1.5: Conversion Table for Distance, Volume and Mass

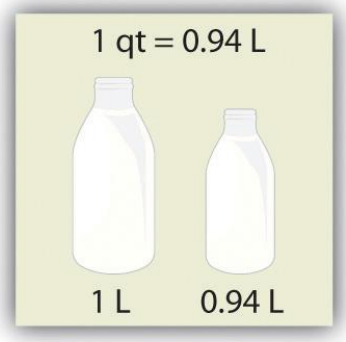
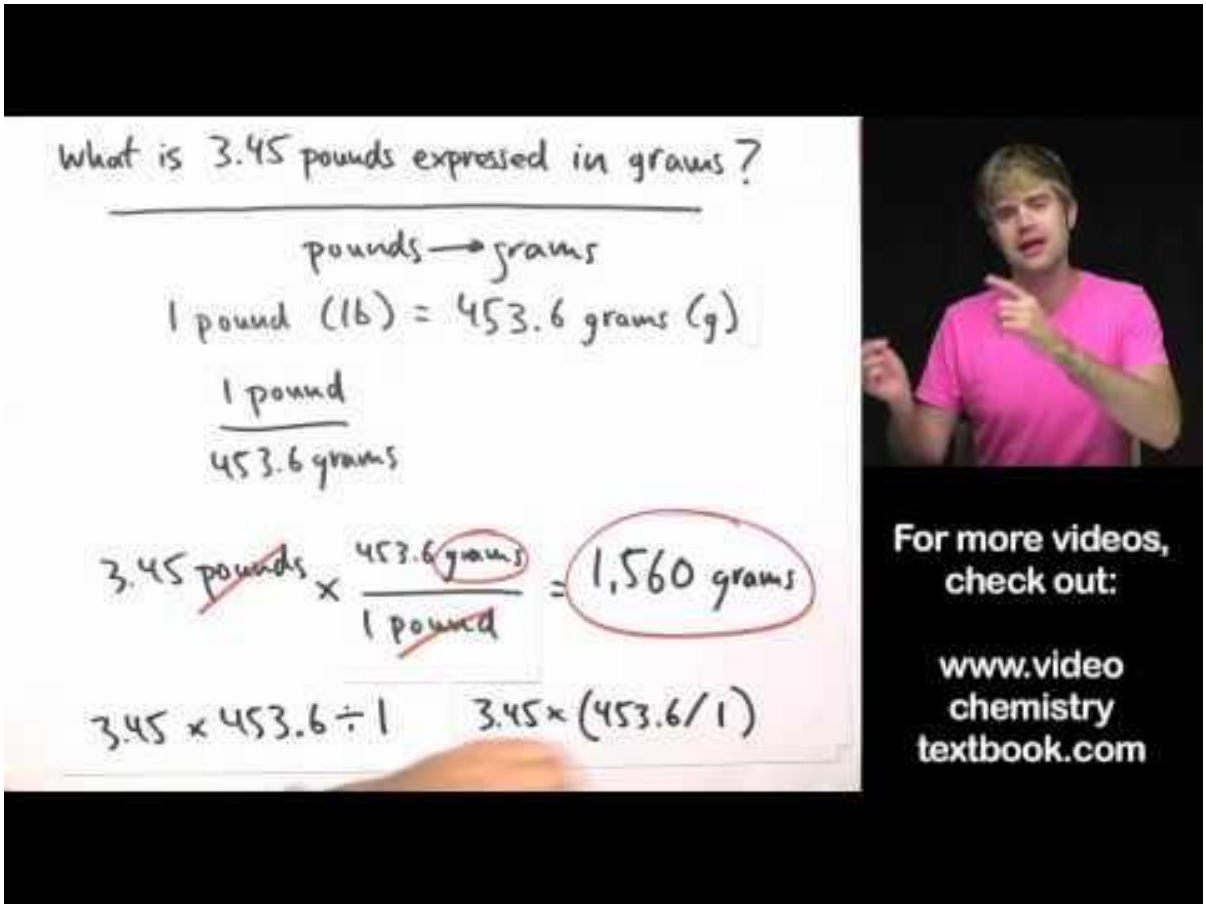


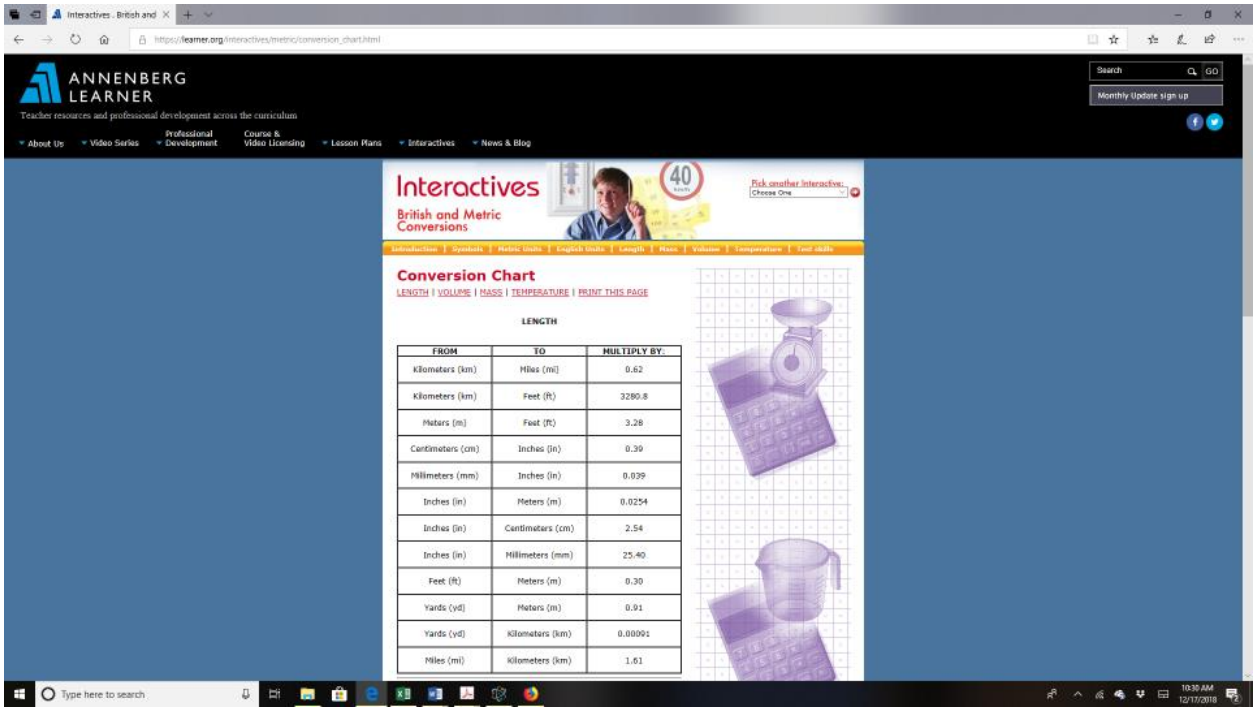
Figure 1.18: Milk bottles showing volume

For more information watch:



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

For more information visit:



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 milliliter, which is equal to a cubic centimeter. There are thus 1000 cm^3 in 1 dm^3, which is the same thing as saying there are 1000 mL in 1L. The conversion factor of 1 cm^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 = $1 cm^3$

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.

$3.6\ mm^3 \times (??)$

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.

$3.6\ mm^3 \times (1m / 1000\ mm)^3 \times (??)$

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.

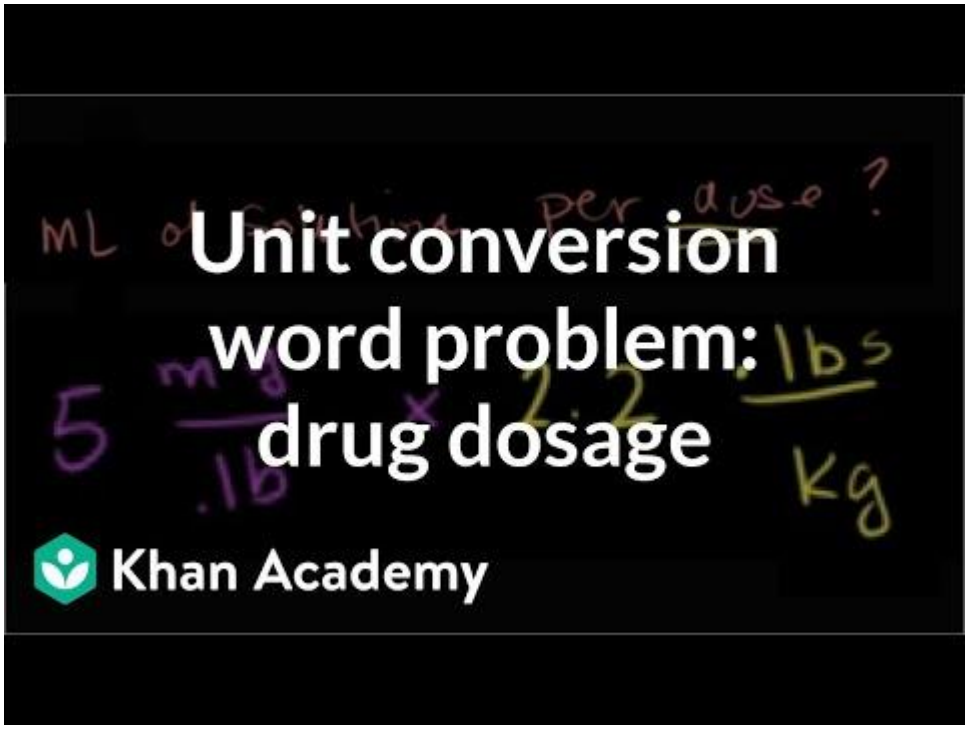
If you find that you forgot to cube numbers as well as units, you can setup the problem in an expanded form which is the equivalent to the previous method to cube the numerical values.

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.



https://www.youtube.com/watch?v=ScvuRb6vsz

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:

Total dosage required = Number of tablets required Dosage per tablet

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 $\frac{1}{3}$ 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 $\frac{500}{125} = 4$

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:

$\frac{\text{What you want}}{\text{What you've got}} \times \text{What it's in}$

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.

Total amount of liquid/tablets for day = Amount to be given per dose

Number of doses per day

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 involvinginfusion, 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:

$\frac{500}{10} \times 50 = 2500$ So the patient needs to receive 2500mls.

We now divide the amount to be given by the time to be taken: $\frac{25}{20} = 125$

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 in the form of grams per 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

5/10 1/20

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)

$= 1/2 \times 1000 = 500$.

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:

$$\frac{\text{What you want}}{\text{What it's in}} \times \text{What you've got}$$

This becomes

$$\frac{30}{} \times 100 = 150$$

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

(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: $\frac{3.28\ \text{ft}}{1\ \text{m}}$ & $\frac{0.6214\ \text{mi}}{1\ \text{km}}$

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

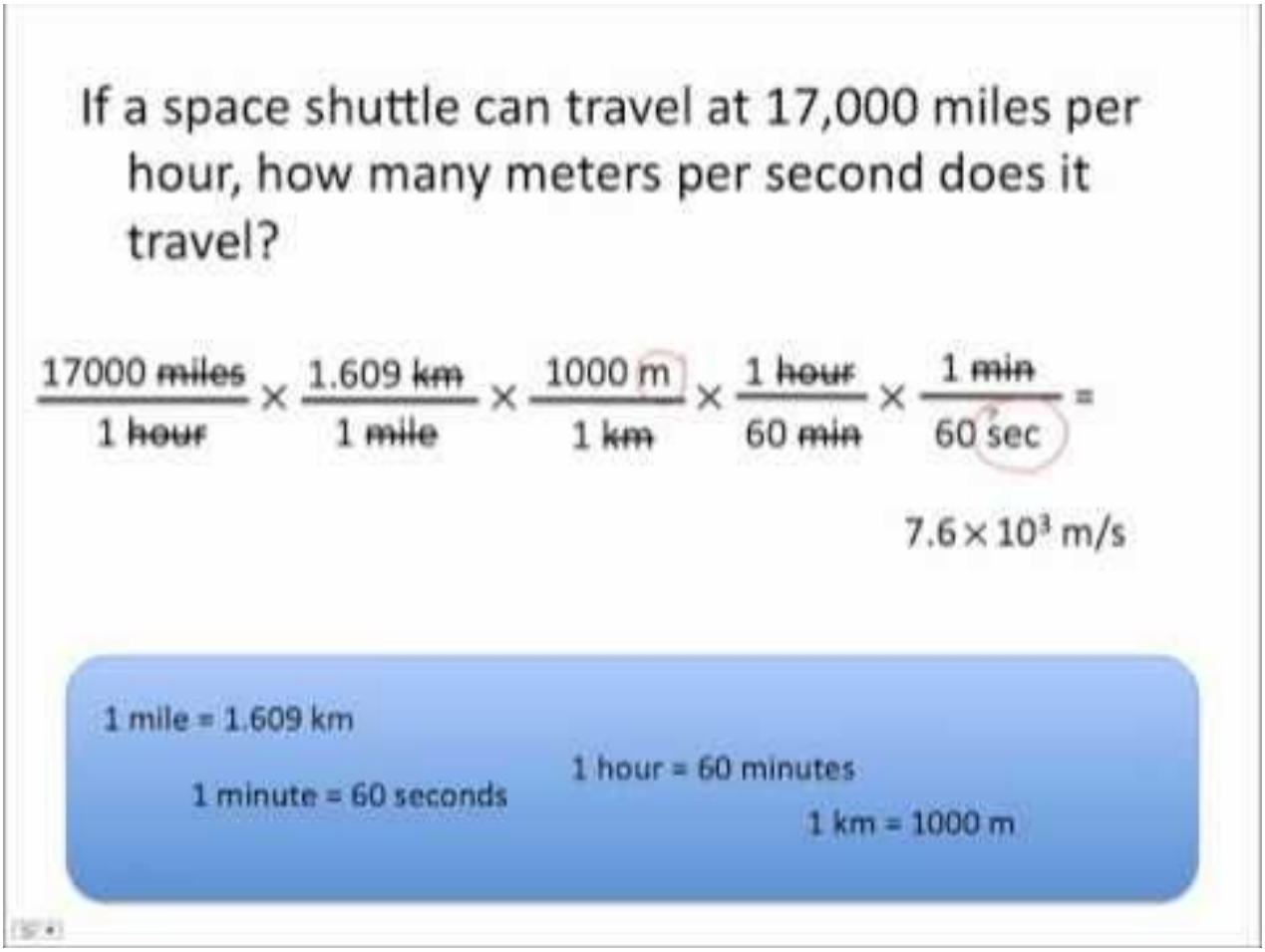
60 min 60 sec

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).

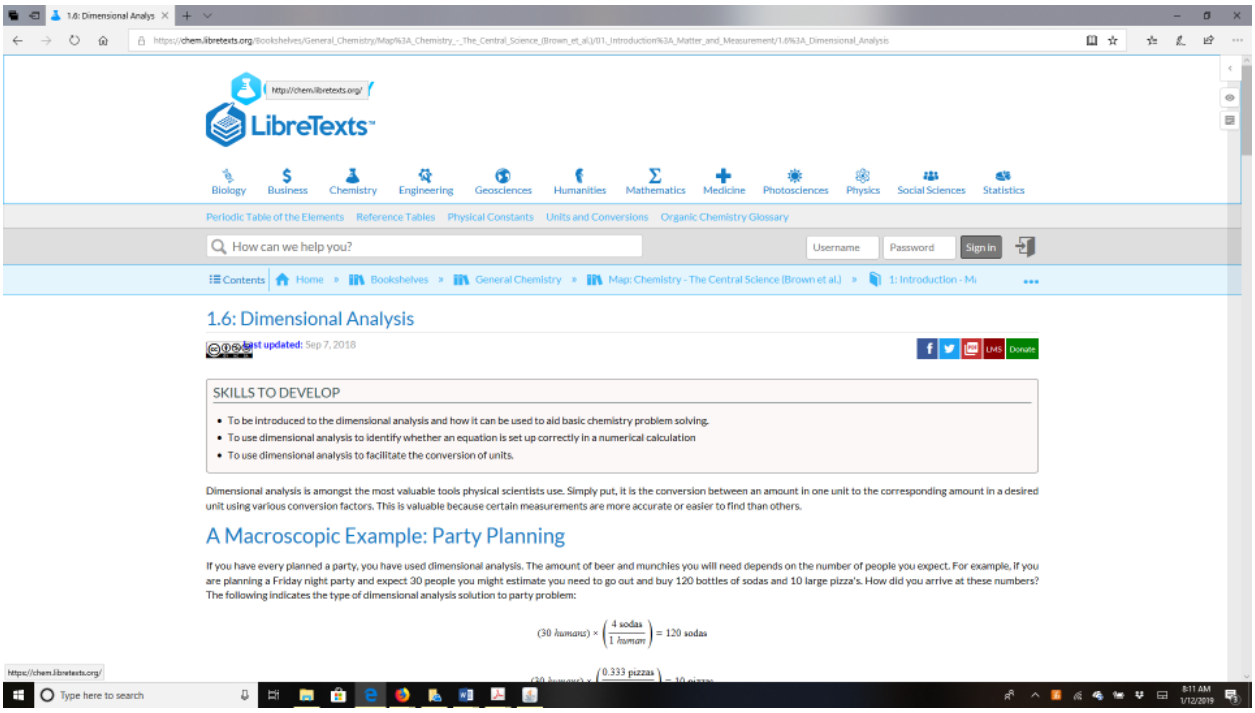
For more information watch this out:



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



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. Finallyyou 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

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

      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.

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.

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 ~~teaspoons of baking powder~~ x4.60 grams = 9.20 g

1.00 ~~teaspoons of baking powder~~

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 ~~Cups of butter~~ x 227.00 grams = 113.5 g

1.00 ~~Cup of butter~~

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 ~~Cups of sugar~~ x 200.00 grams = 150.00 g

1.00 ~~Cup of sugar~~

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.

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

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.

$$1\ \text{cup of milk} \times \frac{473.176\ \text{mL}}{2\ \text{cups of milk}} \times \frac{1.027\ \text{grams}}{1\ \text{mL}} = 242.98\ \text{g}$$

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 ~~tsp vanilla~~ x $\frac{0.15\ \text{~~fl. ounce~~}}{1\ \text{~~tsp~~}}$ *x* $\frac{28.35\ \text{grams}}{1\ \text{~~fl. ounce~~}}$ *= 4.25 g*

s. 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:

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

°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.

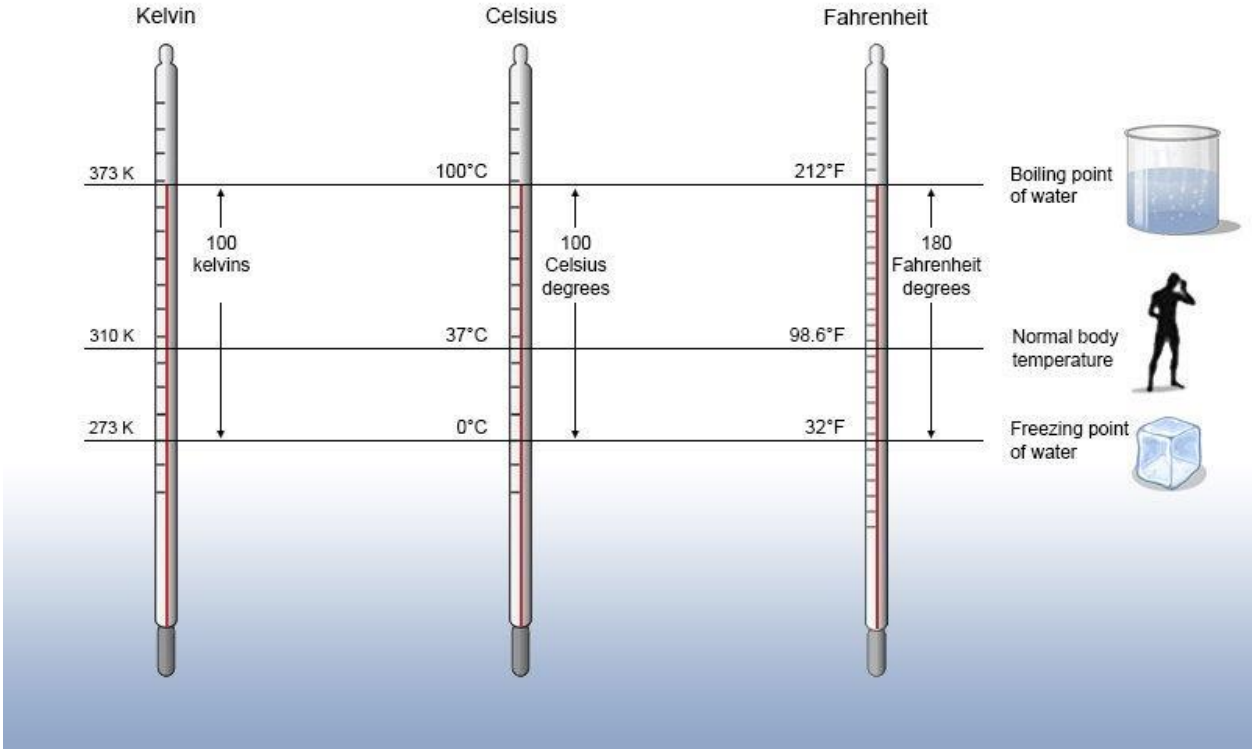
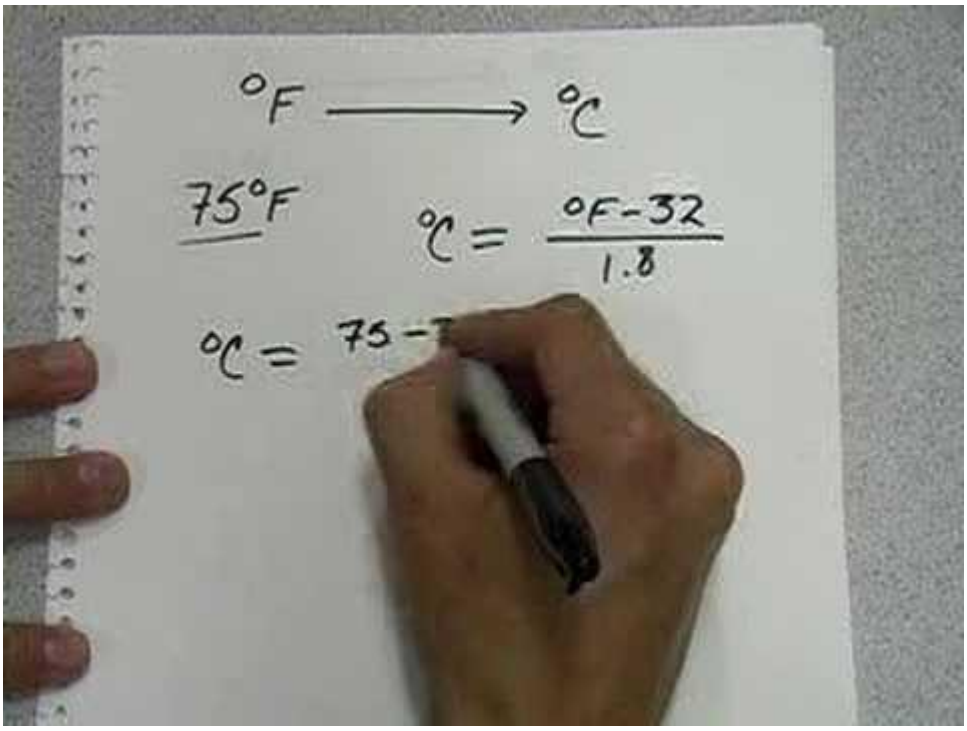


Figure 1.19: Comparision of Temperature in Three Different Units

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°C

Applying the formula: Tf= 1.8Tc+ 32

1.8*61.5 +32= 142.7= 143°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. 12^0F
   b. 32^0F
   c. 40^0F
   d. 212^0F

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

Sample	Volume (mL)	Mass (g)
E	499	438.7

Substance	Density (g/cm3)
benzene	0.8787
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^{0} yards.

45. Determine the number of meters in 1.00 mile.

46. The speed of light is 1.86 x 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 x 10^3 angstroms by 1.0 x 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 Chemical Formulas

2.5 The Periodic Table

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 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.

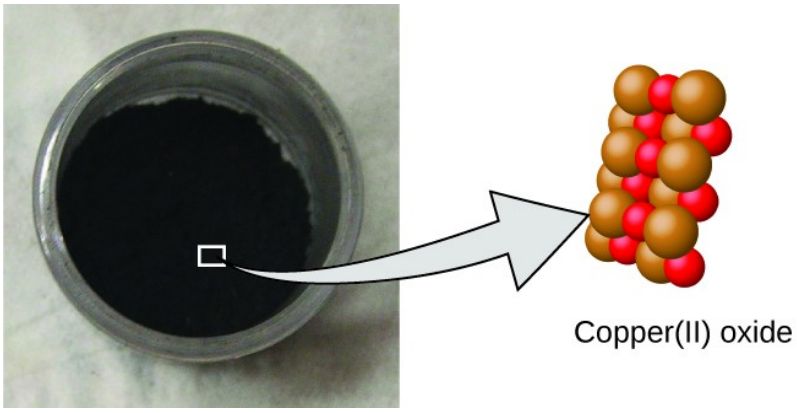


Figure 2. Copper (II) oxide, a powdery, black compound, results from the combination of two types of atoms—copper (brown spheres) and oxygen (red spheres)—in a 1:1 ratio.

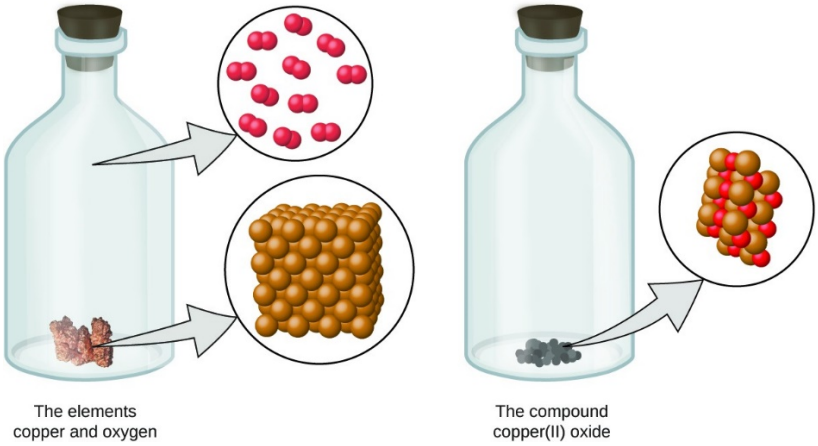
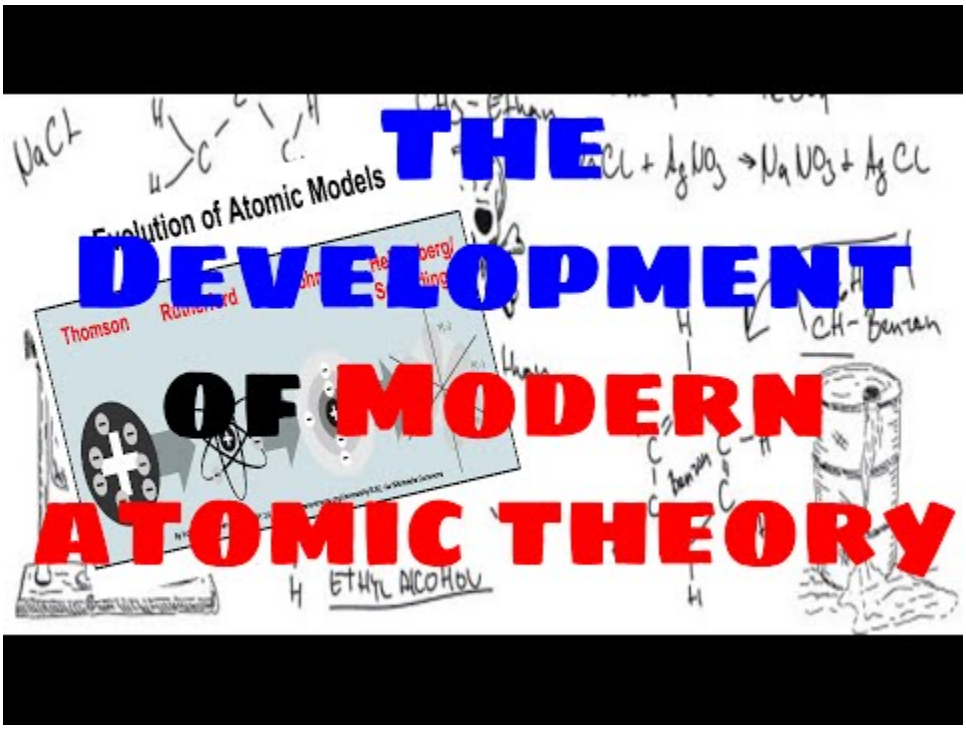


Figure 3. When the elements copper (a shiny, red-brown solid, shown here as brown spheres) and oxygen (a clear and colorless gas, shown here as red spheres) react, their atoms rearrange to form a compound containing copper and oxygen (a powdery, black solid).

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).



https://www.youtube.com/watch?v=nQjkOy7OgMo

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?

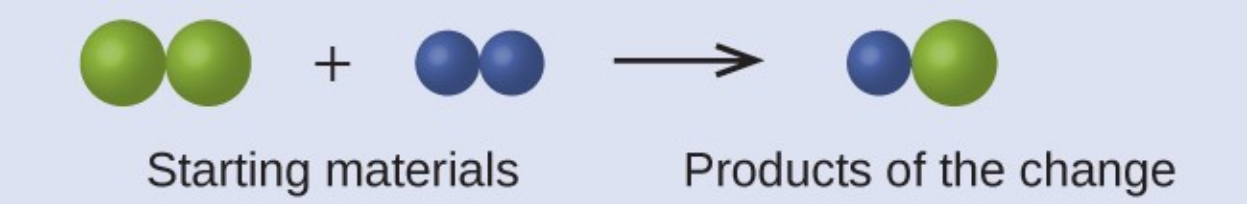


Figure 4: Simple Chemical Reaction

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).

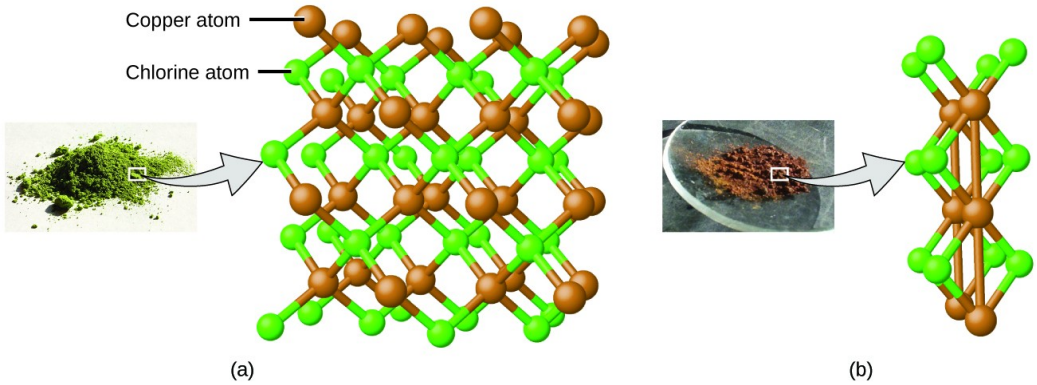


Figure 4. Compared to the copper chlorine compound in (a), where copper is represented by brown spheres and chlorine by green spheres, the copper chlorine compound in (b) has twice as many chlorine atoms per copper atom.

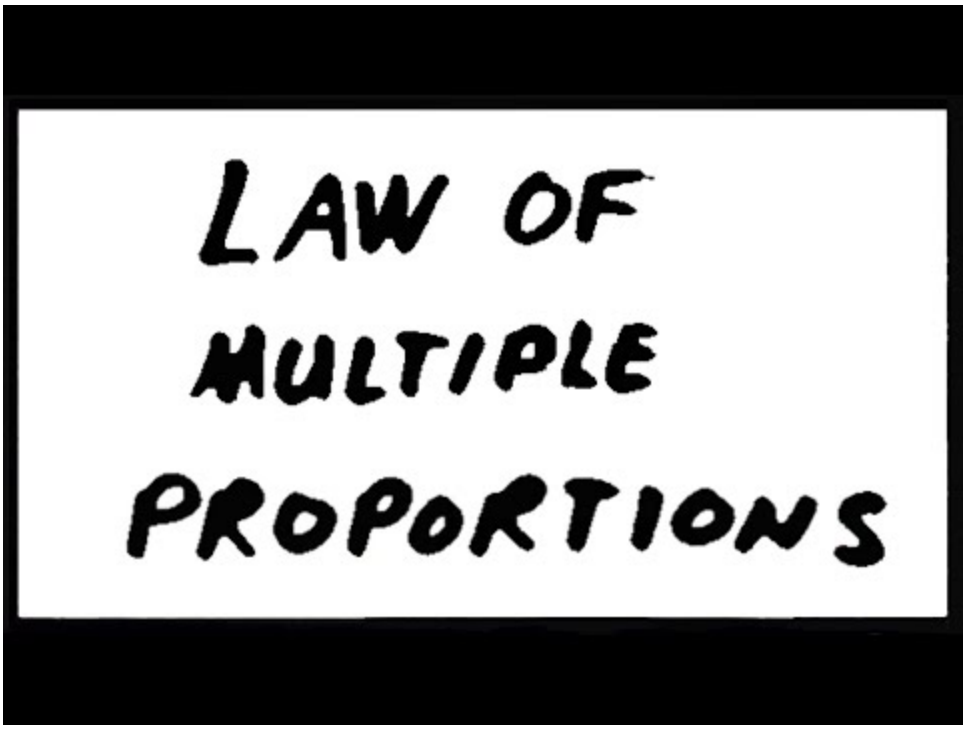
Example 2: Law of definite and multiple proportions

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.

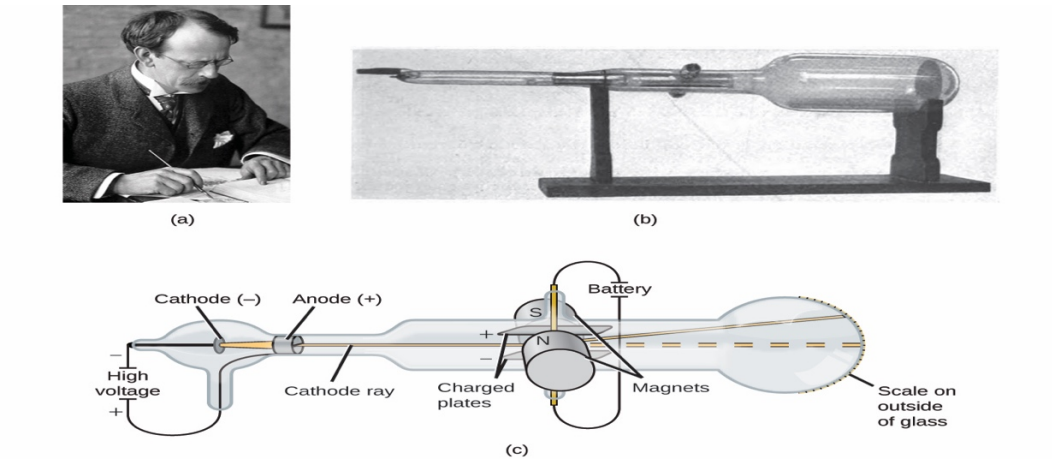
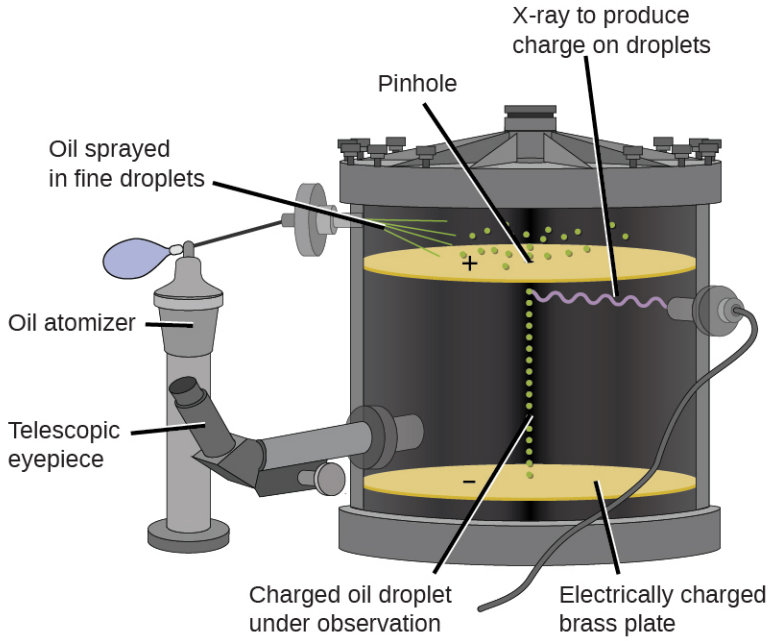


Figure 5. (a) J. J. Thomson produced a visible beam in a cathode ray tube. (b) This is an early cathode ray tube, invented in 1897 by Ferdinand Braun. (c) In the cathode ray, the beam (shown in yellow) comes from the cathode and is accelerated past the anode toward a fluorescent scale at the end of the 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.

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 i*on*."

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 6. Millikan's experiment measured the charge of individual oil drops. The tabulated data are examples of a few possible values.

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.

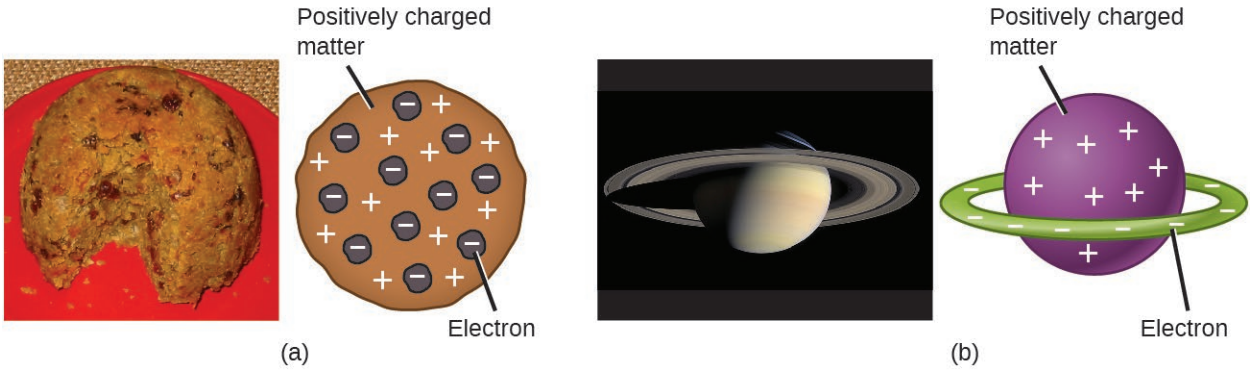


Figure 7. (a) Thomson suggested that atoms resembled plum pudding, an English dessert consisting of moist cake with embedded raisins ("plums"). (b) Nagaoka proposed that atoms resembled the planet Saturn, with a ring of electrons surrounding a positive "planet."

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".

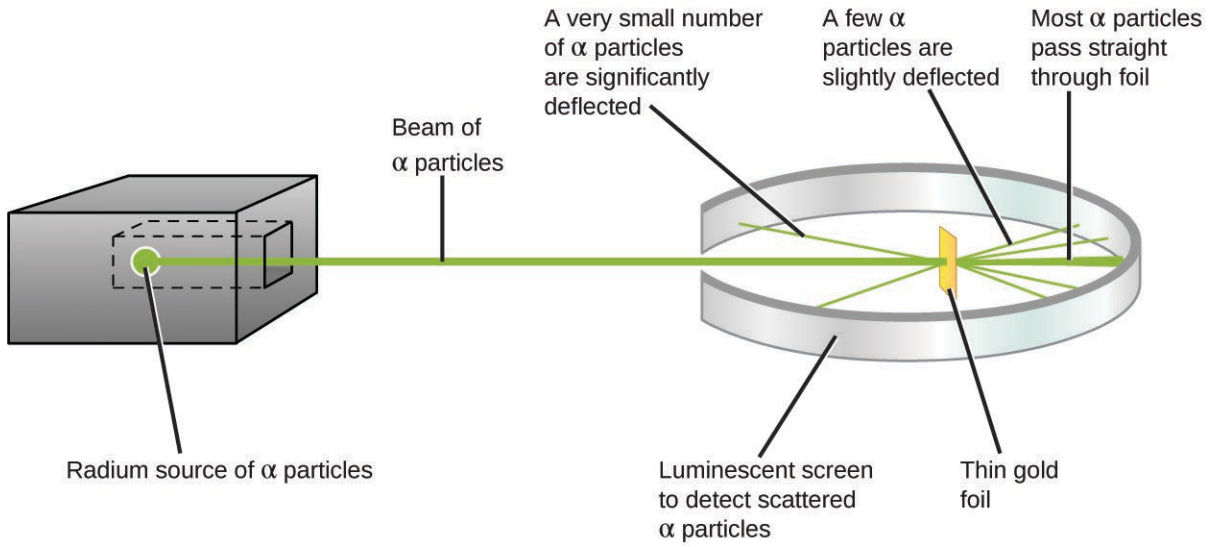


Figure 8. Geiger and Rutherford fired α particles at a piece of gold foil and detected where those particles went, as shown in this schematic diagram of their experiment. Most of the particles passed straight through the foil, but a few were deflected slightly and a very small number were significantly deflected.

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.

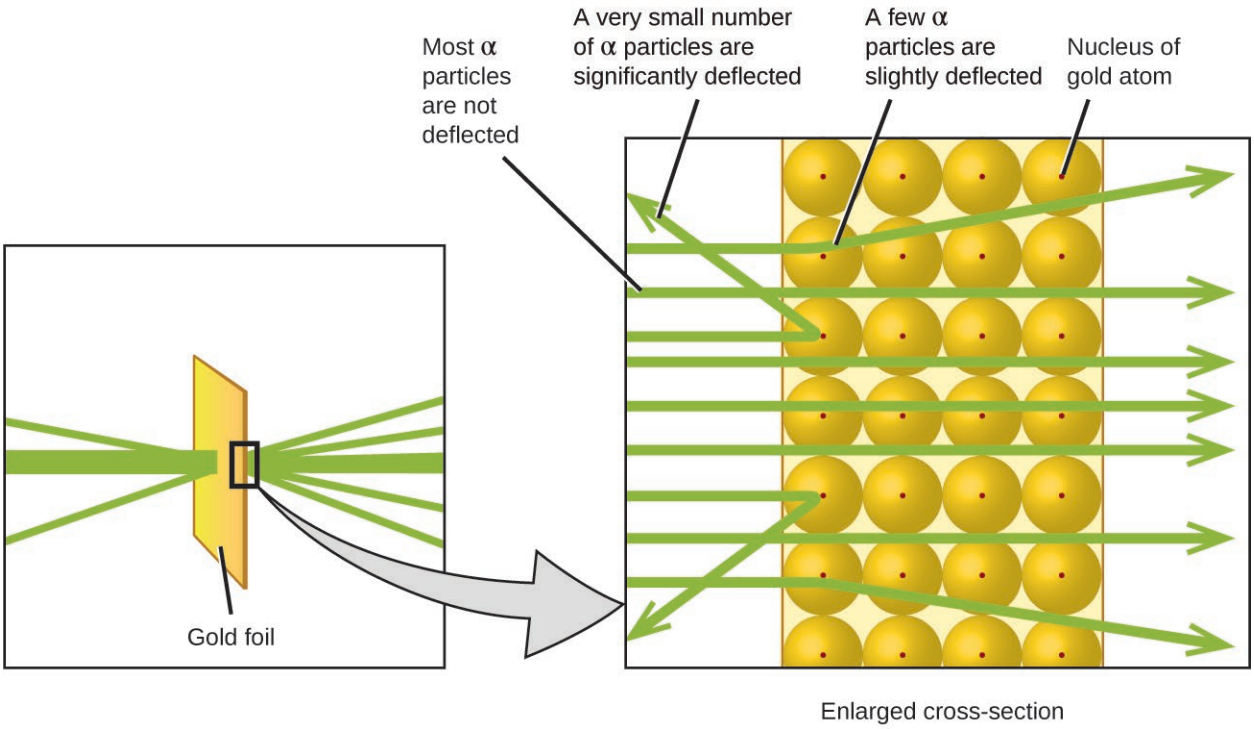
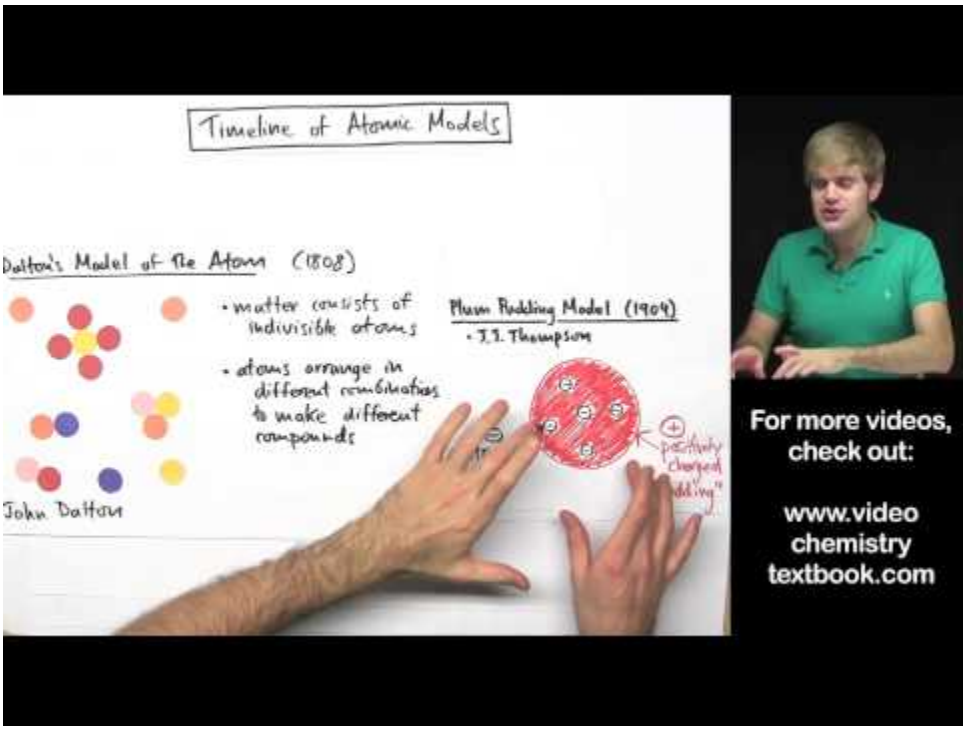


Figure 9. The α particles are deflected only when they collide with or pass close to the much heavier, positively charged gold nucleus. Because the nucleus is very small compared to the size of an atom, very few α particles are deflected. Most pass through the relatively large region occupied by electrons, 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.

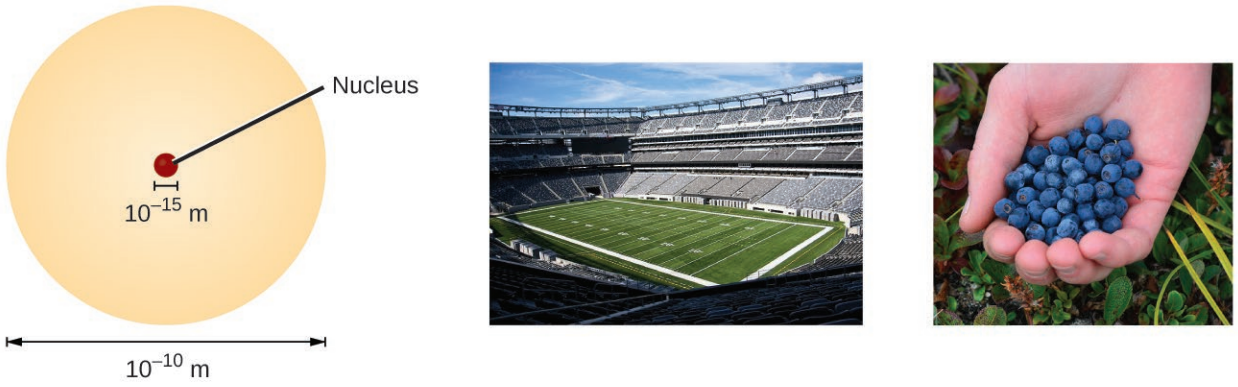


Figure 10. If an atom could be expanded to the size of a football stadium, the nucleus would be the size of a single blueberry.

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 = 1.602×10^{-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}

Properties of Subatomic Particles					
Name	Location	Charge (C)	Unit Charge	Mass (amu)	Mass (g)
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

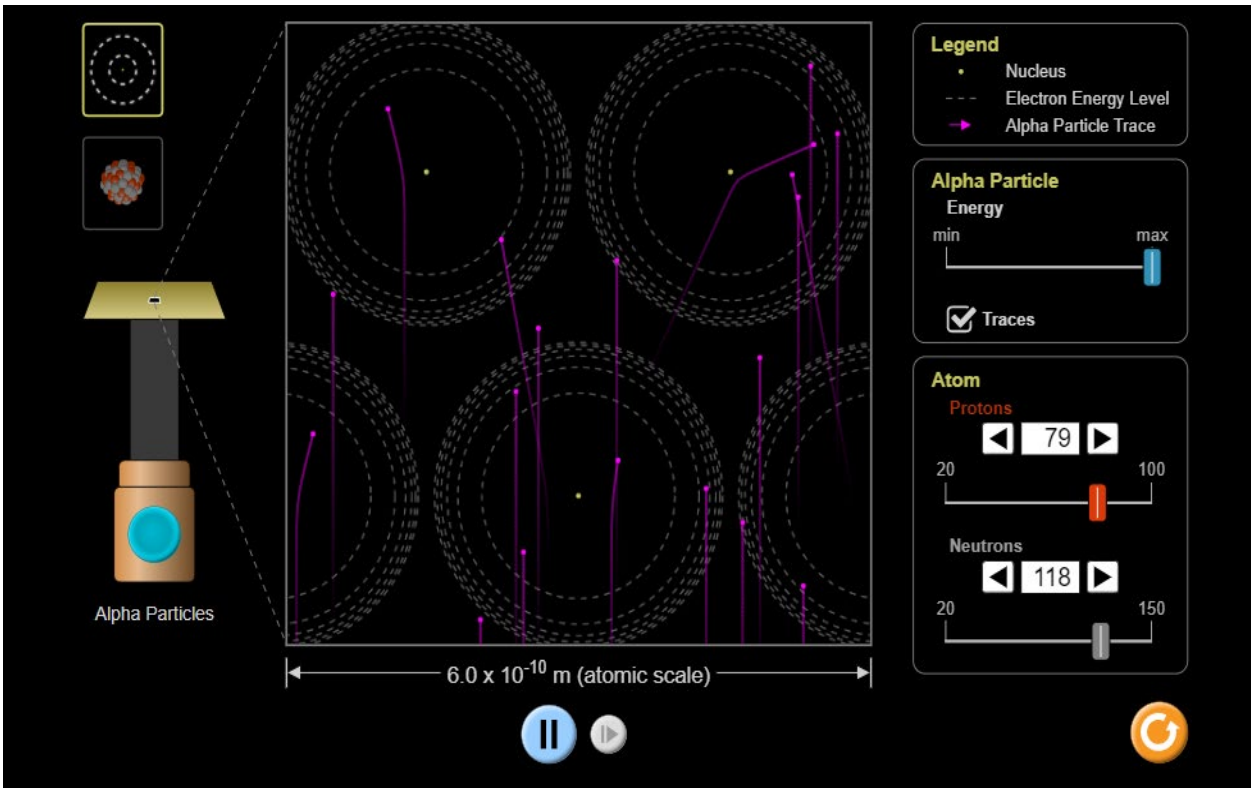


Figure 12A: Phet Simulation

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

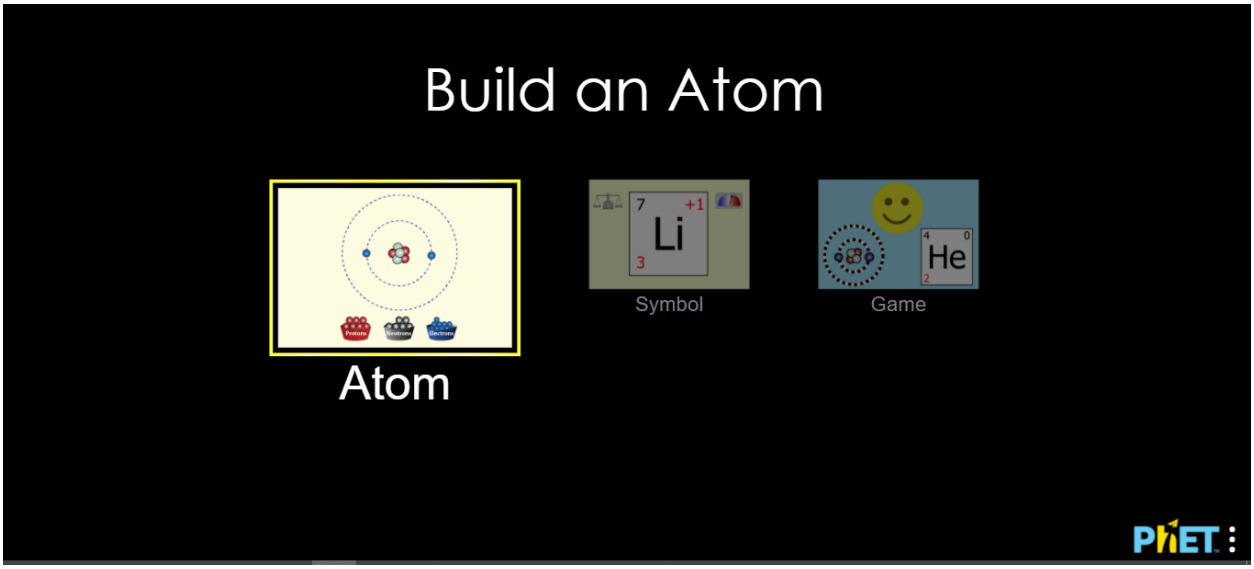


Figure 12: Phet Simulation

- Go to the above activity and hide the mass number box and net charge box
- Drag and drop 7 protons and 7 neutrons from the bucket and put in in the nucleus
- Which element is this?
- What is the atomic number and mass number of the element?
- Now put 6 electrons and predict the charge
- Open the Mass number box, net charge box, click on the element and compare your result
- 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.

(a) (b)

Figure 13: Goiter, a disease caused by deficiency of Iodine in diet

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 11. The element of mercury, its chemical symbol is Hg.

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*)
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

Some Common Elements and Their Symbols			
Element	Symbol	Element	Symbol
fluorine	F	silver	Ag (from *argentum*)
gold	Au (from *aurum*)	sodium	Na (from *natrium*)
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.

Isotopes

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.

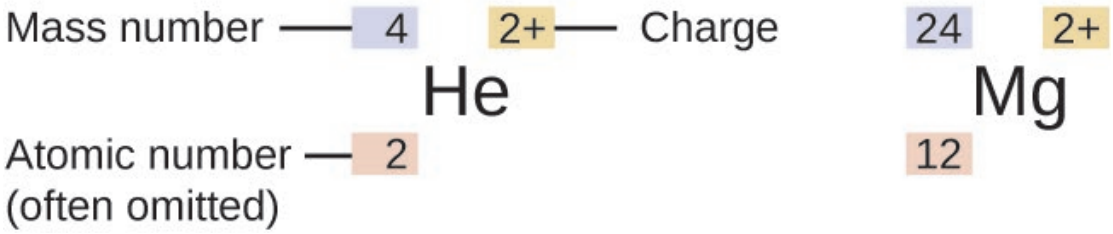


Figure 12. Chemical symbols for atoms.

Atomic Mass

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

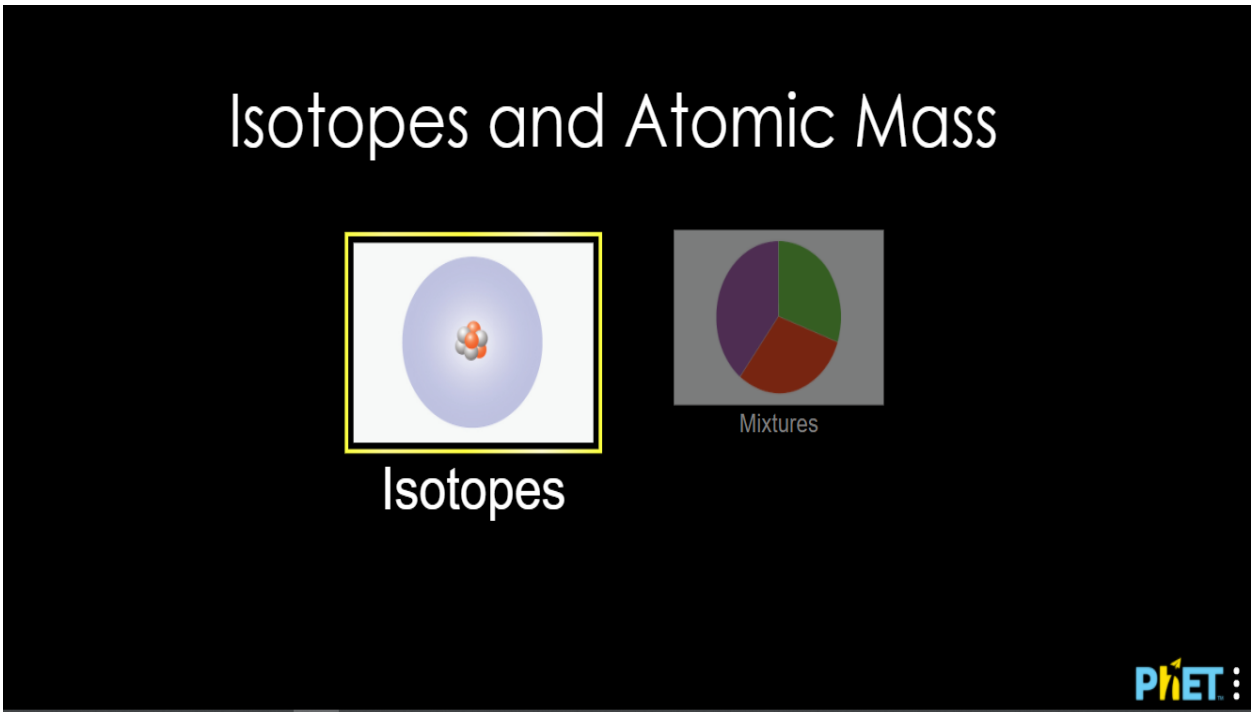


Figure 13: Phet Simulation

- Go to the above activity and click on the mixture.
- Pick the element Nitrogen.
- Drag and drop one atom of each isotope of Nitrogen and then click on Nature's mix.
- Hide the percent composition and average atomic mass boxes.
- Now estimate percent abundance from the visual represented and calculate average atomic mass.
- Open the Percent composition and average atomic mass boxes.
- Compare your value with the values provided in the boxes.

Section 2.4: Chemical Formulas

A molecular formula is a representation of a molecule that uses chemical symbols to indicate the types of atoms followed by subscripts to show the number of atoms of each type in the molecule. (A subscript is used only when more than one atom of a given type is present.) Molecular formulas are also used as abbreviations for the names of compounds.

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.

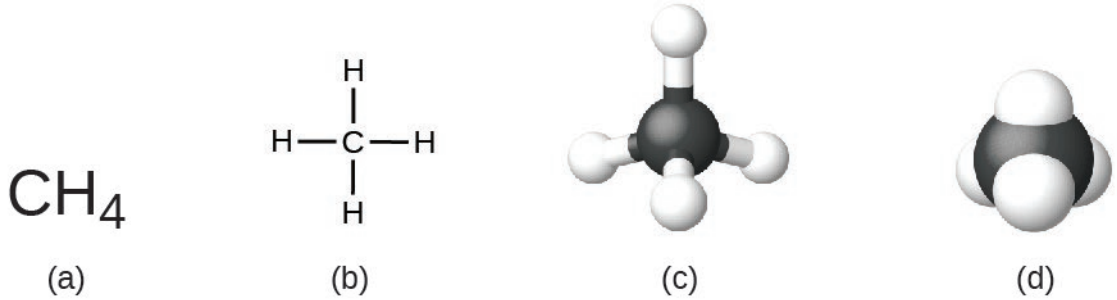


Figure 13. A methane molecule can be represented as (a) a molecular formula, (b) a structural formula, (c) a ball-and-stick model, and (d) a space-filling model. Carbon and hydrogen atoms are represented by black and white spheres, respectively.

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).

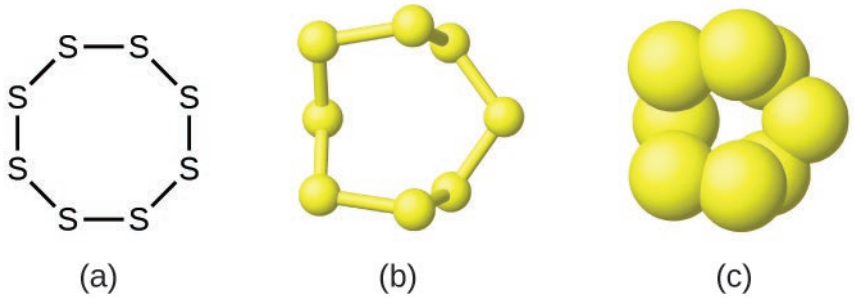


Figure 14. A molecule of sulfur is composed of eight sulfur atoms and is therefore written as S_8. It can be represented as (a) a structural formula, (b) a ball-and-stick model, and (c) a space-filling model. Sulfur atoms are represented by yellow spheres.

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).

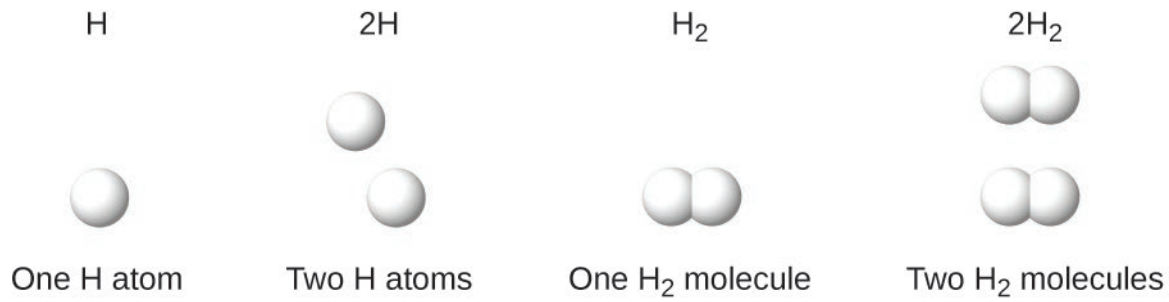


Figure 15. The symbols H, 2H, H_2, and $2H_2$ represent very different entities.

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).

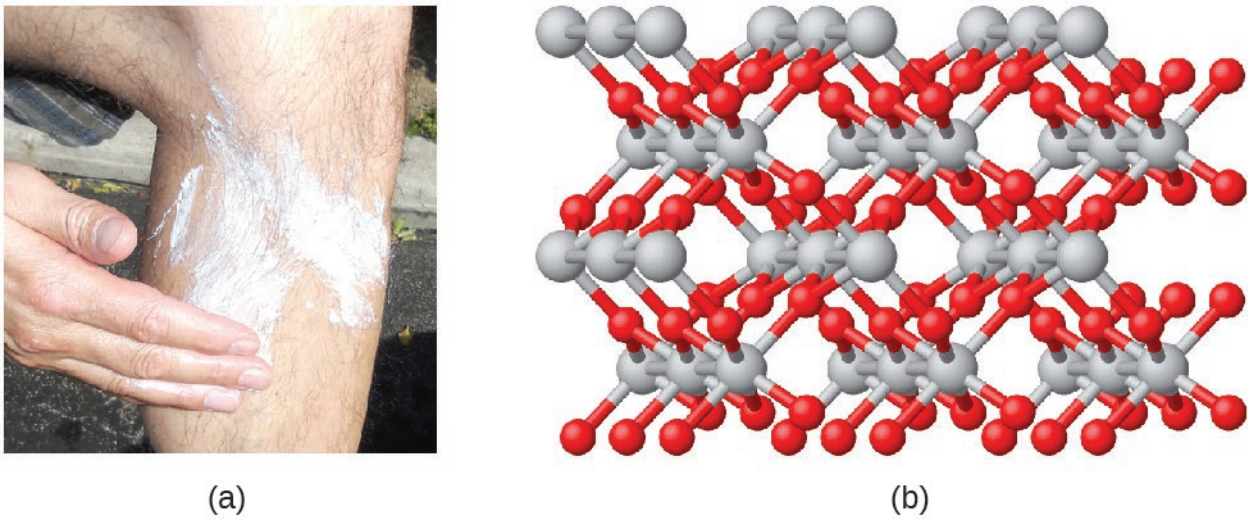


Figure 16. (a) The white compound titanium dioxide provides effective protection from the sun. (b) A crystal of titanium dioxide, TiO_2, contains titanium and oxygen in a ratio of 1 to 2. The titanium atoms are gray and the oxygen atoms are red. (credit a: modification of work by "osseous"/Flickr).

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).

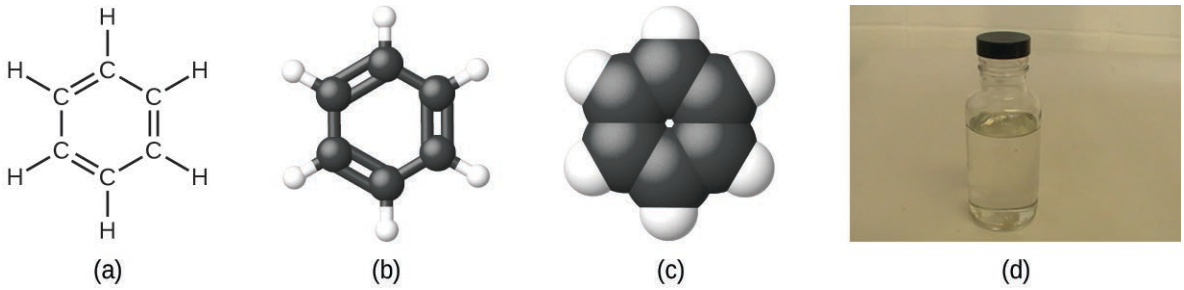


Figure 17. Benzene, C_6H_6, is produced during oil refining and has many industrial uses. A benzene molecule can be represented as (a) a structural formula, (b) a ball-and-stick model, and (c) a space-filling model. (d) Benzene is a clear liquid.

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.

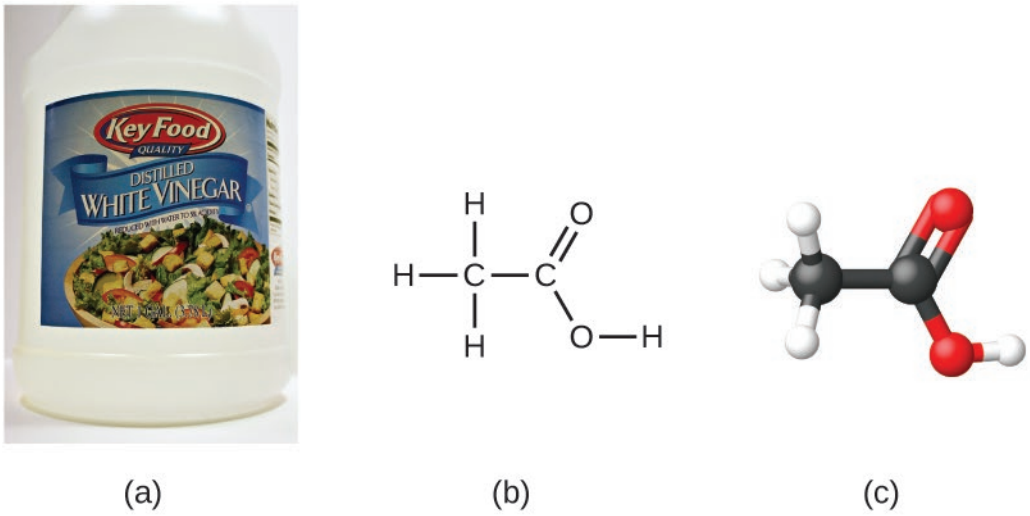


Figure 18. (a) Vinegar contains acetic acid, $C_2H_4O_2$, which has an empirical formula of CH_2O. It can be represented as (b) a structural formula and (c) as a ball-and-stick model.

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.

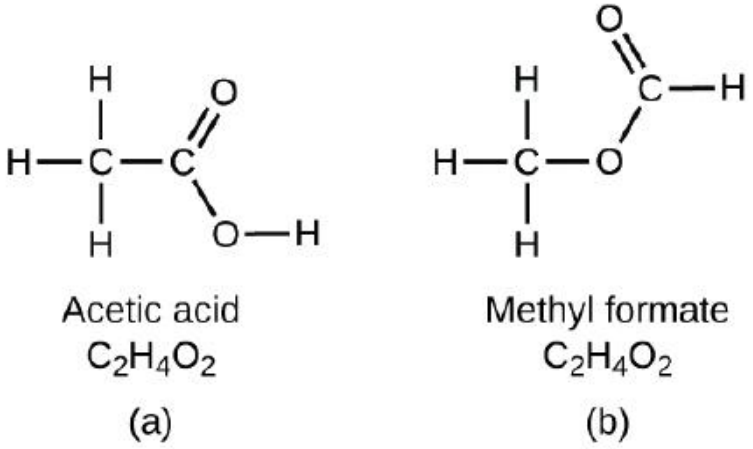


Figure 19. Molecules of (a) acetic acid and methyl formate (b) are structural isomers; they have the same formula ($C_2H_4O_2$) but different structures (and therefore different chemical properties).

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.

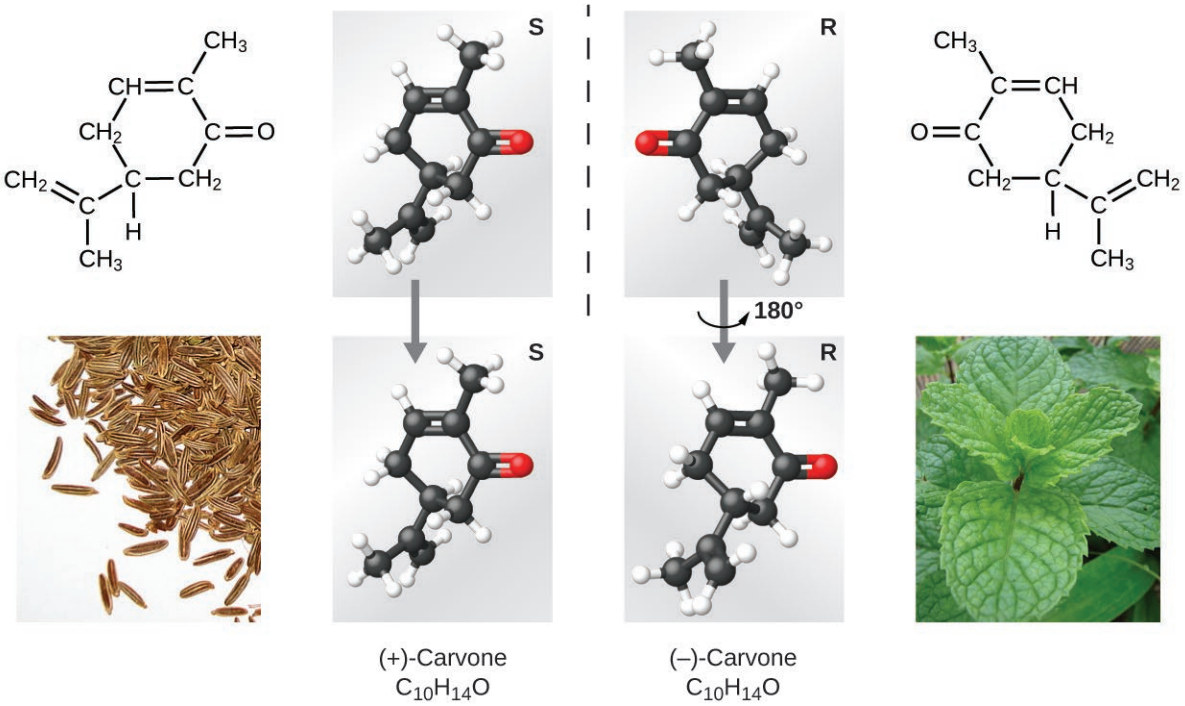


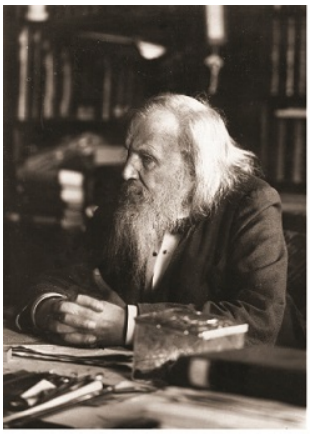
Figure 20: Molecules of carvone are spatial isomers; they only differ in the relative orientations of the atoms in space.

Section 2.5: 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 21).



(a)

Reihen	Gruppo I. — R'0	Gruppo II. — RO	Gruppo III. — R'0³	Gruppo IV. RH⁴ RO²	Gruppo V. RH³ R'0⁵	Gruppo VI. RH² RO³	Gruppo VII. RH R'0⁷	Gruppo VIII. — RO⁴
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	—	— — — —

(b)

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.

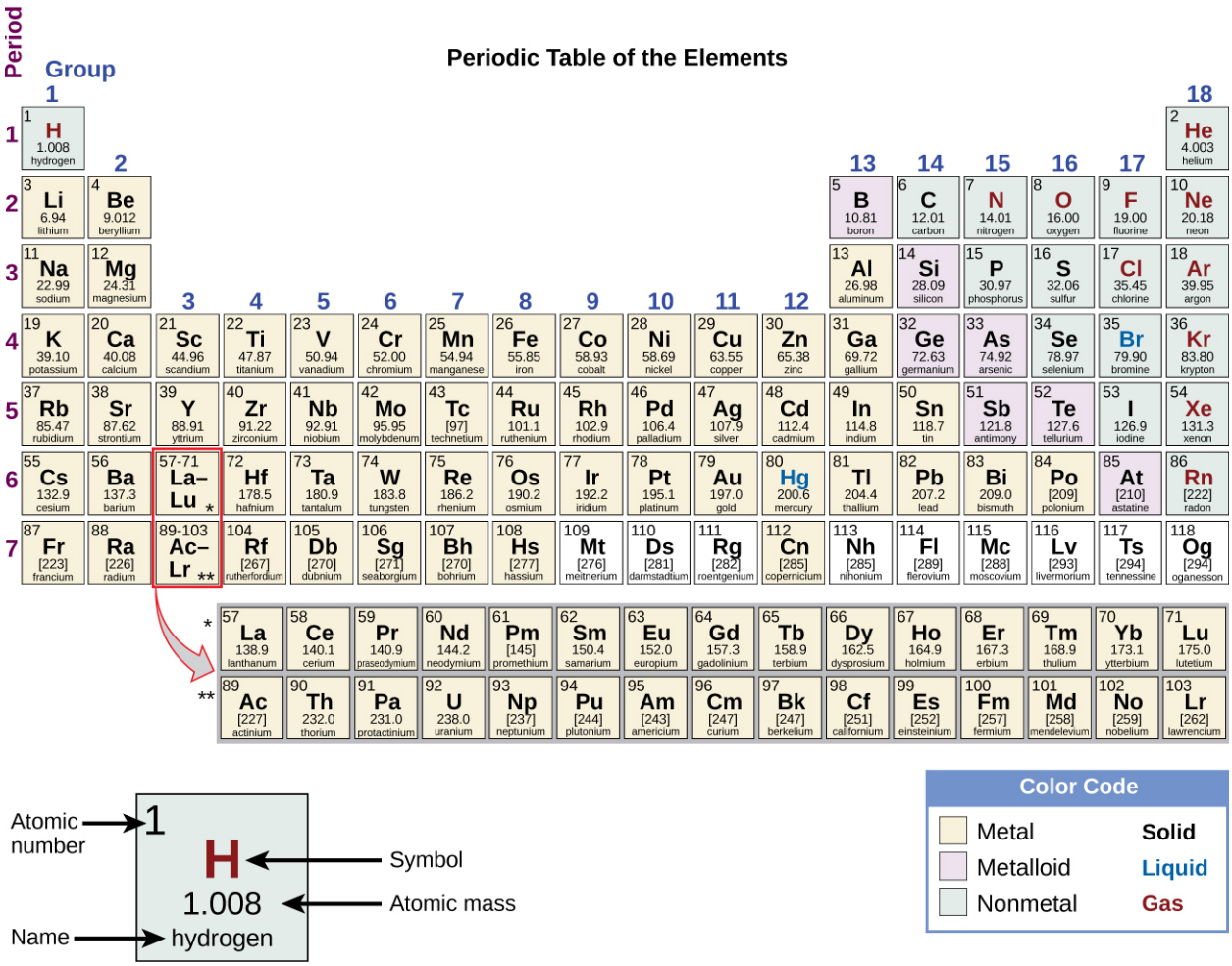


Figure 22. Elements in the periodic table are organized according to their properties.

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.

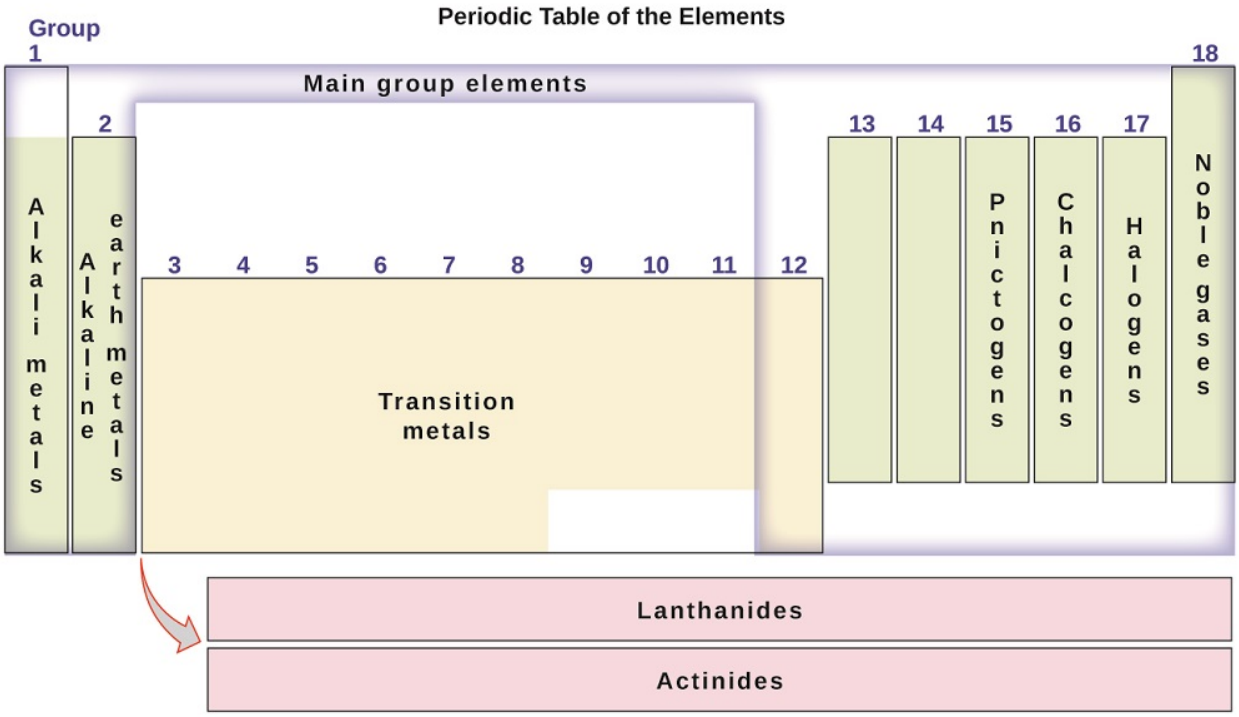


Figure 23: The periodic table organizes elements with similar properties into groups.

Example 6: Naming Groups of Elements

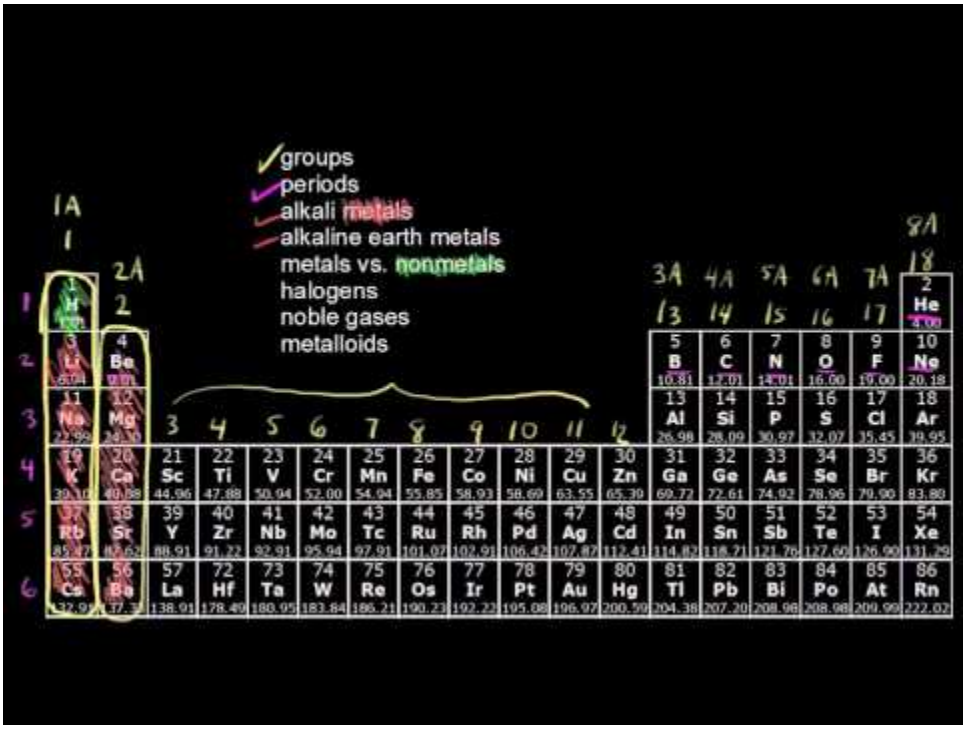
Atoms of each of the following elements are essential for life. Give the group name for the following elements:

chlorine
calcium
sodium
sulfur

Solution

The family names are as follows:

halogen
alkaline earth metal
alkali metal
chalcogen



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.

Figure 24: Periodic table with Atomic Masses of Elements

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.

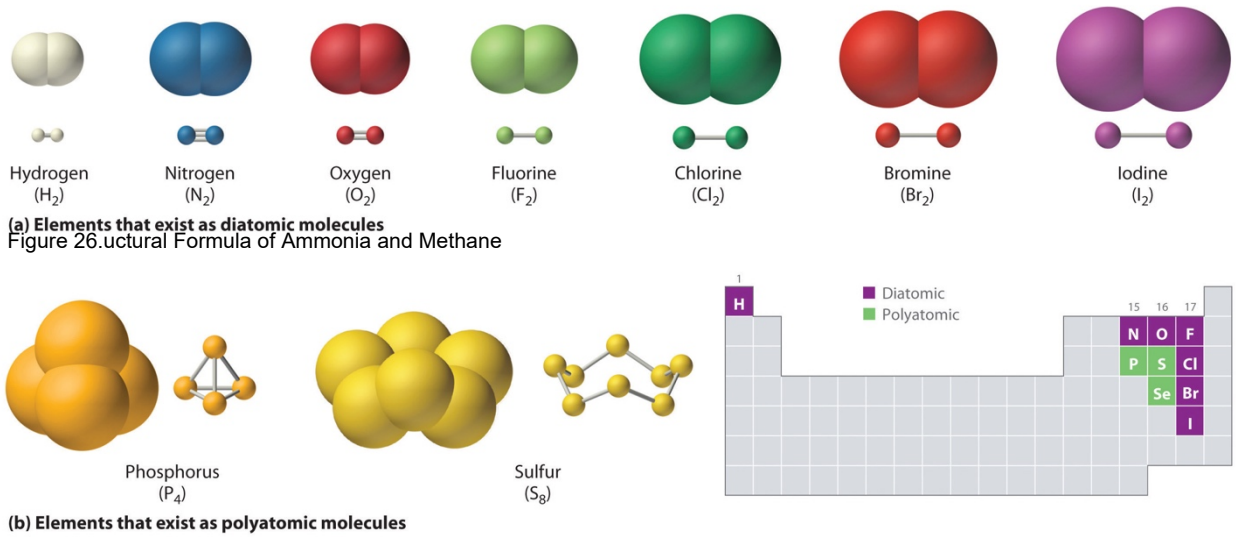


Figure 26.uctural Formula of Ammonia and Methane

Figure 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.

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.

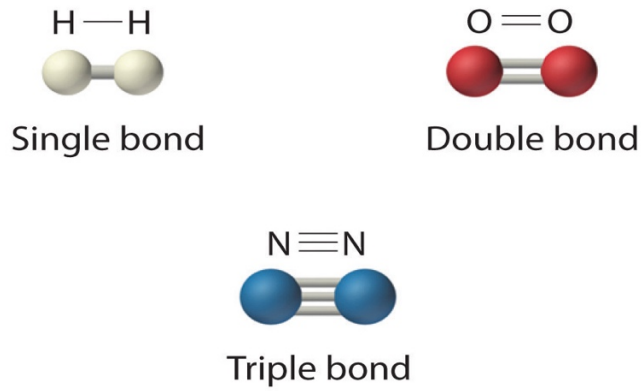


Figure 25. Hydrogen (H_2) has a single bond between atoms. Oxygen (O_2) has a double bond between atoms, indicated by two lines (=). Nitrogen (N_2) has a triple bond between atoms, indicated by three lines (≡). Each bond represents an electron pair.

The structural formula for water can be drawn as follows:

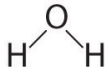


Figure 26.A: Water molecule

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:

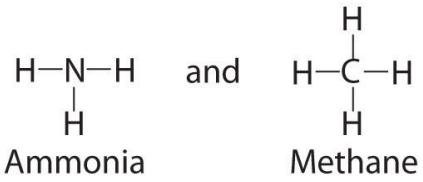


Figure 26.B: Structural Formula of Ammonia and Methane

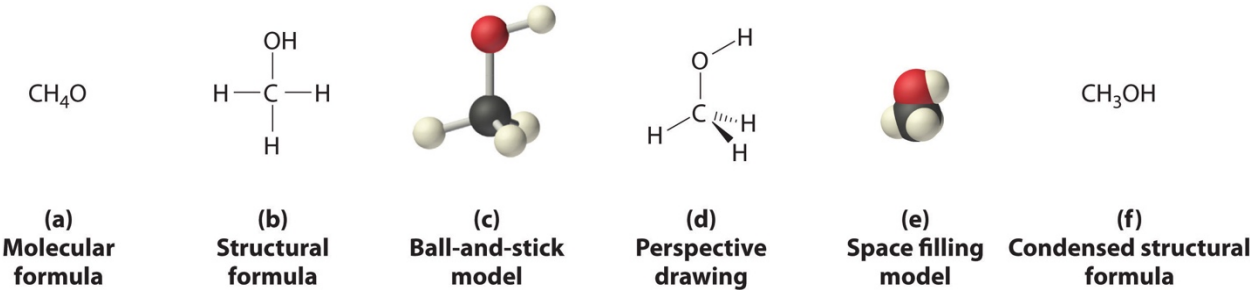


Figure 26. Different ways of representing the structure of a molecule (a) The molecular formula for methanol gives only the number of each kind of atom present. (b) The structural formula shows which atoms are connected. (c) The ball-and-stick model shows the atoms as spheres and the bonds as sticks. (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.

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.

A. Each molecule of sulfur monochloride has two sulfur atoms and two chlorine atoms. Because it does not contain mostly carbon and hydrogen, it is an inorganic compound.
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.

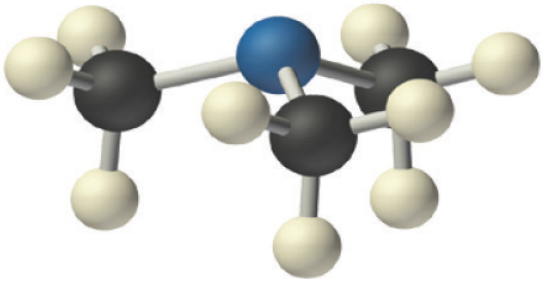


Figure 26.C: Ball and Stick Model

Trimethylamine

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.

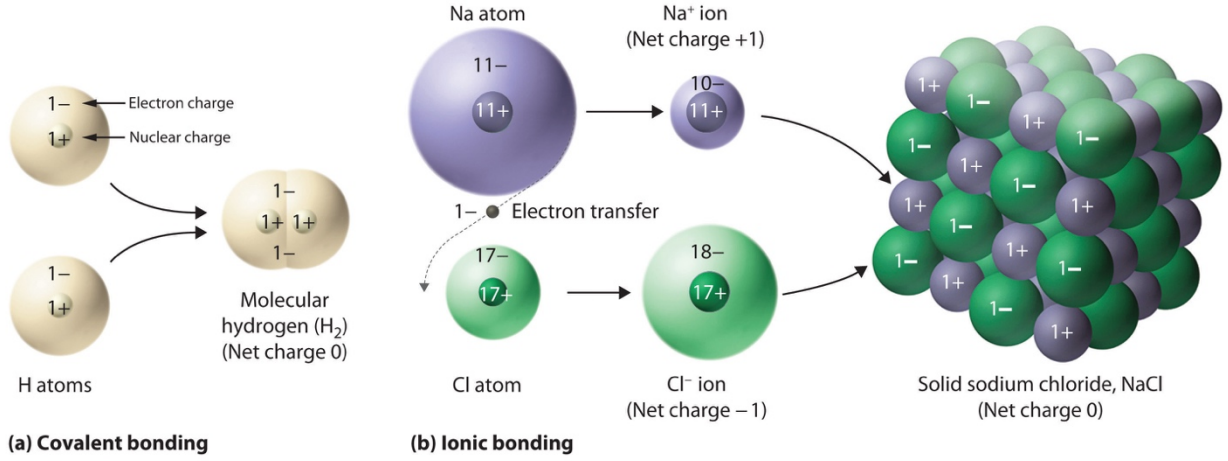


Figure 27. Comparison of covalent and ionic bonding. (a) In molecular hydrogen (H_2), two hydrogen atoms share two electrons to form a covalent bond. (b) The ionic compound NaCl forms when electrons from sodium atoms are transferred to chlorine atoms. The resulting Na^+ and Cl^- ions form a three-dimensional solid that is held together by attractive electrostatic interactions.

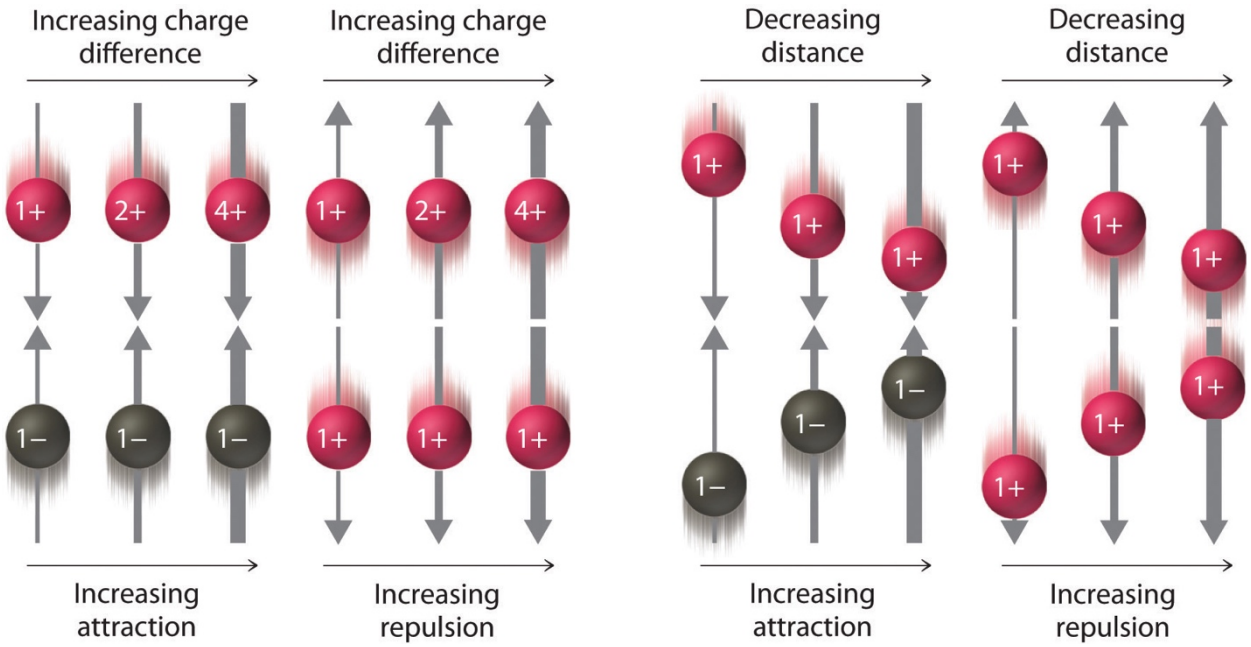


Figure 28. As the charge on ions increases or the distance between ions decreases, so does the strength of the attractive (−…+) or repulsive (−…− or +…+) interactions. The strength of these interactions is represented by the thickness of the arrows.

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	O^{2-} oxide	F^- fluoride

Group 1	Group 2	Group 3	Group 13	Group 15	Group 16	Group 17
				(azide)		
Na^+ sodium	Mg^{2+} magnesium		Al^{3+} aluminum	P^{3-} phosphide	S^{2-} sulfide	Cl^- chloride
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:

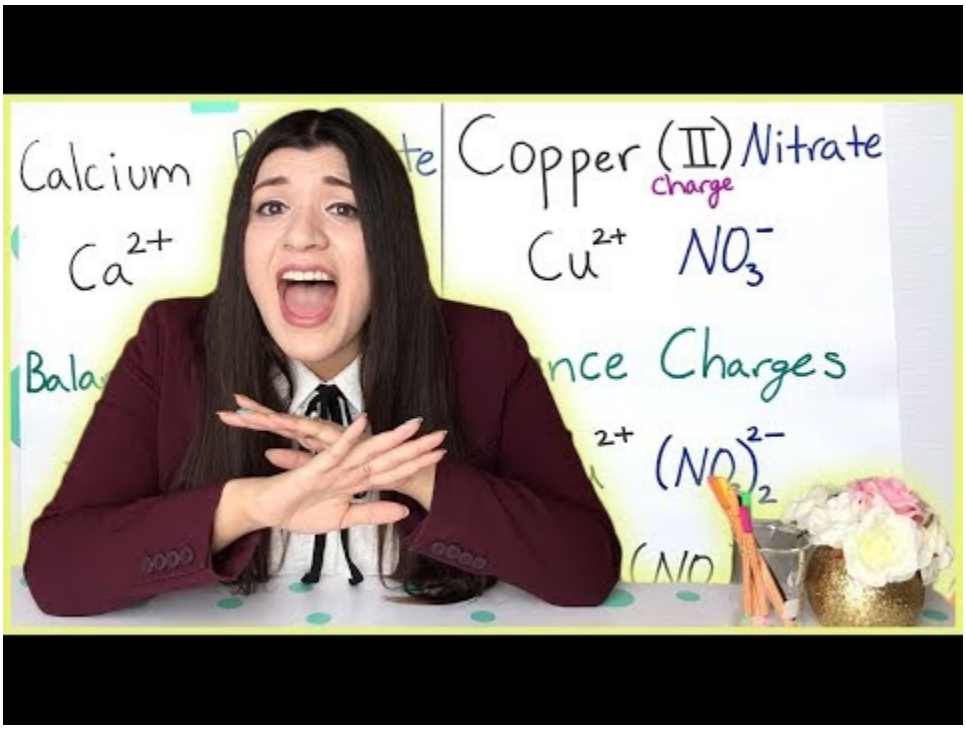
A. Identify the group in the periodic table to which the element belongs. Based on its location in the periodic table, decide whether the element is a metal, which tends to lose electrons; a nonmetal, which tends to gain electrons; or a semimetal, which can do either.
B. After locating the noble gas 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^-		

Table 4: Polyatomic Ions

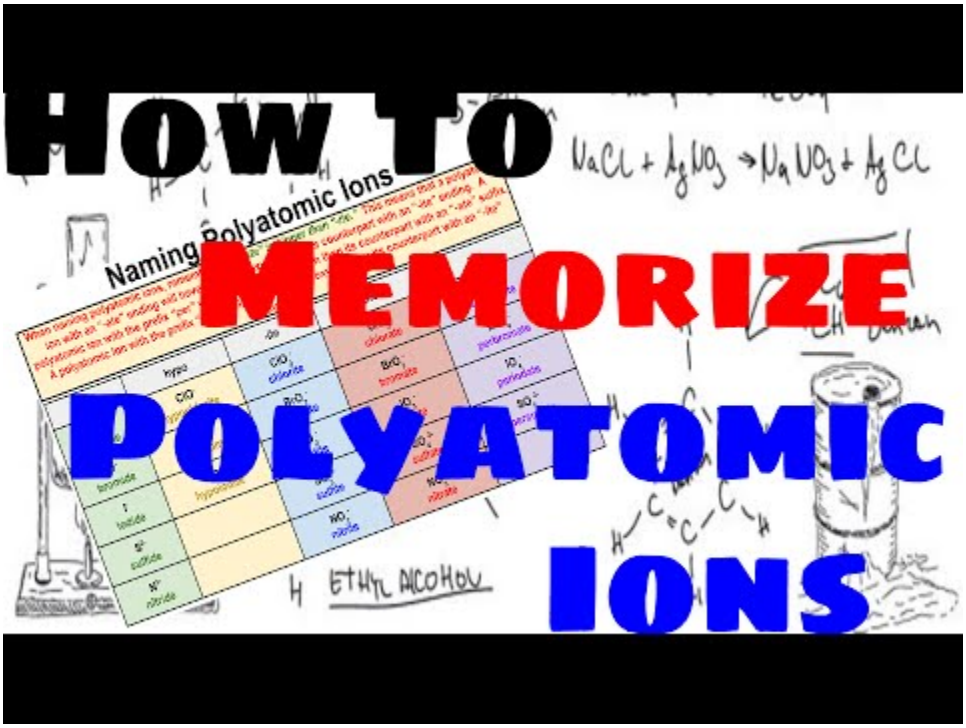
More important polyatomic ions are marked with asterisk below.

Common Polyatomic Ions

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 CH_3COO^-)

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.

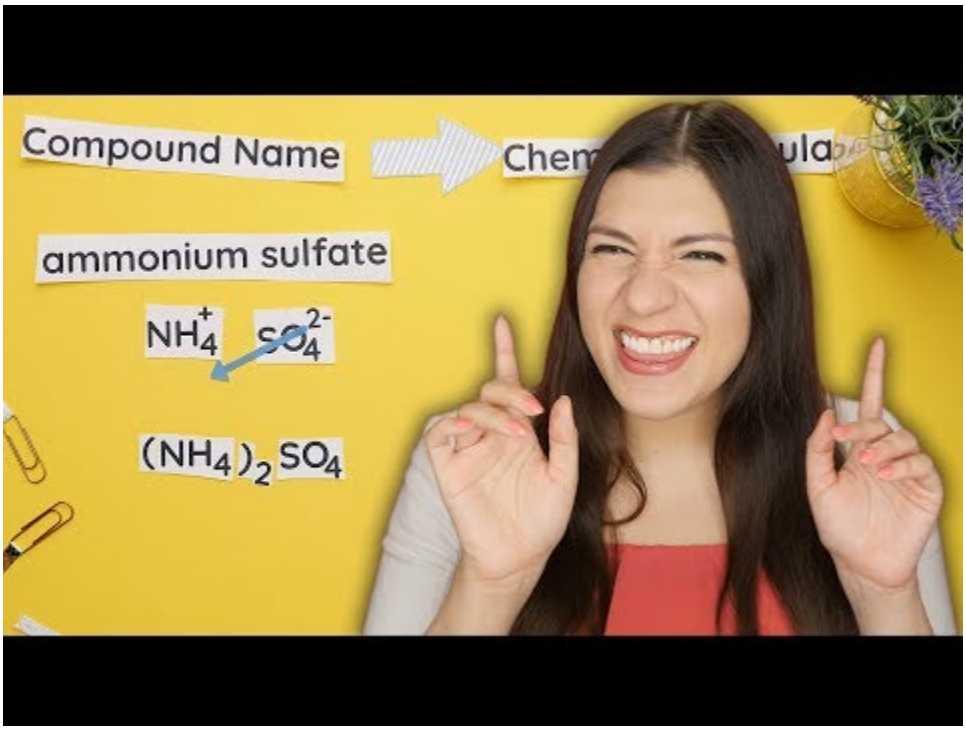
For example: $Na^{+} + SO_4^{2-} \rightarrow Na_2SO4$

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.

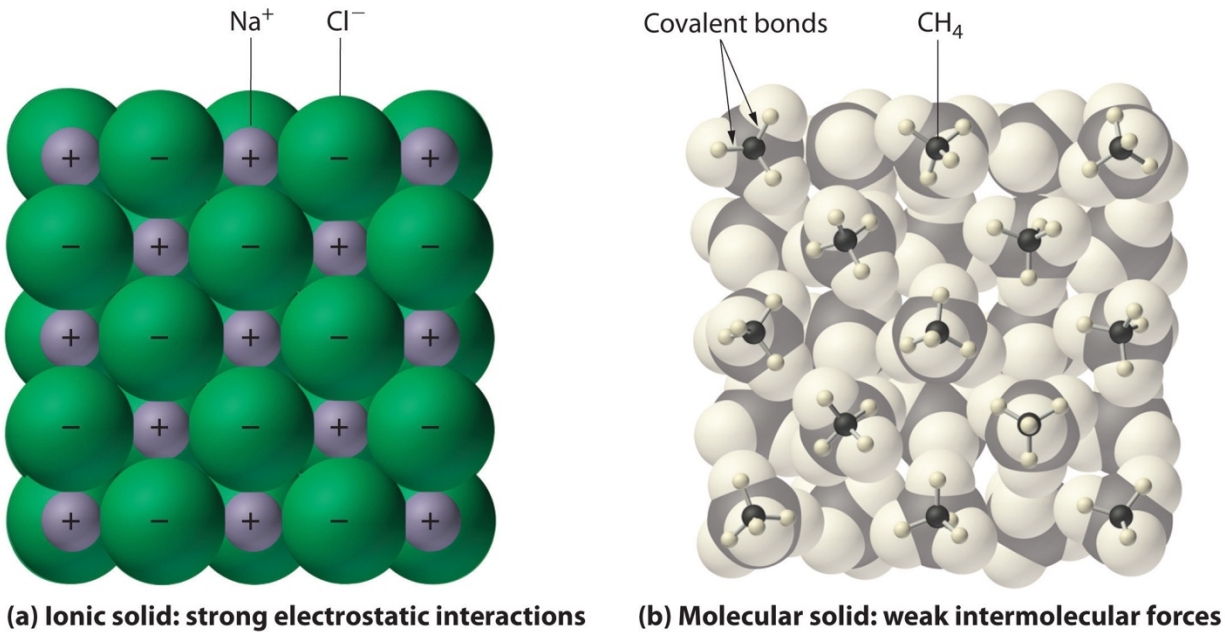


Figure 29. Interactions in ionic and covalent solids. (a) The positively and negatively charged ions in an ionic solid such as sodium chloride (NaCl) are held together by strong electrostatic interactions. (b) In this representation of the packing of methane (CH_4) molecules in solid methane, a prototypical 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.

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:

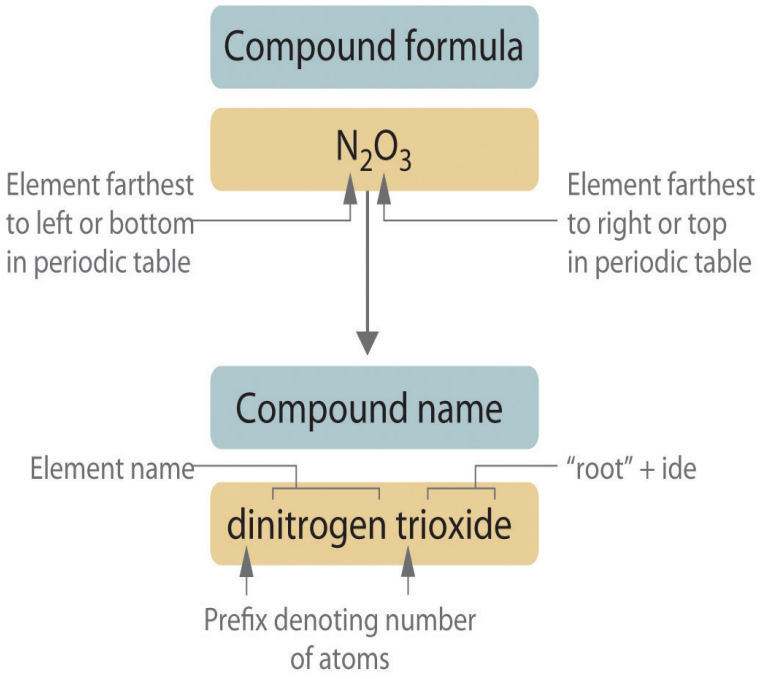


Figure 30. Naming a Covalent Inorganic Compound

1. Place the elements in their proper order.
   a. 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.

b. 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
tri-	3

Prefix	Number
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

a. 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.

b. 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.

. 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.

SF6
N2O4
ClO2

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:

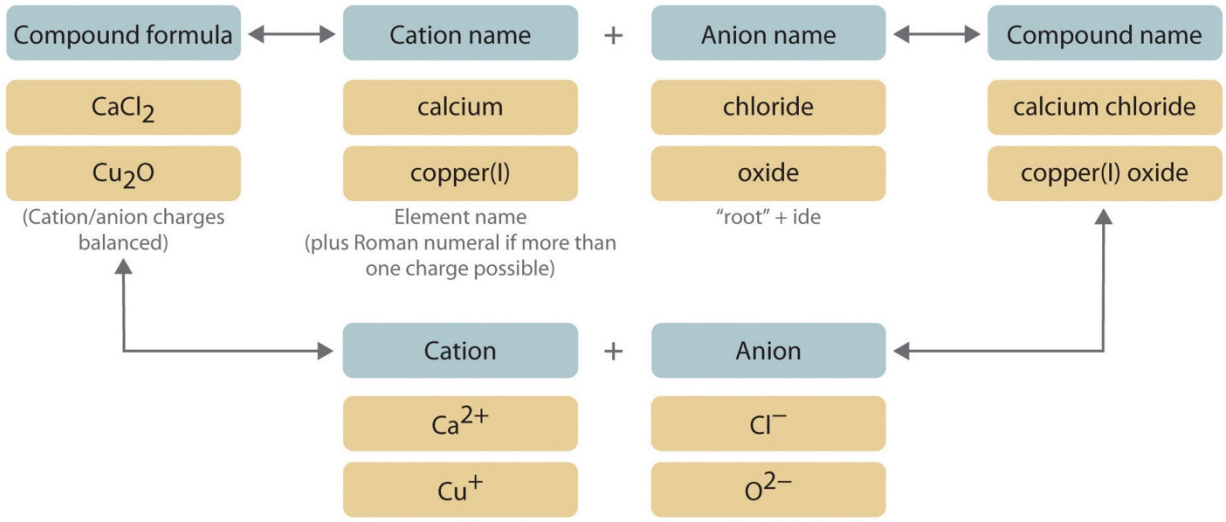


Figure 31. Naming an Ionic Compound

1. Place the ions in their proper order: cation and then anion.
2. Name the cation.

a. 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.

b. 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

c. 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.

. 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.

a. 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.

   It is not necessary to indicate the number of cations or anions present per formula unit in the name of an ionic compound because this information is implied by the charges on the

ions. You must consider the charge of the ions when writing the formula for an ionic compound from its name, however. Because the charge on the chloride ion is −1 and the charge on the calcium ion is +2, for example, consistent with their positions in the periodic table, simple arithmetic tells you that calcium chloride must contain twice as many chloride ions as calcium ions to maintain electrical neutrality. Thus, the formula is $CaCl_2$. Similarly, calcium phosphate must be $Ca_3(PO_4)_2$ because the cation and the anion have charges of +2 and −3, respectively. The best way to learn how to name ionic compounds is to work through a few examples.

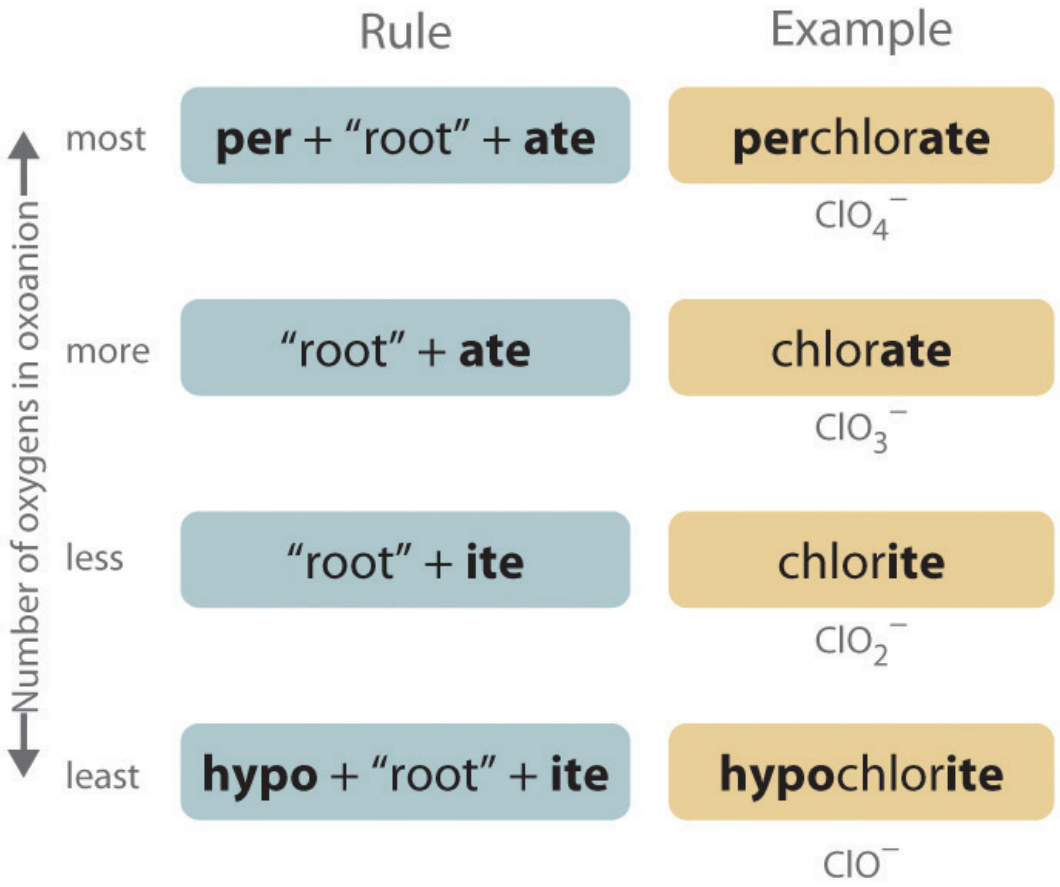
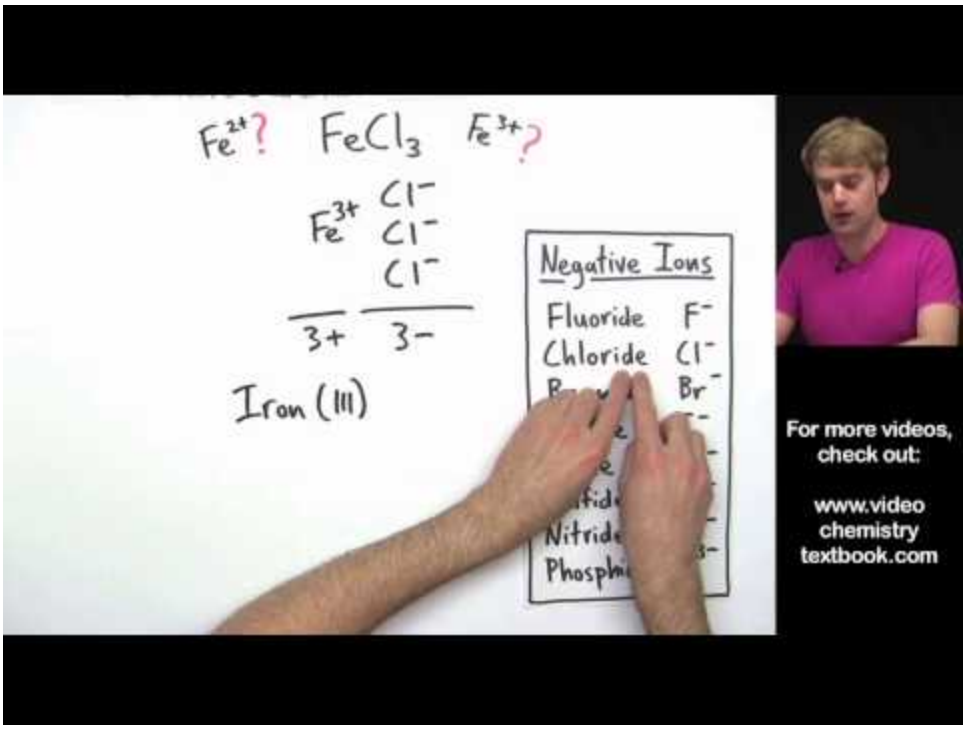


Figure 32. The relationship between the Names of oxoanions and the number of oxygen atoms present

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
MgSO4
(NH4)3PO4
Cu2O

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 5.9.15.9.1: (A) Vinegar comes in a variety of types, but all contain acetic acid. (B) Citrus fruits like grapefruit contain citric and ascorbic acids.

Figure 33: Natural sources of Acids

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*.

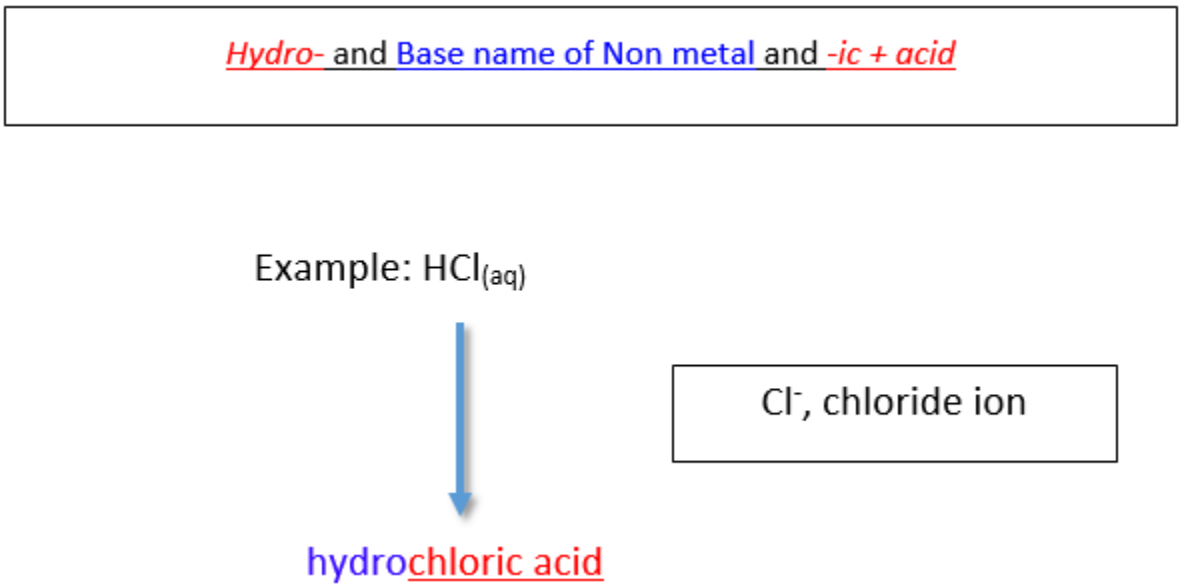


Figure 34A: Naming Binary acid

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.

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

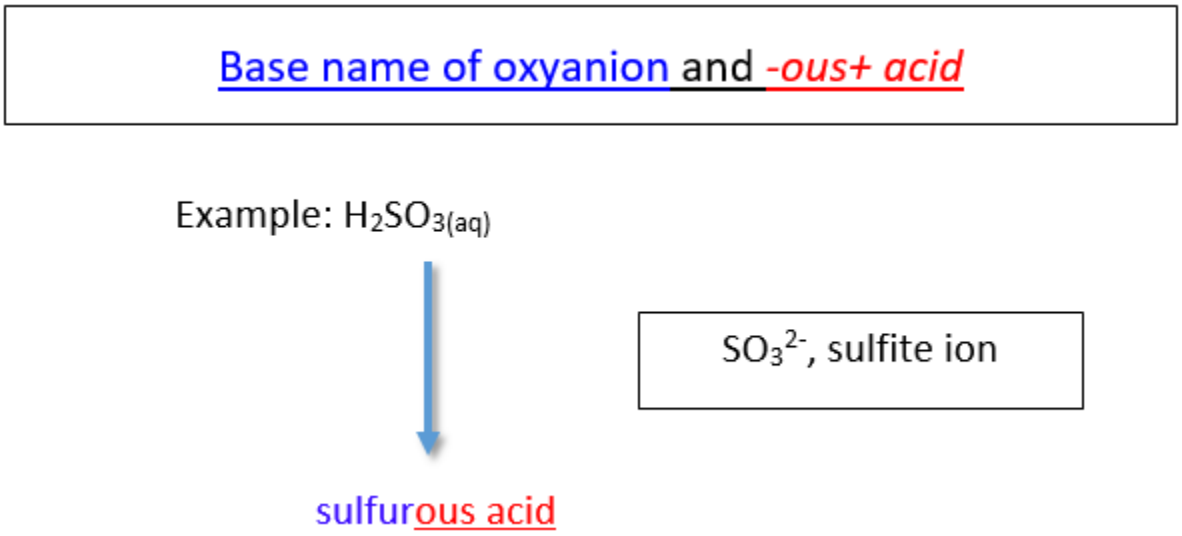


Figure 35 B: Naming Oxy Acids

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.

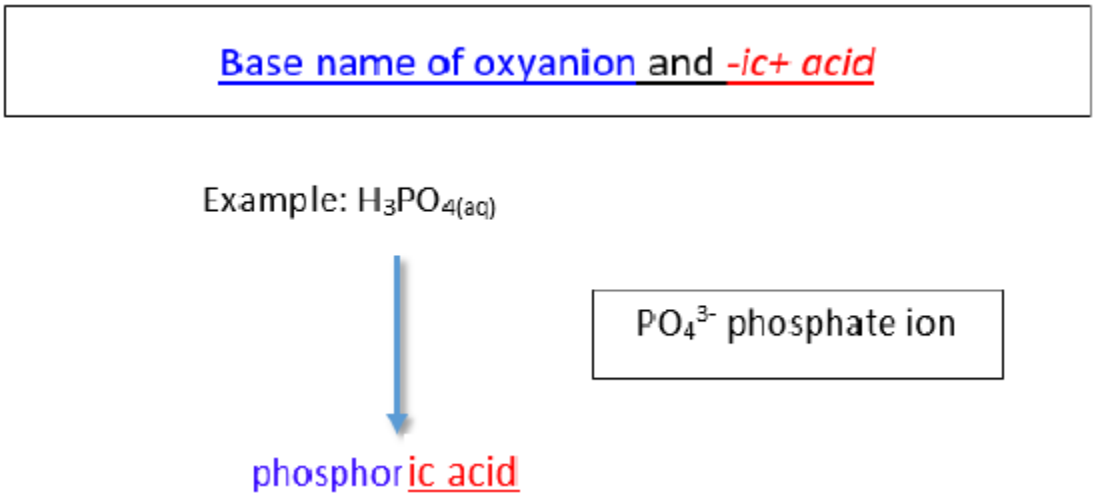


Figure 35 C: Naming Oxy Acids

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

Table 5: Naming oxy acids

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

Like other compounds that we have studied, acids are electrically neutral. Therefore, the charge of the anion part of the formula must be exactly balanced out by the H+H+ ions. Another way to think about writing the correct formula is to utilize the crisscross method, shown below for sulfuric acid.

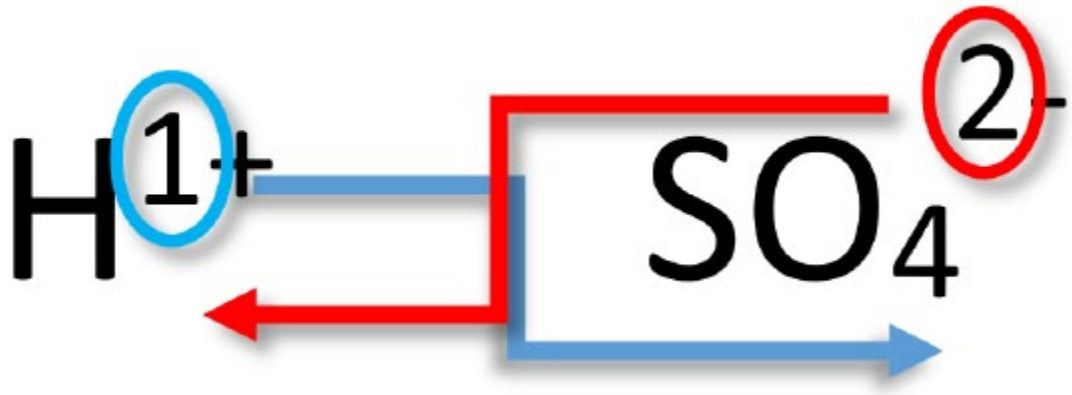
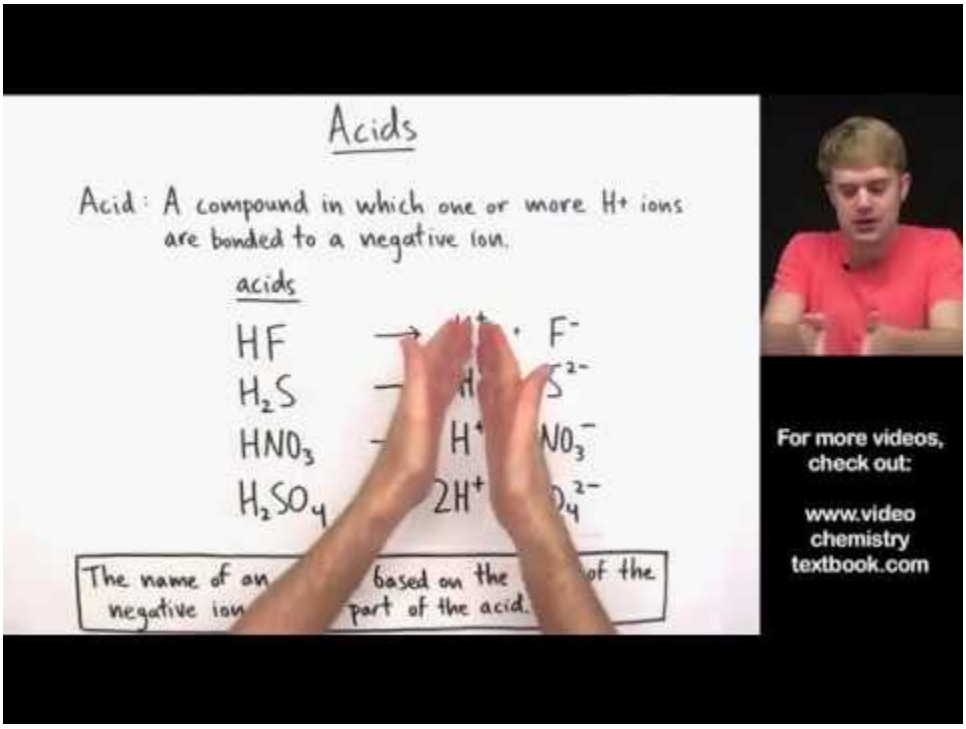


Figure 36: Writing Formula of Acids

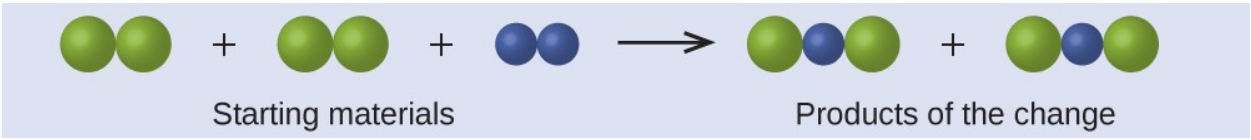
Formula: H_2SO_4

Figure : *Crisscross approach to writing formula for sulfuric acid.*



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

Figure 3: Writing Formula of Acids

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. Ce^{3+}
4. Zr^{4+}
5. Zn^{2+}
6. Kr^{2+}
7. B^{3+}

44. What is the total number of electrons present in each ion?
    1. Ca^{2+}
    2. Se^{2-}
    3. In^{3+}
    4. Sr^{2+}
    5. As^{3+}
    6. N^{3-}
    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. IF_7

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

I. **The Concept of Moles and the Formula Mass**
II. **The Concept of Empirical Formula and Molecular Formula**
III. **Solution's Different Concentrations**
IV. **Concentrations Calculations in Chemical Reactions**
V. **Mole Definition and Mass Percent Calculations and Reviews**

I. The Concept of Moles and the Formula Mass

What is the Mole?

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.

Example:

Each carbon atom weighs about 1.99625 X 10^{-23} g, hence"

[1.99625 X 10^{-23} g / atoms] X [6.02214179 X 10^{23} atoms] = 12.0217 g of Carbon – 12 isotope.

The value of 6.022 X 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 X 10^{23} atoms**
	6.022 X 10^{23} molecules
	6.022 X 10^{23} formula units (ions)

What is the Formula Mass?

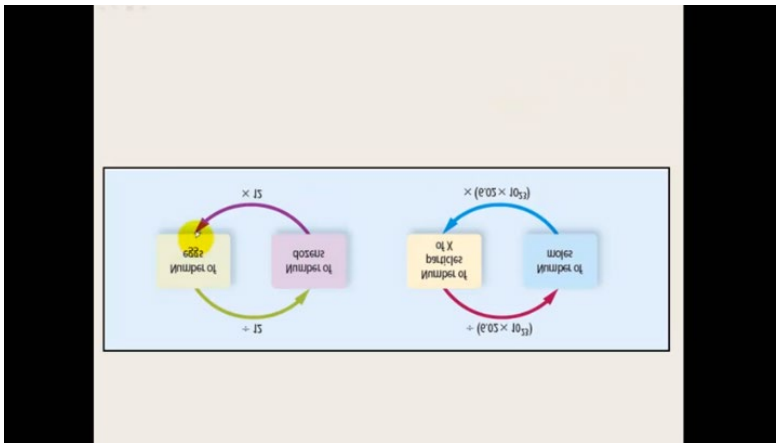
The formula mass of a substance is the sum of the average weighed atomic masses of each atom present in the chemical formula and is expressed in atomic mass units (amu). The formula mass of a covalent compound is also called the molecular mass. The mass in grams of 1 mole of substance is its molar mass and it has the unit of (g/mol)

Examples are posted in table below:

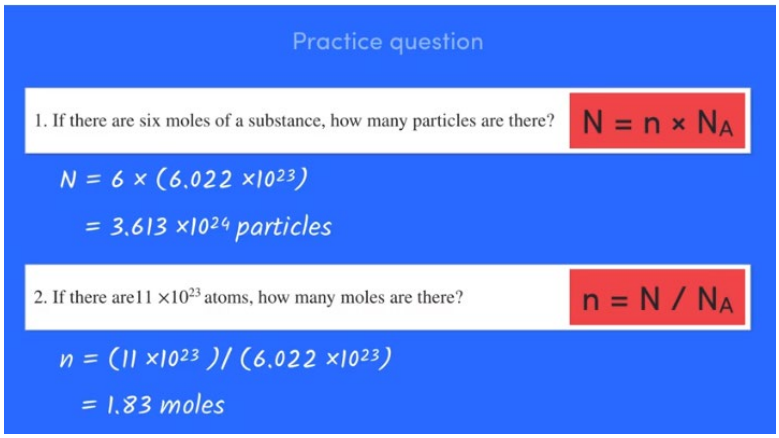
Element Name	**Element Symbol**	**Average Weighed Atomic Mass in amu (atomic mass units)**	**Atomic Mass in g/mol**	**Atoms / 1 mole**
Phosphorous	**P**	**30.973762**	**30.973762**	**6.022 X 10^{23}**
Carbon	**C**	**12.0107**	**12.0107**	**6.022 X 10^{23}**
Uranium	**U**	**238.02891**	**238.02891**	**6.022 X 10^{23}**
Barium	**Ba**	**137.327**	**137.327**	**6.022 X 10^{23}**

Silicon	**Si**	**28.0855**	**28.0855**	**6.022 X 10^{23}**
Xenon	**Xe**	**131.293**	**131.293**	**6.022 X 10^{23}**

The two videos explain the concept of the mole:



https://www.youtube.com/watch?v=wORiAOnvw8g&feature=youtu.be



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.

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 X 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:

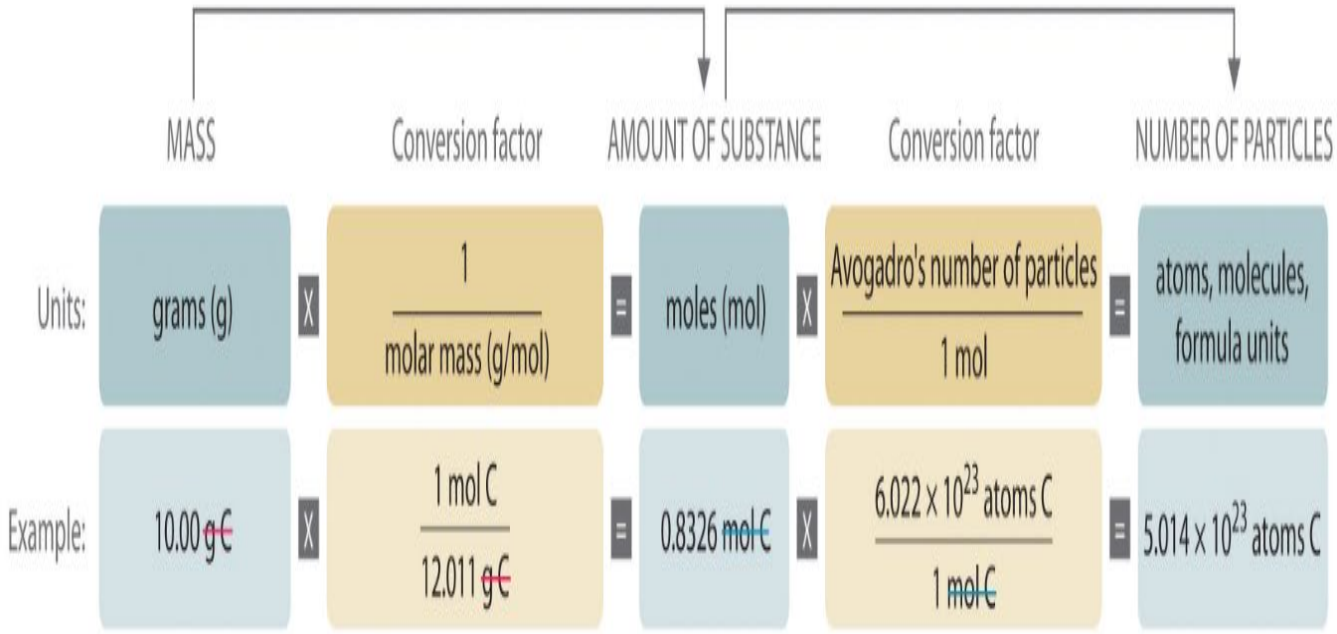
How may moles can be calculated for 1.18 X 10^3 grams NaCl?

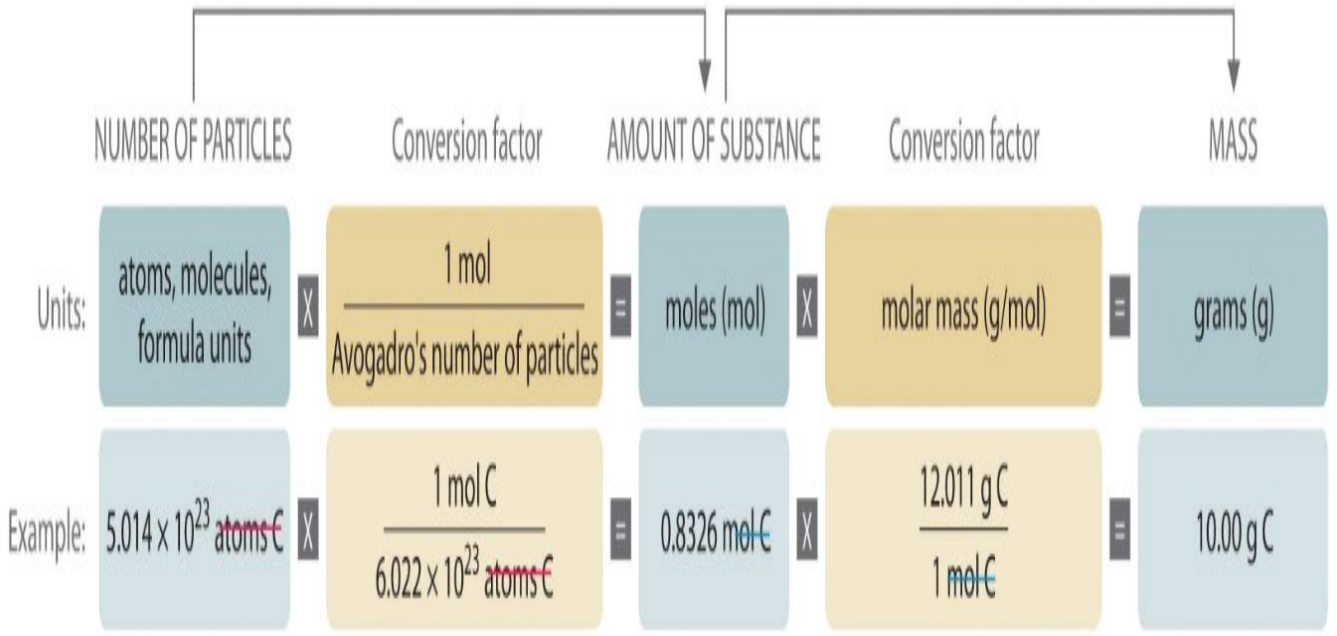
Molar mass of NaCl = Na + Cl = 23.0 g/mole + 35.5 g/mole = 58.5 g/mole

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:





Reference:
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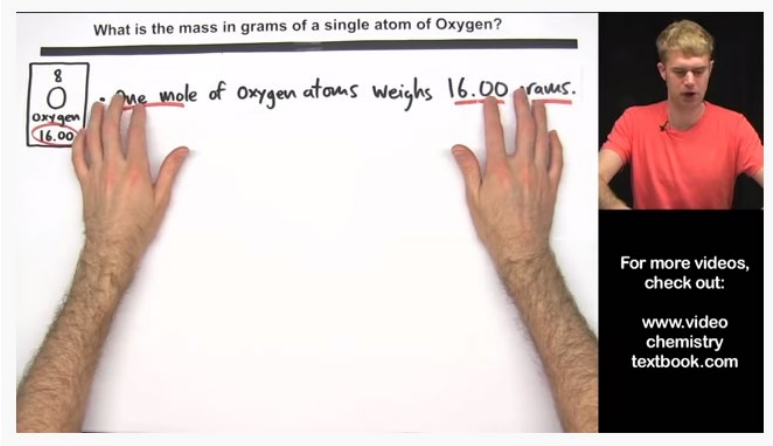
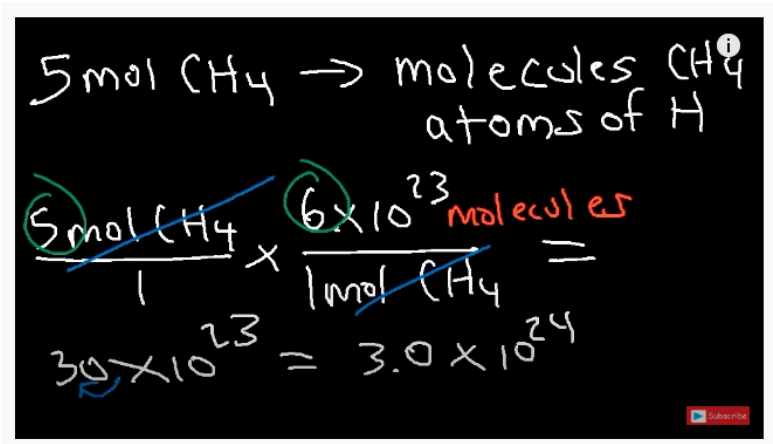
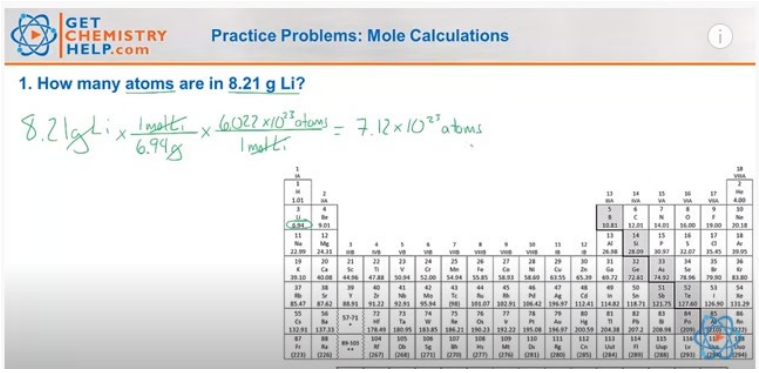
Videos covering the conversion of atoms, molecules, ions (formula units into grams of matter and vice versa are given below:



https://www.youtube.com/watch?v=BO9M1hbs88s

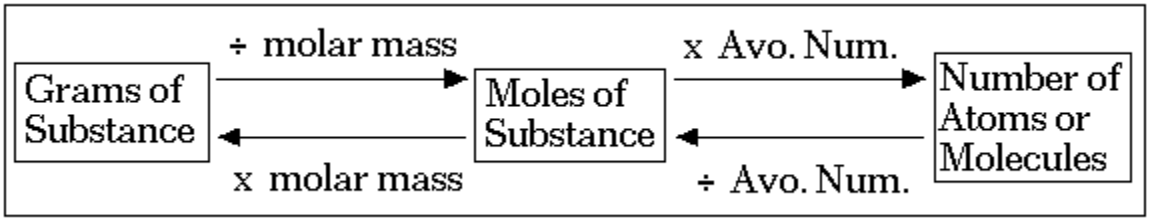


https://www.youtube.com/watch?v=74-X94OP2XI



https://www.youtube.com/watch?v=w2-Pcfj60fA

Examples:



https://www.chemteam.info/Mole/Avogadro-Number-CalcsII.html

Convert 0.450 mole of Fe into atoms of Fe?

[0.450 mole Fe] X [6.022×10^{23} atoms of Fe / mole] = 2.71×10^{23} atoms of Fe

Convert 0.450 gram of Fe into atoms of Fe?

You will need to use the average weighed atom mass of Fe from the periodic table:

Atomic mass of Fe = 55.85 g /mole

[0.450 g of Fe] X [mole / 55.85 g of Fe] X [6.022×10^{23} atoms of Fe / mole] = 4.85×10^{21} atoms of Fe

Convert 0.200 grams of H_2O into molecules of H_2O?

You will need to calculate first the molar mass of H_2O using the atomic masses of H and O from the periodic table:

Molar mass of H_2O = 2 H + 1 O = [2 X 1.00 g/mole] + [1 X 16.0 g/mole] = 18.0 g/mole H_2O

[0.200 g H_2O] X [mole H_2O / 18.0 g H_2O] X [6.022×10^{23} molecules of H_2O / mole H_2O] = 6.68×10^{21} molecules H_2O

Convert 1.058 mole of H_2O into molecules of H_2O

No molar mass incorporation is needed:

[1.058 mole H_2O] X [6.022×10^{23} molecules of H_2O / mole H_2O] = 6.371×10^{23} molecules H_2O

Which contains more molecules: 10.0 grams of O_2 or 50.0 grams of iodine, I_2?

You will need the molar mass of oxygen O_2 (32.0 g/mole) and the molar mass of iodine I_2 (253.8 g/mole)

Number of O_2 molecules = [10.0 g O_2] X [mole O_2/32.0 g O_2] X [6.022 x 10^{23} molecules of O_2 / mole O_2] =

Number of I_2 molecules = [50.0 g I_2] X [mole I_2/253.8 g I_2] X [6.022 x 10^{23} molecules of I_2 / mole I_2] =

No need to do real calculations. Just inspect both equations: Iodine equations has to be divided by the value of 253.8 which is almost 8 times larger than the value 32.0. Therefore, oxygen will have more molecules than iodine.

If 18.0 g of H_2O is present. (a) How many oxygen atoms are present? (b) How many hydrogen atoms are present?

Steps to solve this type of problems:

1. Convert grams to moles:
18.0 g / 18.0 g/mol = 1.00 mol
2. Convert moles to molecules:
(1.00 mol) (6.02 x 10^{23} mol^{-1}) = 6.02 x 10^{23} molecules
3. Determine number of atoms of oxygen present:
(6.02 x 10^{23} molecules) (1 O atom / 1 H_2O molecule) = 6.02 x 10^{23} O atoms
4. Determine number of atoms of hydrogen present:
(6.02 x 10^{23} molecules) (2 H atoms / 1 H_2O molecule) = 1.20 x 10^{24} H atoms

A sample of C_3H_8 has 2.96 x 10^{24} H atoms.

1. **How many carbon atoms does the sample contain?**
2. **What is the total mass of the sample?**

1.The ratio between C and H is 3 to 8, so this:

$$\frac{3}{8} = \frac{y}{2.96 \times 10^{24} \text{ H atoms}}$$

This will tell us the number of carbon atoms present:

y = 1.11 x 10^{24} carbon atoms

The above ratio and proportion can also be written like this:

3 is to 8 as y is to 2.96 x 10^{24}

2. Determine the moles of C_3H_8 present.

$2.96 \times 10^{24} / 8 = 3.70 \times 10^{23}$ molecules of C_3H_8

2) Divide by Avogadro's number:

$3.70 \times 10^{23} / 6.022 \times 10^{23}\ mol^{-1} = 0.614414$ mol

3) Use the molar mass of C_3H_8:

0.614414 mol x 44.0962 g/mol = 27.1 g

Activity:

Particles .. Moles .. Mass

The Particles .. Moles .. Mass Concept Builder includes three scaffolded difficulty levels designed to provide learners comfort with the mathematical relationship between the number of particles of a compound, the number of moles of particles, and the mass of those particles. In each difficulty level, a five row table is presented with unknown cell values. Learners must determine the unknown values. Immediate feedback is given and chances for correction of incorrectly-inputted values is allowed. Help is provided for each difficulty level. Built-in score-keeping makes this Concept Builder a perfect candidate for a classroom activity.

Users are encouraged to open the Concept Builder and explore. There is no need for an activity sheet for this Concept Builder. However, the 12 different groups of questions can be printed. View **Questions**.

Learners and Instructors may also be interested in viewing the accompanying **Notes page**. Technical information, teaching suggestions, and related resources that complement this Concept Builder are provided on the Notes page. View **Notes**.

Particles .. Moles .. Mass - Directions

How it Works:

Using the Particles.. Moles .. Mass Concept Builder is quite simple. You will be presented with a table of numerical values associated with molar mass, number of particles, number of moles, and the mass in grams for a stated substance. Some cells of the table are blank and you will have to use mathematical relationships to solve for the blank cells. You can consider each row of the table as a separate problem. Only information from that row can be used to determine the unknown values. One row is not dependent upon other rows.

To enter numbers into the table, simply tap on a table cell. A Number Pad pops up. You can use the Number Pad to enter answers into the table cell. Once complete, you can tap the Close

Number Pad button (at the bottom of the number pad) or tap on a different table cell. Once you are satisfied with your answers, tap on the **Check Answers** button. Your answers will be evaluated and feedback will be given. Feedback is given in terms of color-coded table cells. Table cells color-coded green were correctly answered and cannot be changed again. If an answer is incorrect, then the table cell will be color-coded red.

The Concept Builder keeps track of the number of misses. A miss is considered any value that is entered into a cell and evaluated as incorrect. If a cell value is incorrect on the first attempt and not changed, it would be marked as a miss on the second attempt. If you do not wish to check that incorrect value again, then you would have to remove the value (tap on the cell to open the Number Pad and tap on the **C** or Clear button) before the next time that your check your answers.

Once all table cells are accurately completed, your Health Percent is shown. It is also shown as you are filling in the table as long as the Number Pad is closed. The Health Percent is based upon the number of misses and on some adjustments made for the use of the **CF** button. The formulas for calculating this are:

Your Health Percent is displayed on the Main Menu. If you wish to repeat the Difficulty Level to improve your Health Percent, you can tap on the provided button to do so. Your best Health Percent is always displayed on the Main Menu. If you repeat a difficulty level and do worse the second time, it is the best Percent that will be displayed.

About the CF Button

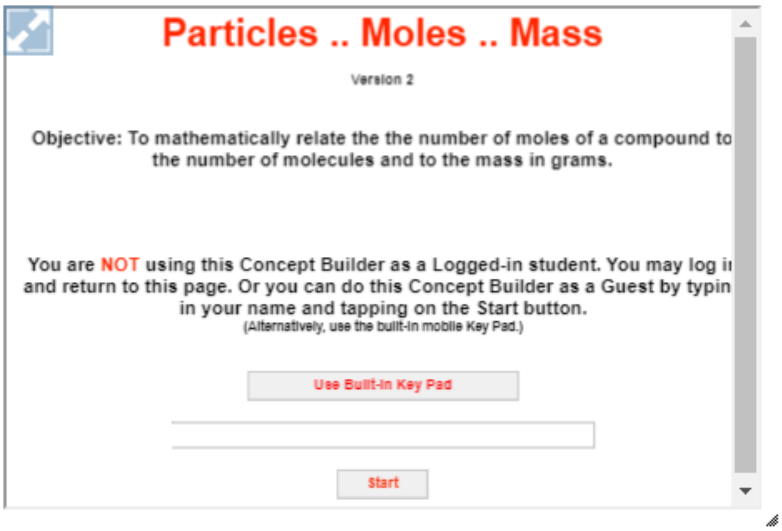
The Concept Builder includes a Hint feature. The Hint feature is marked by a **CF** button that lies between the various columns. Tapping on the **CF** button will slide in a screen that explains how to convert between quantities. An example conversion is shown as part of the Hint. In the Apprentice Difficulty Level, tapping on the **CF** button will not have any effect upon the Heath Percent. In the Master Difficulty Level, tapping on the **CF** button will have no effect for the first two hints. But the third and the fourth tap on the **CF** button will result in a 4% deduction in the Health Percent. In the Wizard Difficulty Level, every viewing of a Conversion Factor Hint will result in a 4% deduction in the Health Percent. When tapping on the **CF** button in the Master and Wizard Difficulty Level, users will be warned that they will have the 4% deduction and be given the opportunity to cancel out. There are four types of conversions and four types of hints: particles to moles, moles to particles, moles to grams, and grams to moles. In the Master and Wizard Difficulty Level, once one of the Hint types has been shown, tapping on a **CF** button for the same type of Hint will display the Hint a second or third or fourth ... time without any warning or 4% deduction.

Now you can start your simulation activity:

Launch Concept Builder

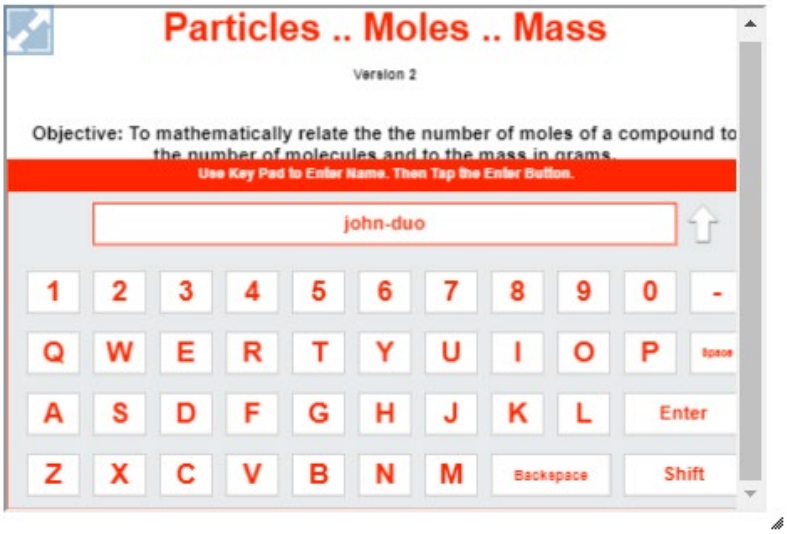
https://www.physicsclassroom.com/Concept-Builders/Chemistry/Mole-Conversions/Concept-Builder

Make the Concept Builder Larger by expand it.

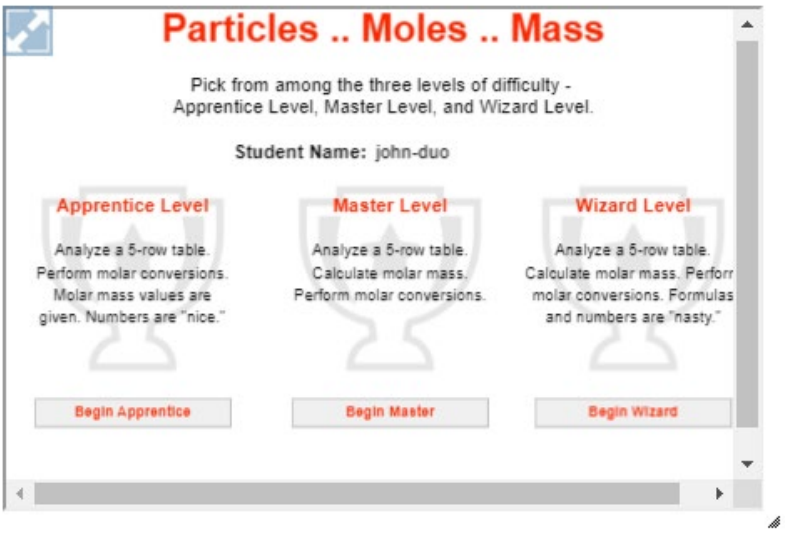


Use the keyboard and type any name (it has not to be your name).

Press Enter.



Click the Start button. Select your desired Level and start the simulation by answering the questions. You can repeat your attempts and you can examine your knowledge regarding the mole concepts.



II. The Concept of Empirical Formula and Molecular Formula

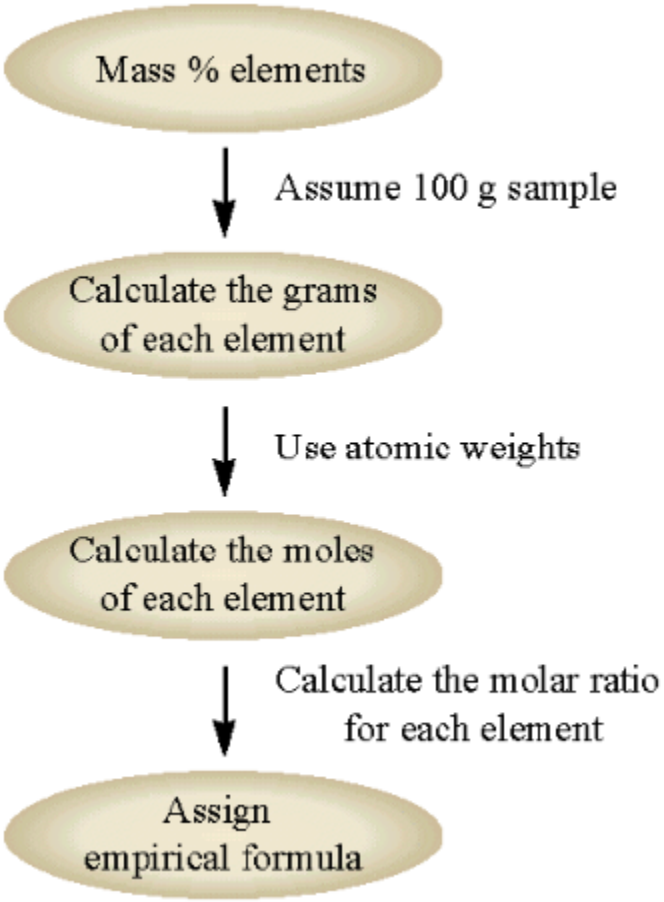
An empirical formula expresses the relative ratios of the atoms in a compound or a molecule. The ratio of the atoms within the compound and molecule is held for the atomic level as well the molar level.

$MgCl_2$ 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)

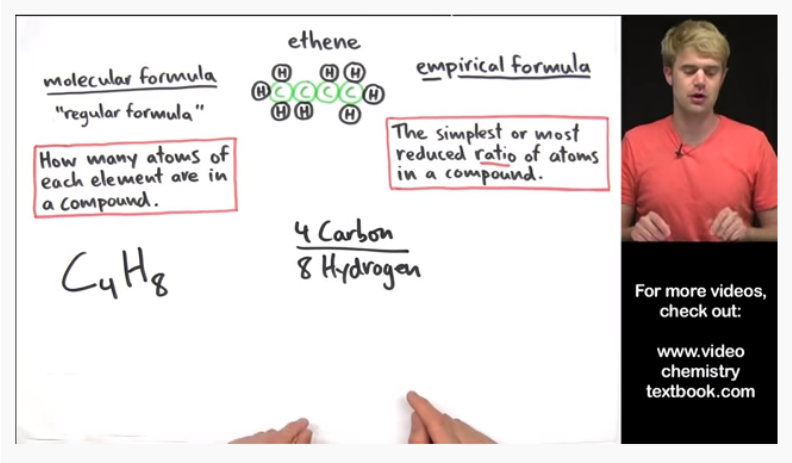
Knowing the molar ratio of each element within a molecule or a compound, one can determine the empirical formula of such molecule or compound.

Steps how to calculate the empirical formula from known mass percent (%):can be seen below:

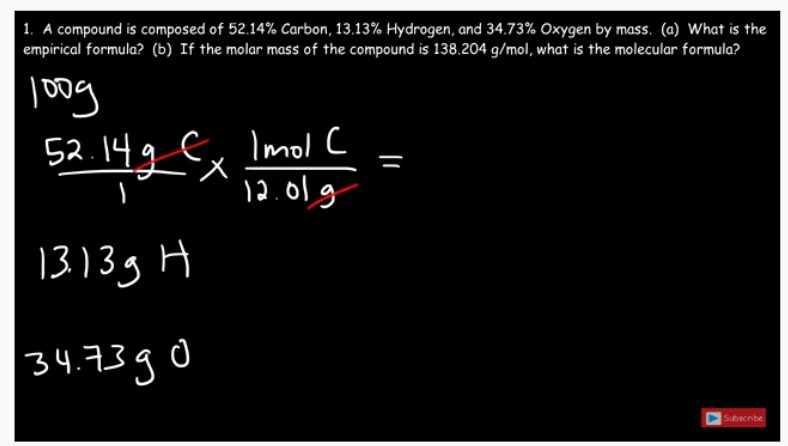


Reference:
https://chem.libretexts.org/Courses/Heartland_Community_College/HCC%3A_Chem_161/3%3A_Chemical_Reactions_and_Quantities/3.4%3A_Determing_an_Empirical_and_Molecular_Formula#:~:text=Chemical%20formulas%20tell%20you%20how,same%20as%20the%20chemical%20formula.

The videos below illustrates with examples the concept of the empirical formula:



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



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:

$P_{0.0235}Cl_{0.0704}$

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).

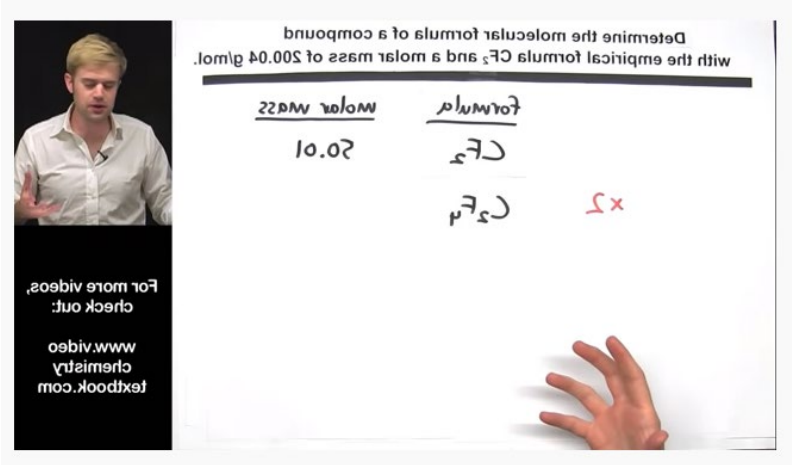
Molecular Formula: The actual number of the atoms of each element within a compound or a molecule or a formula unit (ion).

The relationship between Molecular Formula (molar mass) and Empirical Formula (empirical formula mass) is given below:

$$\frac{\text{molecular or molar mass}\left(\text{amu or }\frac{\text{g}}{\text{mol}}\right)}{\text{empirical formula mass}\left(\text{amu or }\frac{\text{g}}{\text{mol}}\right)} = n\,\text{formula units/molecule}$$

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:



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

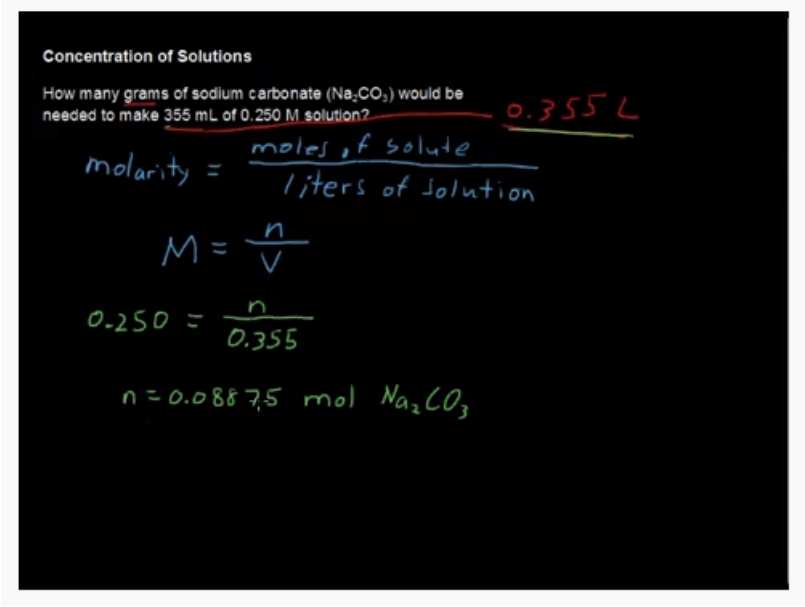
A solution is a homogeneous mixture made of a solute and a solvent. A solute is a chemical compound that is limited in the amount and soluble in the solvent. The solvent in a chemical compound that has the ability to dissolve the solute and it has excess amount compared with the solute amount. To assure solubility both solute and solvent share similar polarity.

An example of a homogenous mixture is the solubility of sodium chloride NaCl in water. Sodium chloride is considered as a solute with the least amount and water is considered as a solvent with a large amount.

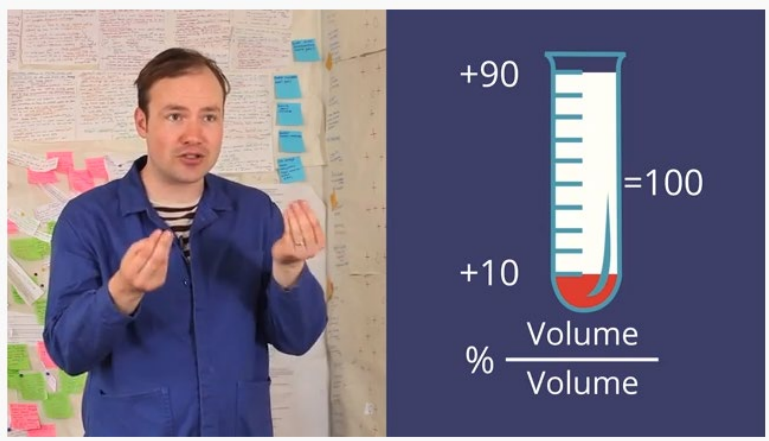
Also solubility of an oil (none polar compound) in cyclohexane solvent (none polar) makes a homogenous mixture.

If the solute and solvent have different polarities, then they form heterogeneous mixture which is not considered as a solution.

The videos below illustrate the concept of solution and its concentrations (molarity).



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 ppb = {[mass of solute] / [mass of solution]} x 1 x 10^9	ppm ppb		

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 with455 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. 10.00×10^{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 = [10.00×10^{26} molecules of acetone] x [1 mole acetone/6.022×10^{23} molecules of acetone]

One has to use the Avogadro's number of 6.022×10^{23} to calculate number of moles:

1 mole of acetone = 6.022×10^{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

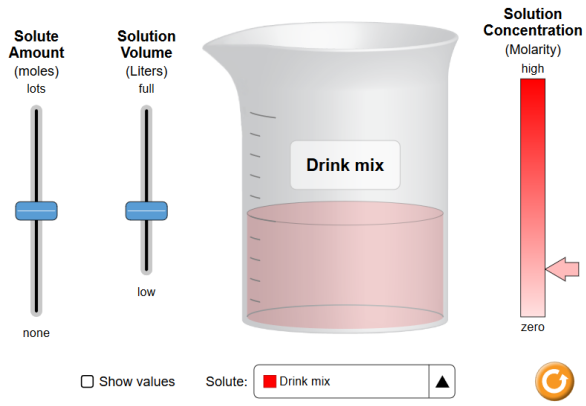
c. How much water should be added to 985 mL of a 6.55 M NaOH solution to make a 1.00 M solution?
   $C_1xV_1 = C_2xV_2$
   Total volume = V_2 = X + 985 mL
   X = volume of water
   6.55 M x 985 mL = 1.00 M x V_2
   V_2 = [6.55 M x 985 mL] / [1.00 M] = 6451.75 mL
   X + 985 mL = 6451.75 mL
   X = 5466.75 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 thequalitative 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:

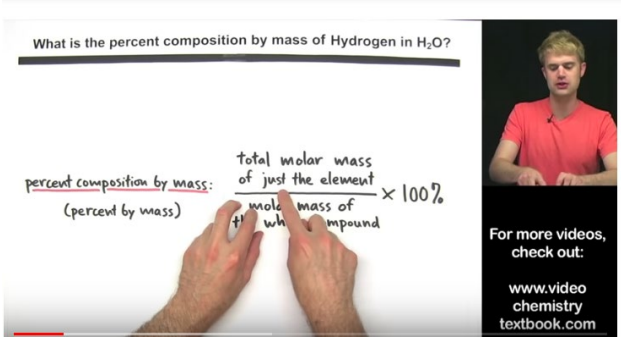
1. Which one of the salts (solutes) used has the largest saturation concentration

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).

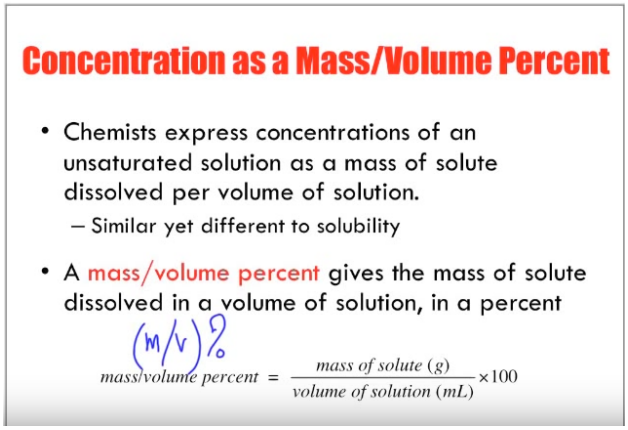
Several You Tube videos discussing the concentration of solution:

(Mass) %



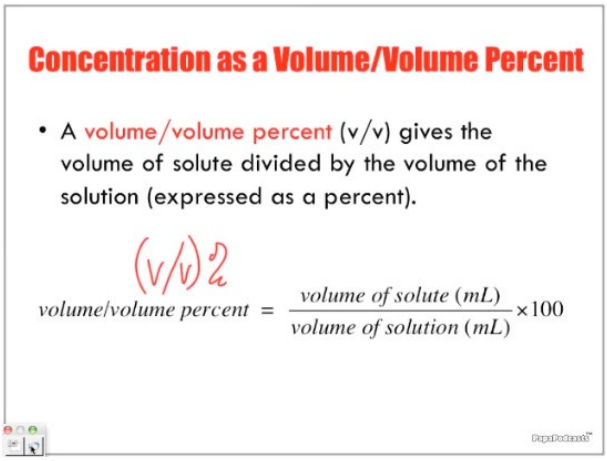
https://www.youtube.com/watch?v=lywmGCfIUIA

(Mass/volume) %:



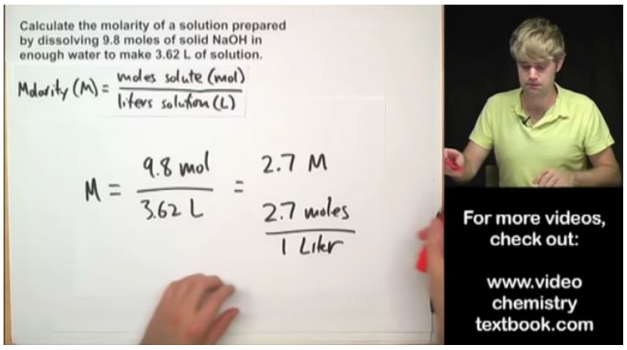
https://www.youtube.com/watch?v=dl6G_p6gsJc

(Volume/volume) %



https://www.youtube.com/watch?v=RCbhk3yyM88

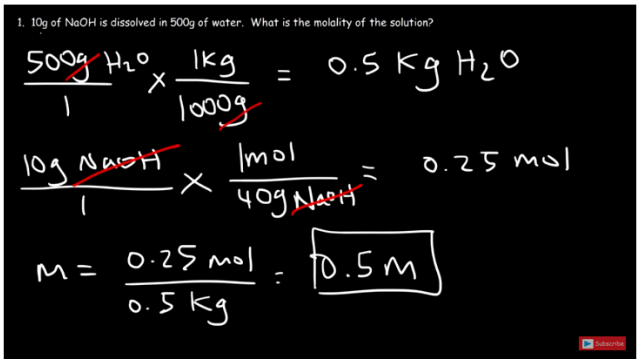
Molarity:



https://www.youtube.com/watch?v=SXf9rDnVFao

Molality:

https://www.youtube.com/watch?v=uj1u7Nx9JUc



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?

$\frac{284}{100}$ X 1,000,000 = **2840000 ppm**

The solubility of AgCl is 0.008 grams/100 grams of water. What is this concentration in ppm?

$\frac{.008}{100}$ X 1000000 = **80 ppm**

A certain pesticide has a toxic solubility of 5.0 grams/Kg of body weight. What is this solubility in ppm?

$\frac{1\ \cancel{Kg}}{1}$ X $\frac{1000\ g}{1\cancel{Kg}}$ = 1000 g $\frac{5}{1000}$ X 1,000,000 = **5000 ppm**

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

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	6.022×10^{23} atoms
	6.022×10^{23} molecules
	6.022×10^{23} formula units (ions)

Examples:

1) How many moles are in 40.0 grams of water?

$$40.0 \text{ g } H_2O \times \frac{1 \text{ mole } H_2O}{18.01 \text{ g } H_2O} = 2.22 \text{ mole } H_2O$$

2) How many grams are in 3.7 moles of Na_2O?

$$3.7 \text{ moles } Na_2O \times \frac{62 \text{ g } Na_2O}{1 \text{ mole } Na_2O} = 230 \text{ g } Na_2O$$

3) How many atoms are in 14 moles of cadmium?

14 mole Cd x $\frac{6.022 \times 10^{23} \text{ atoms Cd}}{1 \text{ mole Cd}}$ = 8.4 x 10^{23} atoms Cd

4) How many moles are in 4.3 x 10^{22} molecules of H_3P0_4?

4.3 x 10^{22} molecules H_3PO_4 x $\frac{1 \text{ mole } H_3PO_4}{6.022 \times 10^{23} \text{ molecules } H_3PO_4}$ = 7.1 x 10^{-2} moles H_3PO_4

5) How many molecules are in 48.0 grams of NaOH?

48.0 molecules NaOH x $\frac{1 \text{ mole NaOH}}{40 \text{ g NaOH}}$ x $\frac{6.022 \times 10^{23} \text{ molecules NaOH}}{1 \text{ mole NaOH}}$

= 7.23 x 10^{23} molecules NaOH

6) How many grams are in 4.63 x 10^{24} molecules of CCl4?

4.63 x 10^{24} molecules CCl_4 x $\frac{1 \text{ mole } CCl_4}{6.022 \times 10^{23} \text{ molecules } CCl_4}$ x $\frac{153.8 \text{ g } CCl_4}{1 \text{ mole } CCl_4}$ = 1180 g CCl_4

7) How many moles are in 15 grams of lithium? **(molar mass of lithium is 6.94 g/mole)**

~~15~~ grams x $\frac{1 \text{ mole}}{\sim\!\!6.94 \text{ grams lithium}}$ = 2.1614 = 2.2 moles Li

8) How many grams are in 2.4 moles of sulfur? **(molar mass of sulfur is 32.07 g/ mole)**

~~2.4~~ moles x $\frac{32.07 \text{ grams}}{\sim\!\!1 \text{ mole}}$ = 76.97 grams sulfur 77 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)

4.5 moles x $\frac{41.99 \text{ grams}}{1 \text{ Mole}}$ = 188.955 g NaF **= 190 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)

98.3 grams x $\frac{1 \text{ mole}}{78.01 \text{ grams}}$ = 1.2601 moles $Al(OH)_3$ **1.26 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

$$\frac{\textbf{25 g } H_2O \quad | \quad \textbf{1 mol } H_2O}{} = 1.39 \text{ mol } H_2O$$

12) How many grams are in 4.500 moles of Li_2O?

134.6 grams

1 mole Li_2O = 29.90 g Li_2O

$$\frac{\textbf{4.500 mol } Li_2O \quad | \quad \textbf{29.90 g } Li_2O}{} = 134.6 \text{ g } Li_2O$$

13) How many molecules are in 23.0 moles of oxygen?

1.38×10^{25} molecules

1 mole oxygen molecules = 6.02×10^{23} oxygen molecules

$$\frac{\textbf{23.0 mol } O_2 \quad | \quad \textbf{6.02 x } 10^{23} \textbf{ } O_2 \textbf{ molecules}}{\textbf{1 mol } O_2} = 1.38 \times 10^{25} \text{ } O_2 \text{ molecules}$$

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

$$\frac{3.4 \times 10^{23} \text{ molecules } H_2SO_4}{} \times \frac{1 \text{ mol } H_2SO_4}{6.02 \times 10^{23} \text{ molecules } H_2SO_4} = 0.56 \text{ mol } H_2SO_4$$

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

$$\frac{25.0 \text{ g } NH_3}{} \times \frac{1 \text{ mol } NH_3}{17.0 \text{ g } NH_3} \times \frac{6.02 \times 10^{23} \text{ molecules } NH_3}{1 \text{ mol } NH_3}$$

= 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

$$\frac{8.200 \times 10^{22} \text{ molecules } N_2I_6}{} \times \frac{1 \text{ mol } N_2I_6}{} \times \frac{789.4 \text{ g } N_2I_6}{1 \text{ mol } N_2I_6} = 107.5 \text{ g } N_2I_6$$

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 $Al(OH)_3$ = **2.0×10^2 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

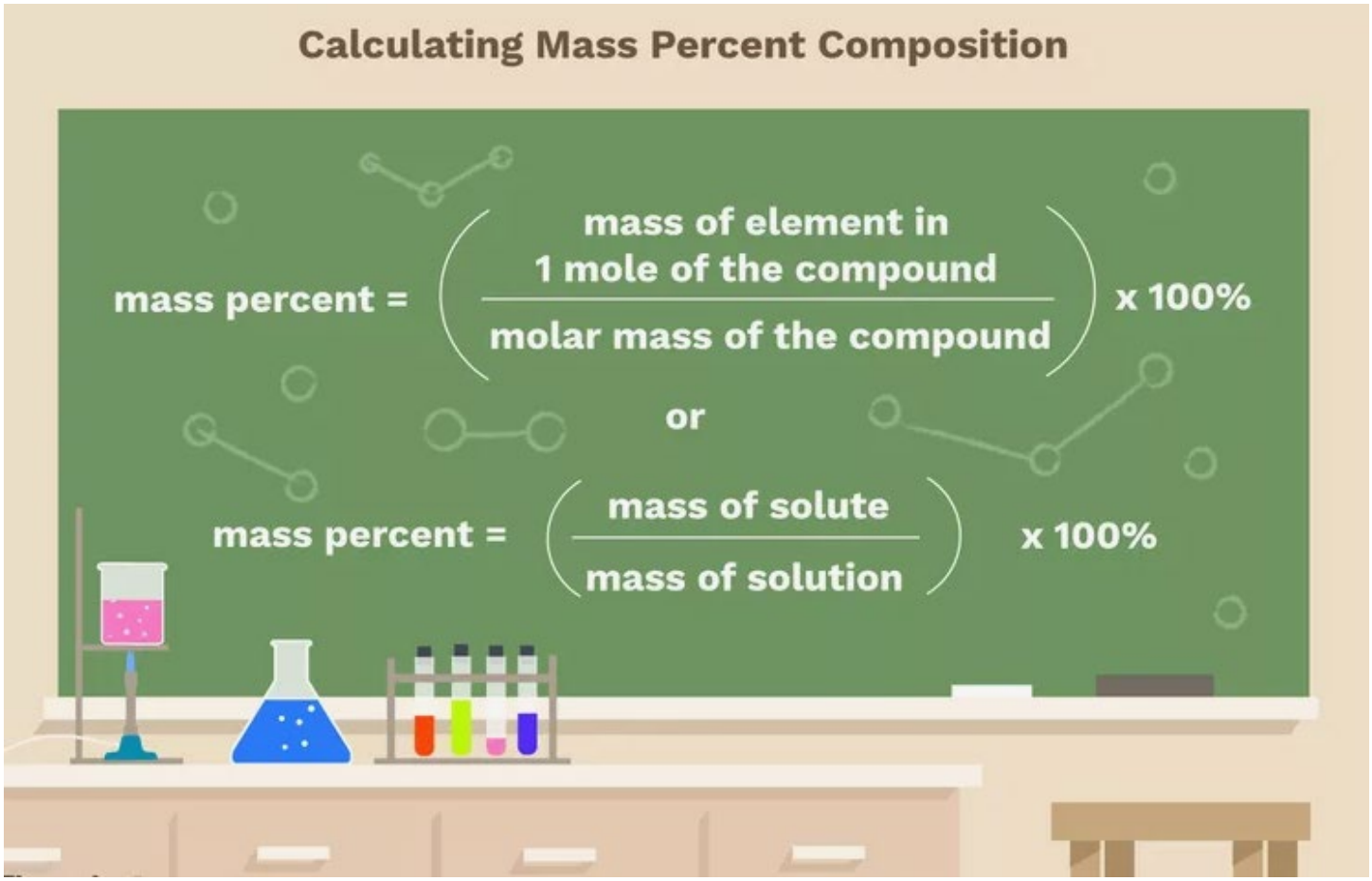
https://www.youtube.com/watch?v=hQ6_BxJwvB0

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_4OH 7 c) NaCl 2 d) N_2O_7 9 e) P_2O_5 7

a) KNO_3 5 b) $Al_2(CO_3)_3$ 14 c) Na_3PO_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_2O_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:

$Cl \rightarrow \frac{0.063mol}{0.063mol} \rightarrow 1$ $\qquad$ $O \rightarrow \frac{0.22mol}{0.063mol} \rightarrow 3.5$

Step 3 is necessary:

Cl = 1•2 = 2 $\qquad$ 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:

$C = 26.1\left|\frac{1mol}{12.01g}\right| = 2.17mol$ $H = 4.3g\left|\frac{1mol}{1.008g}\right| = 4.27mol$

$O = 69.6g\left|\frac{1mol}{16.00g}\right| = 4.35mol$

Step 2:

$C = \frac{2.17mol}{2.17mol} = 1$ $H = \frac{4.27mol}{2.17mol} = 1.9$ $O = \frac{4.35mol}{2.17mol} = 2.0$

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: $N = 30.45g\left|\frac{1mol}{14.01g}\right| = 2.17mol$ $O = 69.55g\left|\frac{1mol}{16.00g}\right| = 4.35mol$

Step 2: $N = \frac{2.17mol}{2.17mol} = 1$ $O = \frac{4.35mol}{2.17mol} = 2.0$

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: g

$$\frac{\frac{92}{mol}}{46.01\frac{g}{mol}} = 2$$

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%

$$Cl = 79.1g\left|\frac{1mol}{35.45g}\right| = 2.23mol \qquad Si = 20.9g\left|\frac{1mol}{28.09g}\right| = 0.744mol$$

$$Cl = \frac{2.23mol}{0.744mol} = 2.99 \qquad Si = \frac{0.744mol}{0.744mol} = 1$$

Empirical: $SiCl_3$

Step 2: $\dfrac{269\frac{g}{mol}}{134.44\frac{g}{mol}} = 2$

Step 3: Si = 1•2 = 2

Cl = 3•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•5 = 21 H = 6•5 = 30 O = 1•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:

$$C = 77.4g\left|\frac{1mol}{12.01g}\right| = 6.44mol \qquad H = 12.9g\left|\frac{8.27mol}{1.008mol}\right| = 12.8mol$$

$$O = 10.2g\left|\frac{1mol}{16.00g}\right| = 0.638mol$$

$$C = \frac{6.44mol}{0.638mol} = 10.1 \qquad H = \frac{12.8mol}{0.638mol} = 20.0 \qquad O = \frac{0.638mol}{0.638mol} = 1$$

Empirical: $C_{10}H_{20}O$

Step 2: $\dfrac{156.3\frac{g}{mol}}{156.26\frac{g}{mol}}$ Step 3: all subscripts will be the same

$C_{10}H_{20}O$ – Menthol

Solution Concentrations

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 X 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 K2SO4 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 a 1.0 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

- I. Introduction to History of Chemical Reactions
- II. Balancing Chemical Reactions
- III. Chemical Reactions Types
- IV. Chemical Reactions Stoichiometry
- V. Yields of Reactions
- VI. 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:

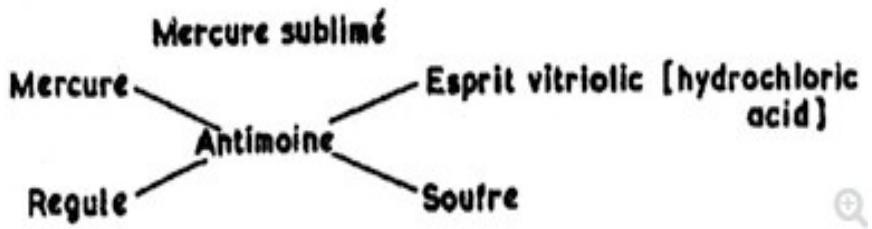


Fig. 4.11 Ancient method describing chemical reaction — Jean Beguin's 1615 diagram from Tyrocinium Chymicum showing the reaction between antimony sulfide and chloride of mercury using labeled lines instead of modern chemical symbols.

Reference: https://www.visionlearning.com/en/library/Chemistry/1/Chemical-Equations/268

Jean Beguin used antimony sulfide to react with chloride of mercury. The mercury became vapor, leaving behind a residue of antimony oxychloride. Jean Beguin first chemical equation is illustrated above.

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:

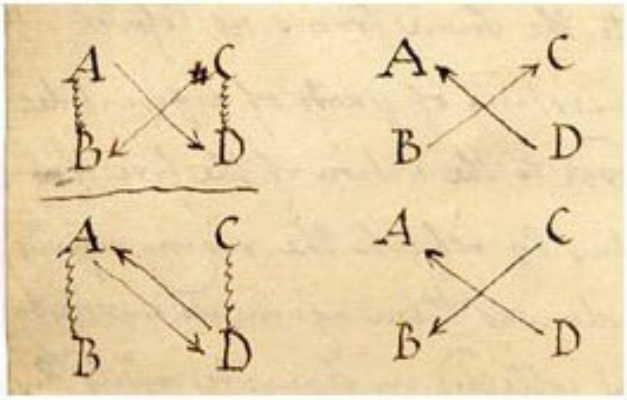


Fig. 4.12 Symbolic method describing chemical reaction — William Cullen's 1747 crossed-line diagrams showing four types of chemical reactions. Each diagram uses letters A, B, C, D to represent chemical species, with crossing lines indicating how reactants transform into products, foreshadowing the modern $A + B \rightarrow C + D$ notation.

Reference: https://www.visionlearning.com/en/library/Chemistry/1/Chemical-Equations/268

The 2 types of reactions diagrammed by Cullen were single and double replacement reactions and the other two were dissolution of salts.

Cullen's diagram was resembling the modern concept of chemical equation where reactants and products were separated by an arrow:

$$A + B \rightarrow C + D$$

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.

At same period of time, Lavoisier, 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.

The history of development of Chemical reactions and equations is given in the figure below:

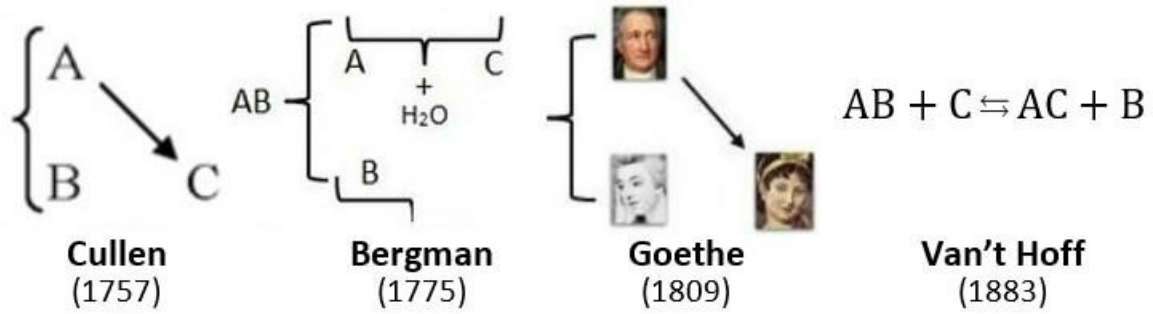


Fig. 4.13 Gradual progression of writing balanced chemical equations — Timeline from Cullen (1757) through Bergman (1775), Goethe (1809), to Van't Hoff (1883), illustrating how chemical notation evolved from simple branching diagrams to the modern symbolic equation $AB + C \rightleftharpoons AC + B$.

Reference: http://www.eoht.info/page/history+of+chemical+equations

II. Balancing Chemical Reactions

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.

Reaction goes to completion: (Using One Arrow to Separate the Reactants from the Products)

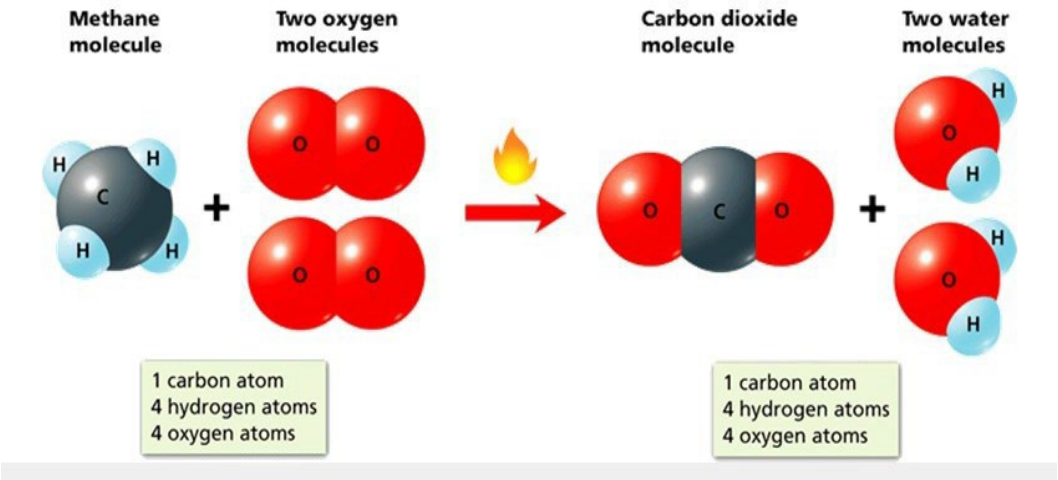


Fig. 4.21 Molecular view of Balancing Chemical Equation — Combustion of methane ($CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$). The diagram shows one methane molecule reacting with two oxygen molecules (4 oxygen atoms) to produce one carbon dioxide molecule and two water molecules. Atom counts on both sides confirm 1 carbon, 4 hydrogen, and 4 oxygen atoms, verifying the equation is balanced.

Reference: https://vhmsscience.weebly.com/chemical-equations--conservation.html

Reaction does not go to completion also known as chemical equilibrium: (Using Double Arrows to Separate the Reactants from the Products)

$$PCl_3 + Cl_2 \rightleftharpoons PCl_5$$

Fig. 4.22 Example of Balanced Chemical Equation — $PCl_3 + Cl_2 \rightleftharpoons PCl_5$. Double arrows (⇌) indicate a chemical equilibrium where the forward and reverse reactions occur simultaneously; both reactants and products are present at equilibrium.

Furthermore, one must 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.

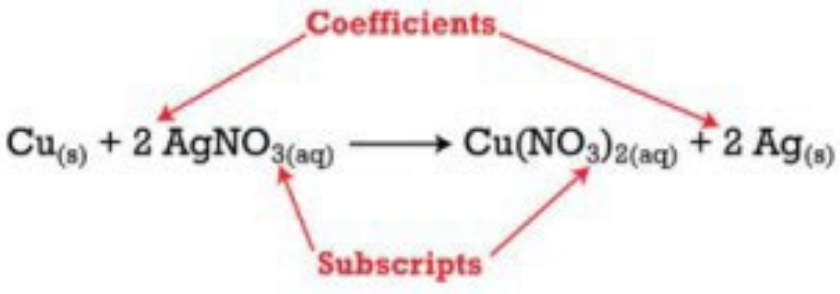


Fig. 4.23 Equation of complete Balanced Chemical Reaction — $Cu(s) + 2AgNO_3(aq) \rightarrow Cu(NO_3)_2(aq) + 2Ag(s)$. Arrows label "Coefficients" (the large numbers in front of formulas that

are adjusted to balance the equation) and "Subscripts" (the small numbers within formulas that indicate fixed atom counts and must never be changed during balancing).

Reference: https://chem.libretexts.org/Bookshelves/Introductory_Chemistry/

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:

$C4H10 + O2 \rightarrow CO2 + H2O + Heat$

Let us make a table:

Table 1: Atom Count for Balancing C_4H_{10} Combustion (Unbalanced)

Atom	Left Side (Reactants)	Right Side (Products)	Status
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.

$C4H10 + O2 \rightarrow 4\ CO2 + 5\ H2O + Heat$

Table 2: Atom Count for Balancing C_4H_{10} Combustion (Balanced)

Atom	Left Side (Reactants)	Right Side (Products)	Status
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 13), one has to go through fraction to balance the chemical equation:

$C4H10 + 13/2\ O2 \rightarrow 4\ CO2 + 5\ H2O$

Since nature does not support fractional atoms, both side of the chemical equations have to be multiplied with the denominator which is 2:

$2 \times [C4H10 + 13/2\ O2 \rightarrow 4\ CO2 + 5\ H2O]$

The final balanced chemical equation is then:

$$2\ C_4H_{10} + 13\ O_2 \rightarrow 8\ CO_2 + 10\ H_2O$$

Chemical equations should exhibit the status of the chemical compounds involved in the chemical reactions such as liquids (l), solids (s), gases (g) and aqueous (aq). Furthermore, the status of the heat being absorbed (taken in) or given away:

$$2\ C_4H_{10}(g) + 13\ O_2(g) \rightarrow 8\ CO_2(g) + 10\ H_2O(g) + \text{Heat [Exothermic]}$$

$$HgCO_3(s) \rightarrow^{(\Delta)} HgO(s) + CO_2(g) \text{ [Exothermic]}$$

$$\text{Heat} + NH_4Cl(g) \rightarrow NH_3(g) + HCl(g) \text{ [Endothermic]}$$

Ionic Chemical Equations

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:

$$NaI(aq) + Pb(NO_3)_2(aq) \rightarrow PbI_2(s) + NaNO_3(aq)$$

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:

$$2\ Na^+(aq) + 2\ I^-(aq) + Pb^{2+}(aq) + 2\ NO_3^-(aq) \rightarrow PbI_2(s) + 2\ Na^+(aq) + 2\ NO_3^-(aq)$$

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.

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:

Net Ionic Chemical Equation:

$$2\ I^-(aq) + Pb^{2+}(aq) \rightarrow PbI_2(s)$$

Example 2:

Complete molecular ionic chemical equation:

$$KI(aq) + Pb(NO_3)_2(aq) \rightarrow PbI_2(s) + KNO_3(aq)$$

Balanced:

$$2\ KI(aq) + Pb(NO_3)_2(aq) \rightarrow PbI_2(s) + 2\ KNO_3(aq)$$

Complete ionic chemical equation:

$$2\ K^+(aq) + 2\ I^-(aq) + Pb^{2+}(aq) + 2\ NO_3^-(aq) \rightarrow PbI_2(s) + 2\ K^+(aq) + 2\ NO_3^-(aq)$$

With K+(aq) and NO3-(aq) are being the spectator ions.

Net ionic chemical equation:

2 I-(aq) + Pb2+(aq) → PbI2(s)

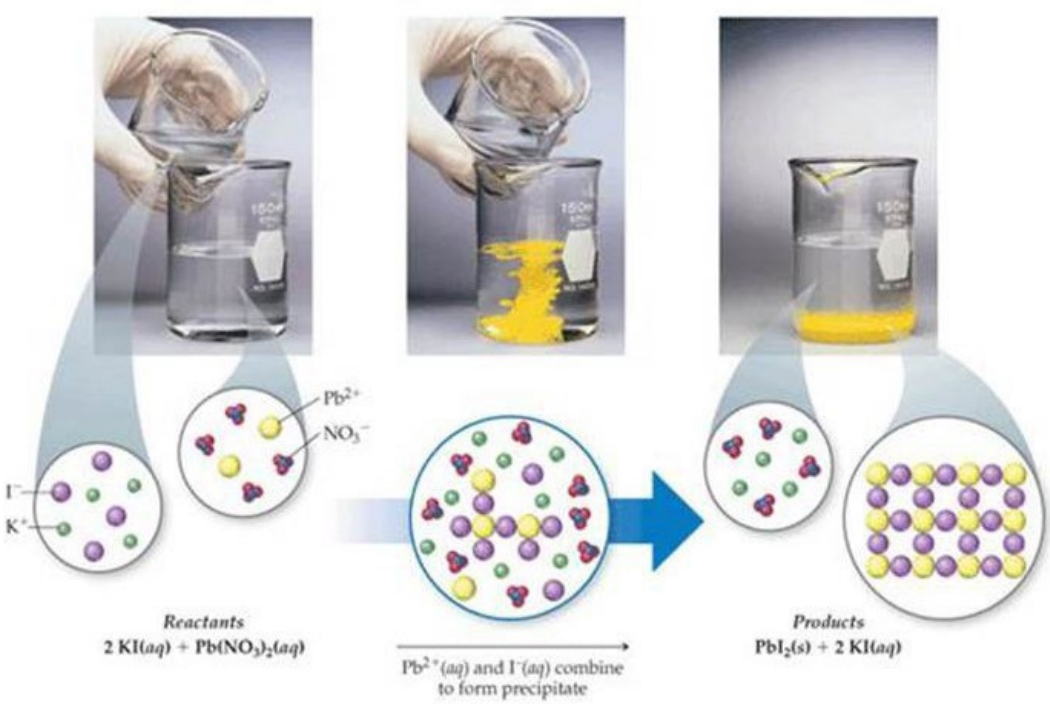


Fig. 4.24 Chemical Reaction Molecular View — Precipitation reaction between potassium iodide (2 KI) and lead(II) nitrate ($Pb(NO_3)_2$). The three-panel image shows: (left) the separated aqueous reactants with their component ions; (center) the mixing process where Pb^{2+} and I^- ions combine to form a yellow precipitate; and (right) the final products — bright yellow lead(II) iodide solid (PbI_2) settled at the bottom of the beaker, with potassium and nitrate spectator ions remaining in solution.

Reference: https://microbenotes.com/introduction-to-precipitation-reaction/

<u>Simulation Activity — Balancing Chemical Equations</u>

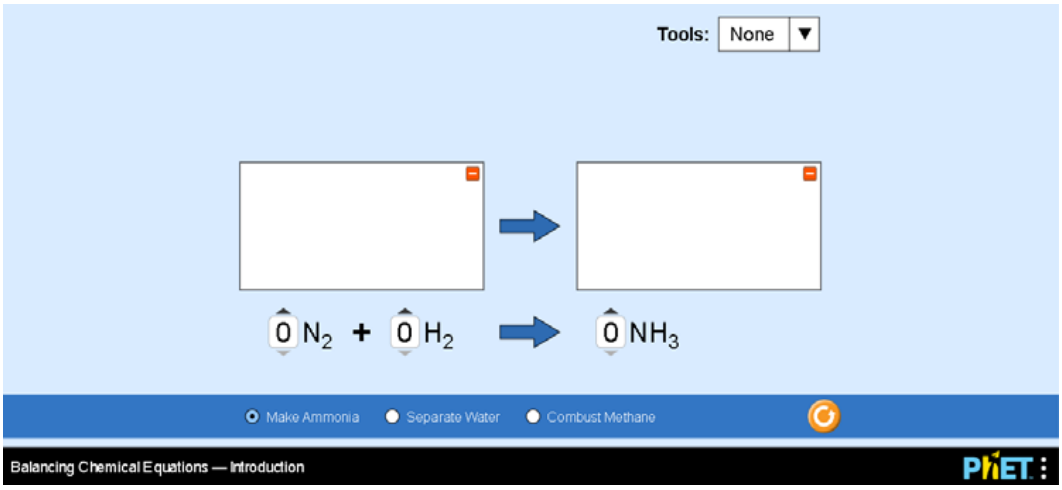


Fig. 4.25 PhET Balancing Chemical Equations Simulation — Introduction Screen. Students can enter coefficients in the boxes above each molecule and use sliders to adjust molecule counts, visually verifying when the number of each type of atom is equal on both sides of the reaction arrow.

Simulation link: 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".

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.

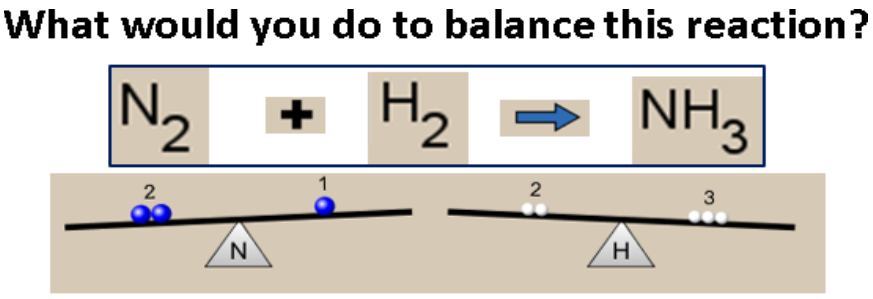
5. Use this reaction to show that you can draw molecular representations of a balanced reaction. Explain how your representations were derived in paragraph form.

$CO_2 + H_2O \rightarrow C_2H_6 + O_2$

(See simulation for molecular representation exercise)

Test your understanding:

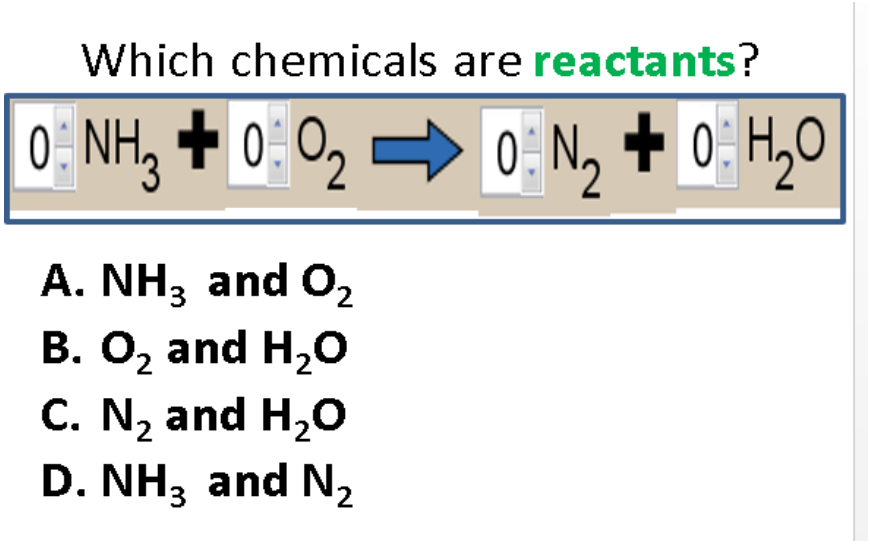
For each question, write your answer and give your reasoning with evidence from the simulation.



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 **($2NH_3$)**

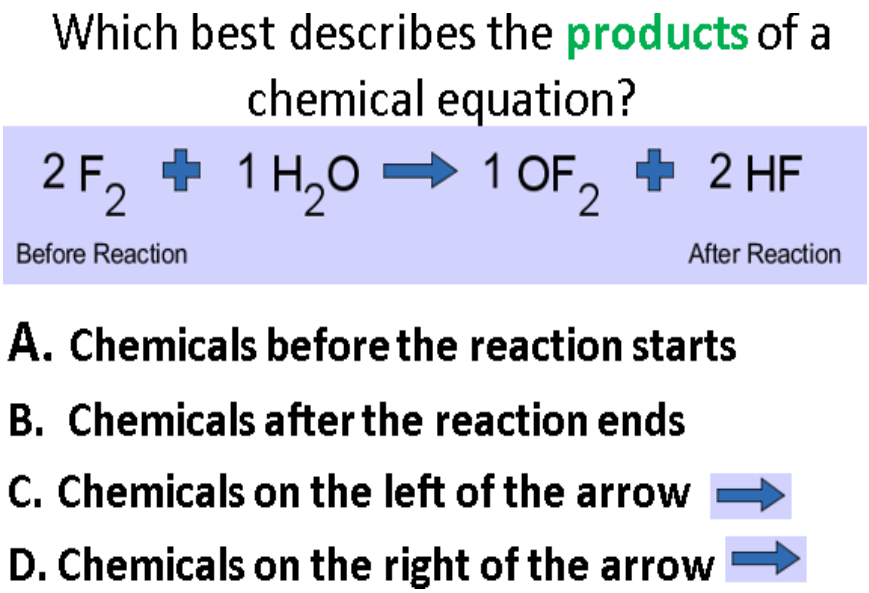
Question 1: What would you do to balance the reaction $N_2 + H_2 \rightarrow NH_3$? The simulation shows current slider values and asks which changes correctly balance the equation. Correct answers involve adjusting coefficients (not subscripts) so atom counts match on both sides.

Your answer and explanation:



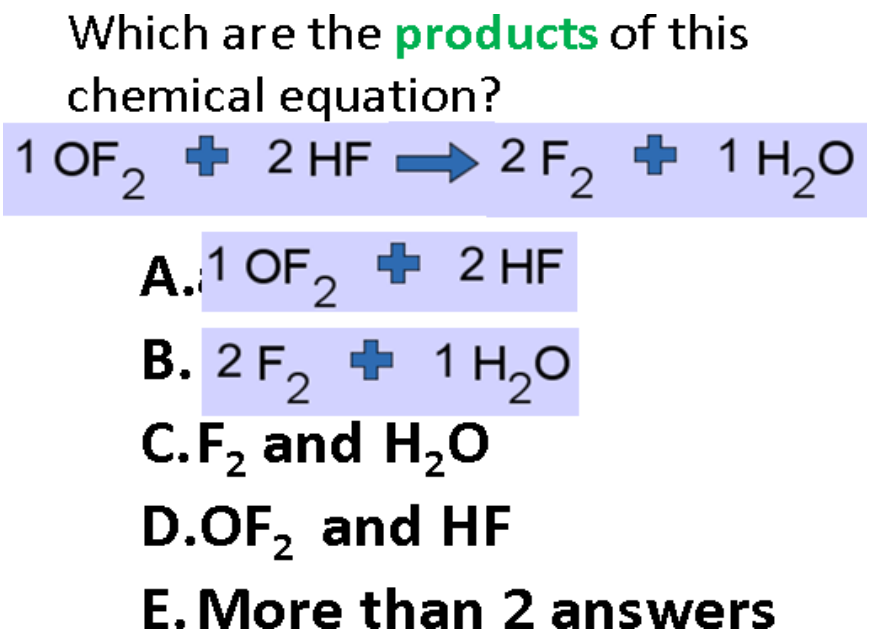
Question 2: Which chemicals are reactants in $NH_3 + O_2 \rightarrow N_2 + H_2O$? Reactants are the substances on the left side of the reaction arrow that are consumed during the reaction. The correct answer is A: NH_3 and O_2.

Your answer and explanation:



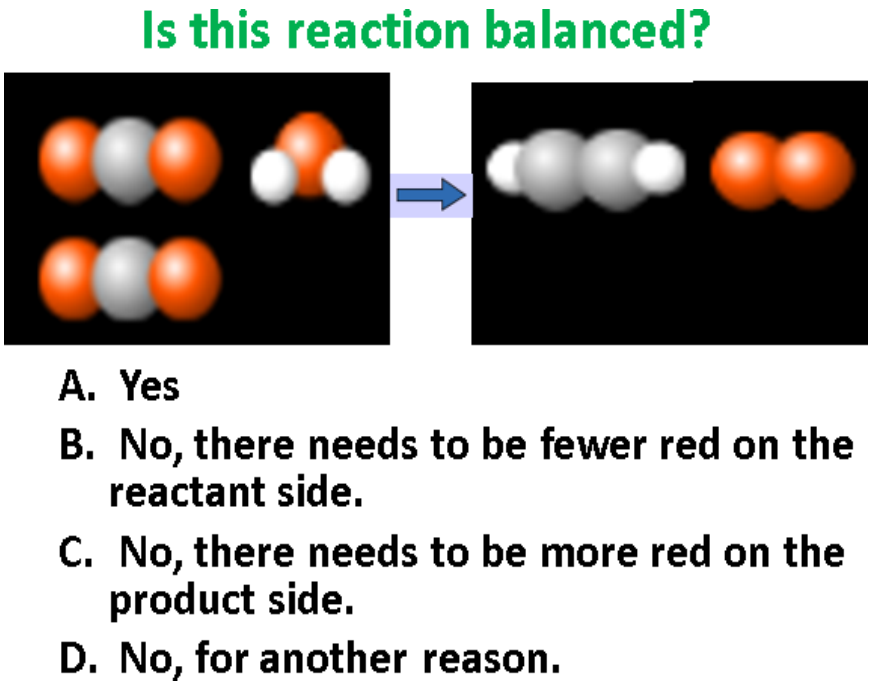
Question 3: Which best describes the products of a chemical equation, using $2F_2 + H_2O \rightarrow OF_2 + 2HF$ as an example? Products are the new substances formed after the reaction — they appear on the right side of the reaction arrow. Correct answers: B (chemicals after the reaction ends) and D (chemicals on the right of the arrow).

Your answer and explanation:



Question 4: Which are the products of the equation $1\ OF_2 + 2\ HF \rightarrow 2\ F_2 + 1\ H_2O$? Products appear on the right side of the reaction arrow. The correct answer is B: $2\ F_2 + 1\ H_2O$, since these are the substances produced after the reaction.

Your answer and explanation:



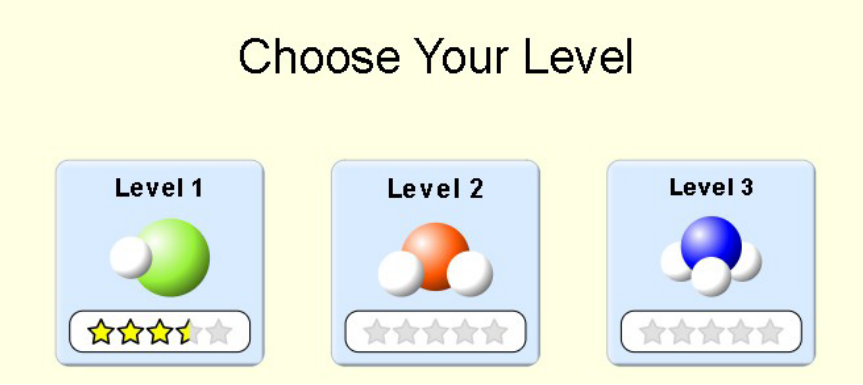
Question 5: Is this reaction balanced? The molecular models show orange (red) and white atoms. Students must count the atoms on each side of the reaction to determine if the equation is balanced. The correct answer requires comparing atom counts for each element on both sides.

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.

Sample game completion screen showing a score of 8 out of 10 with 4 stars — an example of what the level completion screen looks like after playing the Balancing Chemical Equations game.



Balancing Chemical Equations game "Choose Your Level" screen displaying three levels of increasing difficulty. Level 1 (green, basic molecules), Level 2 (red, more complex molecules), and Level 3 (blue, most complex). Star ratings show current progress for each level.

1. Play Level 1 of 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?
    - c. When you complete the level 1 game, capture the screen with your score. Paste it below.
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.

Extra challenge: For an extra challenge, you can turn on the timer and see if you can improve your skills.

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

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:

$$AgNO3(aq) + K2Cr2O7(aq) \rightarrow Ag2Cr2O7(s) + KNO3(aq)$$

Ag2Cr2O7(s) is a ruby red precipitate (solid) insoluble in water. The image below illustrates the Ag2Cr2O7 precipitate:

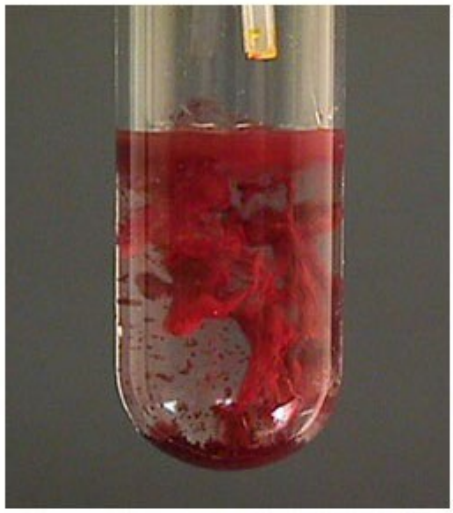


Fig. 4.31 Formation of Precipitation — Photograph of a test tube showing the bright ruby-red precipitate of silver dichromate ($Ag_2Cr_2O_7$) formed from the reaction $AgNO_3(aq) + K_2Cr_2O_7(aq) \rightarrow Ag_2Cr_2O_7(s) + KNO_3(aq)$. The dense red-crimson solid settles in the solution, demonstrating its water insolubility.

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

Reference: https://www.sigmaaldrich.com/technical-documents/articles/chemistry/solubility-rules-solubility-of-common-ionic-compounds.html

Soluble ions in aqueous solutions:

Table 3: Soluble Ions in Aqueous Solutions

Ions	Except
Alkali metals (Group I): Na+, K+, etc.	
Ammonium ions NH4+	
Nitrates, acetates, chlorates, and perchlorate: NO3-, C2H3O2-, ClO3-, ClO4-	
Binary compounds of halogens (Cl-, Br-, I-) with metals	Fluoride: Silver, lead, and mercury (F-, Ag+, Pb2+, Hg2+). *Lead halides are soluble in hot water.
All sulfates SO42-	Barium, strontium, calcium, lead, silver, and mercury: Ba2+, Sr2+, Ca2+, Pb2+, Ag+, Hg2+

Slightly Soluble ions in aqueous solutions:

Table 4: Slightly Soluble Ions in Aqueous Solutions

Ions	Except
Sulfates of lead, silver, and mercury: SO42- with Pb2+, Ag+, Hg2+	*Lead sulfate is poorly soluble.
Hydroxides of alkaline earth metals (Group II): OH- with Ca2+, Sr2+, etc.	Barium Ba2+

Insoluble ions in aqueous solutions:

Table 5: Insoluble Ions in Aqueous Solutions

Ions	Except
Sulfides S2-	Calcium, barium, strontium, magnesium, sodium, potassium, and ammonium: Ca2+, Ba2+, Sr2+, Mg2+, Na+, K+, NH4+
Hydroxides OH-	Alkali metals (Group I), transition metals, aluminum, and ammonium: Na+, K+, etc.; Al3+, NH4+
Carbonates, oxalates, chromates, and phosphates: CO32-, C2O42-, CrO42-, PO43-	Alkali metals (Group I) and ammonium: Na+, K+, etc.; NH4+. *Lithium phosphate is poorly soluble

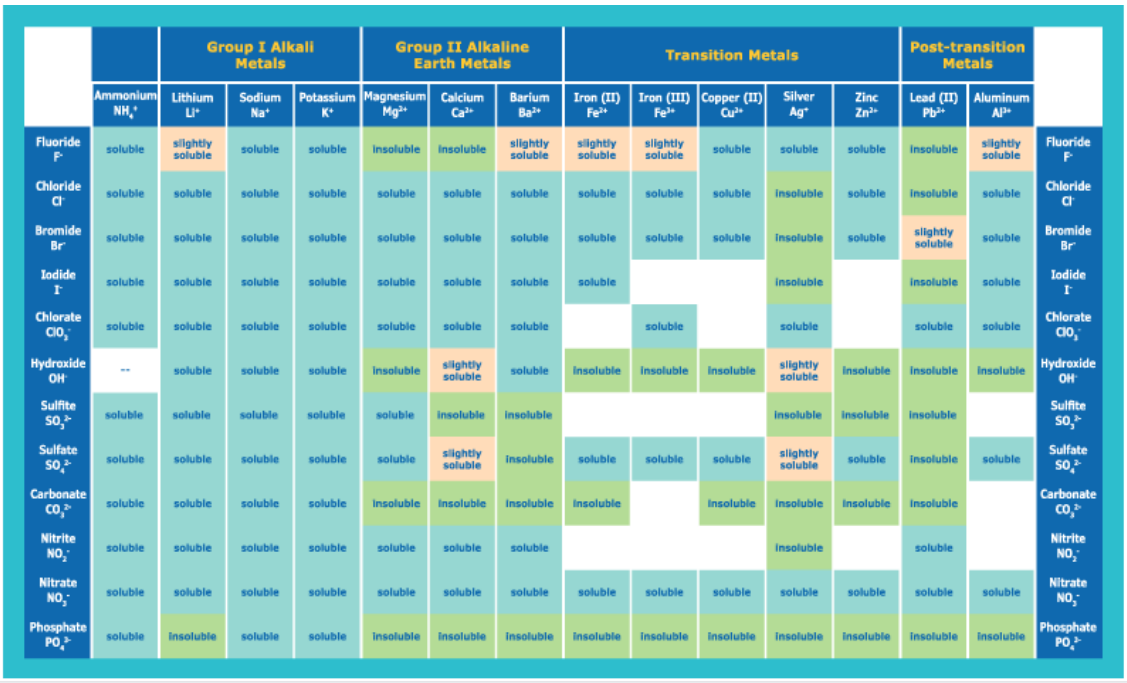


Fig. 4.32 Solubility Rules — Periodic-table-style chart showing the aqueous solubility of common ionic compound combinations. Rows list common anions (fluoride through phosphate) and columns list common cations by periodic group. Each cell indicates whether the resulting compound is soluble, slightly soluble, or insoluble, enabling prediction of whether a precipitation reaction will occur when two ionic solutions are mixed.

Solubility Rule:

- 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 against the solubility table and determine whether this formed ionic compound is soluble or insoluble.

Solubility Activity — Precipitation Reaction

Precipitation Reaction Simulation: https://javalab.org/en/precipitation_reaction_en/

AgNO3(aq) + BaCl2(aq) → AgCl(s) + Ba(NO3)2(aq)

AgCl is a solid and called a precipitate. It settles at the bottom of the reaction container.

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.

Table 6: Precipitation Reaction Matrix — Identifying Double Displacement Reactions

Compounds	BaCl2	CaCl2	NaCl	Na2SO4	Na2CO3	K2SO4	KNO3	AgNO3
BaCl2	No Reaction							

Compounds	BaCl2	CaCl2	NaCl	Na2SO4	Na2CO3	K2SO4	KNO3	AgNO3
CaCl2		No Reaction						
NaCl			No Reaction					
Na2SO4				No Reaction				
Na2CO3					No Reaction			
K2SO4						No Reaction		
KNO3							No Reaction	
AgNO3								No Reaction

Acid – Base Reactions

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.

Example:

$$HCl(aq) + NaOH(aq) \rightarrow NaCl(aq) + H2O(l) + Heat$$

Complete ionic chemical equation:

$$H+(aq) + Cl-(aq) + Na+(aq) + OH-(aq) \rightarrow Na+(aq) + Cl-(aq) + H2O(l) + Heat$$

Net ionic chemical equation [Cl-(aq) and Na+(aq) spectator ions]:

$$H+(aq) + OH-(aq) \rightarrow H2O(l) + Heat$$

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 H3O hydronium ions with hydroxide ions.

Types of Acids

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 (7 known):

- Perchloric acid: HClO4
- Chloric acid: HClO3
- Hydrochloric acid: HCl
- Hydroiodic acid: HI
- Hydrobromic acid: HBr

- Nitric acid: HNO3
- Sulfuric acid: H2SO4

Weak acids (examples):

- Acetic Acid: CH3COOH
- Hydrofluoric acid: HF
- Phosphoric acid: H3PO4
- Oxalic acid: H2C2O4
- Carbonic acid: H2CO3

Fruits are very rich with weak acids:

Fig. 4.33 Common Acidic Substances — These photographs show a variety of fruits and vegetables that naturally contain weak organic acids. Citrus fruits contain citric acid, apples contain malic acid, berries contain ascorbic acid (vitamin C), and grapes contain tartaric acid. All of these are weak acids that partially dissociate in water.

Weak acids are also found in vegetables: Asparagus, Beans, Corn, Cucumbers, Garlic, Green beans, Greens (lettuce, kale, collards, spinach, etc.), Onions, Peas, Pumpkins, Squash

Types of Bases

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 (Group 1A and 2A):

- 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

Weak bases (examples):

- Ammonium hydroxide: NH4OH
- Iron-III-hydroxide: Fe(OH)3
- Titanium-II-hydroxide: Ti(OH)2
- Aluminum hydroxide: Al(OH)3
- Pyridine: C5H5N
- Aniline: C6H5NH2
- All amines are considered as weak bases such as methyl amine CH3NH2 etc...

Fruits are very rich with weak bases:

Fig. 4.34 Common Weakly Basic Substances — Photographs of alkaline-forming foods: dried chestnuts, bing cherries (top), and almonds (bottom). These foods contain weak base compounds that partially dissociate in water, and they have an alkaline-forming metabolic effect. Reference: nuts.com/healthy-eating/alkaline-diet

Acid-Base Neutralization examples:

$Fe(OH)3(aq) + 3\ HNO3(aq) \rightarrow Fe(NO3)3(aq) + 3\ H2O(l)$ [water produced as by product]

This type of reaction is considered neutralization reaction as well as double Replacement/Displacement Reaction.

$C6H5NH2(aq) + HCl(aq) \rightarrow C6H5NH3+\ Cl-\ (s)$

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.

Redox Reactions

Redox Reactions have several sub types: 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 adjacent 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:

- 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 O2, N2, Cl2, NaCl, and Na2CO3 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 Ca2+ ion is +2, Al3+ has the oxidation of +3, and P3- has the oxidation number of -3, S2- has the oxidation number of -2. NH4+ 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: NH3, HNO3, C2H6
- 4. The oxidation number of hydrogen is -1 when hydrogen is forming ionic bonds (combined itself with another metal(s)). Examples: KH, BaH2, AlH3 and LiAlH4.
- 5. The metals in Group IA has the oxidation number of +1. Examples: Na3P and K2S
- 6. The metals in Group IIA has the oxidation number of +2. Examples: Ba3P2 and Ba(HCO3)2
- 7. Generally oxygen has the oxidation number of -2. Exceptions include molecules and polyatomic ions that contain O-O bonds, such as O2, O3 and H2O2, and the O22- ions.
- 8. Group VIIA elements have in general the oxidation number of -1. Examples: FeCl3, HF, and VI3

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 adjacent 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)

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:

$Na^0 \rightarrow Na^+ + e^-$ [first half reaction: oxidation reaction]

$e^- + Cl^0 \rightarrow Cl^-$ [second half reaction: reduction reaction]

$Na^0 + Cl^0 \rightarrow Na^+ + Cl^-$ [Complete Redox Reaction]

Oxidizing and Reducing Agents

Example: $K^0 + Br^0 \rightarrow K^+ + Br^-$

K is forcing Br to be reduced. K is said to be Reducing Agent. K is providing the valence electrons to Br.

Br is forcing K to be oxidized. Br is said to be Oxidizing Agent. Br is removing valence electrons from K.

Worked Examples — Oxidation Numbers

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.

Table 7: Oxidation States of Nitrogen in Common Compounds

Name	Formula	Oxidation State of N
Ammonia	NH_3	-3
Nitrogen	N_2	0

Name	Formula	Oxidation State of N
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. $N_2(g) + 3\ H_2(g) \rightarrow 2\ NH_3(g)$

N in N_2 = 0; in NH_3 = -3 (oxidation number decreases → N_2 is reduced)

H in H_2 = 0; in NH_3 = +1 (oxidation number increases → H_2 is oxidized)

Reducing agent: H_2 (gets oxidized). Oxidizing agent: N_2 (gets reduced).

Balancing Redox Reactions in Acidic Medium

Oxidation/Reduction (Redox) reactions can be balanced using the half-reaction method:

Example: $Br^- + MnO_4^- \rightarrow Br_2 + Mn^{2+}$

Step 1: Split into half-reactions

Bromine: $Br^- \rightarrow Br_2$

Manganese: $MnO_4^- \rightarrow Mn^{2+}$

Step 2: Balance Br:

$2\ Br^- \rightarrow Br_2 + 2e^-$ (oxidation)

Step 3: Balance Mn (add H_2O for O, H^+ for H, e^- for charge):

$5e^- + 8H^+ + MnO_4^- \rightarrow Mn^{2+} + 4H_2O$ (reduction)

Step 4: Equalize electrons (multiply Br half ×5, Mn half ×2):

$10\ Br^- \rightarrow 5\ Br_2 + 10e^-$

$10e^- + 16H^+ + 2\ MnO_4^- \rightarrow 2\ Mn^{2+} + 8H_2O$

Final balanced equation (acidic):

$10\ Br^- + 16\ H^+ + 2\ MnO_4^- \rightarrow 2\ Mn^{2+} + 5\ Br_2 + 8\ H_2O$

Oxidizing agent: MnO_4^- (gets reduced). Reducing agent: Br^- (gets oxidized).

Balancing Redox Reactions in Basic Medium

To carry out in basic solution, add enough OH^- to each side to neutralize H^+. The H^+ and OH^- form H_2O.

From the acidic equation above, add 16 OH^- to each side:

Left side: $16\ H^+ + 16\ OH^- = 16\ H_2O$

Final balanced equation (basic):

$10\ Br^- + 2\ MnO_4^- + 8\ H_2O \rightarrow 5\ Br_2 + 2\ Mn^{2+} + 16\ OH^-$

IV. Chemical Reactions Stoichiometry

The stoichiometry of chemical reactions is based on the mole ratios among the reactants and the products. A general outline summarizes different stoichiometry calculations is given in the figure below:

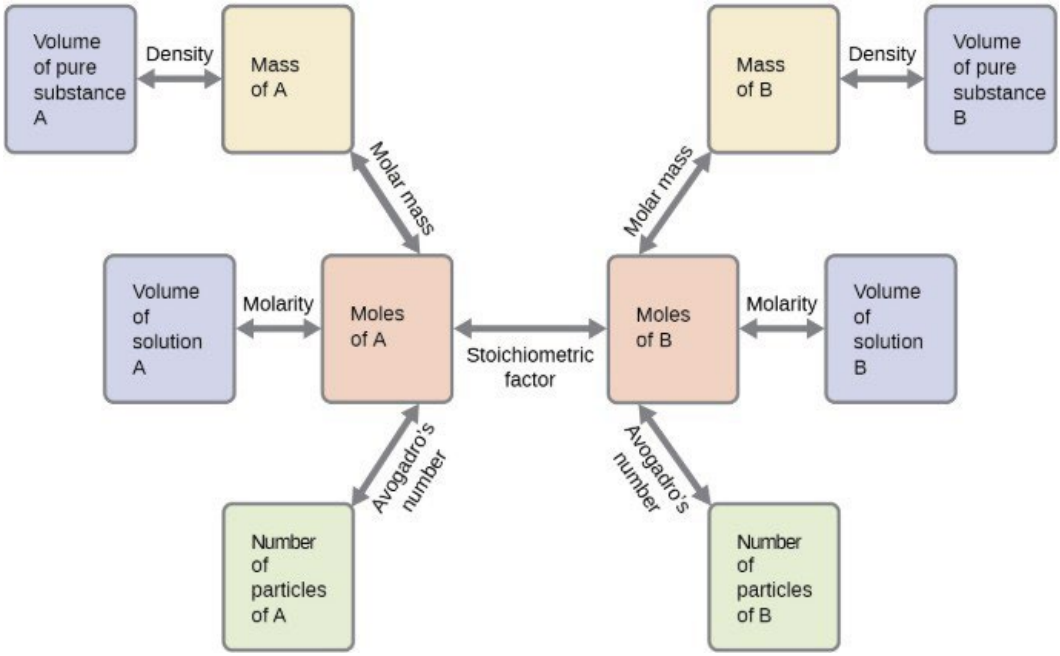


Fig. 4.41 Flow Chart for Reaction Stoichiometry — Diagram showing the mathematical pathways for converting between quantities in a chemical reaction. To convert from one substance (A) to another (B): start with the known quantity (mass, volume, or particles), convert to moles using molar mass, molarity, or Avogadro's number, apply the stoichiometric factor (mole ratio from the balanced equation) to find moles of B, then convert moles of B to the desired quantity. Reference: pressbooks-dev.oer.hawaii.edu/chemistry

Reference: https://pressbooks-dev.oer.hawaii.edu/chemistry/chapter/reaction-stoichiometry/

Example: 2 KClO3 → 2 KCl + 3 O2

The stoichiometry expresses the mole ratios among the reactants and products:

- 2 moles of KClO3 / 2 moles of KCl
- 2 moles of KClO3 / 3 moles O2

$$2\ H_2O \rightarrow 2\ H_2 + O_2$$

7. How many moles of O_2 are produced when 1.26 moles of H_2O is reacted?

$$1.26 \text{ mol } H_2O \left| \frac{1 \text{ mol } O_2}{2 \text{ mol } H_2O} \right. = \frac{.630}{} \text{ mol } O_2$$

How many moles of H_2O are needed to produce 55.7 moles of H_2?

$$55.7 \text{ mol } H_2 \left| \frac{2 \text{ mol } H_2O}{2 \text{ mol } H_2} \right. = \frac{55.7}{} \text{ mol } H_2O$$

Worked stoichiometry examples using the mole ratio (dimensional analysis) method for 2 $KClO_3$ → 2 KCl + 3 O_2. (a) 1.65 mol $KClO_3$ produces 2.48 mol O_2; (b) 3.50 mol KCl requires 3.50 mol $KClO_3$; (c) 2.73 mol $KClO_3$ produces 2.73 mol KCl.

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)

$$\frac{3.40 \text{ mol } H_2 \quad | \quad 1 \text{ mol } O_2}{2 \text{ mol } H_2} = 1.70 \text{ mol } O_2$$

Stoichiometry problems for 2 H_2O → 2 H_2 + O_2. Problem 7: 1.26 mol H_2O produces 0.630 mol O_2. Conversion: 55.7 mol H_2 requires 55.7 mol H_2O.

$$2\ KClO_3 \rightarrow 2\ KCl + 3\ O_2$$

9. How many **grams** of O_2 will be formed from 3.76 grams of $KClO_3$?

$$\frac{3.76 \text{g } KClO_3 \quad | \quad 1 \text{ mol } KClO_3 \quad | \quad 3 \text{ mol } O_2 \quad | \quad 32.00 \text{ g } O_2}{122.55 \text{ g } KClO_3 \quad | \quad 2 \text{ mol } KClO_3 \quad | \quad 1 \text{ mol } O_2} = 1.47 \text{ g } O_2$$

Worked stoichiometry problems using gram conversions for 2 $KClO_3$ → 2 KCl + 3 O_2. Problem 9: 3.76 g $KClO_3$ → 1.47 g O_2. Problem 10: 30.0 g KCl requires 49.3 g $KClO_3$. Problem 11: 2.73 g $KClO_3$ → 1.66 g KCl. Molar masses used: $KClO_3$ = 122.55 g/mol, KCl = 74.55 g/mol, O_2 = 32.00 g/mol.

Number of molecules produced from moles of reactants

Consider the reaction: N2 + 3 H2 ⇌ 2 NH3 + Heat

a) How many molecules of NH3 produced if 0.750 moles of N2 is used.

Molecules of NH3 = [0.750 mol N2] × [2 mol NH3 / 1 mol N2] × [6.022×10^{23} molecules/mol] = 9.033×10^{23} molecules NH3

b) How many molecules of NH3 produced if 1.80 moles of H2 is used.

Molecules of NH3 = [1.80 mol H2] × [2 mol NH3 / 3 mol H2] × [6.022×10^{23} molecules/mol] = 7.23×10^{23} molecules NH3

Gram (mass) stoichiometry calculations

Consider: ZnSO4 + SrCl2 → SrSO4 + ZnCl2

a) Mass of SrCl2 consumed when 55.0 g of ZnCl2 is produced:

= [55.0 g ZnCl2] × [mol ZnCl2 / 136.3 g ZnCl2] × [1 mol SrCl2 / 1 mol ZnCl2] × [158.5 g SrCl2 / mol SrCl2] = 64.0 g SrCl2

b) Mass of SrSO4 when 88.5 g of ZnSO4 reacts:

= [88.5 g ZnSO4] × [mol ZnSO4 / 161.5 g ZnSO4] × [1 mol SrSO4 / 1 mol ZnSO4] × [183.7 g SrSO4 / mol SrSO4] = 0.101×10^3 g SrSO4

V. Yields of Reactions

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.

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.

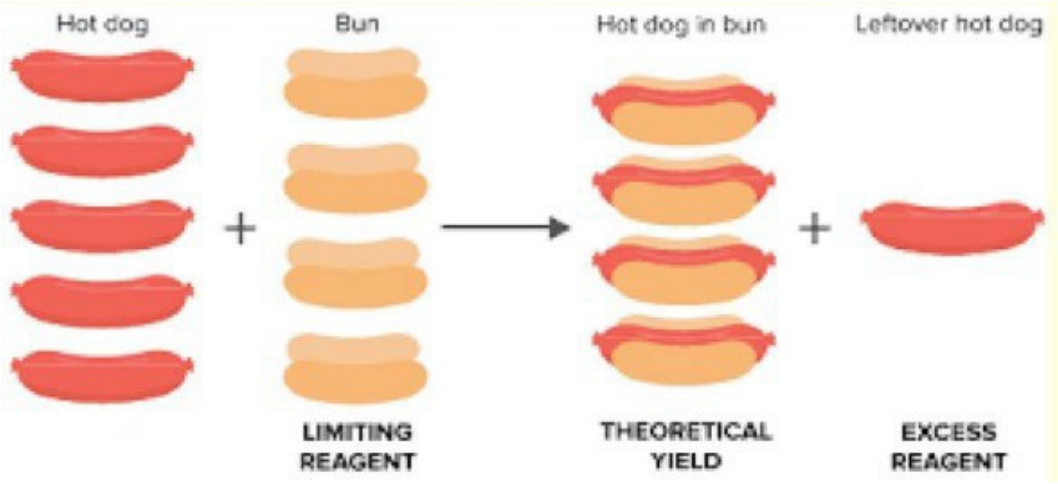


Fig. 4.51 Theoretical Yield Analogy Using Hot Dogs — The hot dog analogy illustrates limiting and excess reactants. With 5 hot dogs and 3 buns: the buns are the limiting reagent (they determine the maximum product), 3 assembled hot dogs represent the theoretical yield, and 2 leftover hot dogs are the excess reagent. Reference: slideplayer.com/slide/12627403/

Reference: https://slideplayer.com/slide/12627403/

Example: CO + 2 H2 → CH3OH

If 12.0 g H2 and 74.5 g CO are used, determine the limiting reactant.

Moles of CH3OH based on CO:

[74.5 g CO] × [mol CO / 28.0 g CO] × [1 mol CH3OH / 1 mol CO] = 2.66 moles CH3OH

Moles of CH3OH based on H2:

[12.0 g H2] × [mol H2 / 2.00 g H2] × [1 mol CH3OH / 2 mol H2] = 3.00 moles CH3OH

Since 2.66 moles < 3.00 moles → CO is the limiting reactant and H2 is the excess reactant.

Theoretical yield:

[2.66 mol CH3OH] × [32.0 g CH3OH / mol CH3OH] = 85.1 g CH3OH

Example: C3H8 + 5 O2 → 3 CO2 + 4 H2O

If 0.550 g C3H8 is reacting with 0.550 g O2. Calculate:

a) CO2 produced based on limiting reactant:

Based on C3H8: [0.550 g C3H8] × [1 mol / 44.0 g] × [3 mol CO2 / 1 mol C3H8] = 0.0375 mol CO2

Based on O2: [0.550 g O2] × [1 mol / 32.0 g] × [3 mol CO2 / 5 mol O2] = 0.0103 mol CO2

O2 produces fewer moles of CO2 → O2 is the limiting reactant.

b) Theoretical yield:

[0.0103 mol CO2] × [44.0 g CO2 / mol CO2] = 0.572 g CO2

c) Overall yield (if actual yield = 0.550 g CO2):

Overall yield = [0.550 g / 0.572 g] × 100% = 96.2%

d) Percent error:

% error = |[0.572 g - 0.550 g] / 0.572 g| × 100% = 3.85%

VI. Quantitative Chemical Analysis

Quantitative chemical analysis is a branch of chemistry that oversees the determination of the amount or percentage of one or more the components of a chemical compound. 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.

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.

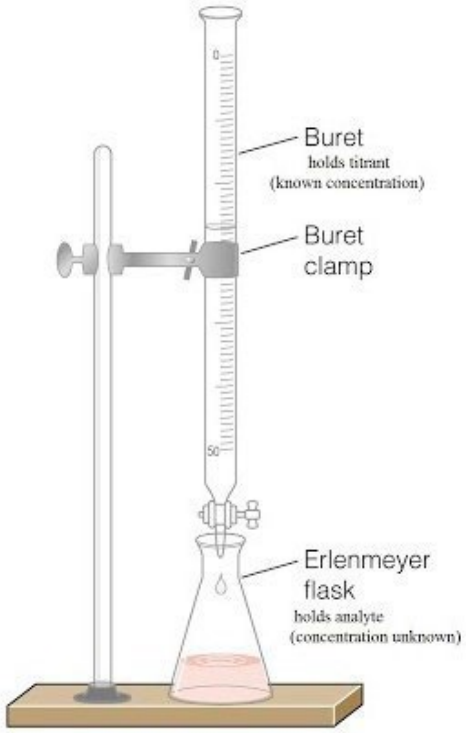


Fig. 4.61 Titration Setup — Standard laboratory titration apparatus consisting of a buret (filled with the titrant of known concentration) held vertically by a clamp and stand, positioned above an Erlenmeyer flask containing the analyte or titrand (solution of unknown concentration). Drops of titrant are added gradually until the indicator signals the endpoint, indicating neutralization is complete.

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 titrand.

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 difference between the indicator end point and the equivalent point is very minimal.

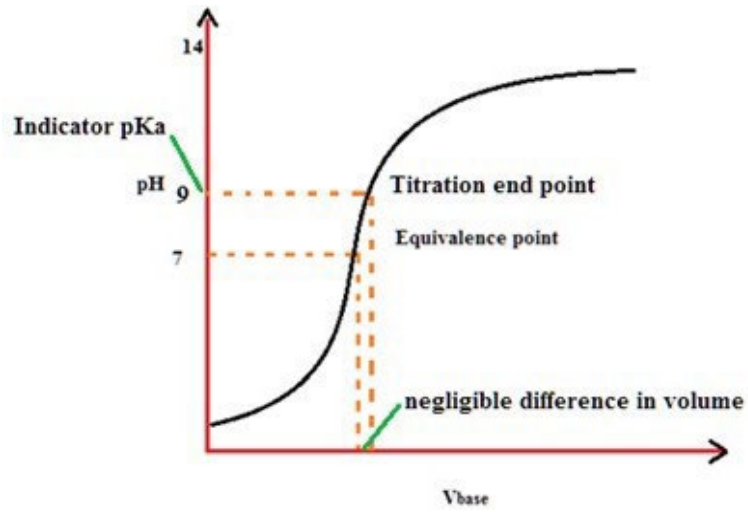


Fig. 4.62 Titration Plot with Indicator — S-shaped pH titration curve showing pH versus volume of base added. The equivalence point (where moles of acid = moles of base, ~pH 7) and titration endpoint (where indicator changes color, slightly above pH 7) are marked with dotted lines. The negligible volume difference between them confirms the indicator endpoint closely approximates the true equivalence point. Reference: assignmentexpert.com

Titration Definition, Method and Calculations

Titration is the process by which an unknown concentration of an acid or a base (called the analyte or titrand) is neutralized with exact known concentration of a base or an acid (called the titrant) which is introduced in the buret. The analyte is placed in an Erlenmeyer flask with a few drops of the appropriate indicator.

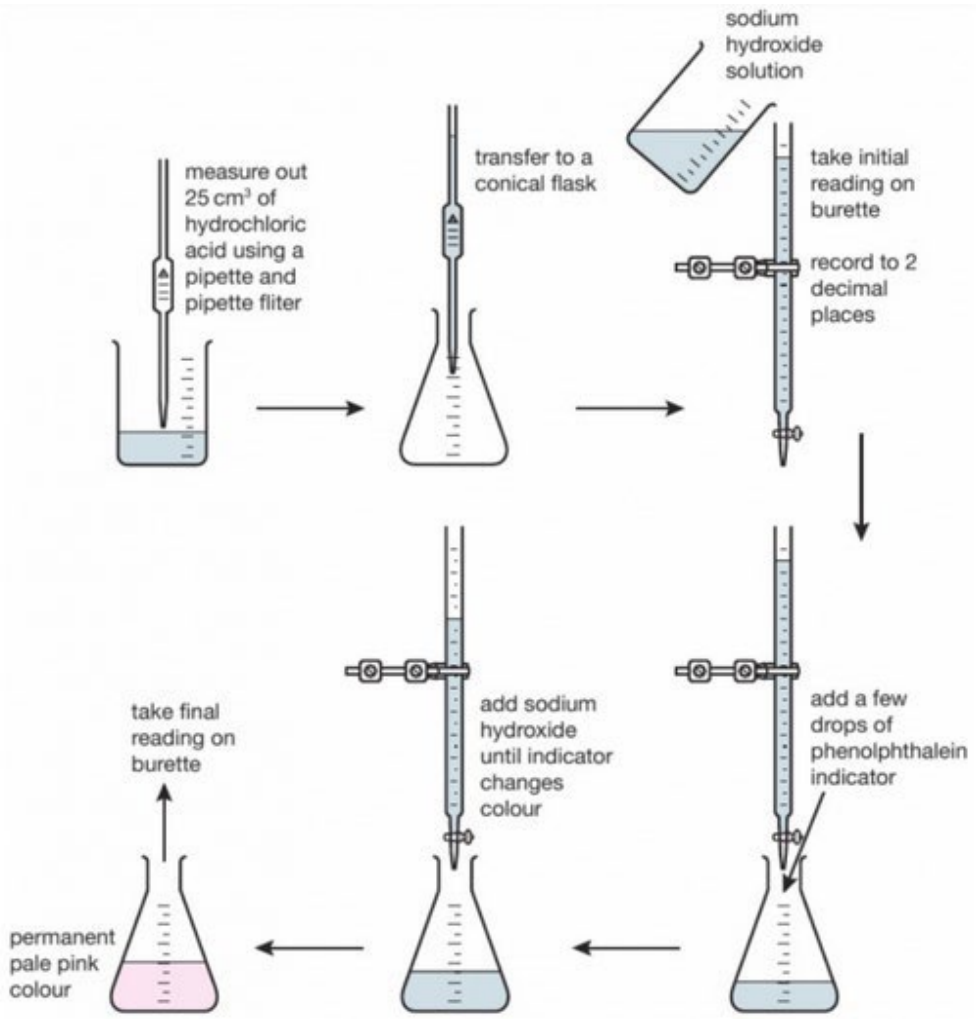


Fig. 4.63 Process of Titration — Step-by-step illustration of a standard acid-base titration procedure: (1) Measure 25 cm³ of hydrochloric acid using a pipette; (2) Transfer to conical flask; (3) Take initial burette reading; (4) Add a few drops of phenolphthalein indicator; (5) Slowly add sodium hydroxide from the burette until the indicator changes colour; (6) Record the final burette reading when a permanent pale pink colour appears, indicating the endpoint. Reference: tutormyself.com

Example Calculations

Acid – Base Ratio = 1 mol : 1 mol

1) Calculate the molarity of 35.5 mL HCl titrated with 2.50 M NaOH. Endpoint = 26.5 mL NaOH.

$HCl(aq) + NaOH(aq) \rightarrow NaCl(aq) + H2O(l)$

Using the Dilution Law ($M1 \times V1 = M2 \times V2$):

$M(HCl) = [2.50\ M \times 26.5\ mL] / [35.5\ mL] = 1.87\ M\ HCl$

2) 83 mL of 0.45 M NaOH neutralizes 235 mL of HCl. Find M(HCl):

$M(HCl) = [0.45\ M \times 83\ mL] / [235\ mL] = 0.16\ M$

8) 50.0 mL of 0.500 M LiOH neutralizes 125 mL H2SO4. Find M(H2SO4):

$H_2SO_4(aq) + 2\ LiOH(aq) \rightarrow Li_2SO_4(aq) + 2\ H_2O(l)$ [Mole ratio 1:2 — cannot use Dilution Law]

Step 1: mol LiOH = [0.5000 mol/L] × [0.0500 L] = 0.0250 mol LiOH

Step 2: mol H_2SO_4 = [0.0250 mol LiOH] × [1 mol H_2SO_4 / 2 mol LiOH] = 0.0125 mol H_2SO_4

Step 3: M(H_2SO_4) = [0.0125 mol] / [0.125 L] = 0.100 M H_2SO_4

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.

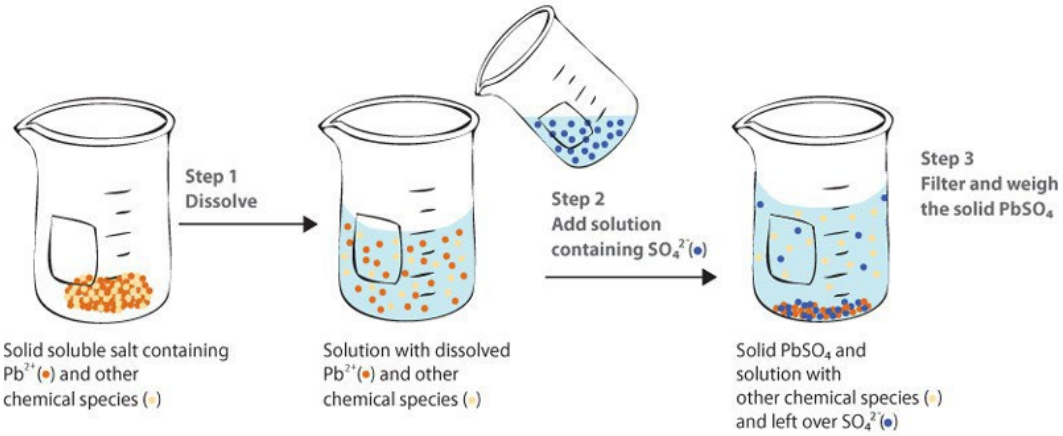


Fig. 4.67 Process of Gravimetric Separation — Three-step diagram illustrating how gravimetric analysis works to isolate and quantify Pb^{2+} ions: (1) Dissolve the solid sample containing Pb^{2+} and other species in water; (2) Add a solution containing SO_4^{2-} ions to precipitate all Pb^{2+} as insoluble $PbSO_4$; (3) Filter the mixture to collect the $PbSO_4$ precipitate, dry it, and weigh it to calculate the original Pb^{2+} concentration. Reference: chemcollective.org

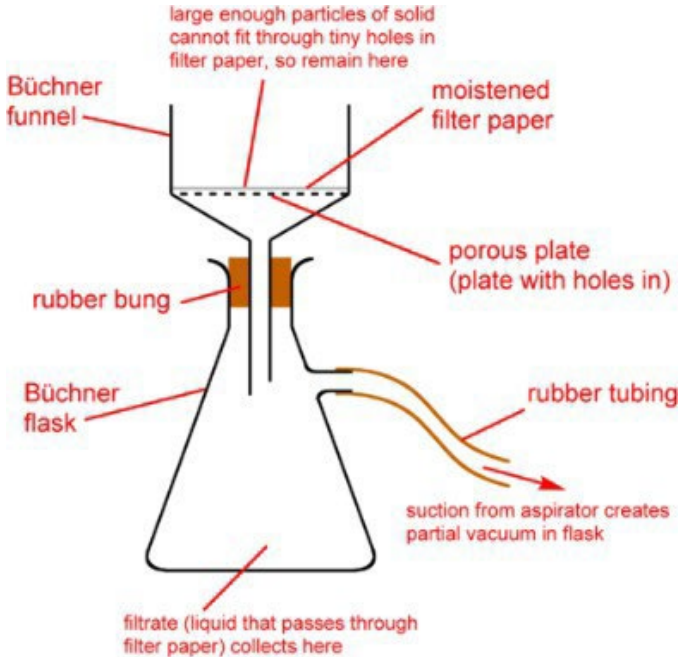


Fig. 4.68 Gravimetric Analysis — Vacuum Filtration Apparatus (Buchner Funnel). The diagram shows a Buchner funnel with moistened filter paper over a porous plate, sealed with a rubber bung onto a Buchner flask connected to vacuum suction. The suction pulls filtrate (liquid) through the filter paper into the flask below, while the solid precipitate remains trapped on the filter paper for collection and weighing. Reference: chem.libretexts.org

Example: A 0.955 g solid mixture containing K_2SO_4 is dissolved in water and treated with excess $Ba(NO_3)_2$, resulting in precipitation of 0.850 g of $BaSO_4$.

$$K_2SO_4(aq) + Ba(NO_3)_2(aq) \rightarrow BaSO_4(s) + 2\ KNO_3(aq)$$

Amount of K_2SO_4 = [0.850 g $BaSO_4$] × [1 mol $BaSO_4$ / 233.38 g] × [1 mol K_2SO_4 / 1 mol $BaSO_4$] × [174.259 g K_2SO_4 / mol] = 0.635 g K_2SO_4

% K_2SO_4 = [0.635 g / 0.955 g] × 100% = 66.5%

Combustion Analysis

Combustion analysis is a method used in both organic chemistry and analytical chemistry to determine the elemental composition (empirical formula) of a pure organic compound by combustion reaction.

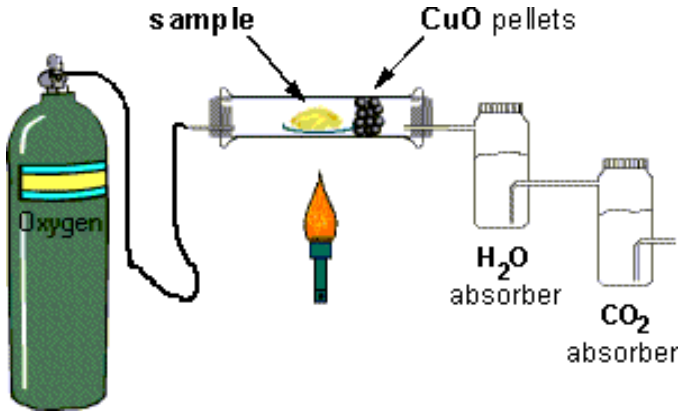


Fig. 4.69 Combustion Analysis Setup — Diagram showing the apparatus used to determine elemental composition of organic compounds. Excess oxygen from the tank passes through a heated tube containing the organic sample and CuO catalyst pellets. The combustion converts all carbon to CO_2 and all hydrogen to H_2O. Products flow into sequential absorbers: the H_2O absorber (magnesium perchlorate) traps water, and the CO_2 absorber (sodium hydroxide) traps carbon dioxide. Mass changes in each absorber reveal the masses of H and C in the original sample. Reference: chem.wilkes.edu

The combustion reaction is carried out under excess oxygen. H2O is collected in an absorber filled with magnesium perchlorate, Mg(ClO4)2. CO2 is collected in a separate absorber filled with sodium hydroxide, NaOH.

$$2.6406\ \text{g}\ CO_2 \times \frac{1\ \text{mol}\ CO_2}{44.01\ \text{g}\ CO_2} \times \frac{1\ \text{mol C}}{1\ \text{mol}\ CO_2} = 0.06000\ \text{mol C}$$

$$0.5400\ \text{g}\ H_2O \times \frac{1\ \text{mol}\ H_2O}{18.00\ \text{g}\ H_2O} \times \frac{2\ \text{mol H}}{1\ \text{mol}\ H_2O} = 0.06000\ \text{mol H}$$

Combustion analysis stoichiometric calculations showing conversion of measured masses to moles of elements. From 2.6406 g CO_2: 0.06000 mol C. From 0.5400 g H_2O: 0.06000 mol H. Equal mole ratio gives empirical formula CH.

Example: Elemental analysis yields 2.6406 g CO2 and 0.5400 g H2O. Molar mass of compound = 78.11 g/mol.

Mol C = [2.6406 g CO2] × [1 mol CO2 / 44.01 g] × [1 mol C / 1 mol CO2] = 0.06000 mol C

Mol H = [0.5400 g H2O] × [1 mol H2O / 18.00 g] × [2 mol H / 1 mol H2O] = 0.06000 mol H

Empirical formula = CH (mol ratio C:H = 1:1)

Molar mass of empirical formula CH = 12.0 + 1.00 = 13.0 g/mol

Empirical formula units = [78.11 g/mol] / [13.0 g/mol] = 6 units

Molecular formula = 6 × CH = C6H6

Confirmation: Molar mass of C6H6 = 78.0 g/mol ✓

End of Chapter Questions

Balancing Chemical Equations

- 1) _Mg(OH)2 + _2_ HCl → MgCl2 + _2_ H2O [Double replacement]
- 2) _Na2CO3 + _2_ HCl → _2_ NaCl + H2CO3 [Double replacement]
- 3) _NH4NO2 → _N2 + _2_ H2O [Decomposition]
- 4) _2_ N2 + _5_ O2 → _2_ N2O5 [Synthesis]
- 5) _MgCO3 → MgO + CO2 [Decomposition]
- 6) _2_ KBr + Cl2 → _2_ KCl + Br2 [Single replacement]
- 7) _Zn + CuSO4 → Cu + ZnSO4 [Single replacement]
- 8) _4_ P + _3_ O2 → P4O6 [Synthesis]
- 9) _SrBr2 + (NH4)2CO3 → SrCO3 + _2_ NH4Br [Double replacement]
- 10) _2_ AgNO3 + (NH4)2CrO4 → Ag2CrO4 + _2_ NH4NO3 [Double replacement]
- 11) _2_ K + _2_ H2O → _2_ KOH + H2 [Single replacement]
- 12) _2_ Al + _3_ Pb(NO3)2 → _2_ Al(NO3)3 + _3_ Pb [Single replacement]
- 13) _3_ Fe + _2_ O2 → Fe3O4 [Synthesis]
- 14) _4_ Li + O2 → _2_ Li2O [Synthesis]
- 15) _ZnCl2 + _2_ KOH → Zn(OH)2 + _2_ KCl [Double replacement]
- 16) _Fe3O4 + _4_ H2 → _3_ Fe + _4_ H2O [Single replacement]
- 17) _Pb(NO3)2 → Pb + _2_ NO2 + O2 [Decomposition]
- 18) _2_ H2O → _2_ H2 + O2 [Decomposition]
- 19) _3_ Mg + N2 → Mg3N2 [Synthesis]

Net Ionic Equations

1. 2NaCl(aq) + Pb(NO3)2(aq) → PbCl2(s) + 2NaNO3(aq) Net Ionic: 2Cl-(aq) + Pb2+(aq) → PbCl2(s)

2. Na2CO3(aq) + FeCl2(aq) → FeCO3(s) + 2NaCl(aq) Net Ionic: CO32-(aq) + Fe2+(aq) → FeCO3(s)

3. Mg(OH)2(aq) + 2HCl(aq) → MgCl2(aq) + 2H2O(l) Net Ionic: 2OH-(aq) + 2H+(aq) → 2H2O(l)

4. K2(CrO4)(aq) + CaCl2(aq) → 2KCl(aq) + Ca(CrO4)(aq) Net Ionic: NA — all spectator ions

5. 2(NH4)3PO4(aq) + 3Zn(NO3)2(aq) → 6NH4NO3(aq) + Zn3(PO4)2(s) Net Ionic: 2PO43-(aq) + 3Zn2+(aq) → Zn3(PO4)2(s)

Oxidation Reduction

1. Oxidation numbers:

    a. H2CO3: H=+1, O=-2, C=+4

    b. N2: N=0

    c. Zn(OH)42-: Zn=+2, H=+1, O=-2

    d. NO2-: N=+3, O=-2

    e. LiH: Li=+1, H=-1

    f. Fe3O4: Fe=+8/3, O=-2

Limiting Reactant, Percent Yield, Mole Stoichiometry — Multiple Choice

- 1. Combustion of 0.800 g hydrocarbon yields 2.613 g CO_2 and 0.778 g H_2O. Percent composition: Answer: C — 89.1% C; 10.9% H
- 2. Mass of Na reacting with excess water to produce 15 g NaOH: Answer: C — 8.6 g
- 3. $2\ Al_2O_3 \rightarrow 4\ Al + 3\ O_2$: If 12 moles Al_2O_3 consumed, moles O_2 produced: Answer: E — 18
- 4. $2\ H_2 + O_2 \rightarrow 2\ H_2O$ with 8.0 g H_2 and 9.0 g O_2: O_2 is the limiting reactant (Answer: C)
- 5. $Mg + I_2 \rightarrow MgI_2$: 25.0 g Mg and 25.0 g I_2: Answer: C — 27.4 g MgI_2
- 6. $2\ Cs + Cl_2 \rightarrow 2\ CsCl$: 70.9 g Cl_2, theoretical yield: Answer: D — 337 g
- 7. AgCl dissolves in water in large amounts? Answer: D — No (AgCl is insoluble)
- 8. Na_2SO_4 dissolves in water in large amounts? Answer: C — Yes

Acid – Base Titration — Multiple Choice

- 1. $H_2SO_4 + NaOH$: 27.4 mL of 0.768 M NaOH titrates 16.7 mL H_2SO_4: Answer: B — 0.630 M
- 2. $NaOH + HCl$: 24.5 mL HCl titrates 33.0 mL of 0.112 M NaOH: Answer: A — 0.151 M
- 3. $Ba(OH)_2 + HClO_4$: mL of 1.2 M $HClO_4$ to neutralize 5.8 mL of 0.44 M $Ba(OH)_2$: Answer: D — 4.3 mL

Gravimetric Analysis — Multiple Choice

- 1. $CaCO_3 + 2HNO_3 \rightarrow Ca(NO_3)_2 + CO_2 + H_2O$: mL of 0.1015 M HNO_3 for 0.9857 g $CaCO_3$: Answer: C — 194.1 mL
- 2. Acetic acid titration with $Mg(OH)_2$: concentration: Answer: B — 1.25 mol/L

Combustion Analysis — Multiple Choice

- 1. Hydrocarbon combustion with 18.214 g O_2 yields 23.118 g CO_2 and 4.729 g H_2O: empirical formula: Answer: C — CH
- 2. 12.501 g petroleum compound yields 38.196 g CO_2 and 18.752 g H_2O: empirical formula: Answer: D — C_5H_{12}
- 3. Compound with C, H, N: 12.923 g CO_2, 6.608 g H_2O, 2.501 g NH_3: empirical formula: Answer: C — C_2H_5N
- 4. Compound with C, H, O: 18.942 g CO_2 and 7.749 g H_2O from 12.915 g: Answer: A — CH_2O
- 5. Hydrocarbon combustion: 33.057 g CO_2 and 10.816 g H_2O: Answer: B — C_5H_8

Chapter 5: Thermochemistry

Key Concepts

1. I. Historical Background of Thermochemistry Concepts
2. II. Basic Concept of Energy
3. III. Calorimetry Concept
4. IV. Enthalpy and the First Law of Thermodynamics

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 includes everything belonging 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

Chemical reactions can give heat (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 endothermic chemical reactions changes:
https://www.youtube.com/watch?v=L-G7pLufXAo
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:

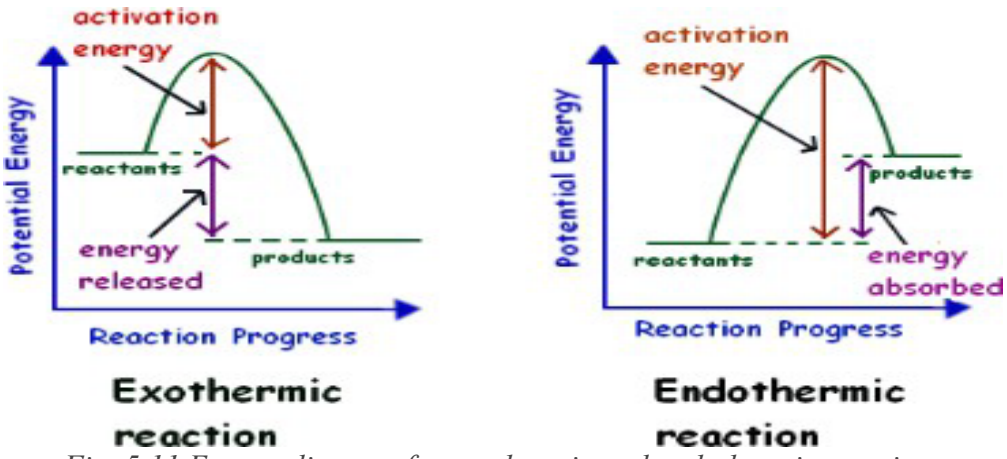


Fig. 5.11 Energy diagram for exothermic and endothermic reactions

Reference: https://sites.google.com/site/mrlowesscience/home/year-12-chemistry/structure-andbonding-as24/exothermic-and-endothermic

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:
$C(s) + O_2(g) \rightarrow CO_2(g) + Heat$

Endothermic Equation Example:
$Heat + C(s) + H_2O(g) \rightarrow H_2(g) + CO(g)$

2. Using a value instead of the "Heat"

Exothermic Equation Example:
$C(s) + O_2(g) \rightarrow CO_2(g) + 393\ kJ/mole$

Endothermic Equation Example:
$131\ kJ/mole + C(s) + H_2O(g) \rightarrow H_2(g) + CO(g)$

3. Using the "Enthalpy Symbol" with negative or positive values to replace the word heat

Exothermic Equation Example:
$C(s) + O_2(g) \rightarrow CO_2(g) \quad \Delta H = -393\ kJ/mole$ [Exothermic: Negative Value]

Endothermic Equation Example:
Heat + C(s) + $H_2O(g)$ → $H_2(g)$ + CO(g) $\Delta H = +131$ kJ/mole [Endothermic: Positive Value]

The term "Enthalpy" will be discussed later.

Exothermic and Endothermic Applications

Cold (Ice) pack (endothermic chemical reaction) and Hot pack (exothermic chemical reaction)

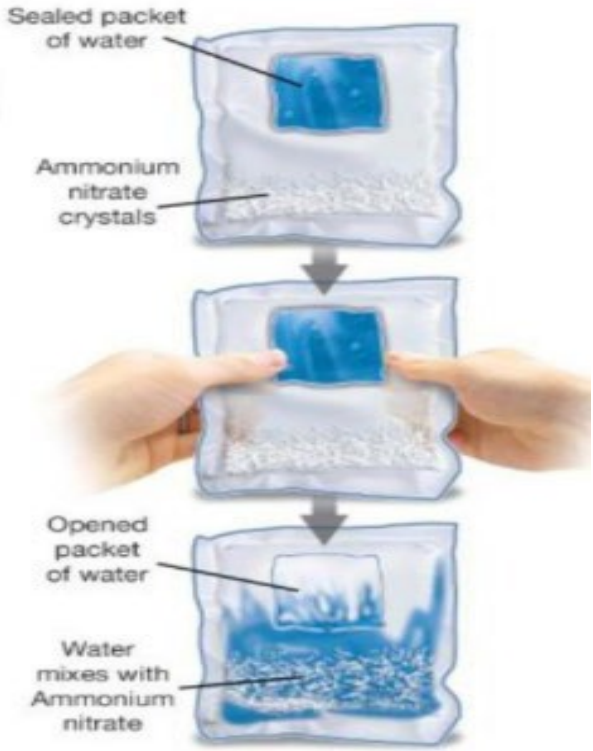


Fig. 5.12 Cold (Ice) pack – endothermic chemical reaction

Fig. 5.12b Detailed diagram of cold pack operation showing water and ammonium nitrate components

Ammonium nitrate 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 starts 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:

$$\text{Heat} + NH_4NO_3(s) + H_2O(l) \leftrightarrow NH_4^+(aq) + NO_3^-(aq) + H_2O(l)$$
or
$$25.7\ \text{kJ/mole} + NH_4NO_3(s) + H_2O(l) \leftrightarrow NH_4^+(aq) + NO_3^-(aq) + H_2O(l)$$
or
$$NH_4NO_3(s) + H_2O(l) \leftrightarrow NH_4^+(aq) + NO_3^-(aq) + H_2O(l) \quad \Delta H = +25.7\ \text{kJ/mole}$$

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 starts 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 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

$CaCl_2(s) + H_2O(l) \leftrightarrow Ca^{2+}(aq) + 2\ Cl^-(aq) + H_2O(l) + 82.8$ kJ/mole
or
$CaCl_2(s) + H_2O(l) \leftrightarrow Ca^{2+}(aq) + 2\ Cl^-(aq) + H_2O(l)$ $\Delta H = -82.8$ kJ/mole

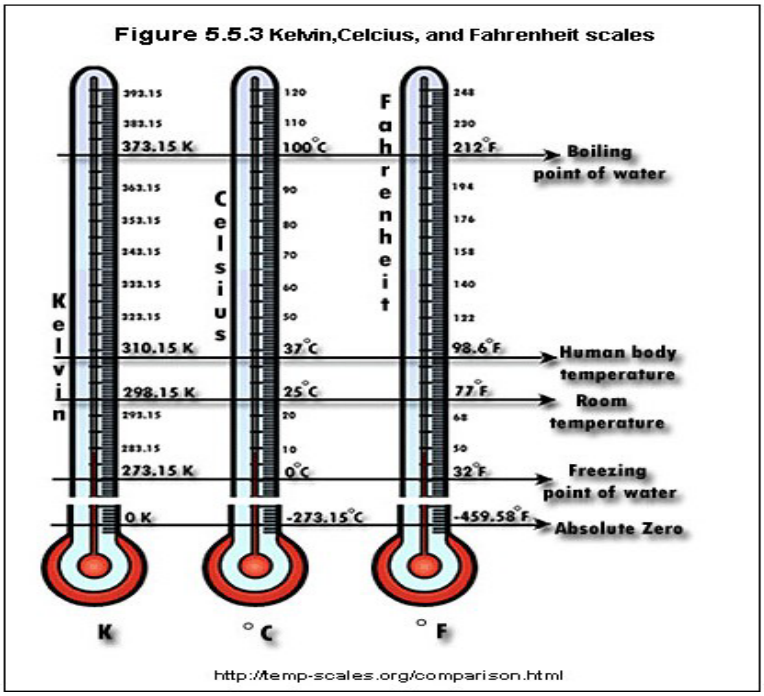


Fig. 5.13 Hot pack (exothermic chemical reaction) — calcium chloride dissolving in water releases heat

Reference: https://www.youtube.com/watch?v=leonysaMIRo

Heat, Temperature and Thermal Energy

Heat:
A term used to describe the transfer of thermal energy between molecules within a system. Heat measures how thermal energy flows, moves or transfers.

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 used to measure the heat. It is measured in different systems as follows:
English System: Fahrenheit (°F)
Metric System: Centigrade Celsius (°C)
International System (SI): Kelvin (K)

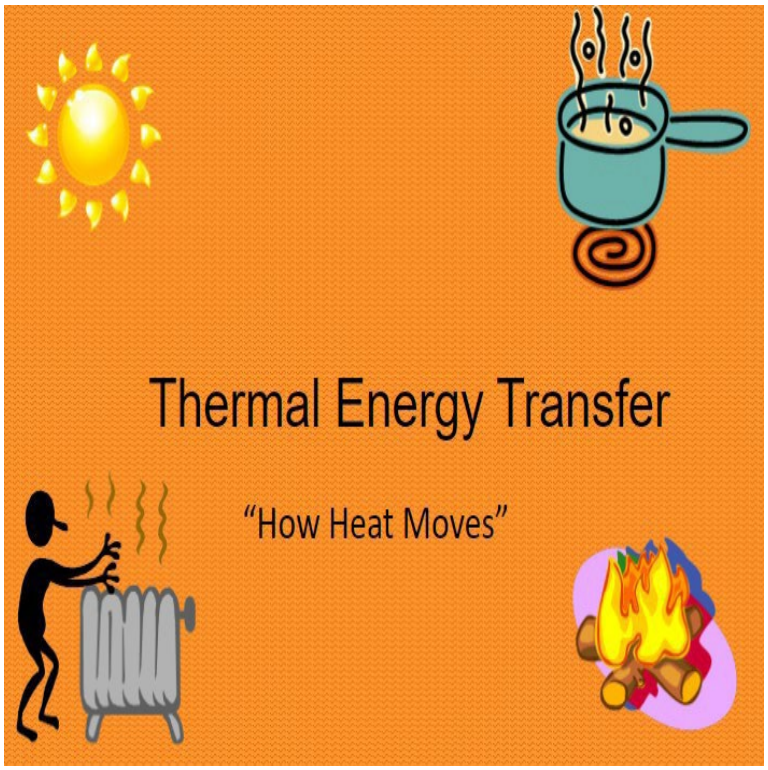


Fig. 5.14 Different temperature scales — Kelvin, Celsius, and Fahrenheit with key reference points

Reference: https://legacy.etap.org/demo/chem5/instruction5tutor.html

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:

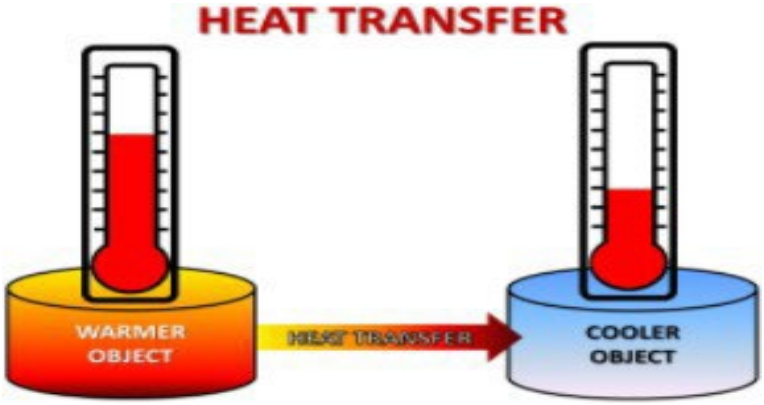


Fig. 5.15 Heat energy flowing diagram illustrating various modes of thermal energy transfer

Reference: https://slideplayer.com/slide/8214047/

Heat Transfer:

Heat transfers from hot to cold and never in reverse. The figure below shows this movement:

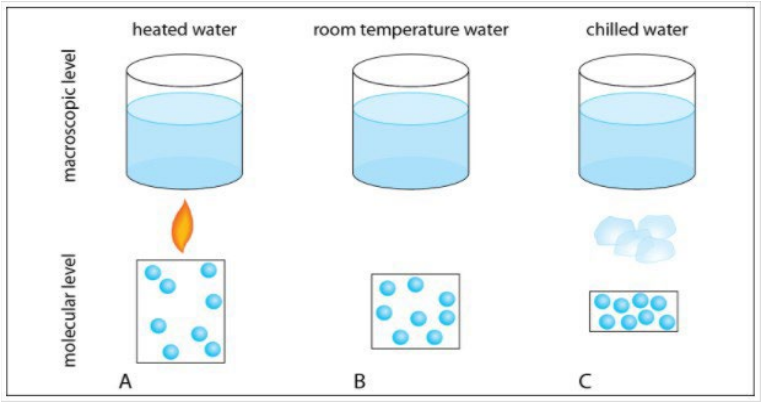


Fig. 5.16 Transfer of heat — heat flows from a warmer object to a cooler object
Reference: https://sites.google.com/a/wyckoffschools.org/solar-cooker-challenge/heattransfers

Hot matter expands while cold matter shrinks:

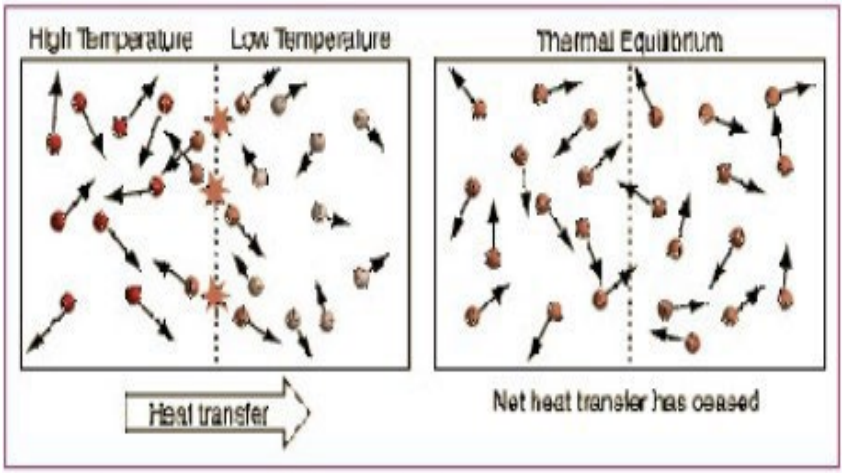


Fig. 5.7 Molecular view of hot and cold water — heated water expands (spread molecules) and chilled water contracts (packed molecules)

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 phenomenon:

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

Fig. 5.8 Molecular view of thermal equilibrium — heat transfer continues until both regions reach the same temperature

Reference: https://legacy.etap.org/demo/chem5/instruction5tutor.html

Now we can introduce 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°C 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 Iron.

We expand the formula further by looking at the concept of the specific heat and the molar heat capacity of a matter which is defined as follows:

Specific Heat

$c = q / m \Delta T$ and $q = m c \Delta T$

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°C or 1 K). The unit of the specific heat is cal / g × °C or 4.184 J / g × °C. 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 × °C or 0.902 J / g × °C

Example of the Specific Heats for some substances is given below:

Table 5.17 Specific Heat values of common substances

Table 1: Specific Heat Values of 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
Copper	0.385
Zinc	0.385
Tin	0.222
Lead	0.129

Reference: Reference: Metal HeatLAB.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:

$C_n = q / n \Delta T$ and $q = n c_n \Delta T$

Where:
C_n = molar heat capacity
q = heat
ΔT = temperature change
n = number of moles of the matter

The molar heat capacity cn is defined as the amount of energy needed to raise the temperature of 1.0 mole of a matter 1.0 degree (1.0°C or 1 K). The unit of the molar heat is cal / mole × °C or

4.184 J / mole × °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 × °C or 24.3 J / mole × °C

The videos below explain the terms of heat capacity, the specific heat of capacity and the molar heat capacity:
https://www.youtube.com/watch?v=IoHXMaiwT80
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 × °C = 4.184 J / g × °C
$q = m c \Delta T$ = [250.0 g × 4.184 J/g × °C] × [55.0 – 25.0]°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°C to 13.50°C?
$c = q / m \Delta T$ $m = q / c \Delta T$
c = specific heat of water = 1 cal/g × °C = 4.184 J / g × °C
m = [585.0 × 10^3 J] / [4.184 J/g × °C] × [70.00°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.
$c = q / m \Delta T$
c = [455 J] / [25.0 g] × [155 – 25]°C = 0.14 J / g × °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?
$c = q / m \Delta T$
c = [47.3 cal] / [55.00 g] × [15.0°C] = 0.0573 cal / g × °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 × °C?
$c = q / m \Delta T$
$\Delta T = q / m \times c$
ΔT = [1.00 × 10^3 J] / [150.0 g] × [0.960 J / g × °C] = 6.944°C
ΔT = T(final) – T(initial) = 6.944°C = T(final) – 25.0°C = 31.9°C

Reference: https://www.youtube.com/watch?v=4RkDJDDnIss

III. Calorimetry Concept

Calorimetry

Calorimetry is a method by which heat transfer into and out of 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 two major types of calorimeters:

5. Adiabatic Calorimeters
6. 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 surroundings and function at zero heat exchange conditions also known as adiabatic conditions.

The video below illustrates the function of the adiabatic calorimeter:

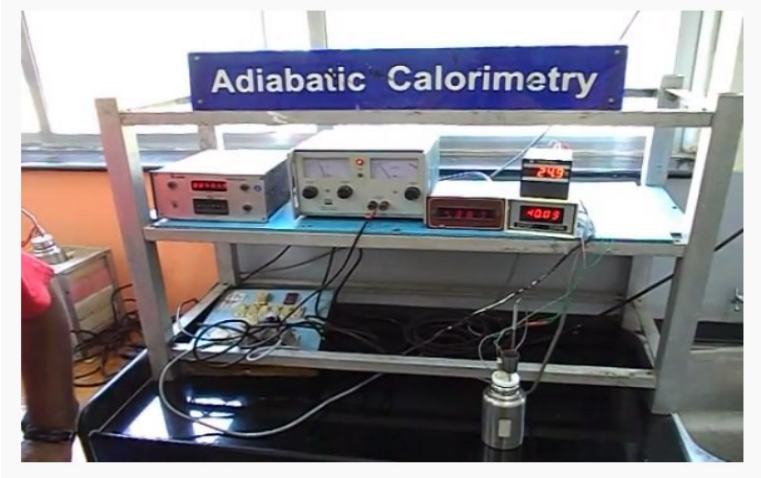


Fig. 5.21 Adiabatic Calorimeter — used to measure enthalpy changes under zero heat exchange (adiabatic) conditions

Reference: https://www.youtube.com/watch?v=44X1z0_snIY

2. Reactions Calorimeters

There are several reactions calorimeters available in the market and in 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:

7. Heat-flow
8. Heat-balance
9. Constant flux
10. Power compensation

Detailed functionalities: https://www.azosensors.com/article.aspx?ArticleID=798

A. Foam Cup (Coffee Cup) Calorimeter

This type of calorimeter is used mostly at undergraduate physics and chemistry labs because it is 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 a 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°C to 60°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.

Figure 5.221 Coffee Cup Calorimeter — simple polystyrene foam cup used in undergraduate chemistry labs

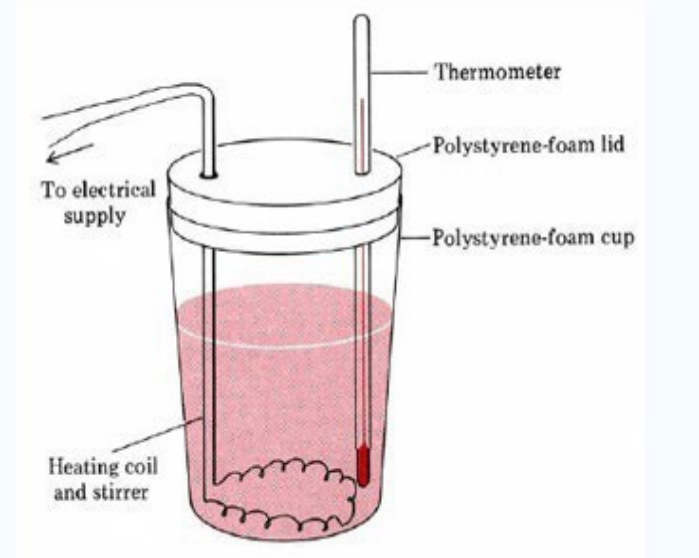


Figure 5.222 Inside view of Coffee-cup calorimeter — showing thermometer, foam lid, foam cup, heating coil, and stirrer

Reference: https://commons.wikimedia.org/wiki/File:Coffee_cup_calorimeter_pic.jpg

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 the outer sealed mantle of the combustion chamber. The heat will warm up the water and the temperature is monitored and recorded and the heat of the combustion is calculated.

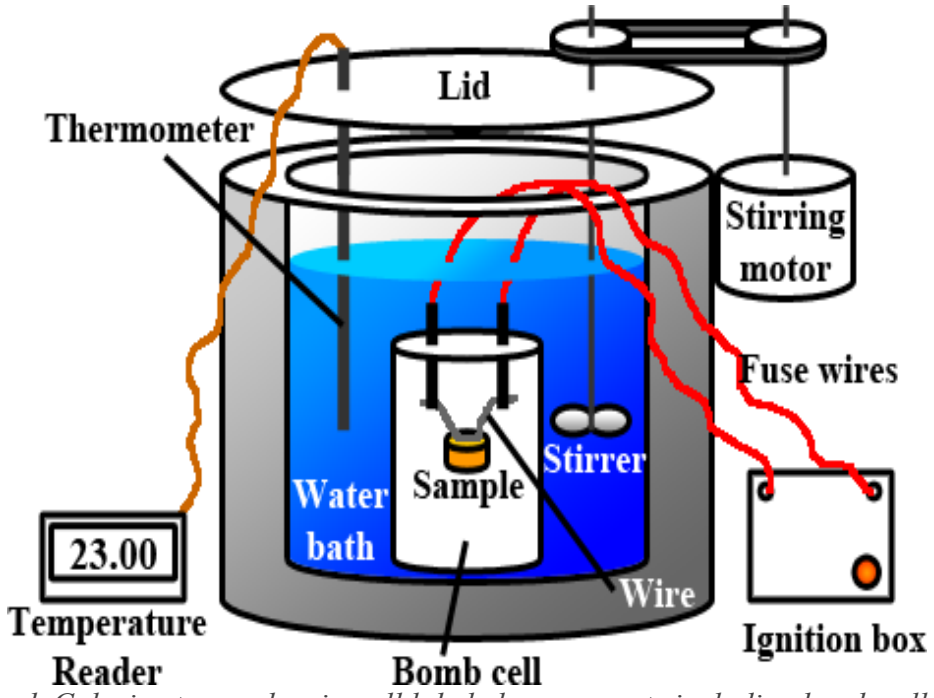


Fig. 5.23 Bomb Calorimeter — showing all labeled components including bomb cell, water bath, thermometer, stirring motor, and ignition system

Reference: https://commons.wikimedia.org/wiki/File:Bomb_Calorimeter_Diagram.png

The videos below illustrate the bomb calorimeter concept:
https://www.youtube.com/watch?v=F2cMvNDRqQA
https://www.youtube.com/watch?v=wwJG2JVg6qM

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

Solution Calorimeter

This type of calorimeter is used to measure the heat of solution of dissolving a solid compound 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.

https://www.youtube.com/watch?v=HnYZh69HJqU
https://www.youtube.com/watch?v=dpmr0665FFA

The Heat of Solution, Dilution, and Neutralization Calculations

The temperature is followed till there is no rise in the temperature and an equilibrium temperature of the system is attained.

The 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

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) × c(metal) × ΔT(metal) = -mass(water) × c(water) × ΔT(water)
[59.047 g] × c(metal) × [100°C – 27.8°C] = -[100.0 mL × 1.00 g/mL] × [4.184 J/(g × °C)] × [27.8°C – 23.7°C]
[59.047 g] × c(metal) × [72.2°C] = 1713.8 J
c(metal) = [1713.8 J] / {[59.047 g] × [72.2°C]} = 0.402 J/g × °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°C and the water was originally at 24.6°C. After the reaction, the temperature of both substances is 31.3°C.
A) Was the reaction exothermic or endothermic? Explain.
For the water — endothermic. The temperature increased from 24.6°C to 31.3°C indicating energy was absorbed by the water.
For the HCl — exothermic. The temperature decreased from 44.6°C to 31.3°C indicating energy was released by the HCl.

B) Calculate how much heat the water lost or gained.
q(water) = mass(water) × c(water) × ΔT(water) = [100.0 g] × [4.184 J/(g × °C)] × [31.3°C – 24.6°C] = 2803.3 J = 2.80×10^3 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) × c(water) × ΔT(water)
840.0 J = [10.0 g] × [4.184 J/(g × °C)] × ΔT(water)
ΔT(water) = 840.0 J / {[10.0 g] × [4.184 J/(g × °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.
$q = c(\text{calorimeter}) \times \Delta T = [11.4\ \text{kJ/°C}] \times [24.2 - 21.5\text{°C}] = [11.4\ \text{kJ/°C}] \times (2.7\text{°C}) = 30.78\ \text{kJ}$
$(30.78\ \text{kJ}) / (0.88\ \text{g}) = 34.98\ \text{kJ/g}$

5. A piece of metal weighing 85.5 g was heated to 100.0°C and then put into 100.0 mL of water (initially at 23.7°C). Calculate the final equilibrium temperature if the specific heat of the metal is 0.350 J/(g × °C).
Heat is lost by the metal = -Heat is gained by water
$[85.5\ \text{g}] \times [0.350\ \text{J/(g} \times \text{°C)}] \times [T(\text{final}) - 100.0\text{°C}] = -[100.0\ \text{mL} \times 1.00\ \text{g/mL}] \times [4.184\ \text{J/(g} \times \text{°C)}] \times [T(\text{final}) - 23.7\text{°C}]$
$[29.925/\text{°C}] \times [T(\text{final}) - 100.0\text{°C}] = -[418.4/\text{°C}] \times [T(\text{final}) - 23.7\text{°C}]$
$29.925\ T(\text{final}) - 2992.5 = -418.4\ T(\text{final}) + 9916.08$
$448.325\ T(\text{final}) = 3016.2$
$T(\text{final}) = 3016.2 / 448.325 = 6.73\text{°C}$

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 changes from 22°C to 25.1°C. How much heat is generated per gram of potassium?
$q = m \times c(\text{solution}) \times \Delta T(\text{solution}) = [100\ \text{g}] \times [4.184\ \text{J/g-°C}] \times [25.1\text{°C} - 22\text{°C}] = 1297\ \text{J}$
$q = (1297\ \text{J}) / (0.258\ \text{g}) = 5027\ \text{J/g}$

7. 25.0 mL of 0.15 M HCl is neutralized with 30.0 mL of 0.25 M NaOH inside a foam cup calorimeter. Both acid and base were initially at 23.5°C. The final temperature recorded is 26.5°C. Calculate the heat of neutralization reaction.
$HCl(aq) + NaOH(aq) \rightarrow NaCl(aq) + H_2O(l)$
Total volume = 25.0 mL + 30.0 mL = 55.0 mL
Mass of solution = 55.0 mL × 1.00 g/mL = 55.0 g
$\Delta T = 26.5\text{°C} - 23.5\text{°C} = 3.0\text{°C}$
$q(\text{solution}) = q(\text{neutralization}) = [55.0\ \text{g}] \times [4.184\ \text{J/(g} \times \text{°C)}] \times [3.0\text{°C}] = 690.36\ \text{J} = 690\ \text{J}$

8. A 1.5 kg block of Ni at 100°C is placed into 500 mL of water at 21°C. What is the final temperature assuming the specific heat of Ni is 0.44 J/g-°C and water is 4.184 J/g-°C?
$[1500\ \text{g Ni}] \times [0.44\ \text{J/g} \times \text{°C}] \times [100\text{°C} - Tf] = [500\ \text{mL} \times 1\text{g/1mL}] \times [4.184\ \text{J/g} \times \text{°C}] \times [Tf - 21\text{°C}]$
Tf = 40°C

9. 25.6 g of ethanol was combusted in a bomb calorimeter with a heat of 6.53 kJ. The initial temperature was 24.0°C. Find its final temperature.
$C_2H_5OH + 3\ O_2 \rightarrow 2\ CO_2 + 3\ H_2O$
$6.53\ \text{kJ} = 6.53 \times 1000\ \text{J} = -[25.6\ \text{g}] \times [4.184\ \text{J/g} \times \text{°C}] \times [T(\text{final}) - T(\text{initial})]$
$6.53 \times 1000\ \text{J} = -[107\ \text{J/°C}] \times [T(\text{final}) - 24.0\text{°C}]$
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?
c = q(combustion) / m × ΔT = [2200. J] / [100. g × 10.0°C] = 2.20 J/g × °C

11. When 3.12 g of glucose, $C_6H_{12}O_6$, is burned in a bomb calorimeter, the temperature increases from 23.8°C to 35.6°C. The calorimeter contains 775 g of water and the bomb has a heat capacity of 893 J/°C. How much heat was produced?
qrxn = -(qwater + qbomb)
qwater = [775 g] × [4.184 J/g × °C] × [35.6°C – 23.8°C] = 38262.68 J
qbomb = [893 J/°C] × [35.6°C – 23.8°C] = 10537.4 J
Add both: qwater + qbomb = 48,800.08 J ≈ 48.8 kJ
This reaction released 48.8 kJ of heat when 3.12 g of glucose was burned.

IV. Enthalpy and the First Law of Thermodynamics

Enthalpy

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) under constant pressure conditions will equal 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 ΔV represents the work (w) with the ΔV positive. Then: $P\,\Delta V = -w$
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. 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:
$CH_4 + O_2 \rightarrow CO_2 + 2\ H_2O$ $\Delta H = -802.3$ kJ/mol [for 1 mole]
If 2 moles of CH_4 are used then:
$2\ CH_4 + 2\ O_2 \rightarrow 2\ CO_2 + 4\ H_2O$ $\Delta H = -2 \times 802.3$ kJ/mol $= -1604.6$ 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:
$Mg(s) + 2\ HCl(aq) \rightarrow MgCl_2(aq) + H_2(g)$
Number of moles of Mg = (1.50 g) / (24.3 g Mg/mole) = 0.0617 moles
ΔH = 1 mole Mg × [5.15 kJ / 0.0617 moles] = -83.5 kJ/mole [Heat is produced]
Thermochemical equation: $Mg(s) + 2\ HCl(aq) \rightarrow MgCl_2(aq) + H_2(g)$ $\Delta H = -83.5$ 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.

By the endothermic process: the system is gaining heat from the surrounding and $q > 0$, and $\Delta H > 0$.
By the exothermic process: the system is giving off heat to the surrounding and $q < 0$, and $\Delta H < 0$.

Effect of the temperature on the enthalpy: When temperature increases, the molecular interactions increase the internal energy and the enthalpy of the system.
$c = q / \Delta T$ At constant pressure: $cp = [\Delta H / \Delta T]p$

Standard Enthalpy

A standard state is defined by IUPAC as the state where 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 ΔH is given the superscript "o".

The symbol of the standard enthalpy is $\Delta H°$
There is no standard temperature but usually the temperature used and considered is 298.15 K.

https://www.youtube.com/watch?v=wZYOGgc25yQ
https://www.youtube.com/watch?v=RI7xCYBmDqQ

The table below shows the standard enthalpy of the combustions:

Table 2: Standard Enthalpy of Combustion

Substance	Combustion Reaction	ΔH°c (kJ/mol) at 25°C
carbon	$C(s) + O_2(g) \rightarrow CO_2(g)$	−393.5
hydrogen	$H_2(g) + ½O_2(g) \rightarrow H_2O(l)$	−285.8
magnesium	$Mg(s) + ½O_2(g) \rightarrow MgO(s)$	−601.6
sulfur	$S(s) + O_2(g) \rightarrow SO_2(g)$	−296.8
carbon monoxide	$CO(g) + ½O_2(g) \rightarrow CO_2(g)$	−283.0
methane	$CH_4(g) + 2O_2(g) \rightarrow CO_2(g) + 2H_2O(l)$	−890.8
acetylene	$C_2H_2(g) + 5/2\ O_2(g) \rightarrow 2CO_2(g) + H_2O(l)$	−1301.1
ethanol	$C_2H_5OH(l) + 3O_2(g) \rightarrow CO_2(g) + 3H_2O(l)$	−1366.8
methanol	$CH_3OH(l) + 3/2\ O_2(g) \rightarrow CO_2(g) + 2H_2O(l)$	−726.1
isooctane	$C_8H_{18}(l) + 25/2\ O_2(g) \rightarrow 8CO_2(g) + 9H_2O(l)$	−5461

Table: Standard enthalpies of combustion for common substances at 25°C and 1 atm (all values in kJ/mol)

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: $CH_4 + O_2 \rightarrow CO_2 + 2\ H_2O$ $\Delta H = -802.3$ kJ/mol

If 1.50 L of CH_4 is used for the combustion, calculate the standard enthalpy of combustion.
Density of methane (gas): 0.72 g/L; Molar mass of methane: 16.0 g/mole
$\Delta H° = [1.50\ CH_4\ L] \times [0.72\ CH_4\ g/L] \times [1\ mole\ CH_4 / 16.0\ g\ CH_4] \times [802.3\ kJ/mole\ CH_4] = -54.2$ 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 and 298.15 K) is formed from its pure elements under the same conditions.

$\Delta H°reaction = \Sigma\Delta H°f(products) - \Sigma\Delta H°f(Reactants)$

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 $\Delta H° = 0$.
$Cl_2(l)$ is least stable and therefore will have the highest enthalpy and $\Delta H°$ has a nonzero value.

2. Calculate the ΔH° for the reaction: $2\ SO_2 + O_2 \rightarrow 2\ SO_3$
ΔH°reaction = {2 × ΔH°f[SO_3]} – {[2 × ΔH°f[SO_2] + ΔH°f[O_2]]}
ΔH°f[SO_3] = -395.2 kJ/mole
ΔH°f[SO_2] = -296.1 kJ/mole
ΔH°f[O_2] = 0 kJ/mole
ΔH°reaction = {-2 × 395.2} – {[(-2 × 296.1) + 0]} = -790.4 + 592.2 = -198.2 kJ
ΔH°reaction is negative — the reaction is exothermic.

3. Calculate the ΔH° for the reaction: $2\ NO + O_2 \rightarrow 2\ NO_2$
ΔH°f[NO_2] = 33.18 kJ/mole
ΔH°f[NO] = 90.25 kJ/mole
ΔH°f[O_2] = 0 kJ/mole
ΔH°reaction = {2 mole × 33.18 kJ/mole} – {[(2 mole × 90.25 kJ/mole) + 0]} = 66.36 – 180.50 = -114.14 kJ
ΔH°reaction is negative — the reaction is exothermic.

https://www.youtube.com/watch?v=PJweE3F_mPY
https://www.youtube.com/watch?v=FP-VYfTYi8Y

Table 3: Standard Enthalpy of Formation for Various Compounds — ΔH°f Values (kJ/mol)

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

Compound	ΔH°f (kJ/mol)	Compound	ΔH°f (kJ/mol)	Compound	ΔH°f (kJ/mol)	Compound	ΔH°f (kJ/mol)
$CCl_4(l)$	−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

Table 4: Standard Enthalpy of Formation for Ions — ΔH°f Values (kJ/mol)

Cation	ΔH°f (kJ/mol)	Cation	ΔH°f (kJ/mol)	Anion	ΔH°f (kJ/mol)	Anion	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				

Standard Enthalpy of Formation for Various Compounds and Ions — ΔH°f values (kJ/mol) at 25°C and 1 atm

Reference:
http://sistemas.eel.usp.br/docentes/arquivos/5817712/TDQ%20I/Rstandard_enthalpy_of_formation.pdf

Writing Chemical Equations for ΔH°f

Examples:
Write ΔH°f for the reactions below:

1. $CH_3\text{-}O\text{-}CH_3(l)$
2 C(solid, graphite) + ½ $O_2(gas)$ + 3 $H_2(g)$ → $CH_3\text{-}O\text{-}CH_3(l)$

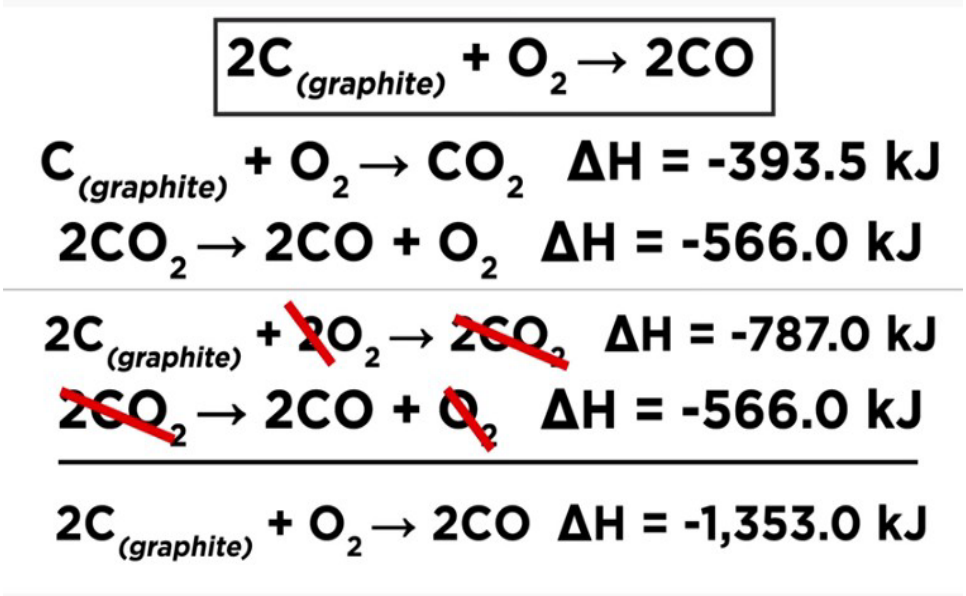
2. $CH_3\text{-}CO\text{-}CH_3(l)$
3 C(solid, graphite) + ½ $O_2(gas)$ + 3 $H_2(g)$ → $CH_3\text{-}CO\text{-}CH_3(l)$

Evaluating an Enthalpy of Formation: Hydrogen gas, H_2, reacts explosively with gaseous chlorine, Cl_2, to form hydrogen chloride, HCl(g). The standard enthalpy of formation of HCl(g) is −92.3 kJ/mol.
$H_2(g) + Cl_2(g) \rightarrow 2\ HCl(g)$ $\quad \Delta H°f = -92.3$ kJ/mole
1 mole of $H_2(g)$ will produce 2 moles of HCl(g)
[2 mole HCl(g)] × [-92.3 kJ/mole] = -184.6 kJ

Hess's Law

Hess was a Russian chemist. This law was named after him in 1840. Hess's law confirms that ΔH° is a 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.

https://www.youtube.com/watch?v=Idv2C8HBbug
https://www.youtube.com/watch?v=2q2u5sj4V00
https://www.youtube.com/watch?v=u7aTBxA7sL8



Hess's Law example — calculating ΔH for 2C(graphite) + O_2 → 2CO by combining known thermochemical equations

Hess's Law Examples

1. Calculate the enthalpy for: $2\ C(s) + H_2(g) \rightarrow C_2H_2(g)$ $\quad \Delta H° = ???$ kJ
Given:
$C_2H_2(g) + \frac{5}{2}O_2(g) \rightarrow 2CO_2(g) + H_2O(l)$ $\quad \Delta H° = -1299.5$ kJ
$C(s) + O_2(g) \rightarrow CO_2(g)$ $\quad \Delta H° = -393.5$ kJ
$H_2(g) + \frac{1}{2}O_2(g) \rightarrow H_2O(l)$ $\quad \Delta H° = -285.8$ kJ

Step 1: a) Flip first equation (put C_2H_2 on product side) b) Multiply second by 2 (get 2C) c) Leave third unchanged
Step 2: Rewritten equations:
$2CO_2(g) + H_2O(l) \rightarrow C_2H_2(g) + \frac{5}{2}O_2(g)$ $\Delta H° = +1299.5$ kJ
$2C(s) + 2O_2(g) \rightarrow 2CO_2(g)$ $\Delta H° = -787$ kJ
$H_2(g) + \frac{1}{2}O_2(g) \rightarrow H_2O(l)$ $\Delta H° = -285.8$ kJ
Step 4: $\Delta H° = +1299.5 + (-787) + (-285.8) = +226.7$ kJ

2. Calculate the enthalpy of: $CS_2(l) + 3O_2(g) \rightarrow CO_2(g) + 2SO_2(g)$
$C(s) + O_2(g) \rightarrow CO_2(g)$ $\Delta H = -393.5$ kJ/mol
$2S(s) + 2O_2(g) \rightarrow 2SO_2(g)$ $\Delta H = -593.6$ kJ/mol
$CS_2(l) \rightarrow C(s) + 2S(s)$ $\Delta H = -87.9$ kJ/mol
$\Delta H° = [-393.5 - 593.6 - 87.9] = -1075.0$ kJ/mole

3. Given: $SrO(s) + CO_2(g) \rightarrow SrCO_3(s)$ $\Delta H = -234$ kJ; $2SrO(s) \rightarrow 2Sr(s) + O_2(g)$ $\Delta H = +1184$ kJ; $2SrCO_3(s) \rightarrow 2Sr(s) + 2C(s,gr) + 3O_2(g)$ $\Delta H = +2440$ kJ
Find ΔH for: $C(s,gr) + O_2(g) \rightarrow CO_2(g)$
$SrCO_3(s) \rightarrow SrO(s) + CO_2(g)$ $\Delta H = +234$ kJ
$SrO(s) \rightarrow Sr(s) + \frac{1}{2}O_2(g)$ $\Delta H = +592$ kJ
$Sr(s) + C(s,gr) + \frac{3}{2}O_2(g) \rightarrow SrCO_3(s)$ $\Delta H = -1220$ kJ
$\Delta H° = +234 + (+592) + (-1220) = -394$ kJ
$C(s,gr) + O_2(g) \rightarrow CO_2(g)$ $\Delta H° = -394$ kJ

4. Given: $2NO(g) + O_2(g) \rightarrow 2NO_2(g)$ $\Delta H = -116$ kJ; $2N_2(g) + 5O_2(g) + 2H_2O(l) \rightarrow 4HNO_3(aq)$ $\Delta H = -256$ kJ; $N_2(g) + O_2(g) \rightarrow 2NO(g)$ $\Delta H = +183$ kJ
Calculate ΔH for: $3NO_2(g) + H_2O(l) \rightarrow 2HNO_3(aq) + NO(g)$
$3NO_2(g) \rightarrow 3NO(g) + \frac{3}{2}O_2(g)$ $\Delta H = +174$ kJ
$N_2(g) + \frac{5}{2}O_2(g) + H_2O(l) \rightarrow 2HNO_3(aq)$ $\Delta H = -128$ kJ
$2NO(g) \rightarrow N_2(g) + O_2(g)$ $\Delta H = -183$ kJ
$\Delta H° = +174 + (-128) + (-183) = -137$ kJ
$3NO_2(g) + H_2O(l) \rightarrow 2HNO_3(aq) + NO(g)$ $\Delta H° = -137$ kJ

First Law of Thermodynamics

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.

$\Delta U = q + w$

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 = -p ΔV (negative value of external pressure P on the system × change in volume):
$\Delta U = q - p\,\Delta V$

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

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 or destroyed:
$\Delta U_{system} + \Delta U_{surroundings} = 0$
$\Delta U_{system} = -\Delta U_{surroundings}$

Table 5: Thermodynamic Processes — Energy, Heat, and Work Summary

The Process	Internal Energy Change (ΔU)	Heat Transfer (q)	Work (w = −PΔV)	Example
q=0 Adiabatic	+	0	+	Isolated system; heat does not enter or leave (e.g., styrofoam)
ΔV=0 Constant Volume	+	+	0	Hard, pressure-isolated system (e.g., bomb calorimeter)
Constant Pressure	+ or −	Enthalpy (ΔH)	−PΔV	Most processes at constant external pressure
ΔT=0 Isothermal	0	+	−	No temperature change (e.g., temperature bath)

Table: Thermodynamic process examples — showing relationships between internal energy change (ΔU), heat transfer (q), and work (w) for adiabatic, constant volume, constant pressure, and isothermal processes

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?
$\Delta U = q + w$
Since the surrounding loses heat, it is gained by the system → q is positive
Since the surrounding does work on the system → w is positive
$\Delta U = 75\ J + 555\ J = 630\ J$

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 $\Delta V = 0$: $w = -p \times (0) = 0$
a) q will be negative: Heat is lost by the system and gained by the surrounding.
b) $\Delta U = q + w = q + 0 = q$
c) $\Delta U = q = -86\ J$

https://www.youtube.com/watch?v=NyOYW07-L5g
https://www.youtube.com/watch?v=7Siv2NNCFag

Questions and Answers

1. Decide whether each reaction is exothermic or endothermic: When two chemicals mix their temperature rises:
a) Exothermic
b) Endothermic
c) None of Above
Answer: A

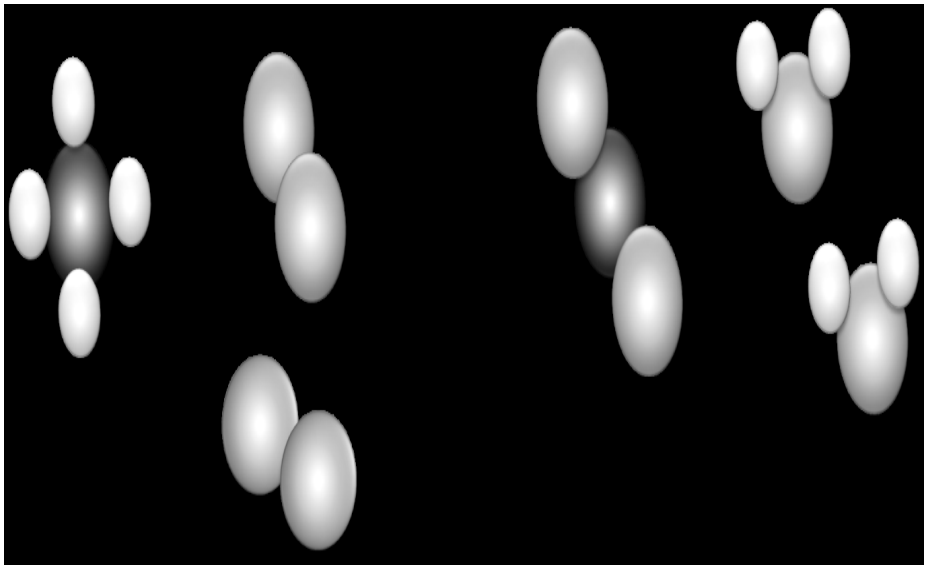
2. Decide whether each reaction is exothermic or endothermic: A solid burns brightly and releases heat, light and sound:
a) Exothermic
b) Endothermic
c) None of Above
Answer: A

3. Decide whether each reaction 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 reaction 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 reaction is exothermic or endothermic: Plants take in light energy for photosynthesis:
a) Exothermic
b) Endothermic
c) None of the above
Answer: B

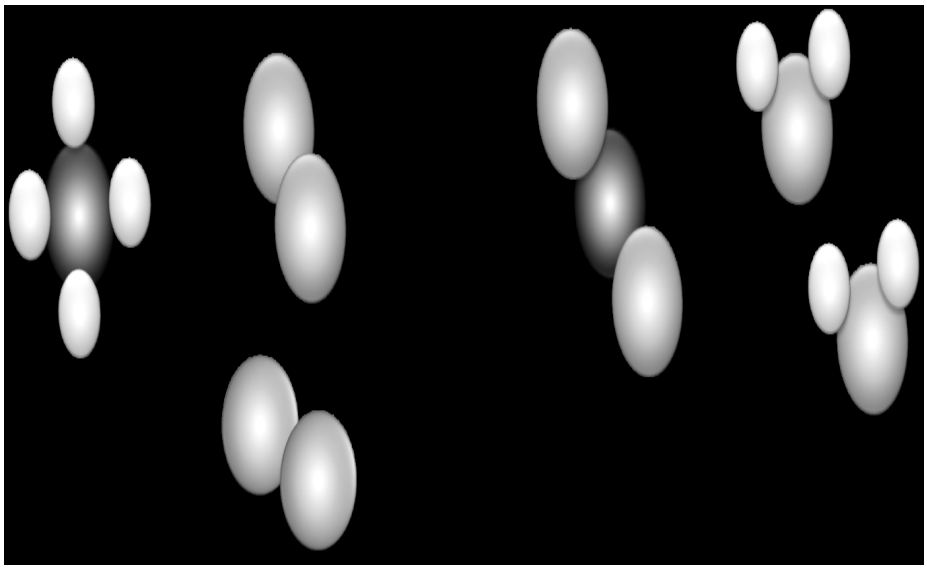
5. Most reactions involve bond breaking and bond making. This equation shows what happens when methane (CH_4) burns in oxygen (O_2):
$CH_4 + 2\ O_2 \rightarrow CO_2 + 2\ H_2O$



Molecular models for methane combustion ($CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$) — illustrating bond breaking and bond making

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

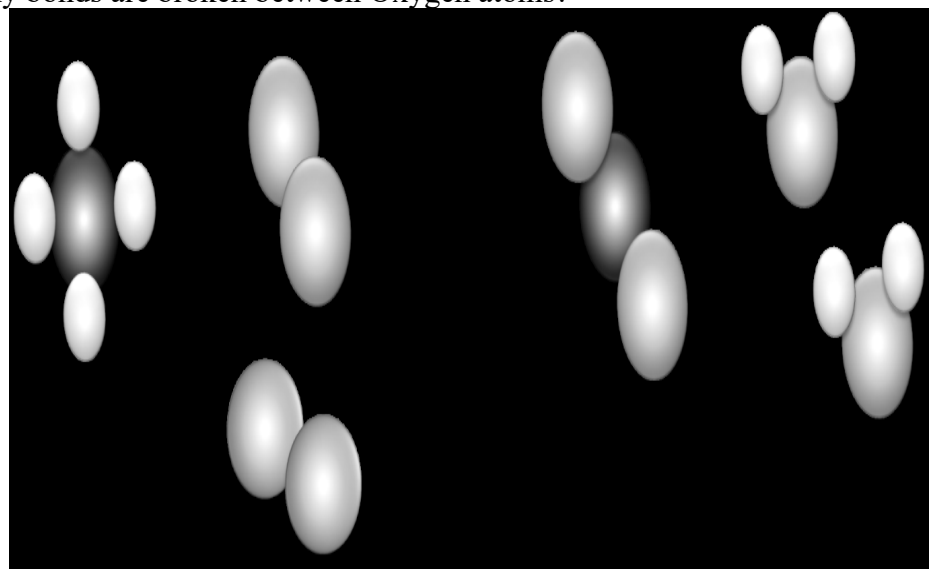
6. How many bonds are broken between Oxygen atoms?



Molecular models for methane combustion — used to identify the number of oxygen-oxygen bonds broken in the reaction

a) 1 b) 2 c) 3 d) 4 e) None of the above
Answer: B

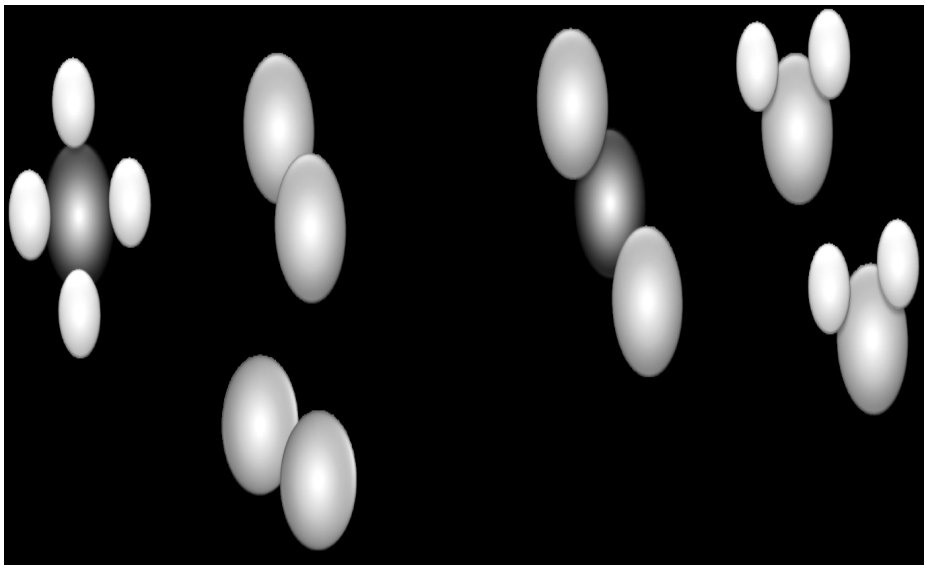
7. How many bonds are broken between Oxygen atoms?



Molecular models for methane combustion — Question 7: identifying number of oxygen-oxygen bonds broken in 2 O_2 molecules

a) 1 b) 2 c) 3 d) 4 e) None of the above
Answer: B

8. How many bonds are broken between Hydrogen and Oxygen atoms?



Molecular models for methane combustion — Question 8: identifying hydrogen-oxygen bonds broken/formed during the reaction

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: $2\ CH_3OH + 3\ O_2 \rightarrow 2\ CO_2 + 4\ H_2O$. 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? ($c = 4.18\ J/g \times °C$)
a) 2.00 kJ b) 2.66 kJ c) 3.55 kJ d) 4.67 kJ e) 5.13 kJ
Answer: B

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 is 28.34°C. What is the specific heat of the metal?

a) 0.755 J/g × °C b) 0.823 J/g × °C c) 0.971 J/g × °C d) 0.235 J/g × °C e) 0.765 J/g × °C
Answer: C

15. A calorimeter has a heat capacity of 1265 J/°C. A reaction changes the temperature from 22.34°C to 25.12°C. How many joules of heat were released?
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 192 J to raise the temperature of 45.0 g of Si by 6.0°C?
a) 0.65 J/g × °C b) 0.79 J/g × °C c) 0.85 J/g × °C d) 0.71 J/g × °C e) 0.54 J/g × °C
Answer: D

17. Aqueous silver ion reacts with aqueous chloride ion. 10.0 mL of 1.00 M $AgNO_3$ + 10.0 mL of 1.00 M NaCl at 25°C. Temperature increases to 32.6°C. Calculate 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. Calculate the heat transferred when one can (~350 g) of Coca Cola is cooled from 25°C to 3°C. (c = 4.18 J/g × °C)
a) 32.2 kJ b) 92.7 kJ c) 49.8 kJ d) 32.6 kJ e) 20.5 kJ
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 × °C b) 0.792 J/g × °C c) 0.855 J/g × °C d) 0.128 J/g × °C e) 0.545 J/g × °C
Answer: D

20. 25 mL of 1.0 M H_2SO_4 + 50 mL of 1.0 M NaOH at 25°C. Temperature increases to 33.9°C. Calculate heat absorbed.
a) 3.09 kJ b) 5.05 kJ c) 9.83 kJ d) 2.56 kJ e) 2.79 kJ
Answer: E

21. What is the specific heat of titanium if 89.7 J raises 33.0 g by 5.20°C? What is the molar heat capacity?
a) 90.0 J/mol × °C b) 13.0 J/mol × °C c) 25.0 J/mol × °C d) 38.0 J/mol × °C e) 42.0 J/mol × °C
Answer: C

22. Sodium has a molar heat capacity of 28.2 J/mol × °C. What is its specific heat?
a) 3.25 J/g × °C b) 4.23 J/g × °C c) 3.55 J/g × °C d) 1.23 J/g × °C e) 2.55 J/g × °C
Answer: D

23. Compound A is burned in a bomb calorimeter with 2.50 L water. Combustion of 0.175 moles causes the temperature to rise 45.0°C. What is the molar heat of combustion?
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 with 1.50 L water. 50.0 g causes 35.0°C rise. Heat of combustion is 2,150 kJ/mol. What is the molar mass?
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. Burning 0.115 moles in a calorimeter with 2.50 L water — what is the temperature increase?
a) 17.40°C b) 13.80°C c) 15.90°C d) 16.70°C e) 19.50°C
Answer: B

26. Compound A: 2.50 L water, 0.175 moles burned, temperature rises 45.0°C. What is the molar heat of combustion?
a) -2.69×10^3 kJ/mole b) -3.75×10^3 kJ/mole c) -2.83×10^3 kJ/mole d) -9.86×10^3 kJ/mole
e) -5.21×10^3 kJ/mole
Answer: A

27. Compound B: 1.50 L water, 50.0 g burned, 35.0°C rise. Heat of combustion is 2150 kJ/mole. What is the molar mass?
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 22.5 kJ, which raised temperature from 22.45°C to 23.97°C. What is its heat capacity?
a) 26.1 kJ/°C b) 35.4 kJ/°C c) 14.6 kJ/°C d) 34.9 kJ/°C e) 14.8 kJ/°C
Answer: E

29. 0.113 g of benzene burns in a calorimeter (551 J/°C), temperature rises 8.60°C. Calculate the reaction enthalpy for combustion of benzene.
a) $C_6H_6(l) + 15/2\ O_2 \rightarrow 6CO_2(g) + 3H_2O(l)$ $\Delta H = -9260$ kJ
b) $C_6H_6(l) + 15/2\ O_2 \rightarrow 6CO_2(g) + 3H_2O(l)$ $\Delta H = -8250$ kJ
c) $C_6H_6(l) + 15/2\ O_2 \rightarrow 6CO_2(g) + 3H_2O(l)$ $\Delta H = -5212$ kJ
d) $C_6H_6(l) + 15/2\ O_2 \rightarrow 6CO_2(g) + 3H_2O(l)$ $\Delta H = -3270$ kJ
e) $C_6H_6(l) + 15/2\ O_2 \rightarrow 6CO_2(g) + 3H_2O(l)$ $\Delta H = -7270$ kJ
Answer: D

30. $\Delta H° = +128.1$ kJ for $CH_3OH(l) \rightarrow CO(g) + 2H_2(g)$. How many kJ consumed when 5.10 g of $H_2(g)$ is formed?
a) 653 kJ b) 62.0 kJ c) 324 kJ d) 162 kJ
Answer: D

31. $\Delta H° = +128.1$ kJ for $CH_3OH(l) \rightarrow CO(g) + 2H_2(g)$. How many kJ consumed when 5.10 g of $CO(g)$ is formed?
a) 533 kJ b) 32.3 kJ c) 43.1 kJ d) 29.5 kJ
Answer: B

32. ΔH° = -1107 kJ for $2Ba(s) + O_2(g) \rightarrow 2BaO(s)$. How many kJ 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 absorbs 9.86 J heated from 23.2°C to 30.5°C. (c = 0.90 J/g × °C). Calculate the mass.
a) 4.73 g b) 3.46 g c) 1.50 g d) 2.80 g
Answer: C

34. Calculate ΔH(reaction) for $C_2H_4(g) + H_2(g) \rightarrow C_2H_6(g)$ using Hess's Law.
a) -242 kJ b) -137 kJ c) -40.1 kJ d) -150. kJ
Answer: B

35. Calculate ΔH for $4NH_3(g) + 5O_2(g) \rightarrow 4NO(g) + 6H_2O(g)$ using Hess's Law.
a) -1425 kJ b) -1375 kJ c) -1628. kJ d) -1983. kJ
Answer: C

36. Find $\Delta H^\circ f$ for acetic acid $HC_2H_3O_2$ using Hess's Law.
a) -525 kJ b) -375 kJ c) -628. kJ d) -486. kJ
Answer: D

37. Calculate ΔH for $CH_4(g) + NH_3(g) \rightarrow HCN(g) + 3H_2(g)$ using Hess's Law.
a) +256.0 kJ b) +1853 kJ c) +3421. kJ d) +1972 kJ
Answer: A

38. Calculate ΔH for $2Al(s) + 3Cl_2(g) \rightarrow 2AlCl_3(s)$ using Hess's Law.
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 with 5.65 L water, water temperature rises 55.4°C. What is the molar heat of combustion?
a) 4160 kJ/mole b) 5893 kJ/mole c) 6812 kJ/mole d) 7356 kJ/mole
Answer: A

40. 22.0 grams of propane (C_3H_8) is combusted in a bomb calorimeter with 3.25 L water, temperature rises 29.5°C. What is the molar heat of combustion?
a) -160 kJ/mole b) -587 kJ/mole c) -872 kJ/mole d) -802 kJ/mole
Answer: D

41. 1.38 g of liquid PCl_3 at 25.55°C added to 100 g water at 25.55°C in a coffee-cup calorimeter; temperature increases to 32.00°C. Calculate the molar heat of solution.
a) -170 kJ/mole b) -271 kJ/mole c) -398 kJ/mole d) -802 kJ/mole
Answer: B

42. Coffee-cup calorimeter: 150 g water at 24.6°C. 110 g molybdenum at 100°C added; final temperature 28.0°C. What is the specific heat of molybdenum?
a) 0.34 J/g × °C b) 0.46 J/g × °C c) 0.39 J/g × °C d) 0.18 J/g × °C e) 0.27 J/g × °C
Answer: E

43. 0.235 g benzoic acid (heat of combustion = 26.38 kJ/g) gives a 3.62°C rise. 0.305 g citric acid gives a 1.83°C rise. 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. 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. d) energy is always conserved.
Answer: D

51. The change in internal energy equals the heat supplied minus:
a) the amount of heat not conserved. b) the amount of work done by the system. c) the original internal energy. d) the volume difference
Answer: B

52. Internal energy is 30 J. Heat is supplied and 20 J of work is done. Final internal energy is 80 J. How many Joules of heat were added?

a) 50 b) 60 c) 70 d) 80
Answer: C

53. Which equation represents the First Law for a closed system (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 system does not allow energy or matter to be exchanged with surroundings?
a) Open b) Closed c) Adiabatic d) Isolated
Answer: D

55. Which system only allows exchange of energy with 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 surroundings?
a) Isolated b) Open c) Adiabatic d) Closed
Answer: B

57. In which case would ΔU in $\Delta U = Q+W$ be less than zero?
a) Work done on the system. b) Work done by the system. c) Magnitudes of heat and work are equivalent. d) Heat magnitude greater than work.
Answer: B

58. Which equation is associated with heat in a thermally isolated system?
a) $Q < 0$ b) $Q > 0$ c) $Q > W$ d) $Q = 0$
Answer: D

59. Which expression 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

6.1 Electromagnetic Energy

6.2 The Bohr Model

6.2.1 Rydberg Equation

6.3 Development of Quantum Theory

6.4 Electronic Structure of Atoms (Electron Configurations)

6.5 Periodic Variations in Element Properties

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 waves
- 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.

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).

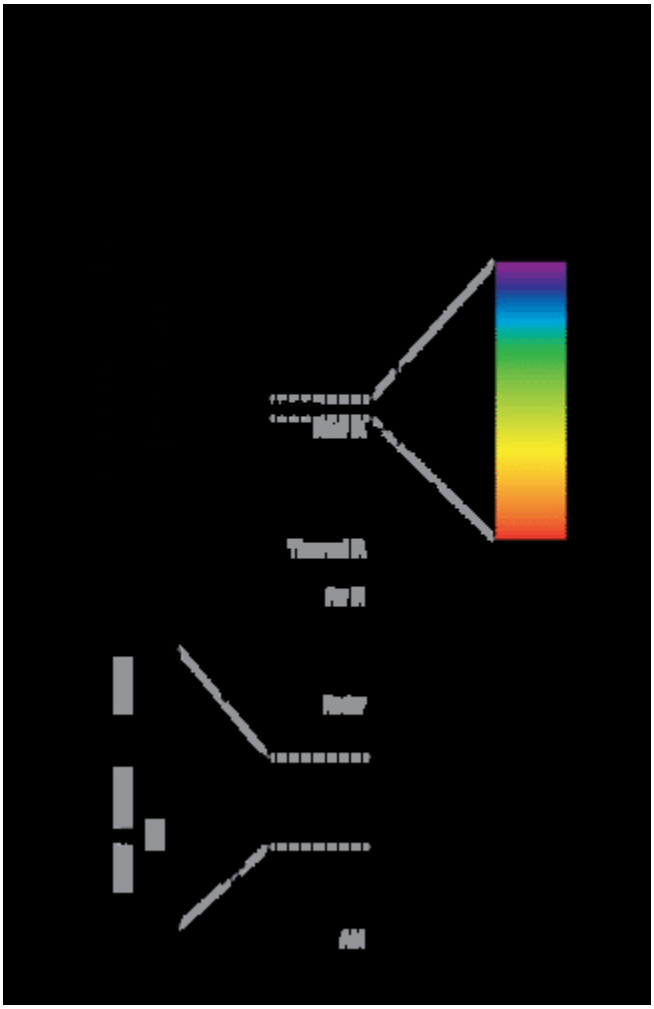


Figure 6.1: The electromagnetic spectrum; short wavelengths are the fastest with the highest energy

Speed of all Electromagnetic Spectrum Waves (c) = 3.0 x 10^8 m/s = speed of light.

c (m/s) = ν x λ = 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)

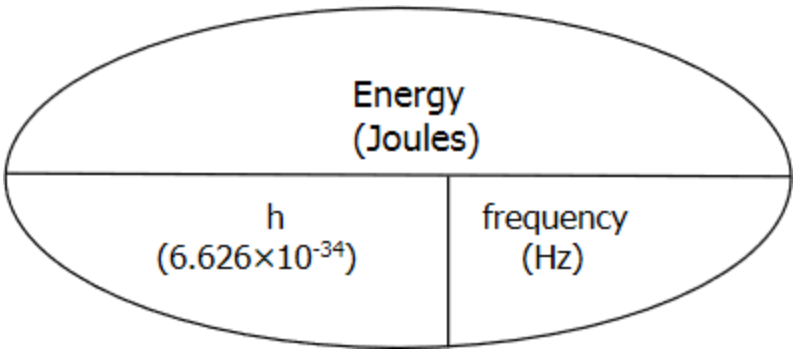


Figure 6.12: Relationship between speed, frequency, and wavelength of electromagnetic waves

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 10^{14} Hz. 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

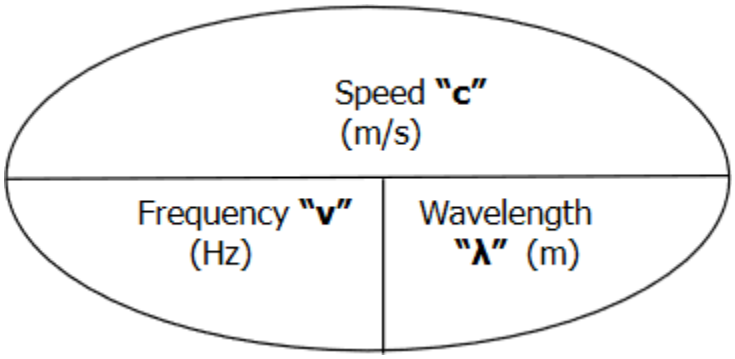


Figure: Relationship between energy, Planck's constant, and frequency (E = hv)

Examples:

a. Calculate the energy of a photon of radiation with a frequency of 8.5 x 10^{14} Hz

Energy (J) = h x ν = [6.626 x 10^{-34} J.s] x [8.5 x 10^{14} Hz] = 5.63 x 10^{-19} J

b. Calculate the energy of a photon of radiation with a wavelength of 6.4 x 10^{-7} m

Energy (J) = h x ν = h x [c / λ] = [6.626 x 10^{-34} J.s] x [(3.0 x 10^{8} m/s) / (6.4 x 10^{-7} m)] = 3.1 x 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.

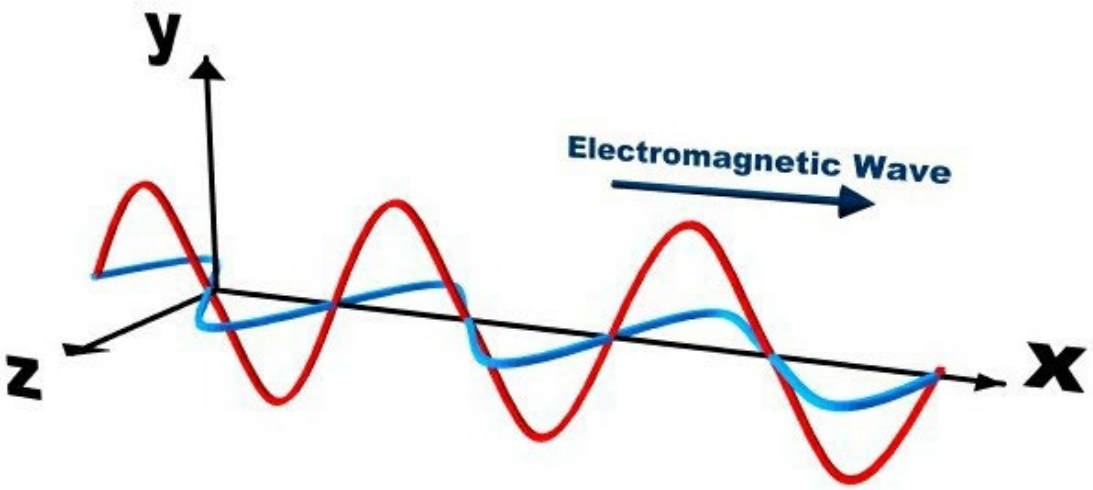


Figure 6.13: Electromagnetic wave characteristics showing perpendicular electric and magnetic fields

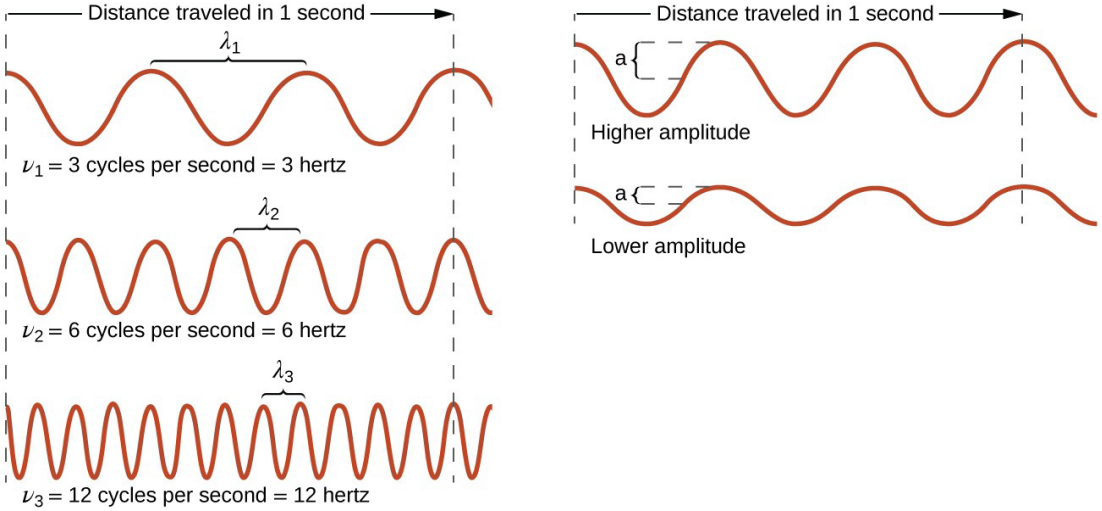


Figure: One-dimensional sinusoidal waves showing the relationship among wavelength, frequency, and speed. The wave with the shortest wavelength has the highest frequency. Amplitude is one-half the height of the wave from peak to trough. Reference: Chemistry 2e OpenStax.

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.

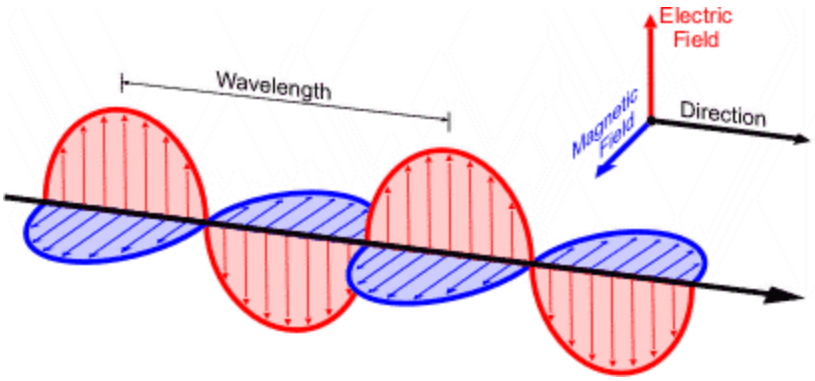


Fig 6.15: Electromagnetic Wave direction showing electric and magnetic field components and direction of travel

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.

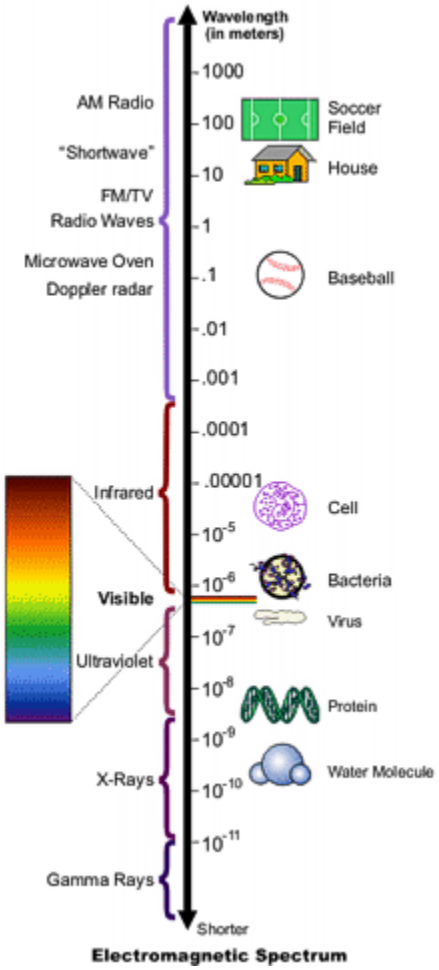


Figure: Electromagnetic Spectrum scale showing wavelengths in meters with corresponding physical object size comparisons

Reference: https://www.youtube.com/watch?v=WNkB8IY-k04

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.

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.

Electromagnetic wave begins when an electrically charged particle vibrates. 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.

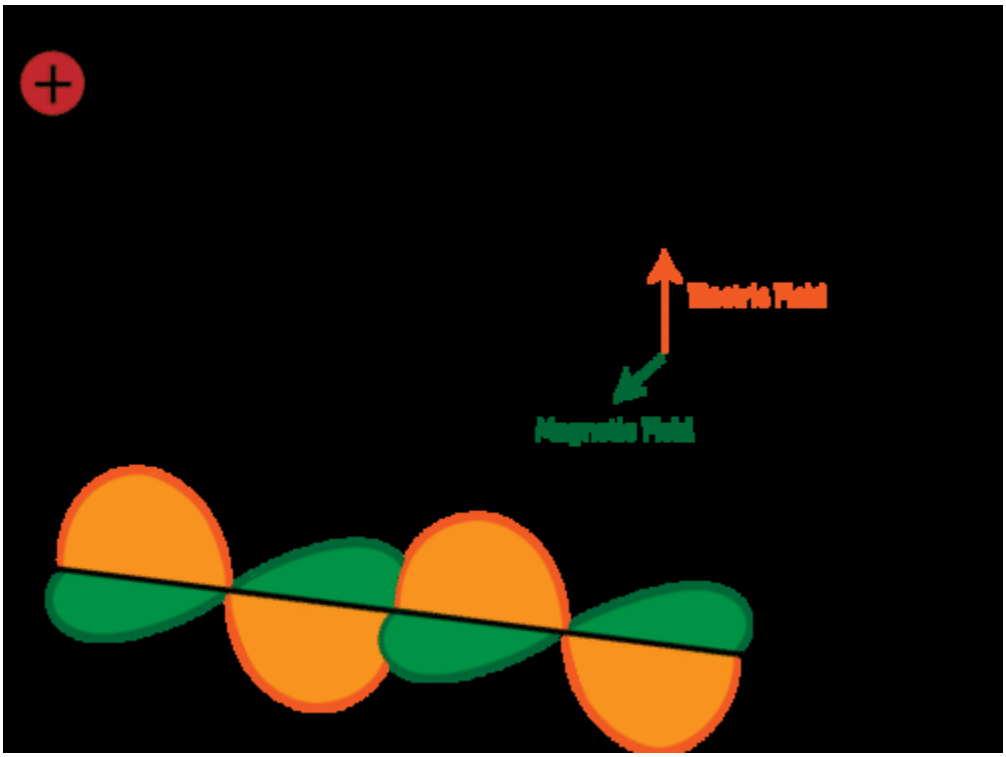


Figure 6.17: Electromagnetic wave travel - A vibrating charged particle generates vibrating electric and magnetic fields that make up an electromagnetic wave

Electromagnetic Wave Travels

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.

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.

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.

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.

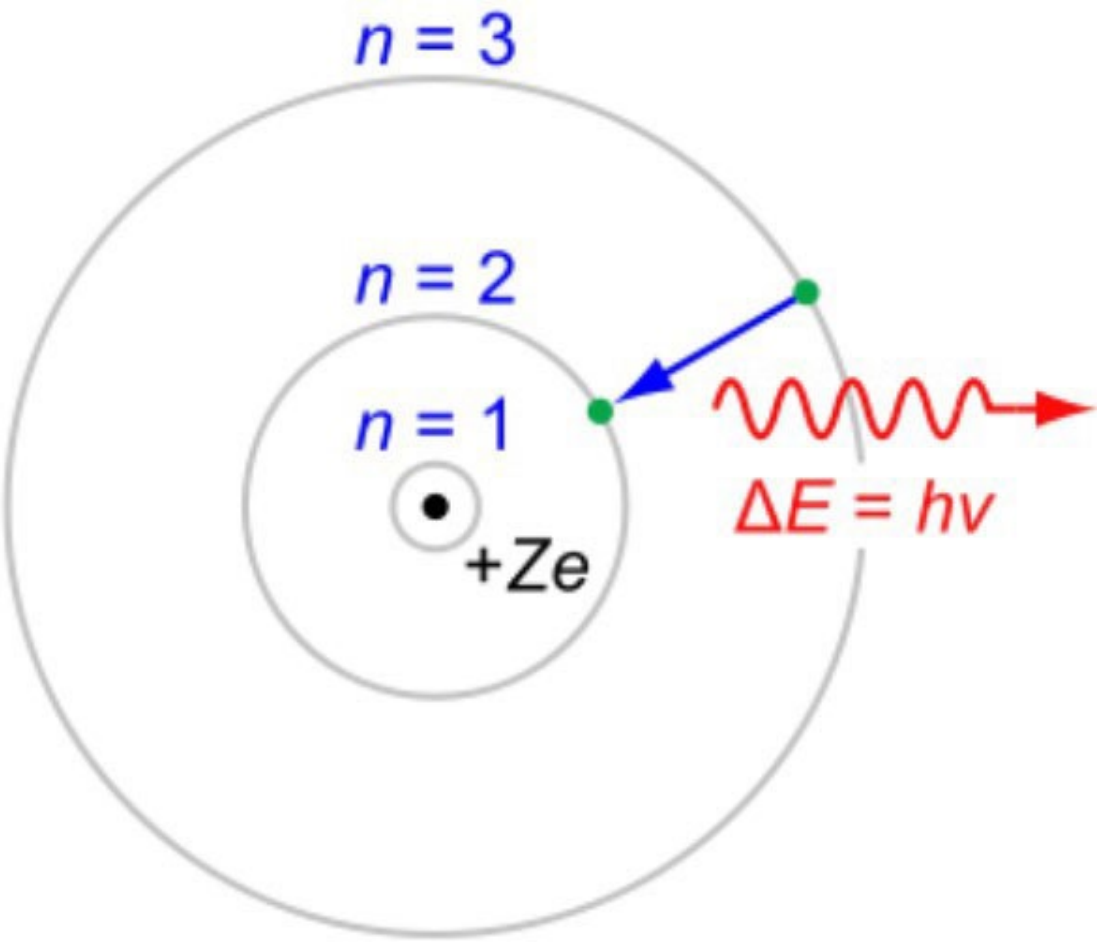


Fig 6.21: Rutherford-Bohr model of the hydrogen atom showing electron energy levels and a photon emission transition

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.

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. The Bohr theory solved this problem and correctly explained the experimentally obtained Rydberg formula for emission lines.

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.

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. Bohr could determine the energy spacing between levels and come to an exactly correct quantum rule—the angular momentum L is restricted to be an integer multiple of a fixed unit:

$$\mathbf{L = n(h/2\pi) = n\hbar}$$

where n = 1, 2, 3, ... is called the principal quantum number and $\hbar = h/2\pi$. The lowest value of n is 1; this gives a smallest possible orbital radius of 0.0529 nm, known as the Bohr radius.

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 Bohr himself did not believe in the concept of photons as explained by Einstein.

Reference: https://en.wikipedia.org/wiki/Bohr_model

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 a 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 in 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 Downtown. Las Vegas was looking very impressive with lots of fancy lights with different colors.

Fig 6.22: Las Vegas at night, showing the colorful lights from various hotel and casino signs

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.

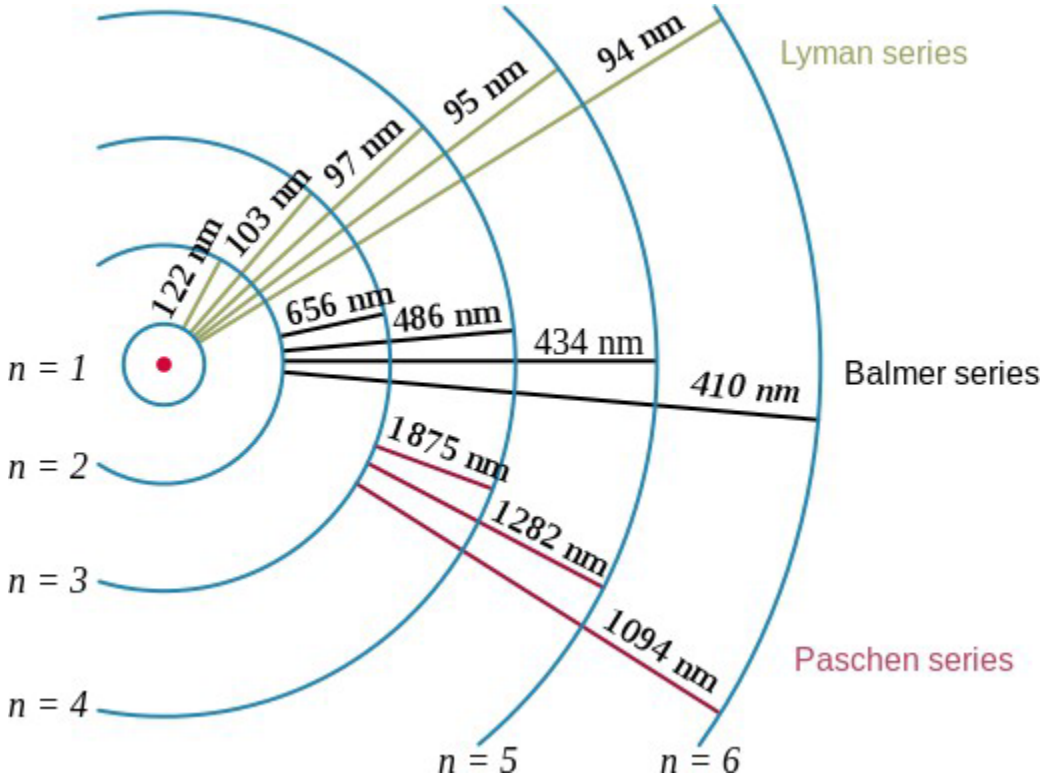


Fig 6.23: Bohr's orbit model showing electron energy level transitions and emission spectrum series for hydrogen (Lyman, Balmer, and Paschen series)

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).

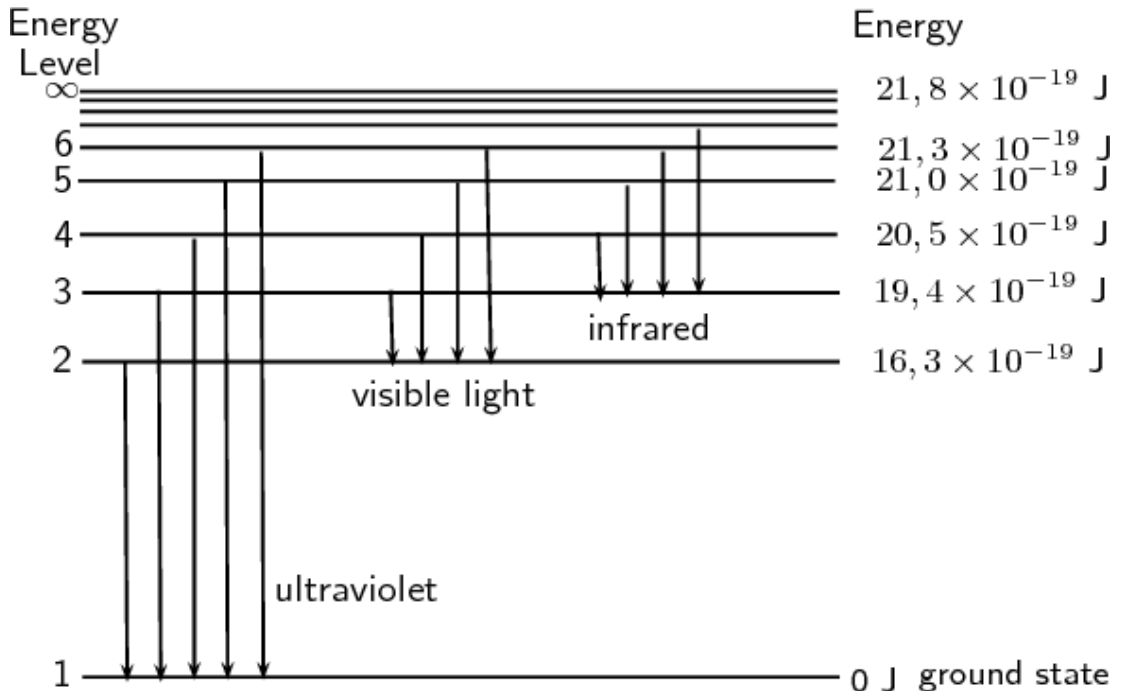


Fig 6.24: Bohr's orbit energy levels showing the energy values in Joules for each electron shell of the hydrogen atom

ΔE(electron) = E(final) − E(initial) = h x ϑ = [h x c / λ]

The above formula is called Planck's formula or Principle

ΔE(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.

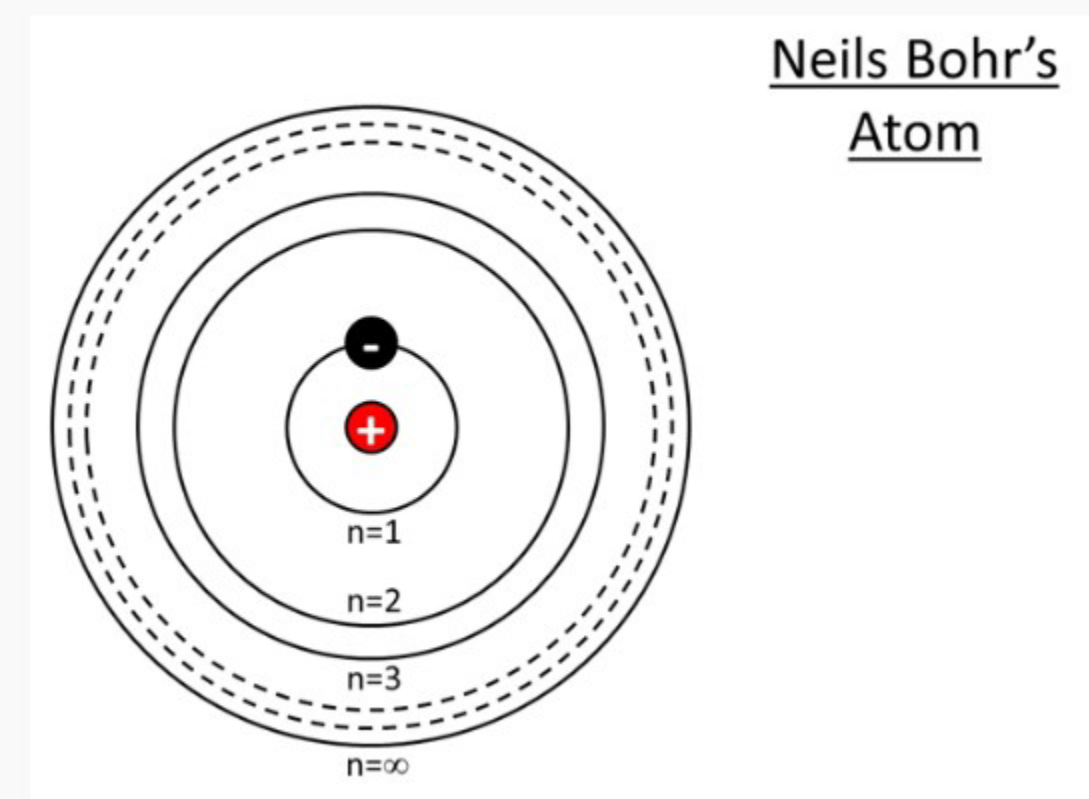


Fig 6.25: Hydrogen Atom Emission Spectrum Lines showing the four visible spectral lines at 410 nm (violet), 434 nm (blue-violet), 486 nm (cyan-green), and 656 nm (red)

The professor went further and recommended his students the following YouTube videos:

https://www.youtube.com/watch?v=XQj0VwM-Hfs

https://www.youtube.com/watch?v=YHmGNDMV1cY

Fig 6.26: Bohr's atomic model showing the nucleus at the center and electron orbits at quantized energy levels n=1, n=2, n=3, and n=infinity

https://www.youtube.com/watch?v=h3E9jNDnrDo

https://www.youtube.com/watch?v=vhxjQ3-gYko

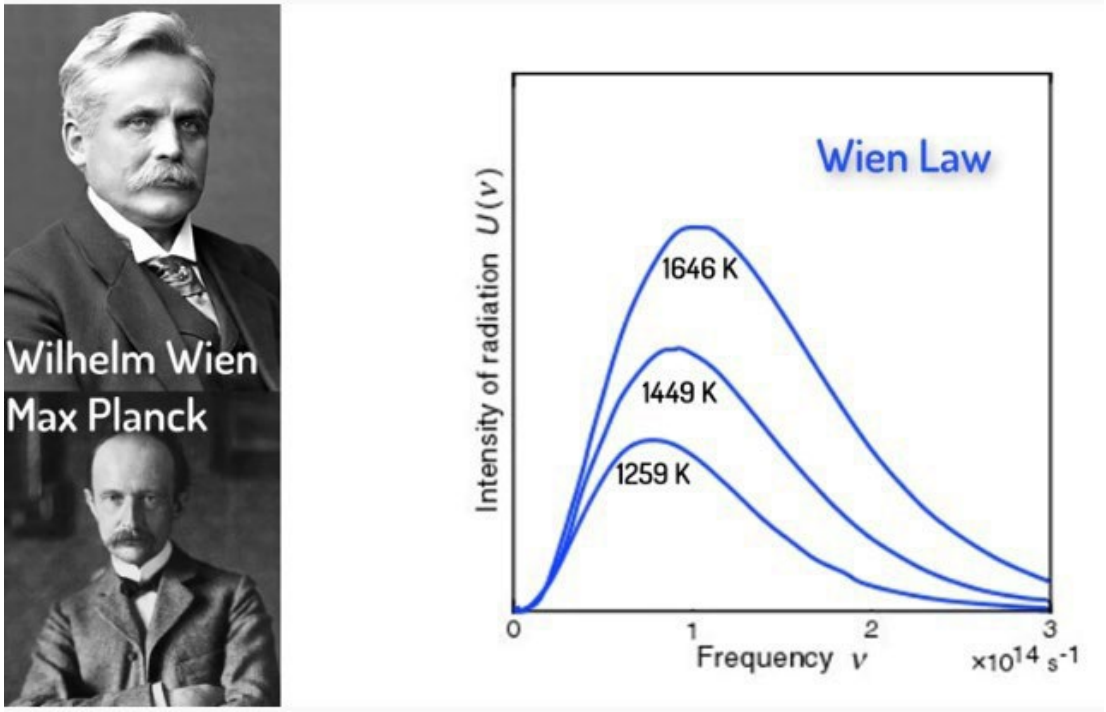


Fig 6.27: Ultraviolet Catastrophe - Photographs of Wilhelm Wien and Max Planck alongside a graph of Wien's Law showing blackbody radiation intensity curves at three different temperatures (1259 K, 1449 K, and 1646 K)

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 below:

$$\frac{1}{\lambda_{\text{vac}}} = R_{\text{H}} \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right),$$

where

λ_{vac} is the wavelength of electromagnetic radiation emitted in vacuum,

R_{H} is the Rydberg constant for hydrogen, approximately $1.096\,775\,83 \times 10^7\ \text{m}^{-1}$,

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.

Figure: Rydberg's Formula showing 1/λ = R_H(1/n1² - 1/n2²), the formula used to calculate spectral emission wavelengths for hydrogen

Reference: https://en.wikipedia.org/wiki/Rydberg_formula

The figure below illustrates the origin of the line spectra of hydrogen:

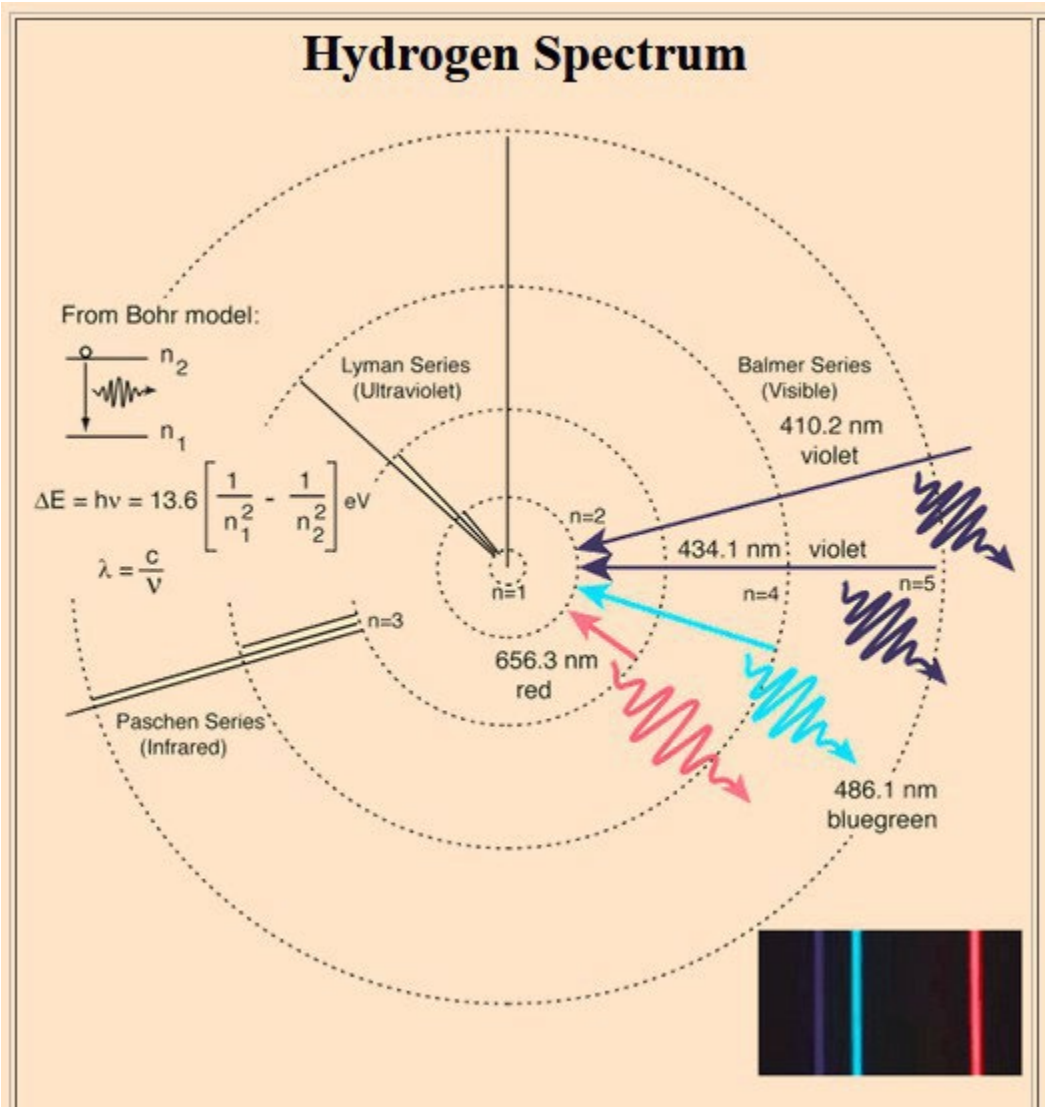


Fig 6.28: Explanation of Emission spectrum in terms of Bohr's model showing the Lyman (ultraviolet), Balmer (visible), and Paschen (infrared) series with specific wavelengths

With the help of Rydberg formula, one can calculate the wavelength of each transition and 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:

https://www.youtube.com/watch?v=mXxsT1ut35Q

https://www.youtube.com/watch?v=DLmnh74MfSA

https://www.youtube.com/watch?v=au2HCVn9IJI

At the end of the professor talk (lecture), the students were very satisfied and happy to cover these materials with lots of details and asked the professor to go back to downtown Las Vegas and enjoy the different colors of lights and were eager to know more about the elements with different emission line spectra (different colors).

Description of Rydberg's Equation

Each element has a distinct spectral fingerprint. When an element in the gaseous state is heated, then it will give off light. When this light passes through a prism, bright lines of different colors can be distinguished. Each element is slightly different from other elements. This discovery was the beginning of the study of spectroscopy.

Johannes Rydberg was a Swedish physicist who found the mathematical relationship between one spectral line and the next of certain elements. He discovered that there was an integer relationship between the wavenumbers of successive lines. His findings were combined with Bohr's model of the atom to create this formula.

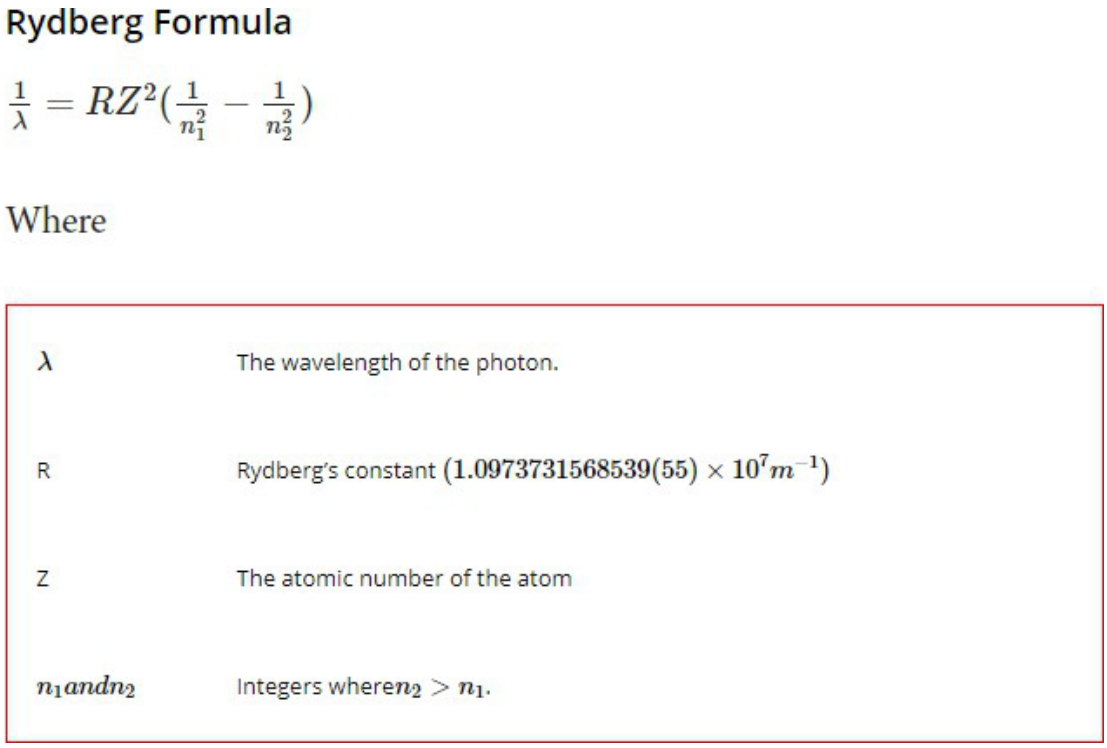


Figure: Rydberg Formula showing 1/λ = RZ²(1/n1² - 1/n2²) with variable definitions in a table

It was later found that n2 and n1 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 n1 to 1 and running n2 from 2 to infinity yields the Lyman series.

For most problems, we will deal with hydrogen so we can use the formula:

$$\frac{1}{\lambda} = R_H\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right)$$

Figure: Hydrogen-specific Rydberg Formula 1/λ = R_H(1/n1² - 1/n2²) with variable definitions

Solution:

We have the Rydberg equation:

$$\mathbf{1/\lambda = R_H(1/n1^2 - 1/n2^2)}$$

Now put the known values, n1 = 1 and n2 = 3.

Use R_H = 1.9074 x 10^7 m^{-1}.

$$\frac{1}{\lambda} = R_H\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right)$$

Now put the known vakues,

$$n_1 = 1$$

and $n_2 = 3$.

Use $R_H = 1.9074 \times 10^7 m^{-1}$.

$$\frac{1}{\lambda} = R_H\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right)$$

$$= 1.0947 \times 10^7\left(\frac{1}{1^2} - \frac{1}{3^2}\right)$$

$$= 1.0947 \times 10^7 \times \frac{8}{9}$$

$$= 0.973 \times 10^7$$

$$\lambda = 1.025 \times 10^{-7}\ meter$$

Figure: Worked example of the Rydberg equation calculation showing step-by-step solution for n1=1 and n2=3, yielding a wavelength of 1.025 x 10^-7 meters

This formula gives a wavelength in meters using this value for Rydberg's constant.

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 won the Nobel Prize in Physics for his theory in 1918.

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, 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.

At the sub-atomic scale, there is no boundary between particles and waves. In fact, both particle 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. Cathode rays were discovered by Michael Faraday. Gustav Kirchhoff in about 1860 had developed 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, it will divide into a number of discrete energy elements ε (epsilon) which direct proportional to the frequency ν:

$$\boldsymbol{\varepsilon = h\nu}$$

h is a numerical value called Planck's constant.

P. Dirac in 1928 had combined both the relativity theory with the quantum mechanics. In 1927, Heisenberg used the quantum mechanics to discover the uncertainty principle which had put theoretical limitation of the accuracy of specific measurements. Einstein and Bose had developed the Bose-Einstein Statistics which put the limitation on the absolute values of the measurements.

So What Is Quantum Mechanics?

Quantum Mechanics is one of the branches of physics dealing with small scale of the atoms and electrons. The classical mechanics deals with the matter and its studies at specific time and place.

Three revolutionary principles

4. Quantized properties: A quantized property is a definite size and the property which may be found in a multiple of that definite size.
5. Particles of light: It was demonstrated experimentally that the light has a dual character: wave and particle.
6. 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 amounts.

Particles of light?

Light particles are called photons by Einstein which means that the light is made of a 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 are fundamental limitations 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 maintain their relative and approximate values.

In general it is not possible to predict the value of a quantity with absolute certainty even if all initial conditions are given.

Reference: https://youtu.be/Usu9xZfabPM

Reference: https://www.youtube.com/watch?v=K0VY9_hB_WU

Reference: https://www.youtube.com/watch?v=8HkPAE_9Q1Y

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 $1s^2 2s^2 2p^6\ 3s^1$.

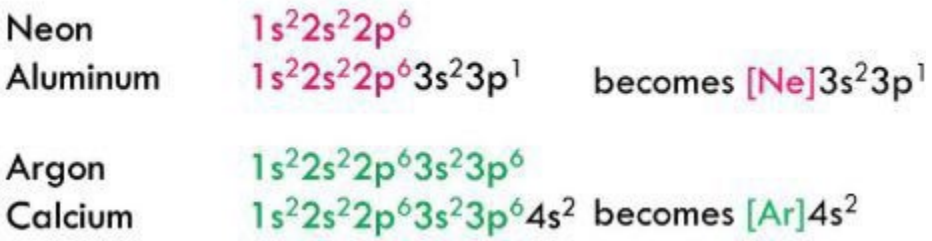


Fig 6.41: Notation for electron configuration showing the three components: energy level (principal quantum number), type of orbital (subshell letter), and number of electrons (superscript)

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 $1s^2 2s^2 2p^6$, which can be abbreviated to $[He]2s^2 2p^6$).

Neon: $1s^2 2s^2 2p^6$

Aluminum: $1s^2 2s^2 2p^6\ 3s^2\ 3p^1$ becomes $[Ne]3s^2 3p^1$

Argon: $1s^2 2s^2 2p^6\ 3s^2 3p^6$

Calcium: $1s^2 2s^2 2p^6\ 3s^2 3p^6\ 4s^2$ becomes $[Ar]4s^2$

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.

Table 6.42: Electron's Shells and Occupancy

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	$2*4^2 = 32$

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.

Table 6.43: Correlation between Quantum numbers and energy levels of Electrons

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.

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.
- For example, 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

Aufbau Principle

The Aufbau principle states that electrons are filling lower energy atomic orbitals before filling higher energy ones (Aufbau is German for "building-up"). By following this rule, we can predict the electron configurations for atoms or ions.

The order in which electrons are filled in atomic orbitals as per the Aufbau principle is:

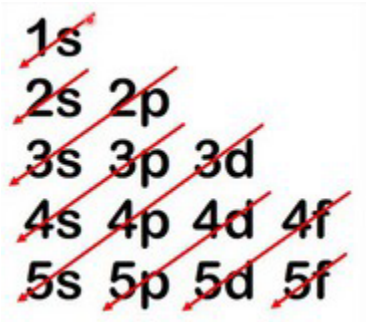


Fig 6.45: Increasing energy level of electrons following Aufbau Principles - diagonal arrow diagram showing the order of subshell filling (1s, 2s, 2p, 3s, 3p, 4s, 3d, 4p...)

Reference: https://www.youtube.com/watch?app=desktop&v=p9Y-Nd4gGAQ

The Aufbau principle has several exceptions such as in copper and chromium atoms. These exceptions are explained by the stability provided by half-filled or completely filled subshells.

Pauli Exclusion Principle

The orbital can only be occupied by a maximum of only two electrons. These two electrons in an orbital should have opposite spin.

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:

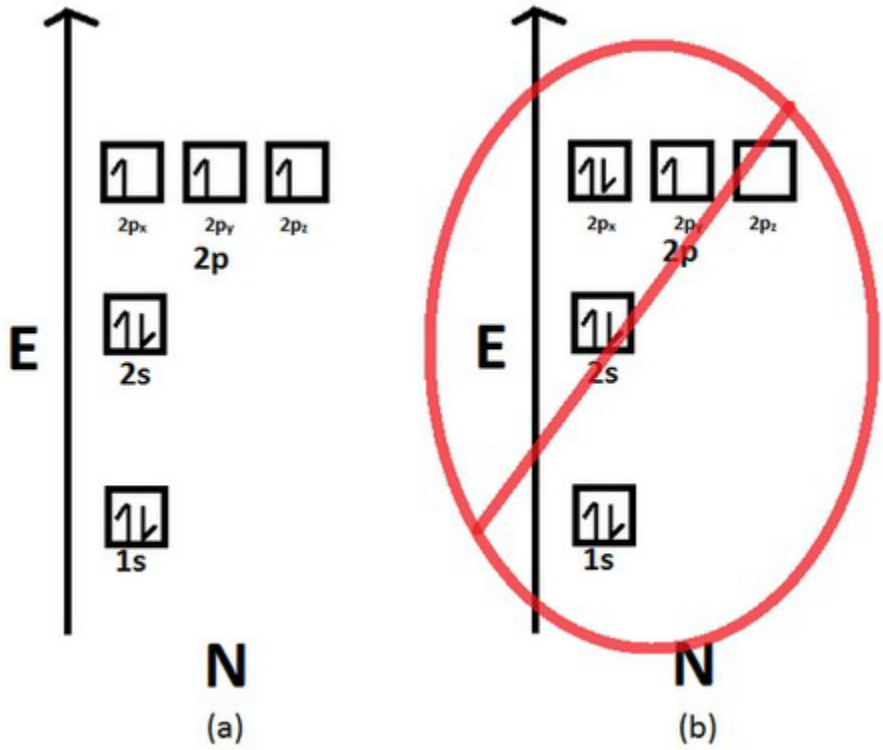


Fig 6.44: Hund's Rule Description showing correct (a) and incorrect (b) electron configurations for nitrogen, demonstrating that electrons fill degenerate orbitals singly before pairing

Examples

The electron configurations of a few elements are provided with illustrations in this subsection.

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:

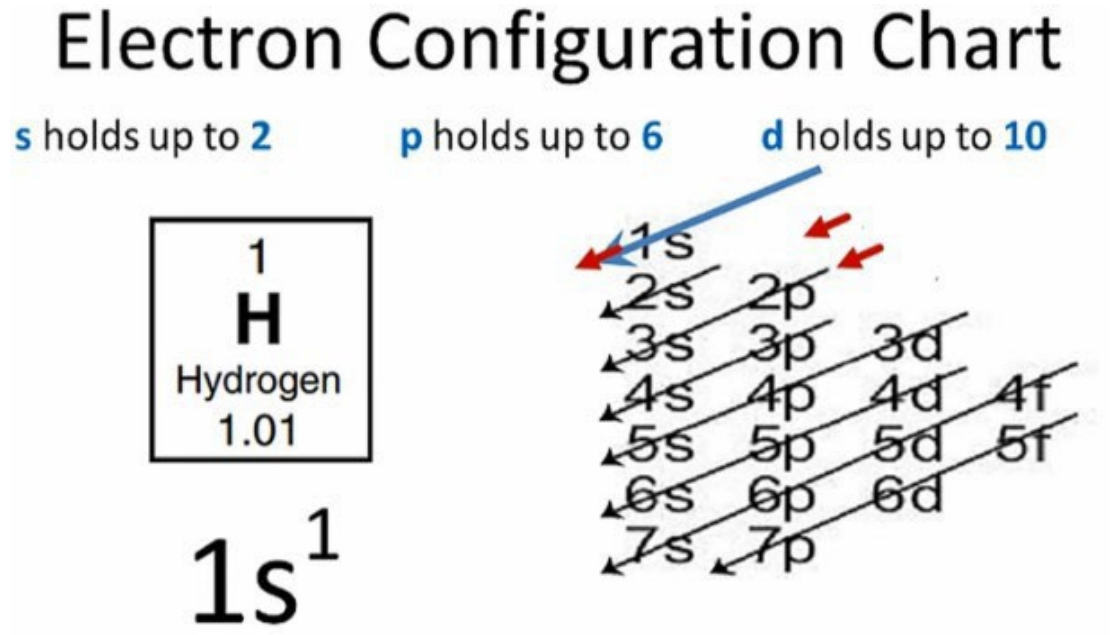


Fig 6.46: Electron Configuration Chart showing hydrogen (1s^1) with the diagonal arrow diagram for the Aufbau filling order

Reference: https://www.youtube.com/watch?v=Wwb8fSXr6oo

Electron Configuration of Oxygen:

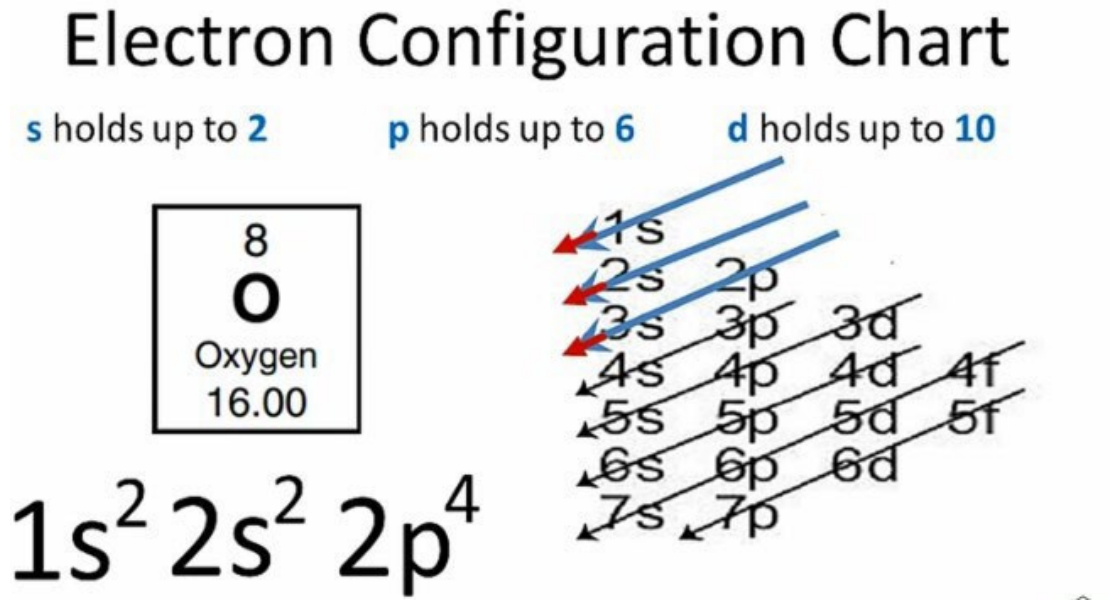


Fig 6.47a: Spectroscopic Notation of Oxygen Atom showing electron configuration $1s^2 2s^2 2p^4$ with the filling order diagram

$1s^2$ 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 $2s^2\ 2p^4$

Electron Configuration of Chlorine:

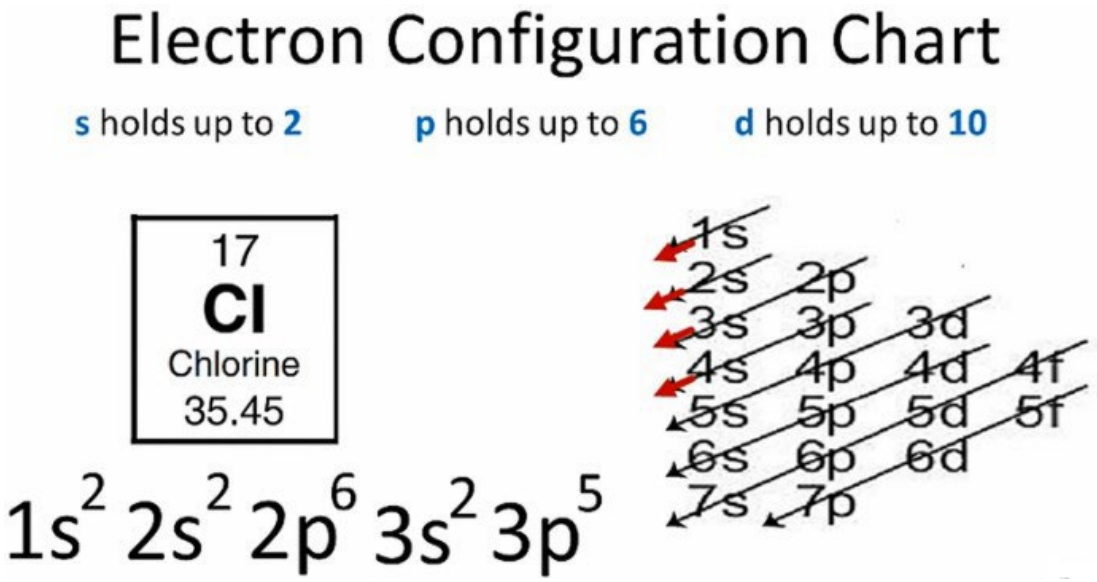


Fig 6.47b: Spectroscopic Notation of Chlorine Atom showing electron configuration $1s^2 2s^2 2p^6\ 3s^2 3p^5$ with the filling order diagram

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 $3s^2\ 3p^5$

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 first way is use the Periodic Table to Write Electron Configurations. Reference: https://youtu.be/ououF9nHUhk

The second way is use the configuration chart. Reference: https://youtu.be/TjVrcw2sZLs

The Aufbau Principle

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 the 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

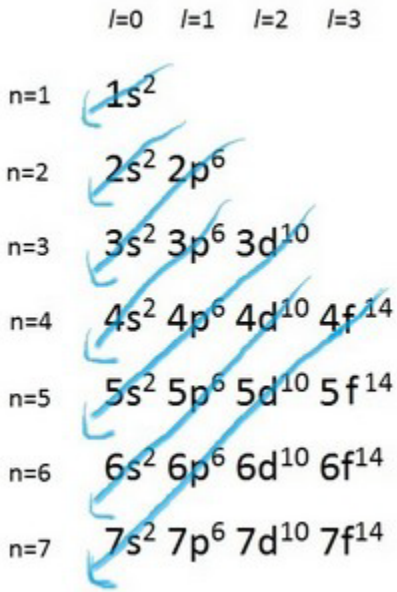


Fig 6.48: Aufbau Diagram showing the energy ordering of subshells from n=1 to n=7, with diagonal arrows indicating the electron filling sequence

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) determines 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.

This periodic table shows the electron configuration for each subshell. By "building up" from hydrogen, this table can be used to determine the electron configuration for any atom on the periodic table.

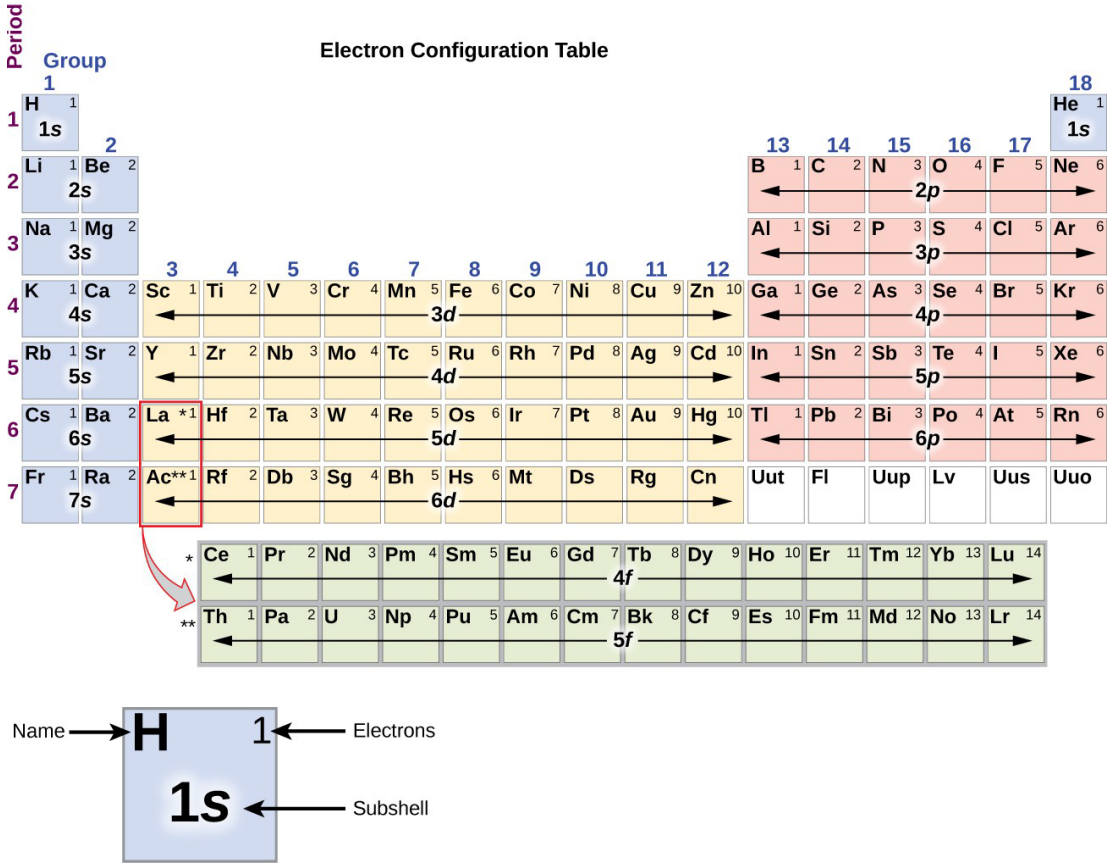


Fig 6.49: Location of shells and subshells in the periodic Table showing each element's subshell electron configuration organized by period and group

This version of the periodic table shows the outer-shell electron configuration of each element. Note that down each group, the configuration is often similar.

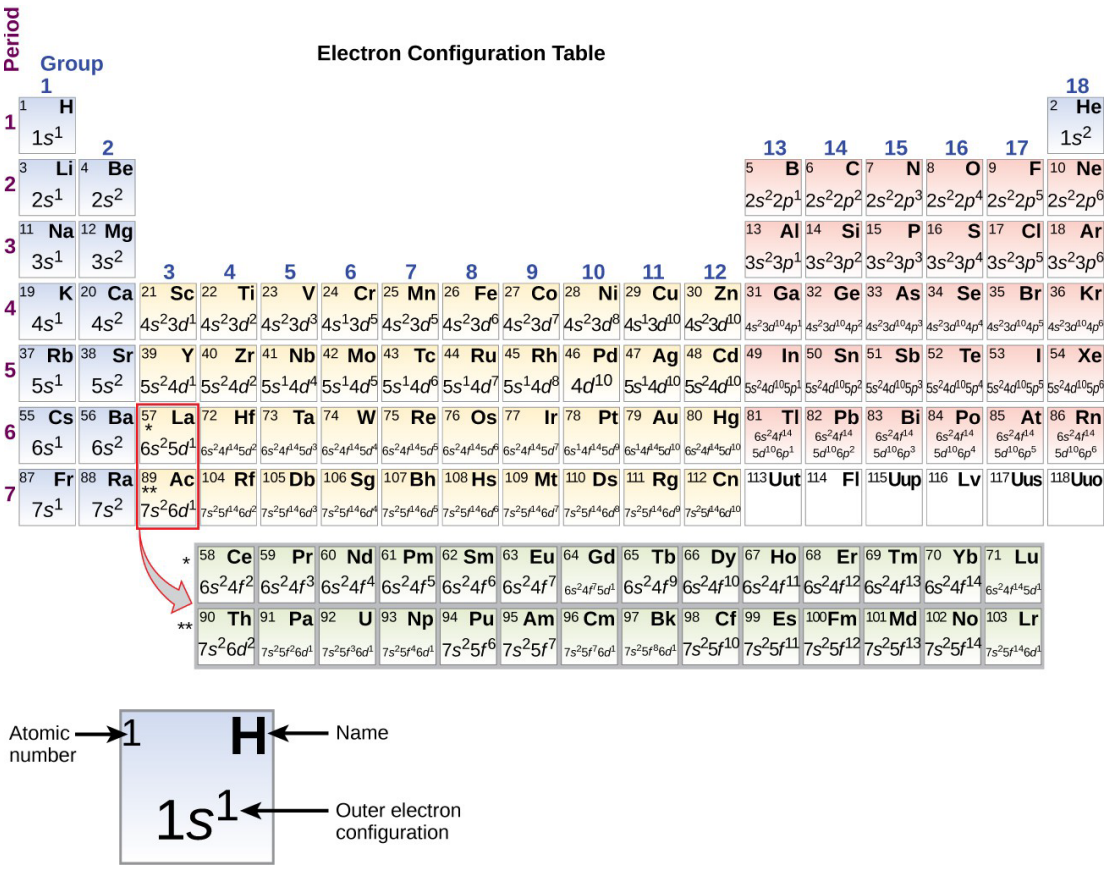


Fig 6.410: Periodic Classification based on electron configuration - complete periodic table showing full outer-shell electron configurations for all elements

Electron Configurations and the Periodic Table

The periodic table arranges atoms based on increasing atomic number so that elements with the same chemical properties recur periodically. When their electron configurations are added to the table we also see a periodic recurrence of similar electron configurations in the outer shells of these elements. Because they are in the outer shells of an atom, valence electrons play the most important role in chemical reactions. The outer electrons have the highest energy of the electrons in an atom and are more easily lost or shared than the core electrons. Valence electrons are also the determining factor in some physical properties of the elements.

Elements in any one group (or column) have the same number of valence electrons; the alkali metals lithium and sodium each have only one valence electron, the alkaline earth metals beryllium and magnesium each have two, and the halogens fluorine and chlorine each have seven valence electrons. The similarity in chemical properties among elements of the same group occurs because they have the same number of valence electrons. It is the loss, gain, or sharing of valence electrons that defines how elements react.

It is important to remember that the periodic table was developed on the basis of the chemical behavior of the elements, well before any idea of their atomic structure was available.

The colored sections show the three categories of elements classified by the orbitals being filled: main group, transition, and inner transition elements. These classifications determine which orbitals are counted in the valence shell, or highest energy level orbitals of an atom.

7. Main group elements (sometimes called representative elements) are those in which the last electron added enters an s or a p orbital in the outermost shell. This category includes all the nonmetallic elements, as well as many metals and the intermediate semimetallic elements. The valence electrons for main group elements are those with the highest n level.
8. Transition elements or transition metals. These are metallic elements in which the last electron added enters a d orbital. The valence electrons in these elements include the ns and (n – 1) d electrons.
9. Inner transition elements are metallic elements in which the last electron added occupies an f orbital. The valence shells of the inner transition elements consist of the (n – 2)f, the (n – 1)d, and the ns subshells. There are two inner transition series: a) The lanthanide series: lanthanide (La) through lutetium (Lu); b) The actinide series: actinide (Ac) through lawrencium (Lr).

Electron Configurations of Ions

We have seen that ions are formed when atoms gain or lose electrons. A cation (positively charged ion) forms when one or more electrons are removed from a parent atom. For main group elements, the electrons that were added last are the first electrons removed. For transition metals and inner transition metals, however, electrons in the s orbital are easier to remove than the d or f electrons, and so the highest ns electrons are lost, and then the (n – 1)d or (n – 2)f electrons are removed. An anion (negatively charged ion) forms when one or more electrons are added to a parent atom. The added electrons fill in the order predicted by the Aufbau principle.

Key Concepts and Summary

The relative energy of the subshells determine the order in which atomic orbitals are filled (1s, 2s, 2p, 3s, 3p, 4s, 3d, 4p, and so on). Electron configurations and orbital diagrams can be determined by applying the Pauli exclusion principle (no two electrons can have the same set of four quantum numbers) and Hund's rule (whenever possible, electrons retain unpaired spins in degenerate orbitals).

Electrons in the outermost orbitals, called valence electrons, are responsible for most of the chemical behavior of elements. In the periodic table, elements with analogous valence electron configurations usually occur within 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 three categories 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

The elements in groups (vertical columns) of the periodic table exhibit similar chemical behavior. These properties vary periodically as the electronic structure of the elements changes. They are (1) size (radius) of atoms and ions, (2) ionization energies, and (3) electron affinities.

The elements in groups (vertical columns) of the periodic table exhibit similar chemical behavior. This similarity occurs because the members of a group have the same number and distribution of electrons in their valence shells. However, there are also other patterns in chemical properties on the periodic table. For example, as we move down a group, the metallic character of the atoms increases. Oxygen, at the top of group 16 (6A), is a colorless gas; in the middle of the group, selenium is a semiconducting solid; and, toward the bottom, polonium is a silver-grey solid that conducts electricity.

As we go across a period from left to right, we add a proton to the nucleus and an electron to the valence shell with each successive element. As we go down the elements in a group, the number of electrons in the valence shell remains constant, but the principal quantum number increases by one each time. An understanding of the electronic structure of the elements allows us to examine some of the properties that govern their chemical behavior. These properties vary periodically as the electronic structure of the elements changes. They are (1) size (radius) of atoms and ions, (2) ionization energies, and (3) electron affinities.

Reference: https://www.youtube.com/watch?v=3tFOr1Jh_bs

The first such property we will consider is atomic size as measured by the atomic radius. The figure below shows how atomic radius varies qualitatively across the Periodic Table.

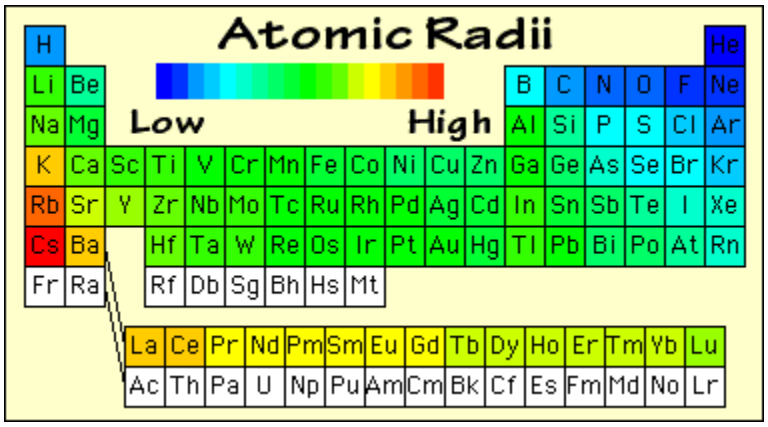


Fig 6.51: Trend in Atomic radii - periodic table showing color-coded atomic radius trends, with larger atoms (low atomic number, lower periods) in red and smaller atoms (higher periods, right side) in blue

The general trend is easy to spot and to understand: heavier atoms (those with large atomic numbers) have more electrons, and increasing the number of electrons means placing electrons into orbitals with ever-increasing principal quantum number—orbitals with ever-increasing size. This clearly explains the trend in increasing size as we go down any one column: H is smaller than Li, etc., ending the first column with the biggest atom for which we have reliable data, Cs. These atoms' sizes are governed by the size of their single highest-energy electron's orbital, which is 1s for H but 6s for Cs.

As we go across a row (look at Li through Ne, for example), the size decreases, but rather slowly: we are adding electrons into orbitals with (for this row) the same principal quantum number. These orbitals are slowly shrinking in size because the nuclear charge is increasing as we go across a row, and increasing nuclear charge means increasing the force attracting electrons to the nucleus, making the orbitals contract.

Next, we look at two energetic properties of atoms, the ionization energy (IE) and the electron affinity (EA). The ionization energy is the energy required to remove the least tightly bound electron from an atom, producing a positive ion and a free electron:

$$\mathbf{A \rightarrow A^{+} + e^{-}}$$

(When we start with a neutral atom, as we have here, we say the energy change is the first ionization energy. If we then remove another electron, as in $A^{+} \rightarrow A^{2+} + e^{-}$, we call the energy need to do so the second ionization energy, and so forth, until we run out of electrons.) The figure below shows the trend in first ionization energies across the Periodic Table.

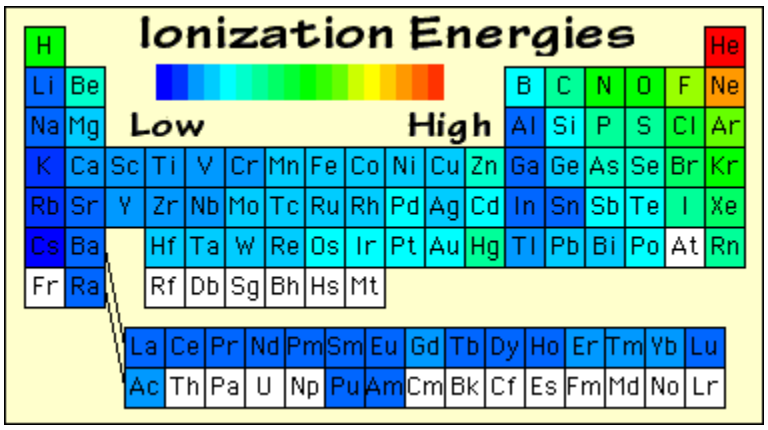


Fig 6.52: Trend in Ionization energy - periodic table showing color-coded first ionization energy trends, with lower values (blue) for alkali metals and higher values (red) for noble gases and halogens

Compare this figure to the earlier figure of Atomic Radii and note that in general, small size means large ionization energy. This trend is easy to understand: small atoms have few electrons that are close to the nucleus. The closer an electron is to a nucleus, the more energy it takes to remove that electron from the atom.

Now look at the trends going across any one row of the Periodic Table: ionization energies increase. For example, the He ionization energy is greater than the H ionization energy. Both have electrons in the 1s orbital, but the increased nuclear charge of He pulls its two 1s electrons closer to the nucleus, and thus more energy is needed to remove either one of them than is needed for H with only a single nuclear proton.

Finally, we focus on the electron affinity. This is the energy required to remove the outermost electron from an atom that has one extra electron stuck to it:

$$\mathbf{A^{-} \rightarrow A + e^{-}}$$

In other words, the electron affinity is the ionization energy of the singly charged atomic anion. The trends in electron affinities are shown below.

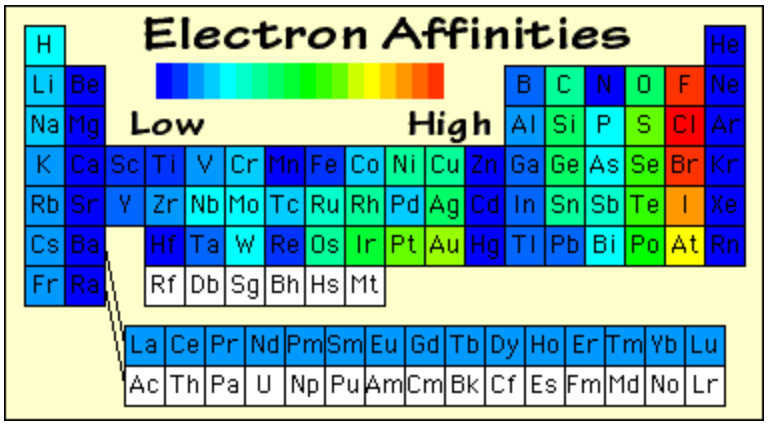


Fig 6.53: Trend in Electron Affinities - periodic table showing color-coded electron affinity trends, with lowest values (blue) for noble gases and alkaline earth metals, and highest values (red) for halogens

Note first the elements that fall in the low end of the range. For these elements, the electron affinity is either zero or very close to zero, which means that these elements do not form stable anions. Those atoms that are spherical because they have closed shells or subshells also have zero or nearly zero electron affinities. Likewise, those that are spherical because they have half-filled shells or subshells also have zero or very small electron affinities.

But for the halogens, F through At, the electron affinity is quite high. These elements are just one electron away from a close shell configuration, and the extra electron can be held by the attractive force of the atom's nucleus. Note as well that Cu, Ag, and Au, which are only one electron away from a closed d subshell, also have high electron affinities.

Reference: General Chemistry, Atomic and Periodic Properties, Trustees of Dartmouth College, 2002.

Reference: https://www.youtube.com/watch?v=A3dTn2at0Hw

Reference: https://www.youtube.com/watch?v=K0YokTyEAMg

Reference: https://www.youtube.com/watch?v=By-n-hPJuDo

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 _____

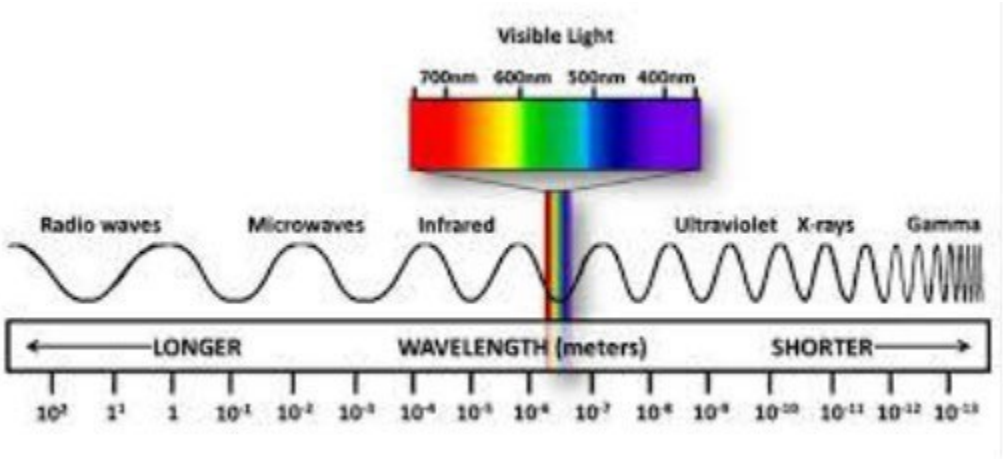


Figure: Electromagnetic Spectrum diagram showing wavelength scale from radio waves to gamma rays with visible light spectrum highlighted

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?

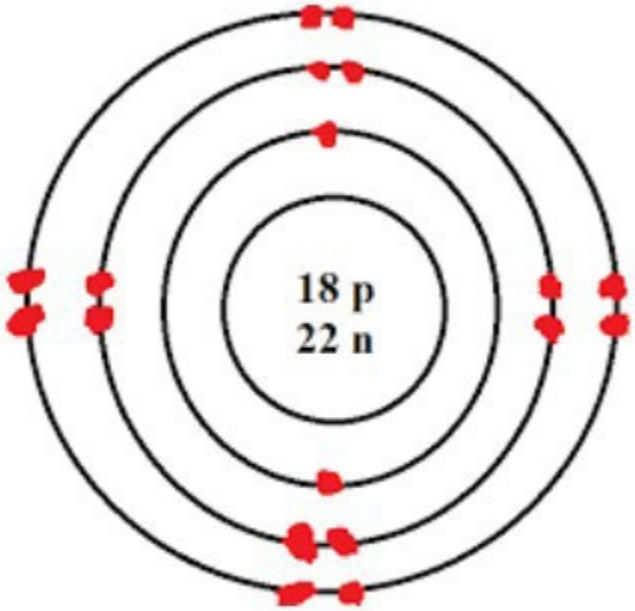


Figure for Q7: Bohr model of an atom with 18 protons and 22 neutrons in the nucleus, surrounded by three electron shells containing 2, 8, and 8 electrons respectively

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 _____

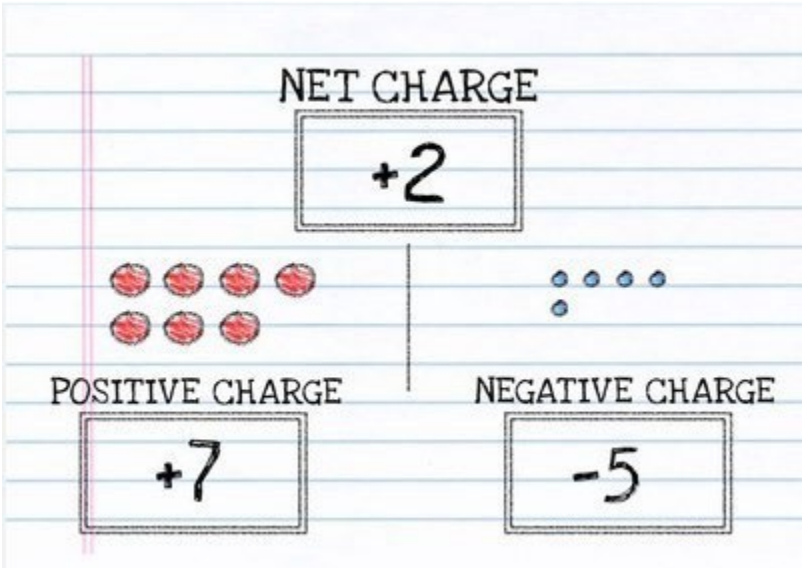


Figure for Q8: Diagram showing an ion with 7 protons and 5 electrons, demonstrating a net positive charge of +2

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 _____

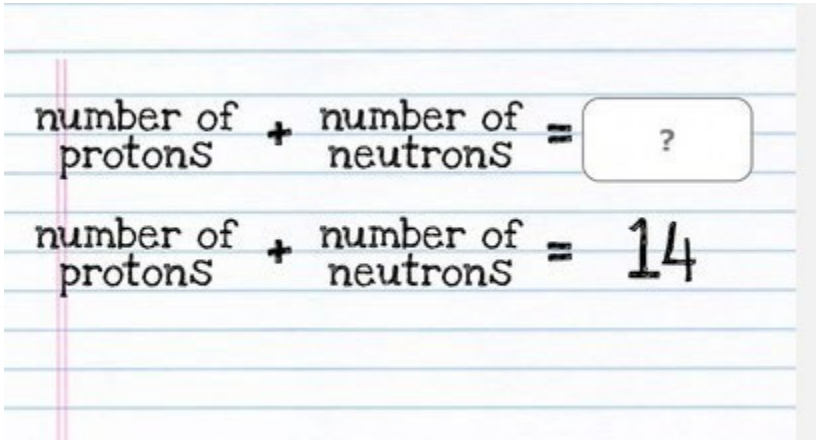


Figure for Q9: Table showing the formula for mass number: protons + neutrons = mass number, with an example result of 14

A- atomic number B- mass number C- isotope number D- average weight

Answer: B

Q 10: What is the mass number of this atom?

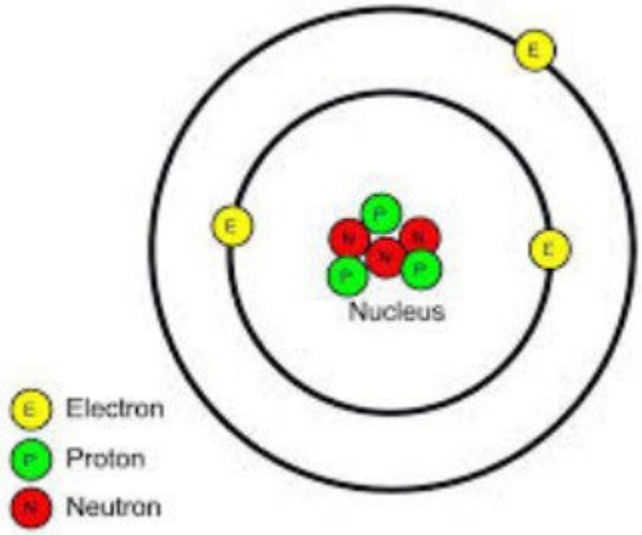


Figure for Q10: Bohr model of Lithium showing 3 protons and 4 neutrons in the nucleus with 3 electrons in two orbital shells, giving a mass number of 7

A- 1 B- 3 C- 4 D- 7

Answer: D

Q 11: What element is represented in this Bohr Model?

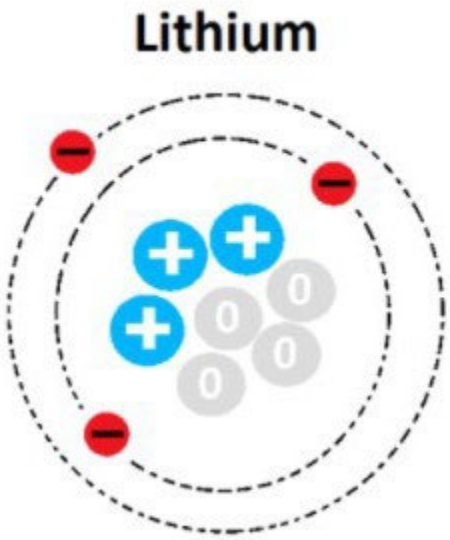


Figure for Q11: Bohr model showing 3 protons and 4 neutrons in the nucleus with 2 electrons in the inner shell and 1 electron in the outer shell, representing Lithium

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- $1s^2 2s^2 2p^6\ 3s^2$, $3p^6\ 4s^2\ 3d^{10}\ 4p^5$ 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?

Figure for Q24: Periodic table element card for Silicon (Si) with atomic number 14 and atomic mass 28.0855

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: Radio waves are about 1m long. Calculate their frequency.

$$\frac{c}{\lambda} = \frac{\nu\lambda}{\lambda} \Rightarrow \frac{c}{\lambda} = \nu = \frac{3.0\times10^{8}\ {}^{m}/_{s}}{1\ m} = 3.0\times10^{8}\ Hz$$

Figure: Solution to Q31 showing calculation of frequency for 1-meter radio waves using v = c/lambda = 3.0 x 10^8 Hz

Q 32: A hypothetical wave has 6.6 J of energy. What is its hypothetical, approximate frequency?

$$E = h\nu \quad \nu = \frac{E}{h} \qquad \nu = \frac{6.6J}{6.626\times10^{-34}\ J{\cdot}s} = 0.9\times10^{34}\ Hz$$

Figure: Solution to Q32 showing calculation of frequency from energy E=6.6 J using v = E/h = 0.9 x 10^34 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

$$green = \frac{hc}{\lambda} = \frac{(6.626\times10^{-34}J\cdot s)(3.0\times10^{8}\ {}^{m}/_{s})}{(500\times10^{-9}m)} = 4.0\times10^{-19}\ J\ for\ green$$

$$red = E = h\nu = \frac{hc}{\lambda} = \frac{(6.626\times10^{-34}J\cdot s)(3.0\times10^{8}\ {}^{m}/_{s})}{(700\times10^{-9}m)} = 0.028\times10^{-17}J = 2.8\times10^{-19}\ J\ for\ red$$

note: $E_{green} > E_{red}$

Figure: Solution to Q33 showing calculation of frequency (1.2 x 10^15 Hz) and wavelength (2.5 x 10^-7 m) for a 5.1 eV photon

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.)

$$\nu = \frac{E}{h} = \frac{(5.1eV)\left(1.60\times10^{-19}\ {}^{J}/_{eV}\right)}{(6.626\times10^{-34}J\cdot s)} = 1.2\times\times10^{15}\ Hz$$

$$\lambda = \frac{c}{\nu} = \frac{(3.0\times10^{8}\ {}^{m}/_{s})}{(1.2\times10^{15}\ {}^{1}/_{s})} = 2.5\times10^{-7}\ m$$

Figure: Solution to Q34 showing energy calculations for green (4.0 x 10^-19 J) and red (2.8 x 10^-19 J) laser photons, confirming green light carries more energy per photon

CHAPTER 7: Chemical Bonding and Molecular Geometry

7.1 Chemical Bonding
7.2 Ionic Bonding
7.3 Octet Rule, Covalent Bonding & Electronegativity
7.4 Lewis Symbols and Structures
7.5 Formal Charges and Resonance
7.6 Strengths of Ionic and Covalent Bonds
7.7 Molecular Structure and Polarity

7.1 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."

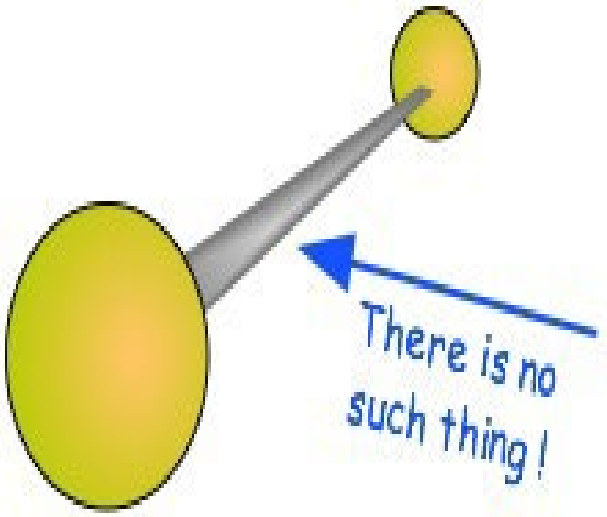


Figure 7.1 Chemical Bond

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 C60 resides in the C60H28 "buckybowl". There are no traditional "chemical bonds" between the ball and the tube.

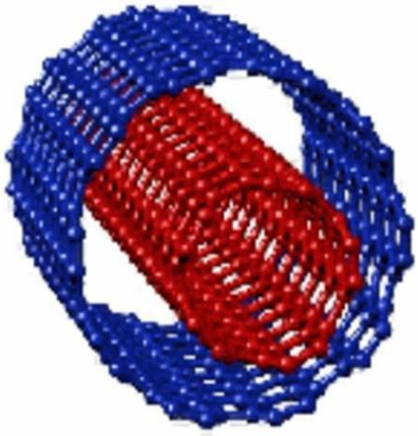


Figure 7.2 Carbon nanotube

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, CH4, 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 He2, 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 C2H6O. The structural formulas reveal the very different connectivity of these two molecules whose physical and chemical properties are quite different:

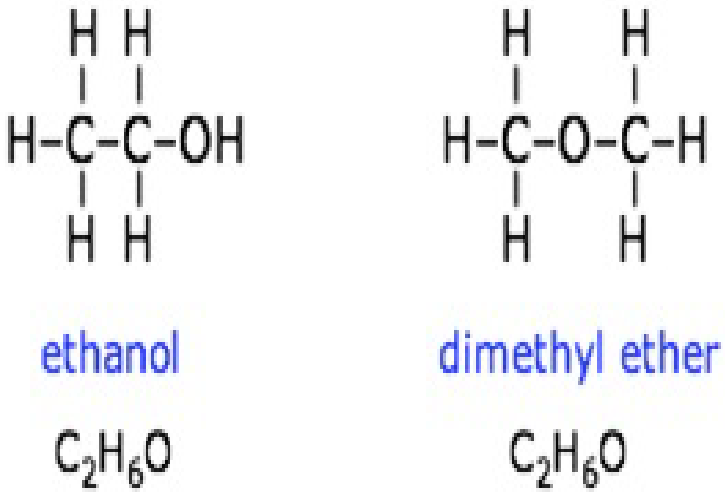


Figure 7.3 Ethanol and Dimethyl ether structure

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) → CH4

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 KrF2 is so weakly bound that it decomposes even at 0°C, and the structure He2 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 CH3, methyl, is a good example: it can be formed by electrical discharge in gaseous CH4, but it is so reactive that it combines with almost any molecule it strikes (even another CH3) 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.

7.2 Ionic Bonding

When a metal loses its valence electrons, it becomes a positively charged ion called a cation, while the nonmetal accepts these valence electrons and becomes negatively charged, called an anion. There are electrostatic forces causing the cation and anion to be attracted to each other.

Reference: https://www.youtube.com/watch?v=zpaHPXVR8WU
Reference: https://www.youtube.com/watch?v=hiyTfhjeF_U

Forming an Ion

An example of ion formation is the sodium cation. Neutral sodium Na has 11 protons and 11 electrons. When Na loses an electron, the number of protons does not change but the number of electrons decreases by one. The number of electrons becomes 10 and therefore Na will have one positive charge: Na^{+}.

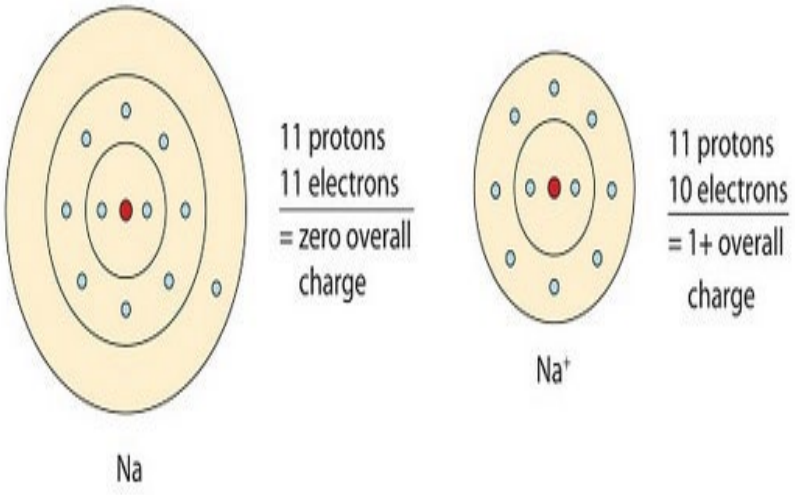


Figure 7.19 Formation of Na^+ Ion

Ref: commons.wikimedia.org/

The nonmetal chlorine Cl has 17 protons and 17 electrons. When the chlorine atom gains an extra electron, the number of protons does not change but the number of electrons increases by one. A negative ion of chlorine called an anion is formed as shown below:

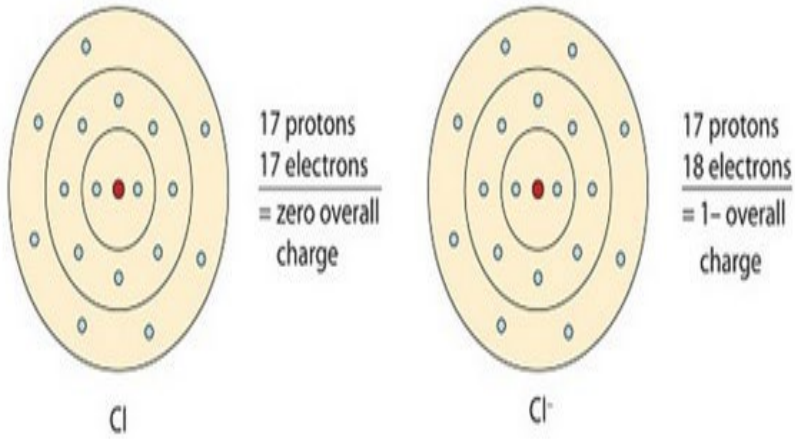


Figure 7.20 Formation of Cl^- Ion

Reference: https://youtu.be/r23klS9fzdc

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 by naming the metal cation, for example Ba^{2+} (barium cation).
2. Then follow the name of the metal cation with the name of the nonmetal anion.
3. Discard the "-ine" ending of the nonmetal chlorine and replace it with the "-ide" ending.

The name of the ionic compound BaCl2 is called barium chloride.

Determining the Formula of Ionic Compound with Metal Having One Positive Charge from a Name

Example: Barium chloride

4. Barium is found in Group 2A. According to the periodic table, barium has +2 positive charges: Ba^{2+}.
5. Chlorine anion called chloride has one negative charge: Cl^{-}.
6. Swap the values of the charges of the ions (not the signs): Ba cation takes value 1 as subscript and chloride takes value 2 as subscript: Ba_1Cl_2 which is written as $BaCl_2$. The value of 1 is understood but not written.

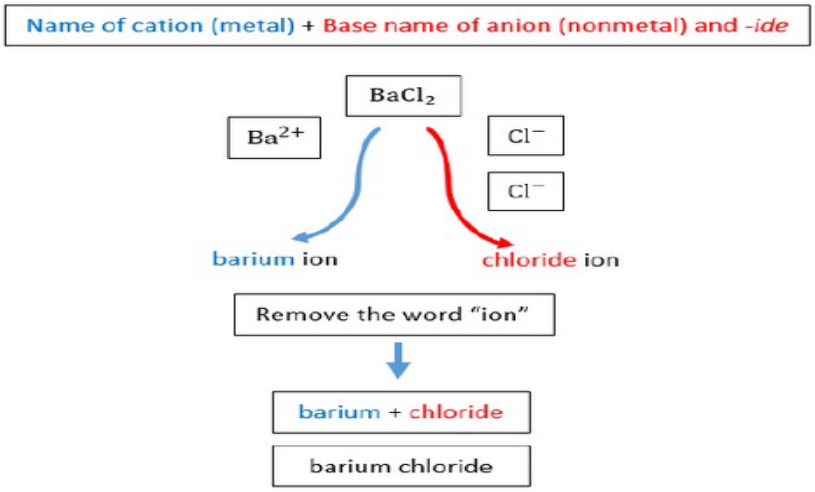


Figure 7.21 Nomenclature of Ionic Compound

Ref: commons.wikimedia.org/

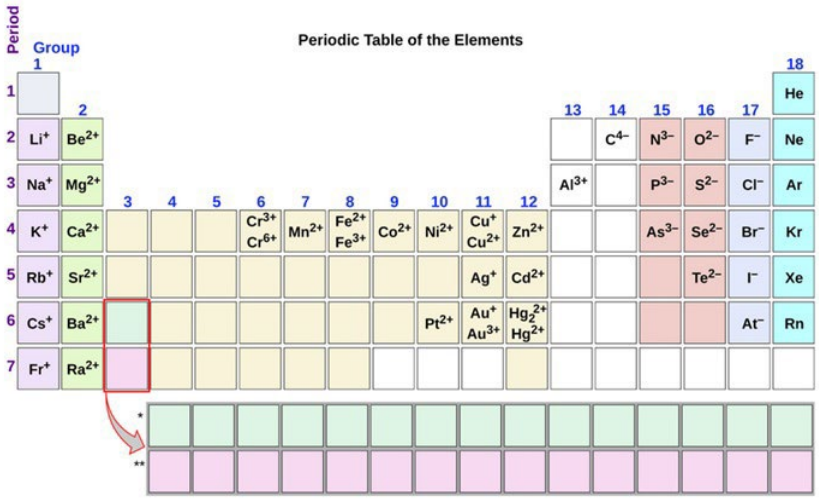


Figure 7.21b Charge of Ions from Periodic Table

Reference: https://chem.libretexts.org/Courses/Oregon_Tech_PortlandMetro_Campus

Determining the Formula of Ionic Compound with Metal Having Multiple Positive Charges from a Name and Determining Its Name from the Formula

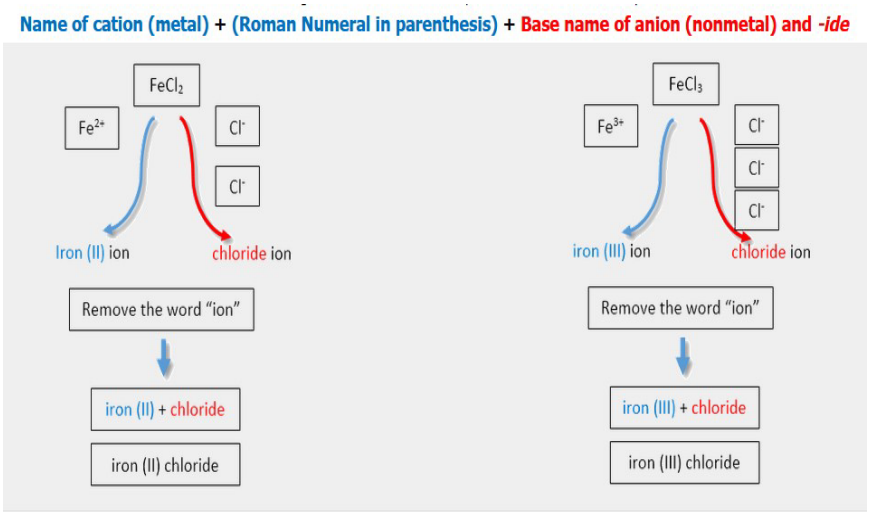


Figure 7.22 Nomenclature of Ionic Compound (Transition Metal)

Reference: https://chem.libretexts.org/Courses/College_of_Marin/CHEM_114

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 Roman numerals 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_1Cl_3. The ionic compound will be $FeCl_3$. The value of 1 is understood but is not written. $FeCl_3$ is named as Iron (III) Chloride. Note that the

subscript of 3 came from Fe and hence Fe has to have 3 positive charges. The same approach can be used to 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

7.3a 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 (D2O), 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 G.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. 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 CH4. 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.

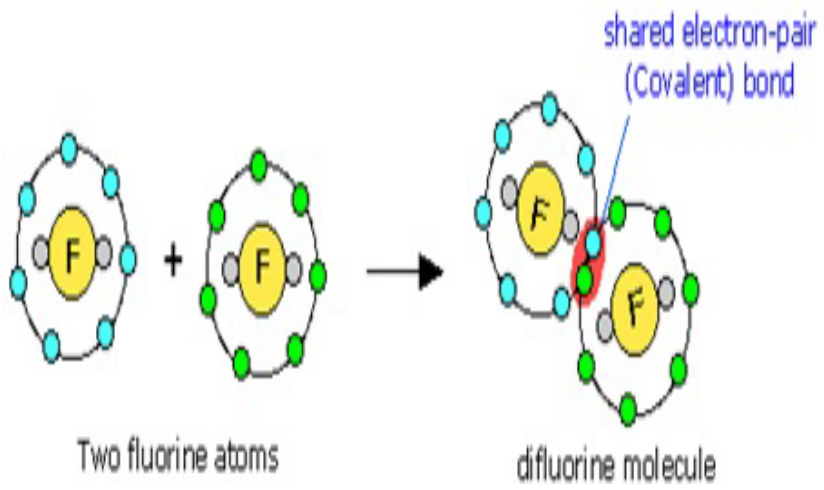


Figure 7.28 Formation of F_2 molecule

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 2s orbital of lithium and the 1s 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.

Reference: https://www.youtube.com/watch?v=6Ecr7m-0E0E

7.3b Covalent Bonding

Covalent bonding is made from the combination of two or more nonmetals. Nonmetals in covalent bonding do not transfer electrons (valence electrons); instead they share them to form single, double, or even triple bonds.

An example is given below depicting the covalent bonding formation of PCl3 between phosphorous and chlorine atoms. The covalent single bonds are designated with shared valence electrons.

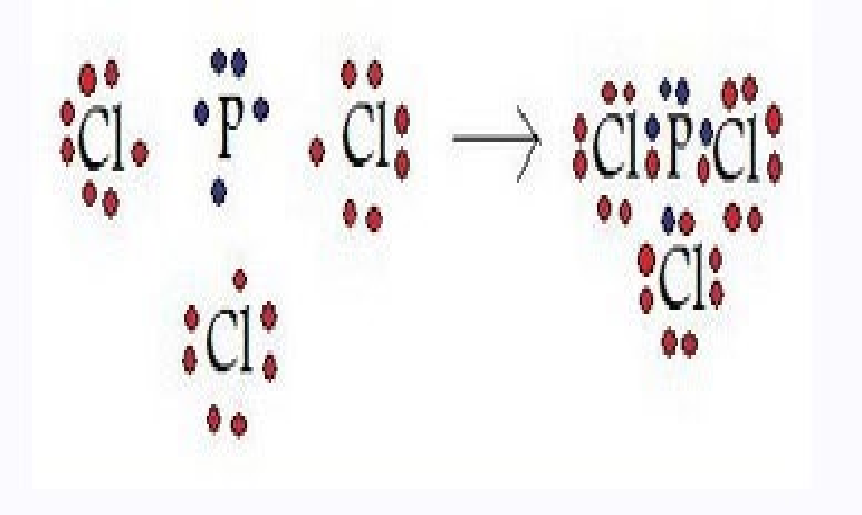


Figure 7.23 Covalent Bond Formation

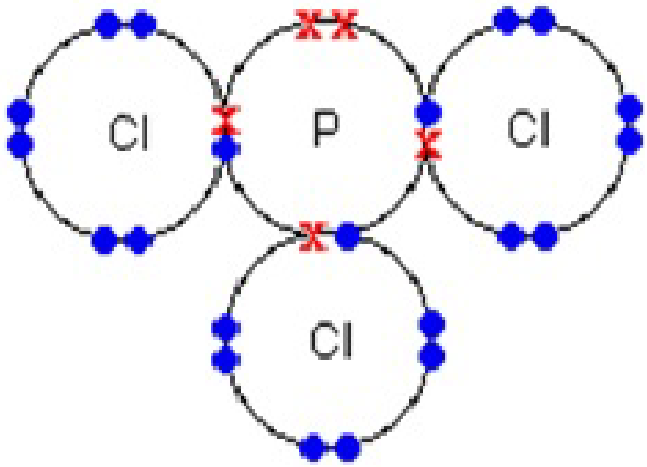


Figure 7.24 Sharing of Electrons in Covalent Bond Formation

There are three single bonds and one set of lone pair in PCl3.

Reference: https://chem.libretexts.org/

Another example: Methane CH4. Hydrogen is in Group 1A, and it has one valence electron. Carbon is in Group 4A, and therefore it has four valence electrons. Methane has four single covalent bonds.

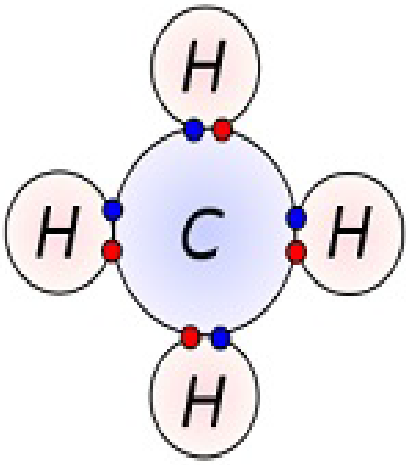


Figure 7.25 Sharing of Electrons in Methane

Reference: https://chem.libretexts.org/

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.

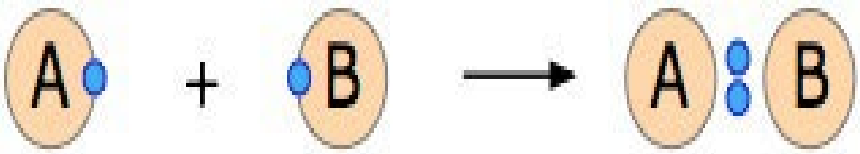


Figure 7.29 Formation of Covalent Bond

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.

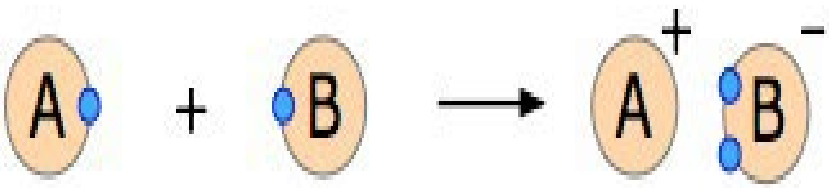


Figure 7.30 Formation of Ion Pair

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.

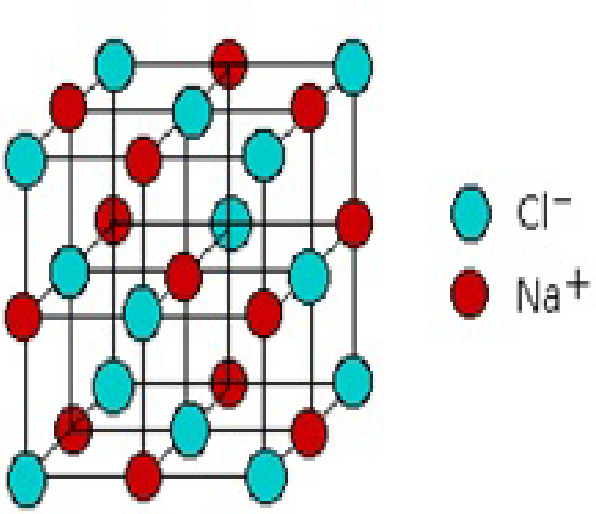


Figure 7.31 Formation of Ionic Crystal

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!

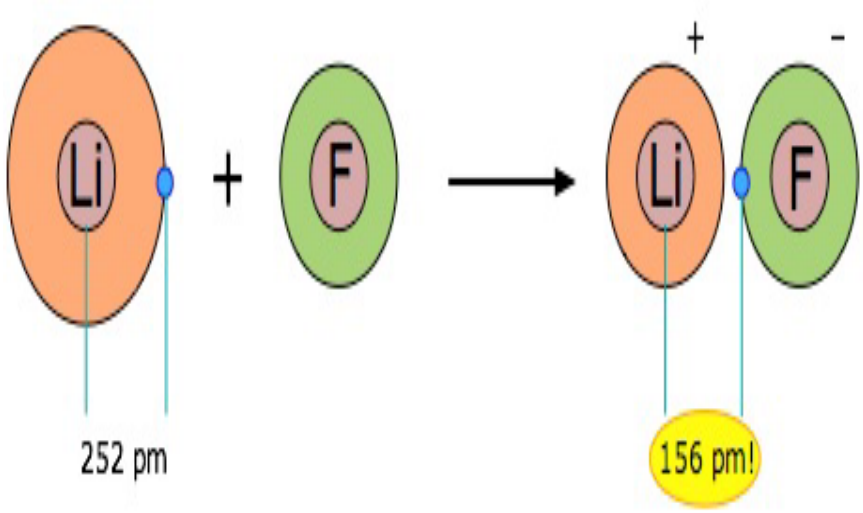


Figure 7.32 Formation of Ionic Bond

So the answer to the above question is both yes and no: yes, the electron that was in the 2s orbital of Li is now within the grasp of a fluorine 2p 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 Cl2, O2, and H2, 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.

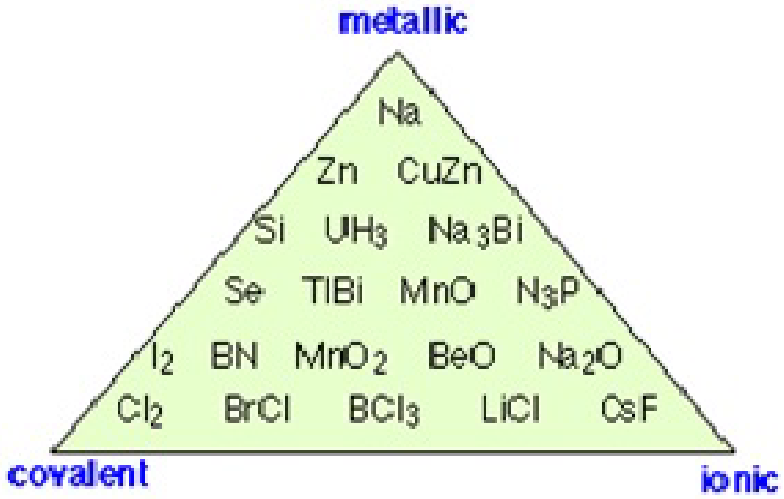


Figure 7.33 Metallic, Covalent and Ionic Compounds of Different Elements

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 the "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.

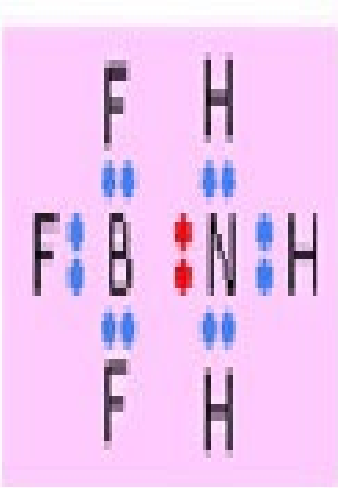


Figure 7.34 Electronic Arrangement in Donor-Acceptor Bond

This is the case, for example, with boron trifluoride and ammonia. In BF3, one of the 2p orbitals is unoccupied and can accommodate the lone pair on the nitrogen atom of ammonia. The electron acceptor, BF3, acts as a Lewis acid here, and NH3 is the Lewis base.

Bonds of this type (sometimes known as coordinate covalent or dative bonds) tend to be rather weak (usually 50-200 kJ/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

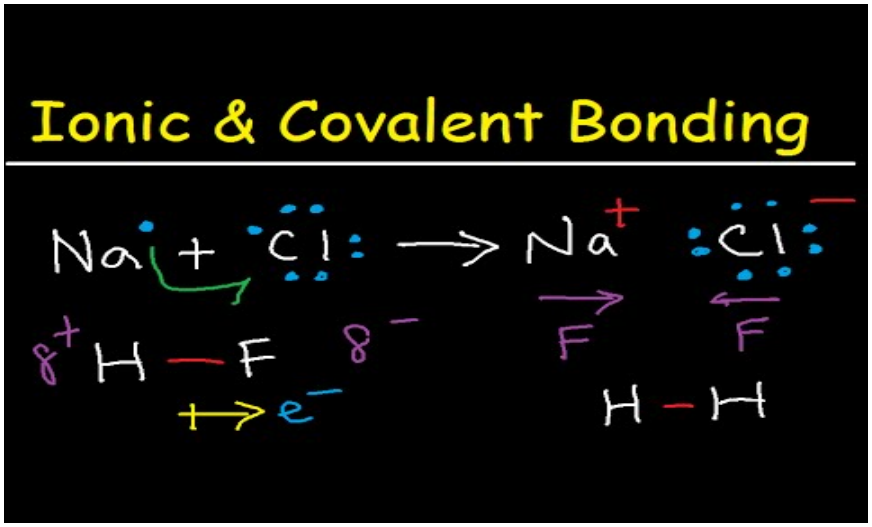
Covalent bonding requires a very discrete and specific orientation to establish the overlap between the bonding orbitals. The overlap can form sigma (single) bonds or pi (double and triple) bonds. The sigma bonds have very strong interaction due to the fact that shared electrons are moving freely along the axis and the overlapping orbitals 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, forming one sigma bond between the two atoms. Double bonds are made when four electrons are shared between the two atoms, forming one sigma bond and one pi bond. Triple bonds occur when six electrons are shared between the two atoms, forming one sigma bond and two pi bonds.

More information on this type of bonding is discussed in the next module (Module 8) Advanced Theories of Bonding.

Reference: https://www.youtube.com/watch?v=ZxWmyZmwXtA
Reference: https://www.youtube.com/watch?v=S_k0kr2eZSQ

Reference video on Covalent Bonds



Reference video on Ionic and Covalent Bonding

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 H2, N2, and CH4.

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 (H2O). 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, H2, 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 PCl3 or PCl5. In both cases, the phosphorus and chlorine atoms are connected by covalent bonds. PCl3 assumes the expected noble gas structure, in which the atoms achieve complete outer electron shells. Yet PCl5 is also stable, so it's important to remember covalent bonds in chemistry don't always abide by the octet rule.

Reference: https://www.youtube.com/watch?v=RK07Bwwxkjg

7.3c 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, 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.

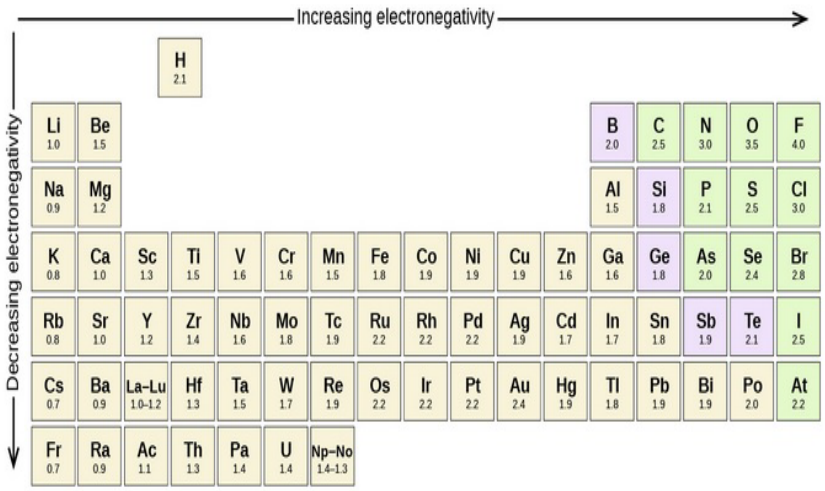


Figure 7.35 Electronegativity Trend on Periodic Table

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 an 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

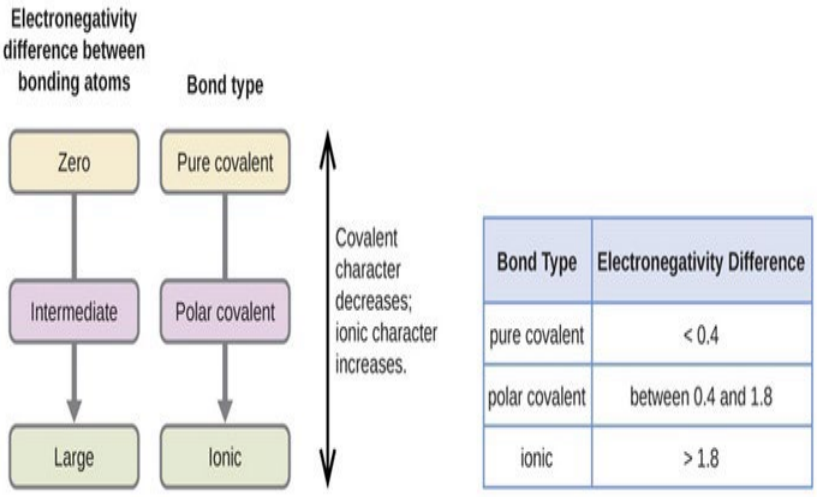
Ionic Compounds vs. Molecular Compounds

A covalent bond that is formed from the same nonmetal atoms will result in a nonpolar covalent bond. The electronegativity difference is zero. A covalent bond that is formed from different nonmetal atoms with different electronegativity will yield a polar covalent bond.

Ionic bonds 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 are dissolved in water.

With the help of the electronegativity difference chart given below, one can determine if the bond is nonpolar covalent, 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/

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 (H2O) 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, C4H10). Properties of ionic and covalent compounds are listed in the following table.

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

Table: Properties of Ionic and Covalent Compounds

The properties listed in the above table are exemplified by sodium chloride (NaCl) and chlorine gas (Cl2). Like other ionic compounds, sodium chloride contains a metal ion (sodium) and a nonmetal ion (chloride), is brittle, and has a high melting temperature. Chlorine gas is similar to other covalent compounds in that it is a nonmetal and has a very low melting temperature.

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

Figure 7.37 (A) Sodium Chloride (NaCl), an Ionic Compound and (B) Chlorine Gas (Cl_2), a Covalent Compound

Reference: Image courtesy of Edal Anton Lefterov from Wikipedia
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.

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 of 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.

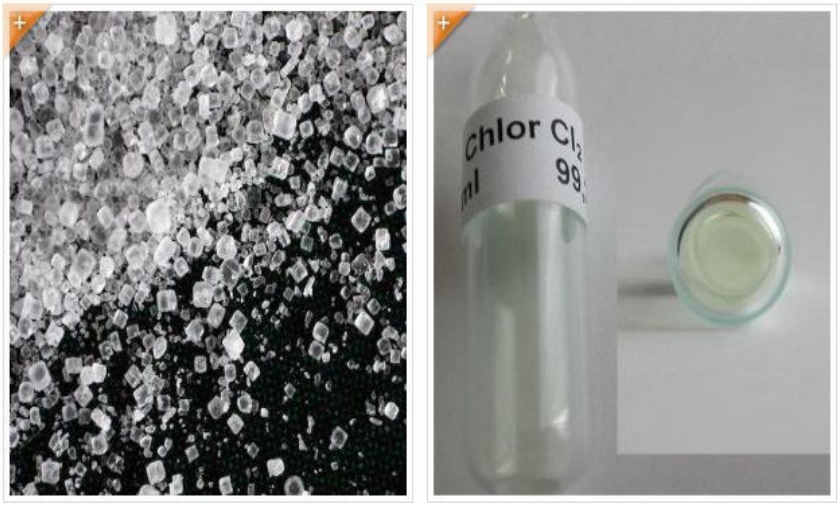


Figure 7.38 Electronegativity in Main Group Elements

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:

$$\mu = (1.6022 \times 10^{-19}\ \text{C}) \times (10^{-10}\ \text{m}) = 1.6 \times 10^{-29}\ \text{C-m} = 4.8\ \text{D}$$

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.

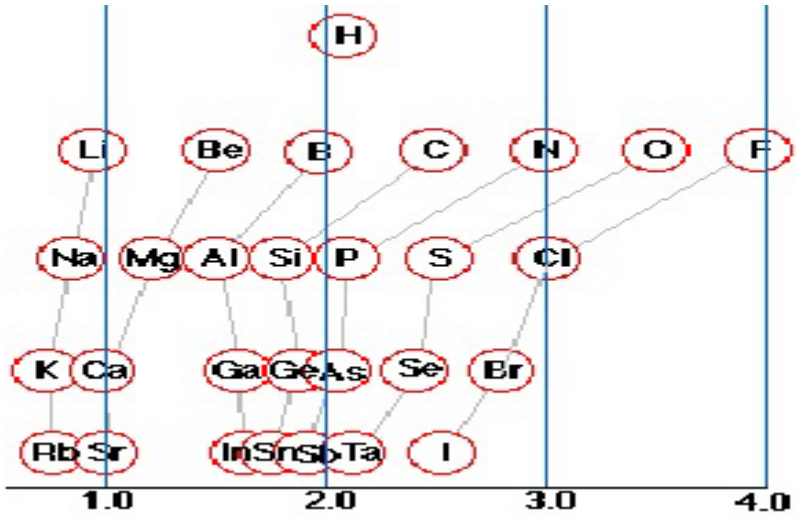


Figure 7.39 Peter Debye

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.

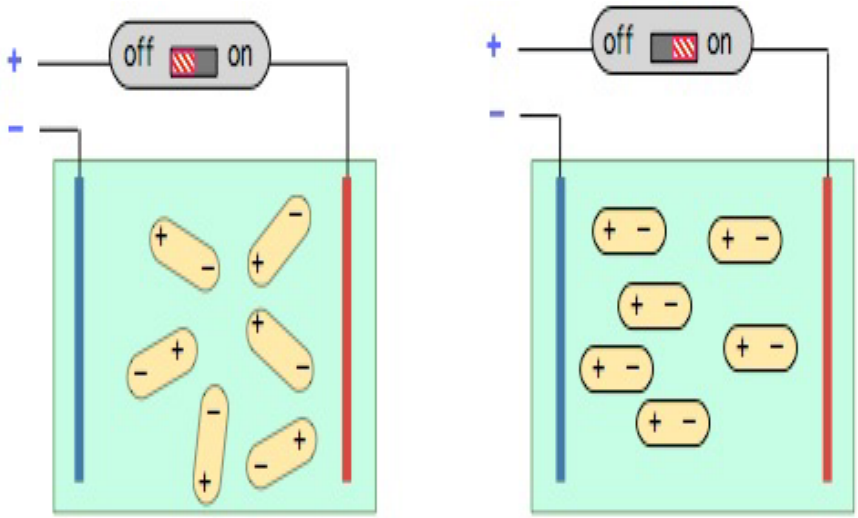


Figure 7.41 Polarity of HF Molecule

Problem Example 1
Estimate the percent ionic character of the bond in hydrogen fluoride from the experimental data shown at the right.

Solution:
6.37E-30 C-m / 92E-12 m = 6.92 E-20 C (charge displaced)
6.92 E-20 C / 1.60E-19 C/electron = 0.43 (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:

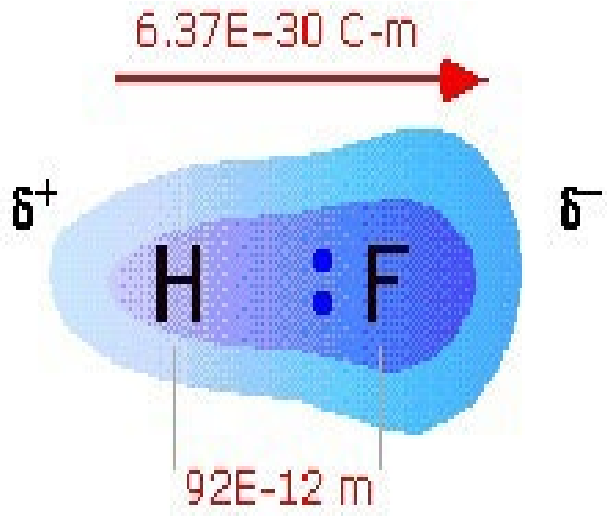


Figure 7.42 Determination of Dipole Moment

The zero dipole moment of CO2 is one of the simplest experimental methods of demonstrating the linear shape of this molecule.

H2O, 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.

$$\frac{6.37\text{E-}30\ \text{C-m}}{92\text{E-}12\ \text{m}} = 6.92\ \text{E-}20\ \text{C}\ \text{(charge displaced)}$$

$$\frac{6.92\ \text{E-}20\ \text{C}}{1.60\text{E-}19\ \text{C/electron}} = 0.43\ \text{(ionic character of bond)}$$

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.

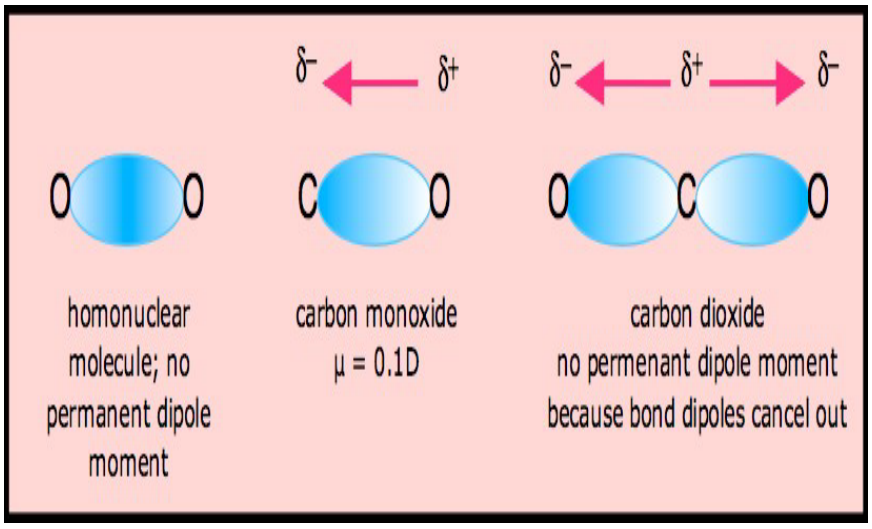


Figure 7.44 Electron Density Map in Ethanol

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 for methanol CH3OH, 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:

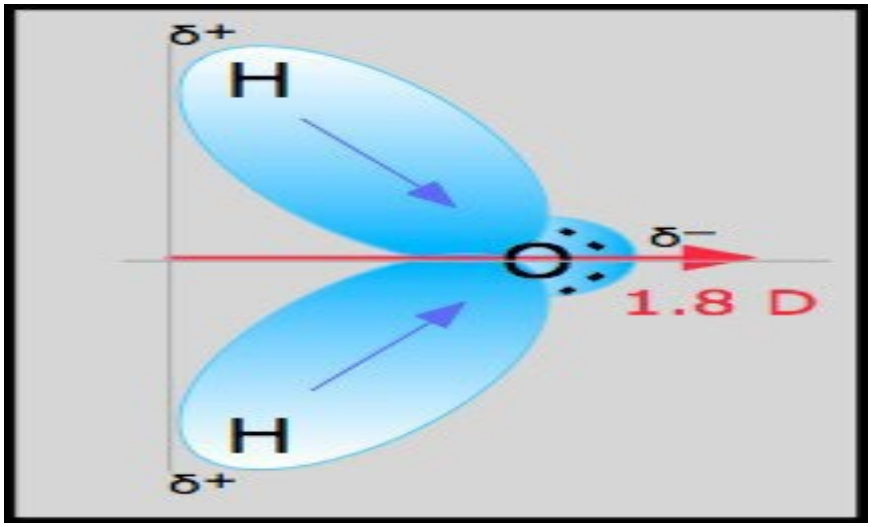


Figure 7.45 Dipole Moments of Different Molecules

(Bear in mind that all four positions around the carbon atom are equivalent in this tetrahedral molecule, so there are only four chloromethane compounds.)

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.

7.4 Lewis Dot and Structures

What is Lewis Electron Dot Structure?

Lewis Dot Structure is a simple presentation of the overlapping orbitals forming sigma and pi bonds. 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.

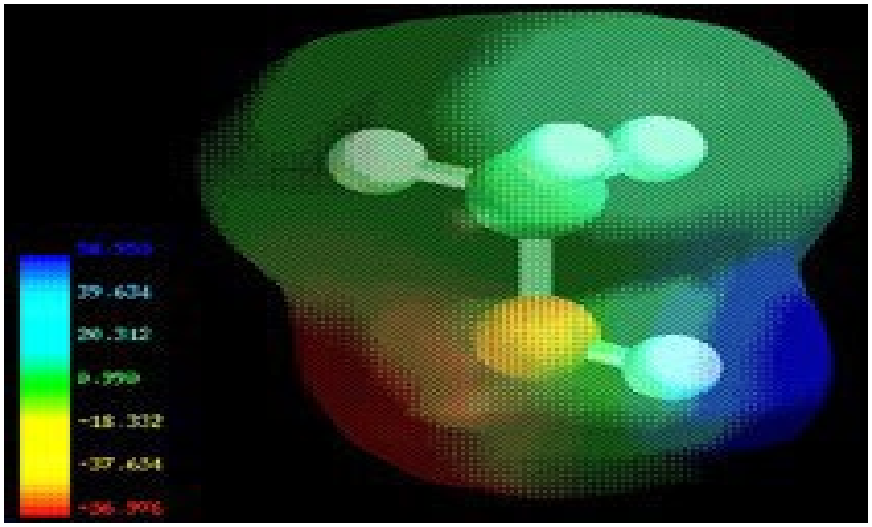


Figure 7.46 Lewis Symbol of Atoms

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:

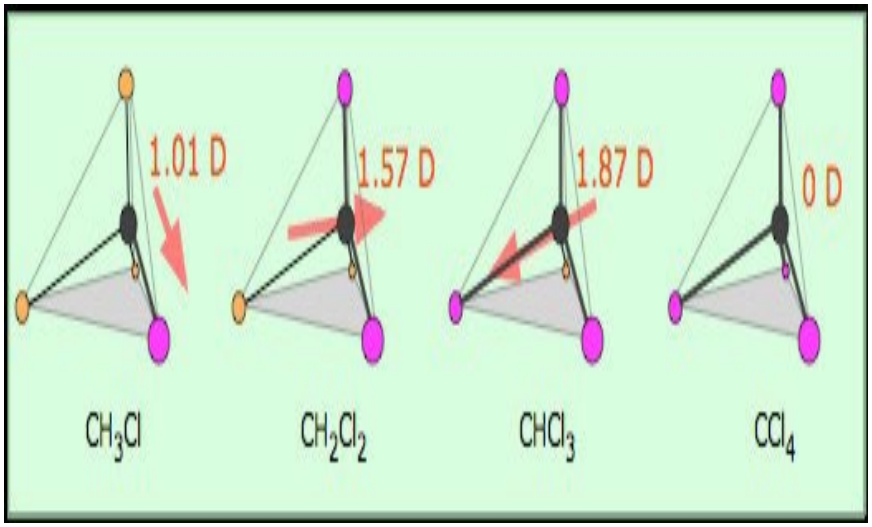


Figure 7.47 Lewis Symbol of Ca

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.

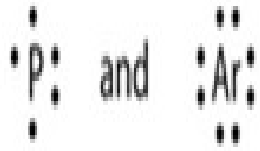


Table showing Lewis Symbols for Third Period Elements with Electronic Configurations

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:

7. First, the total number of valence electrons present in the molecule is calculated by adding the individual valencies of each atom.
8. If the molecule is an anion, extra electrons (number of electrons added = the magnitude of negative charge) are added to the Lewis dot structure.
9. When cationic molecules are considered, electrons are subtracted from the total count in order to make up for the positive charge.
10. The least electronegative atom is made the central atom of the molecule or ion.
11. The atoms are now connected via single bonds.
12. 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.
13. 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.
14. 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.

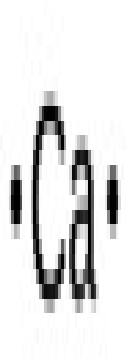


Figure 7.48 Lewis Structure of Covalent Molecules

Ref: commons.wikimedia.org/

After reviewing all these rules, the Lewis Dot Structure of $NO3^-$ will be written as shown below:

Atoms	Electronic Configuration	Lewis Symbol
sodium	$[Ne]3s^1$	Na·
magnesium	$[Ne]3s^2$	·Mg·
aluminum	$[Ne]3s^23p^1$	·Al·
silicon	$[Ne]3s^23p^2$	·Si·
phosphorus	$[Ne]3s^23p^3$	·P·
sulfur	$[Ne]3s^23p^4$	:S·
chlorine	$[Ne]3s^23p^5$	:Cl·
argon	$[Ne]3s^23p^6$	:Ar:

Lewis Dot Structure of Nitrate Ion (NO_3^-) showing 24 total valence electrons

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.
Reference: https://www.youtube.com/watch?v=3nAfsS56yNc

1. Lewis Structure of CO2

- 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.

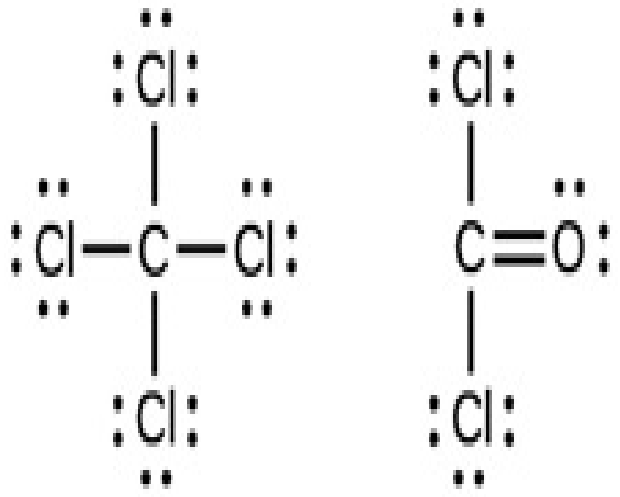


Figure 7.49 Lewis Dot Structure of CO_2

Ref: commons.wikimedia.org/

2. Lewis Structure of O2

- 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 O2 molecule, the atoms form a double bond resulting in the following Lewis electron dot structure.

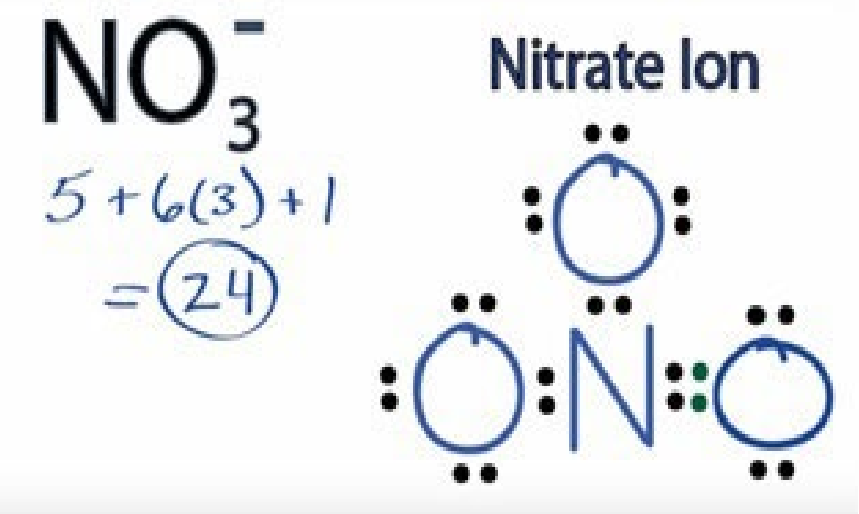


Figure 7.50 Lewis Dot Structure of O_2

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.

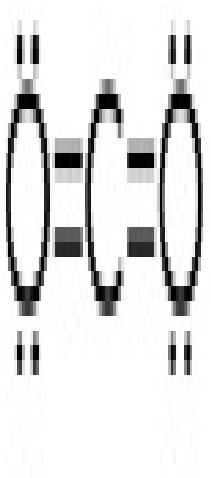


Figure 7.51 Lewis Dot Structure of CO

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.

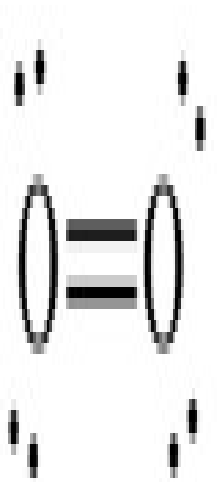


Figure 7.52 The Octet Rule demonstrated in CO_2

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 CO2 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 are carbon in CCl4 (carbon tetrachloride) and silicon in SiH4 (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:

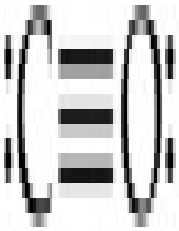


Figure 7.53 Lewis Dot Structures of Carbon Tetrachloride and Silane

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 a 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

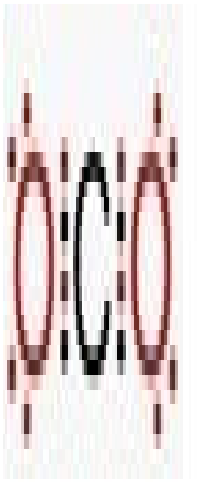


Figure 7.54 Double Bond Examples in Formaldehyde and Ethylene

Ref: commons.wikimedia.org

A triple bond

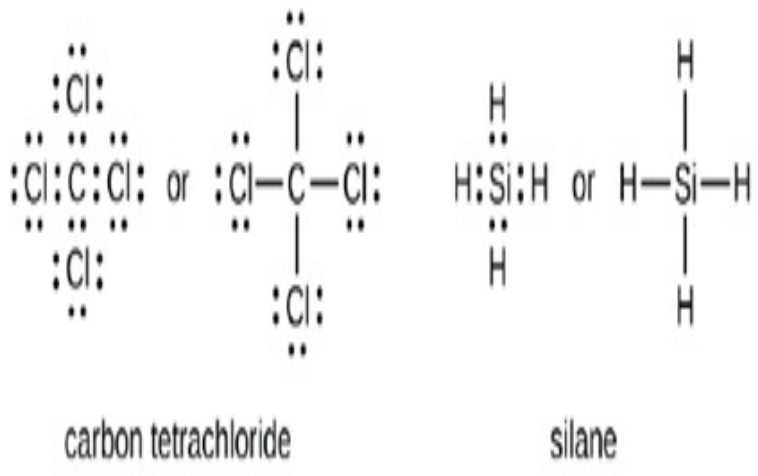


Figure 7.55 Triple Bond Examples in Carbon Monoxide and Cyanide Ion

Ref: commons.wikimedia.org

Reference: https://www.youtube.com/watch?v=aG3di-2Pxmo
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. The 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:

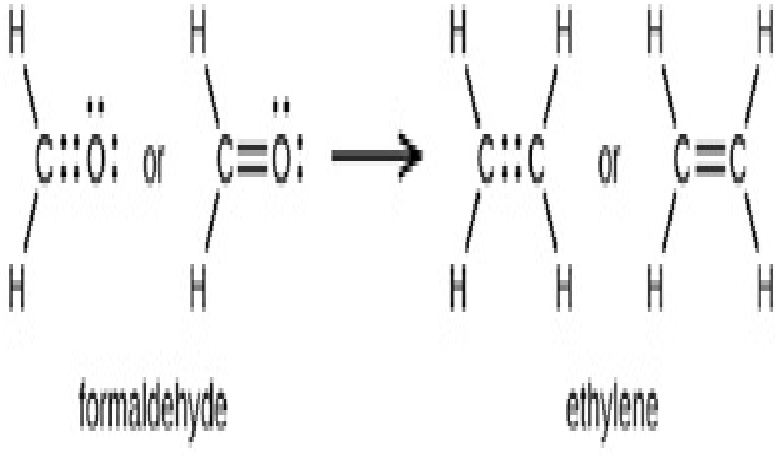


Figure 7.56 Satisfying Octet Rule using Lewis Dot Structures

Ref: commons.wikimedia.org

For more complicated molecules and molecular ions, it is helpful to follow the step-by-step procedure outlined here:

15. 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.
16. 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).
17. Distribute the remaining electrons as lone pairs on the terminal atoms (except hydrogen), completing an octet around each atom.
18. Place all remaining electrons on the central atom.
19. 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

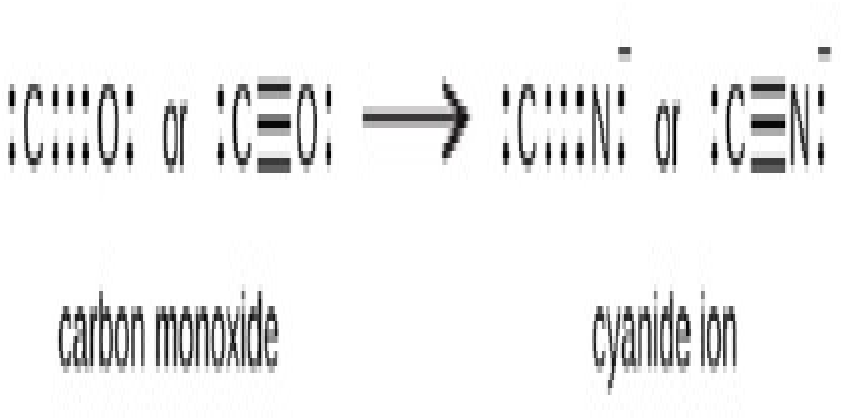


Figure 7.57 Bonding and Nonbonding Electrons in Ammonia (NH_3) and Water (H_2O)

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.

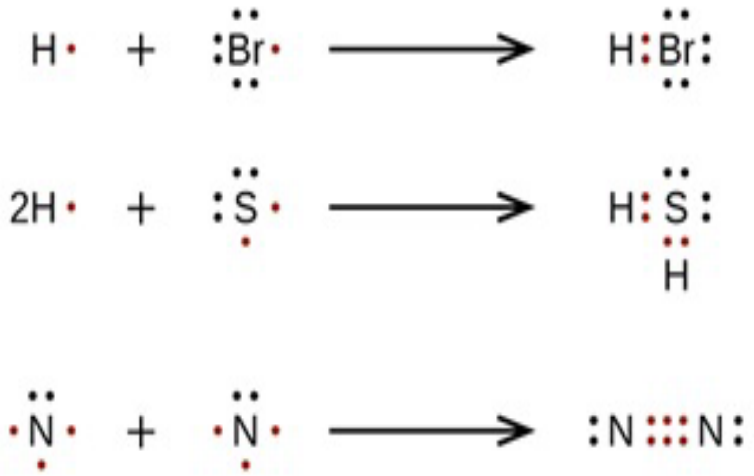


Figure 7.58 Lewis Dot Structures of PCl_5 and SF_6 Showing Expanded Octets

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 4s 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, 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 bond.

Examples of these multivalent, also called hypervalent, molecules are given below:

- Phosphorus pentachloride (PCl5)
- Sulfur hexafluoride (SF6)
- Chlorine trifluoride (ClF3)
- Triiodide ion ($I3^-$)

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 Cl can bond to more than 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 than the 4s orbitals in general, but in reality the difference between 3d and 4s energies is small and hence the 3d orbitals can accommodate more electrons.

The 3d orbitals do participate in forming the covalent bonding and in this process the octet rule is expanded or violated.

Both phosphorous and sulfur are violating the octet rule:

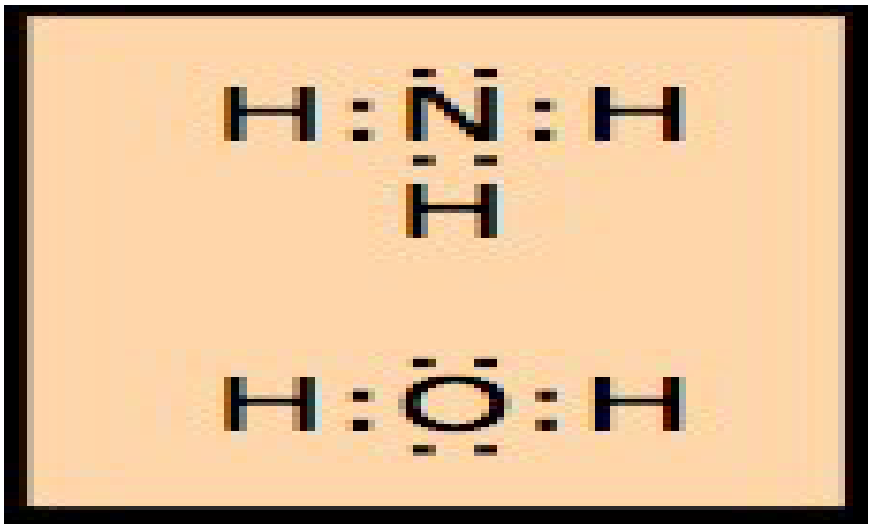


Figure showing PCl_5 (trigonal bipyramidal) and SF_6 (octahedral) as examples of expanded octet molecules

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 Picometers (10^{-12}).

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.

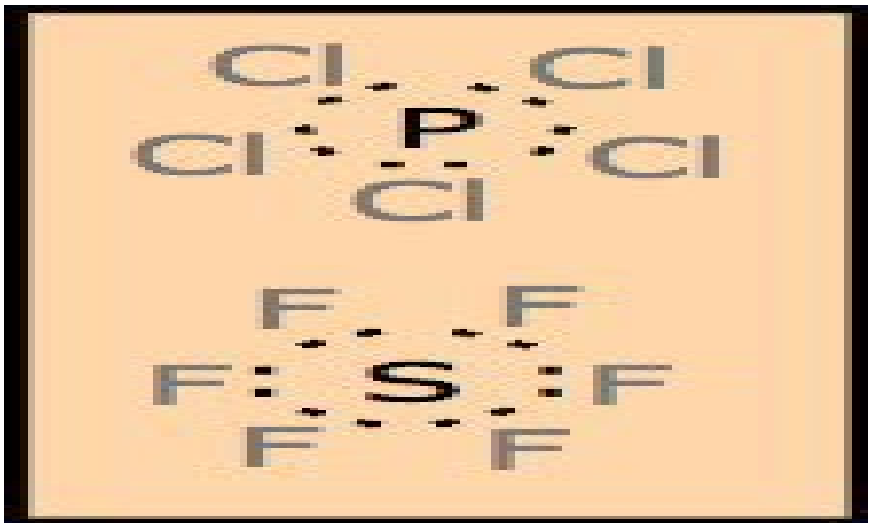


Figure 7.59 Multiple Bonds Formation in CO, Acetylene, N_2, and Cyanide Ion

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!

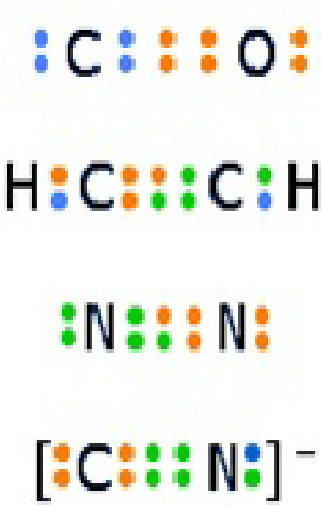


Table: Examples of High-Order Bonds Beyond Triple Bonds

Adding to the fun, a 2006 article presented evidence that the carbon atom in C(PPh3)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.

PCl5: Phosphorous carries 10 valence electrons combined SF6: Sulfur carries 12 valence electrons combined

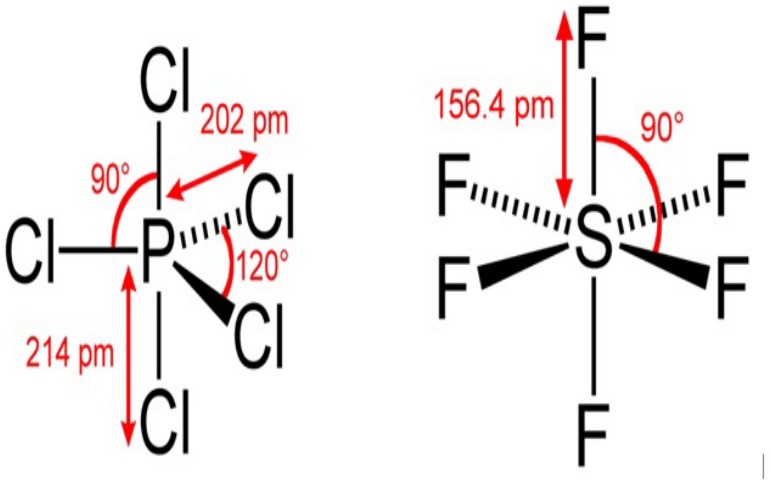


Figure: PCl_5 trigonal bipyramidal and SF_6 octahedral structures showing expanded octets

7.5a Formal Charge

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 always 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:. 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:

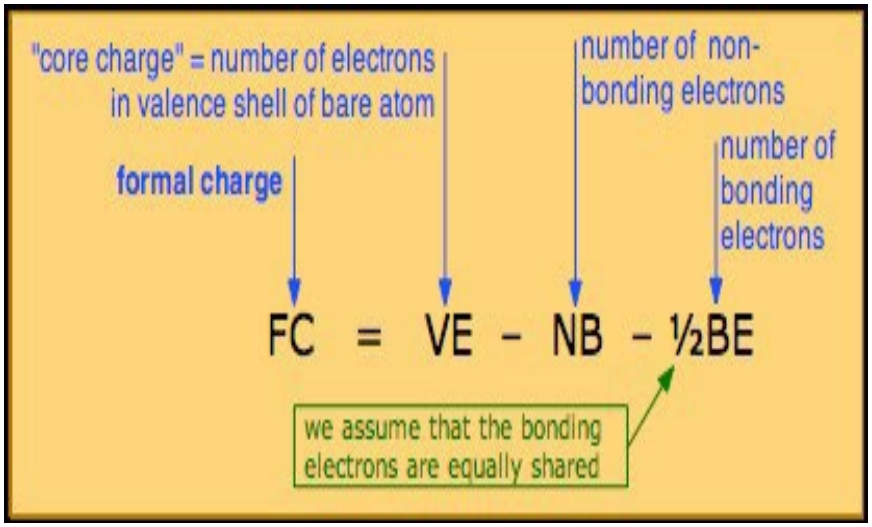


Figure 7.61 Formal Charge Calculation Formula (FC = VE - NB - ½BE)

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 − ½ #bonding electrons

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.

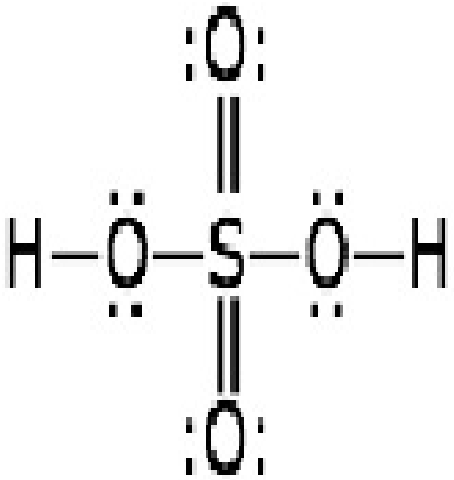


Figure 7.62 Sulfuric Acid H_2SO_4 Lewis Structure

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 bookkeeping 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.

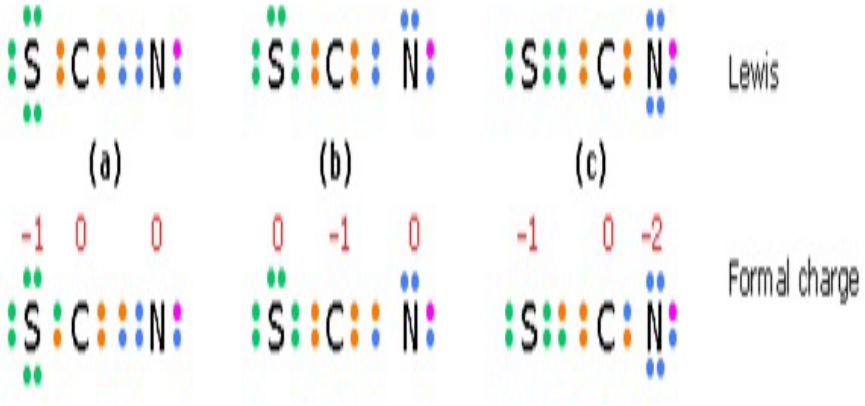


Figure 7.63 Formal Charge Analysis of Thiocyanate Ion (SCN^-) Resonance Structures

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 $NH4^+$, 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 exchanged 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.

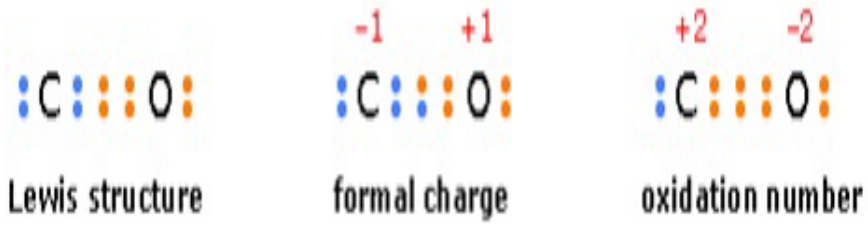


Figure 7.64 Formal Charge vs. Oxidation Number in Carbon Monoxide

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 (NH3) whose Lewis structure is as follows:

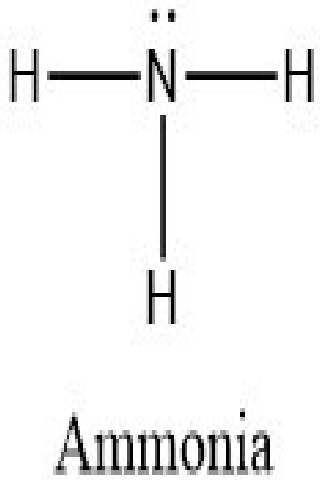


Figure 7.65 Ammonia NH_3 Lewis Structure

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^-) – (½ × 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^-) – (½ × 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 NH3 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

7.5b 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 $NO3^-$. We can develop a Lewis dot formula satisfying the octet rule as follows:

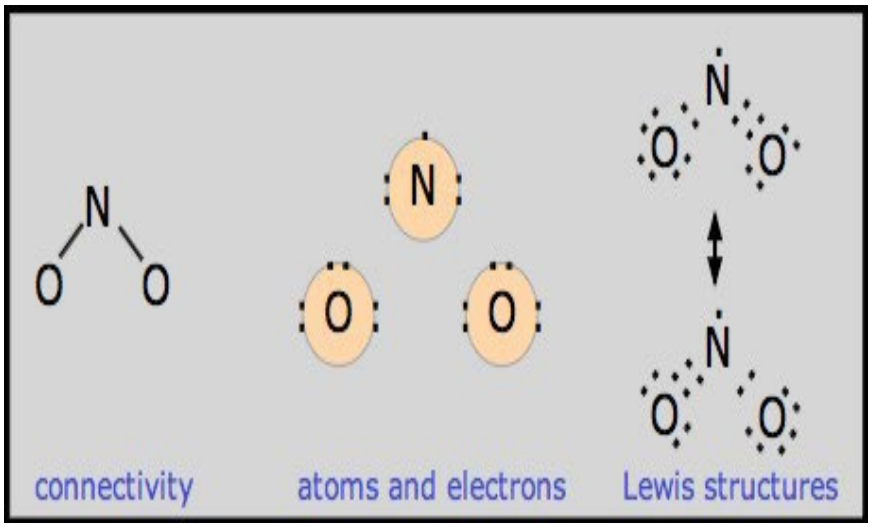


Figure 7.66 Resonance of NO_3^- showing construction of Lewis structures

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:

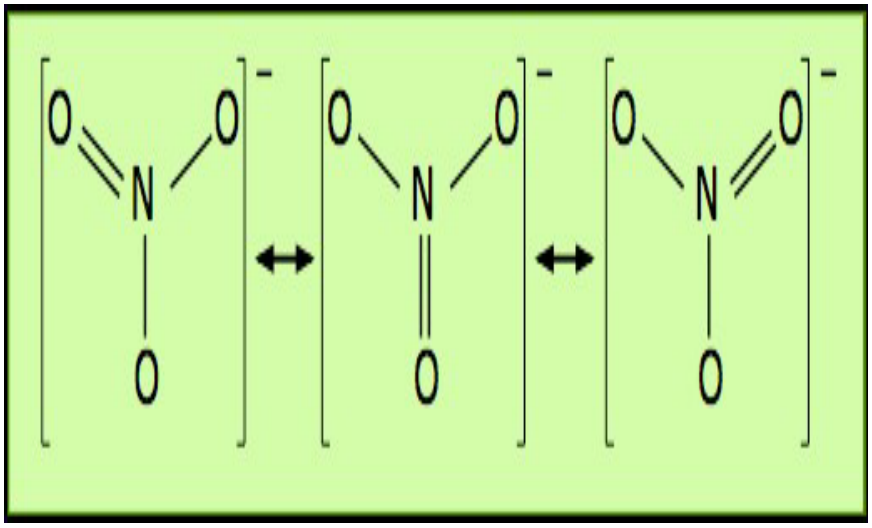


Figure 7.67 Three Resonating Structures of NO_3^-

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.

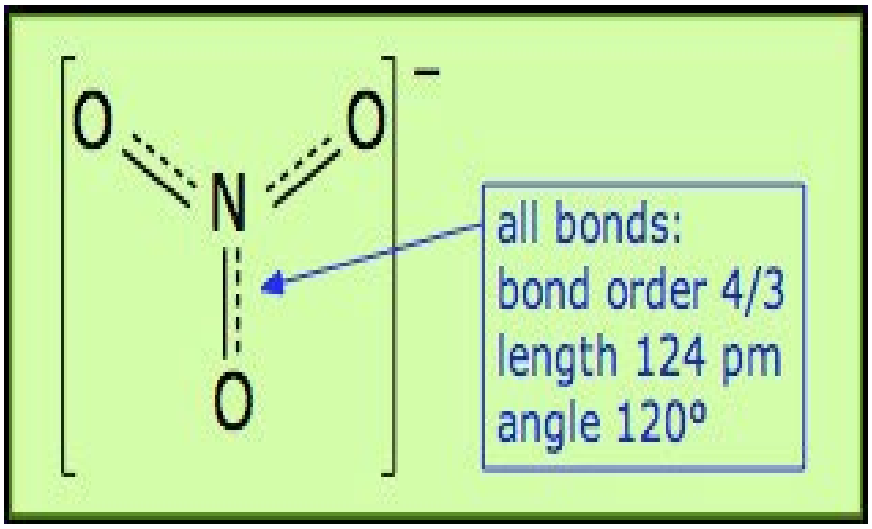


Figure 7.68 Effect of Resonance on NO_3^- Ion showing bond order 4/3, length 124 pm, and 120° angles

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 SO3, and for the carbonate ion $CO3^{2-}$.

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 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:

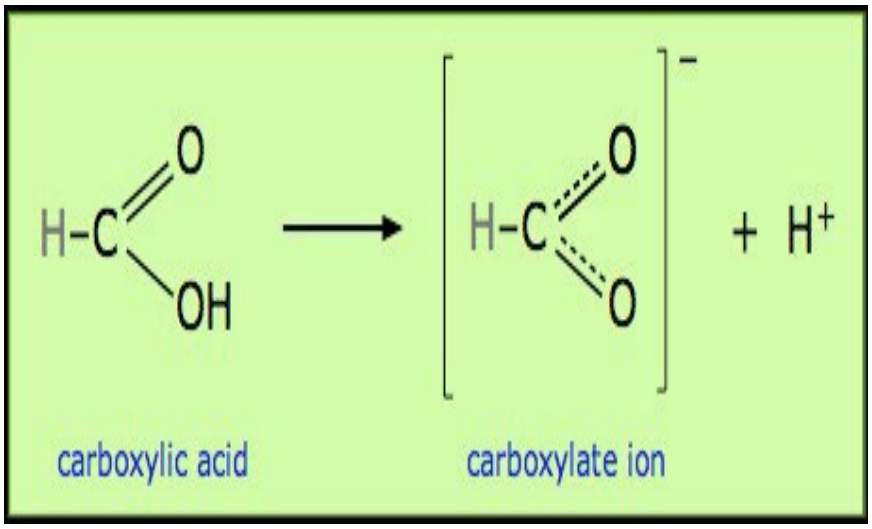


Figure 7.69 Effect of Resonance on Carboxylate Ion Formation in Carboxylic Acids

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 of the 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

Perhaps the most well known molecule whose structure must be represented as a resonance hybrid is benzene, C6H6. 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.

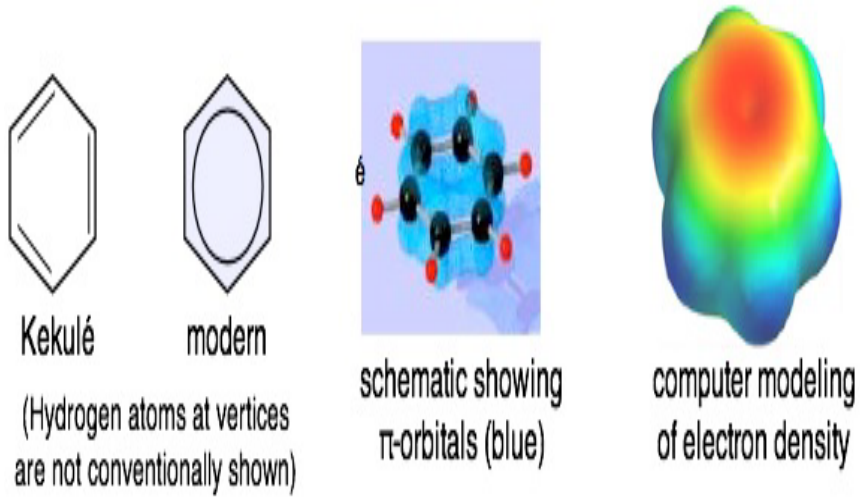


Figure 7.70 Resonating Structures of Benzene: Kekulé, Modern, Schematic (pi-orbitals), and Computer Modeling

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.

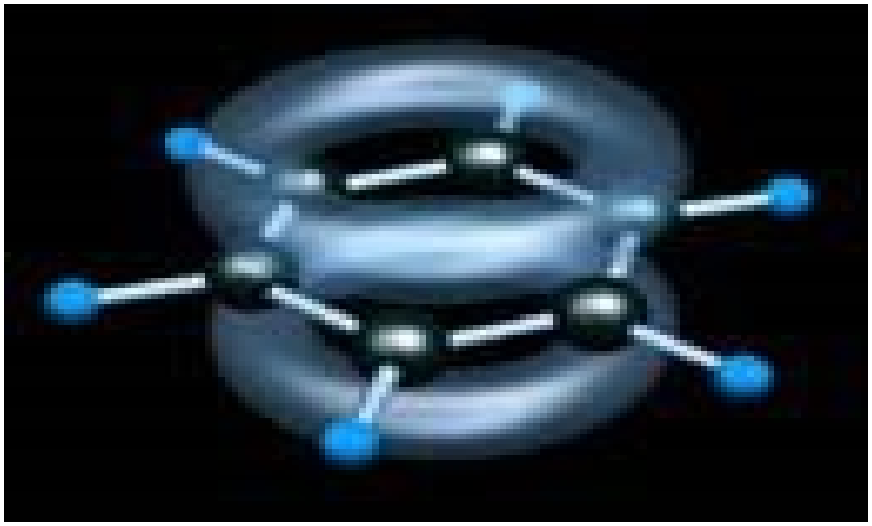


Figure 7.71 3D Shape of Benzene showing delocalized pi-electron system

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:

$2HOF(g) \rightarrow 2HF(g) + O2(g)$

Other molecules having proper Lewis structures but no apparent existence may be stable only at very low temperatures; examples are O4 and H2O4.

The fluorate ion, $FO3^-$, 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 $NO4^{3-}$ and $NO3^{2-}$. 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 $I3^-$, and the bifluoride ion $HF2^-$.

The triiodide ion $[I–I–I]^-$ is a well known species found in aqueous solutions containing iodine and iodide ions: $I2 + I^- \rightarrow I3^-$

The bifluoride ion $[F–H–F]^-$ is formed in a rather similar way in hydrofluoric acid solutions containing fluoride ion: $HF + F^- \rightarrow HF2^-$

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 possess an even number of electrons and are diamagnetic.

Dioxygen

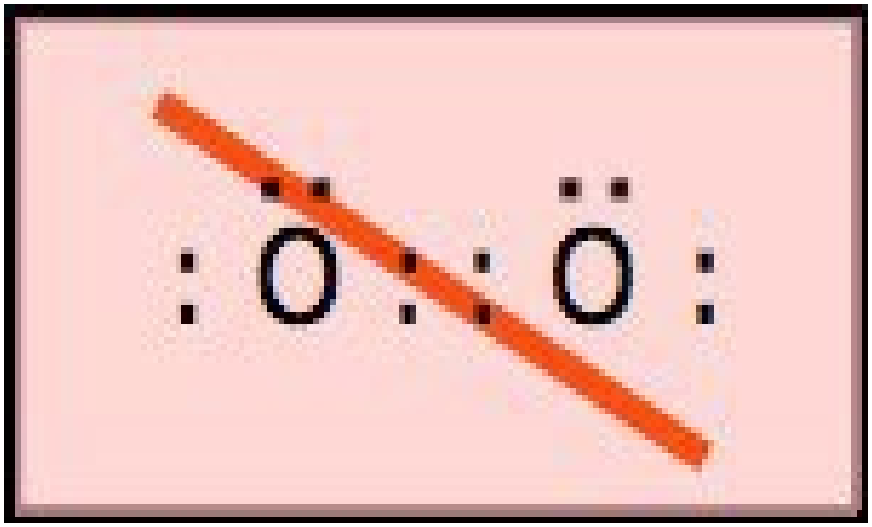


Figure 7.72 Lewis Dot Structure of Dioxygen (O_2) showing why the simple Lewis structure is inadequate

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 O2 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 O2 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

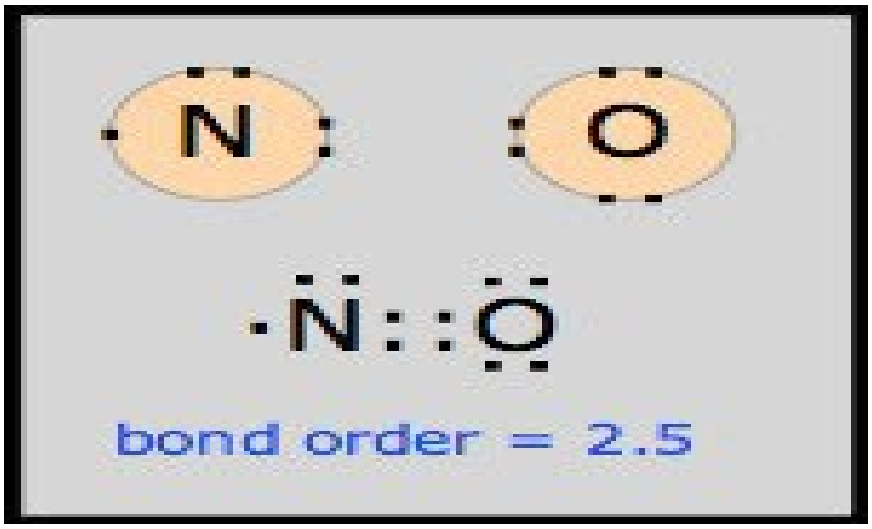


Figure 7.73 Lewis Dot Structure of NO showing the odd-electron molecule with bond order 2.5

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 mammalian 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 NO2 appears to be somewhat local to the nitrogen atom. As a consequence, the dimerization equilibrium:

2 NO2 ⇌ N2O4

is so facile that neither gas can be retained in pure form at ordinary temperatures. Because two equivalent Lewis structures can be written, NO2 is a resonance hybrid in which the N–O bond order is 1.5.

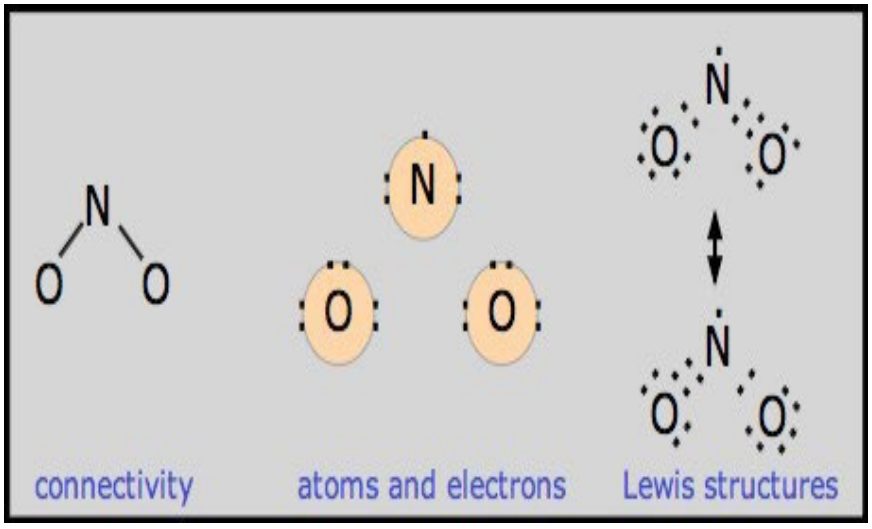


Figure 7.74 Lewis Dot Structure of NO_2 showing resonance and odd-electron nature

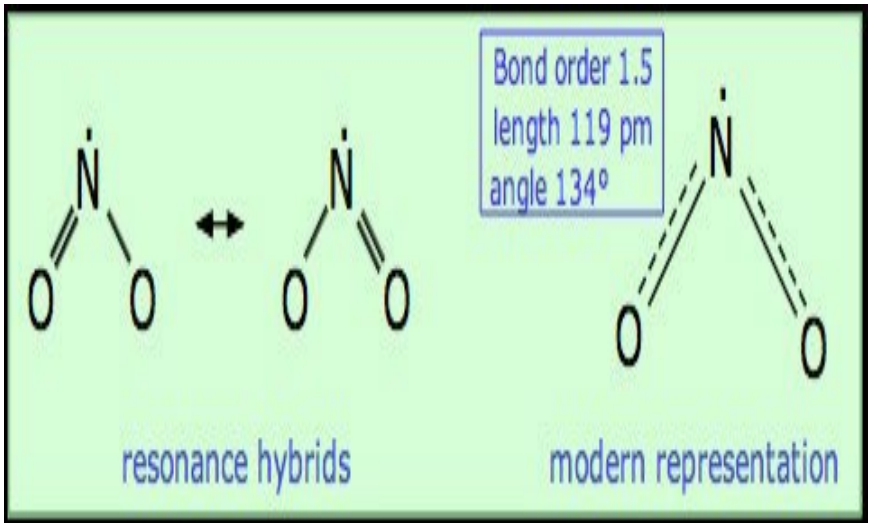


Figure 7.75 Resonating Structure of NO_2 with bond order 1.5, length 119 pm, angle 134°

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).

7.6 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.

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. Conversely, the same amount of energy is released when one mole of H_2 molecules forms from two moles of H atoms.

Reference: https://www.youtube.com/watch?v=5AOblYlknBc

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:

$A—B \rightarrow A(g) + B(g)$
For example, $H—Cl \rightarrow H\cdot(g) + Cl\cdot(g)$

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 CH4 because breaking the second bond might be easier or harder than breaking the first.

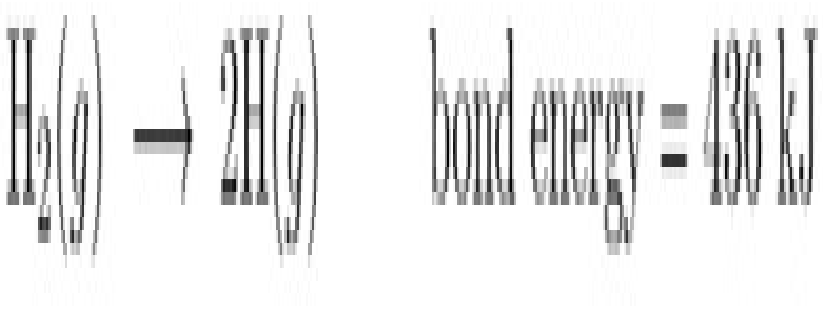


Table 1: Approximate Average Bond Enthalpies (kcal/mol) for Common Chemical Bonds

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 N2 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 (N2H4) 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.

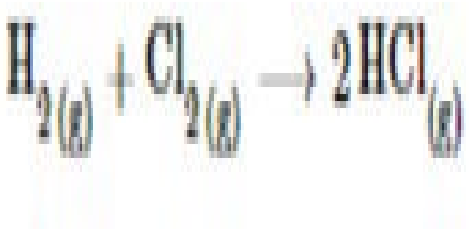


Table 1: Bond Energies (kJ/mol) and Table 2: Average Bond Lengths and Bond Energies for Common Bonds

Reference: https://chem.libretexts.org/Courses/University_of_Kentucky/UK

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:

$$\Delta H = \Sigma D(\text{bonds broken}) - \Sigma D(\text{bonds formed})$$

In this expression, the symbol Σ 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:

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

Enthalpy calculation for $H_2 + Cl_2 \rightarrow 2HCl$ showing $\Delta H = [436 + 243] - 2(432) = -185$ kJ

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.

This excess energy is released as heat, so the reaction is exothermic. The standard molar enthalpy of formation of HCl(g) is –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 is 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	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		

Figure 7.76 Bond Energy vs. Bond Length graph showing inverse relationship

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

Table: Average Bond Lengths (pm) and Average Energies (kJ/mol) for Common Bonds

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. 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 showing H-O bond length 95.8 pm and H-O-H bond angle 104.5°

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.

The Born-Haber Cycle

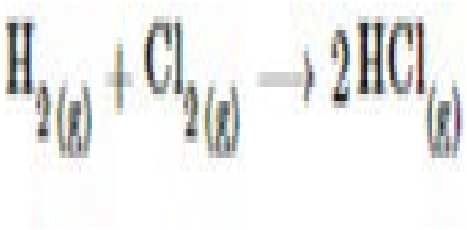
Born-Haber cycle is a cycle of enthalpy change of process that leads to the formation of a solid crystalline ionic compound from the elemental atoms in their standard state and of the enthalpy of formation of the solid compound such that the net enthalpy becomes zero.

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:

- ΔHf°, the standard enthalpy of formation of the compound
- IE, the ionization energy of the metal
- EA, the electron affinity of the nonmetal
- ΔHs°, the enthalpy of sublimation of the metal
- D, the bond dissociation energy of the nonmetal
- $\Delta H_{lattice}$, the lattice energy of the compound

Reference: https://www.youtube.com/watch?v=jIyIhTzA4xI

EXAMPLE



Born-Haber Cycle for $CaCl_2$ formation showing all thermochemical steps

Reference: https://www.youtube.com/watch?v=I61-N0GuSx8

Lattice Energy Comparisons

The precious gem ruby is aluminum oxide, Al2O3, containing traces of Cr^{3+}. The compound Al2Se3 is used in the fabrication of some semiconductor devices. Which has the larger lattice energy, Al2O3 or Al2Se3?

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, Al2O3 would have a shorter interionic distance than Al2Se3, and Al2O3 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.

Reference: https://www.youtube.com/watch?v=DI-bwx8r3r8

7.7 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 BeF2 molecule. The Lewis structure of BeF2 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°.

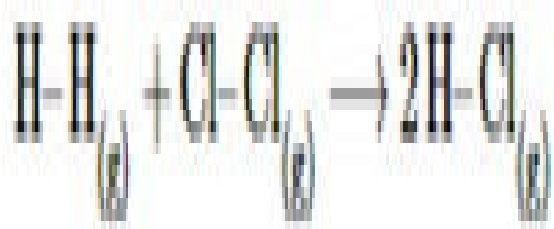


Figure 7.78 BeF_2 showing linear geometry with 180° bond angle

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, CO2

In the CO2 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.

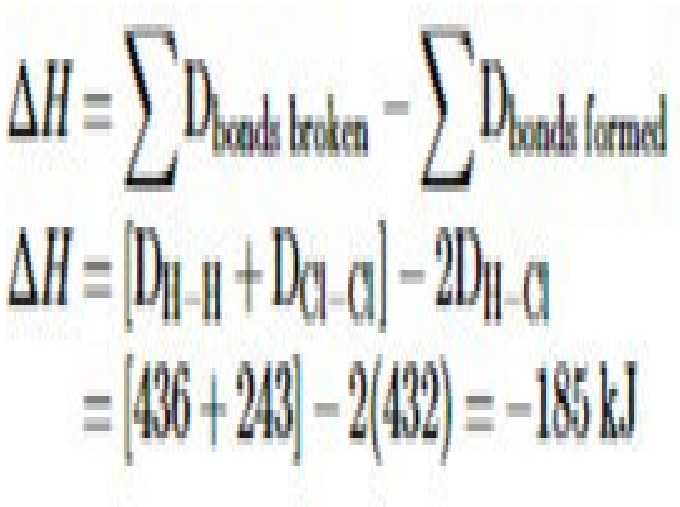


Figure 7.79 Linear CO_2 Molecule as predicted by VSEPR Theory with 180° bond angle

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.

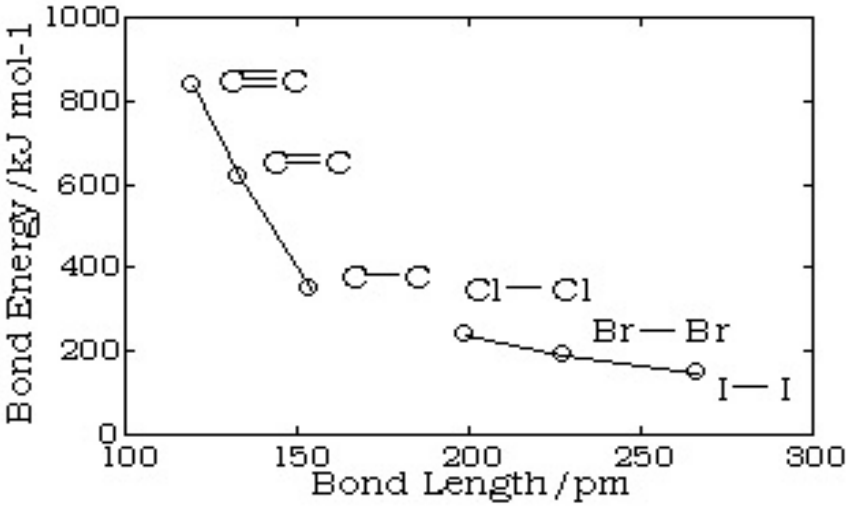


Figure 7.80 Electronic Geometry of CO_2 Molecule showing lone pairs on oxygen atoms

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 that maximize the space around any region of electron density:

Reference: https://chem.libretexts.org/Bookshelves/General_Chemistry

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, CH4, 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

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 7.81 Tetrahedral CH_4 Molecule showing wedge-dash notation for 3D structure

The above Figure-A showing the molecular structure of Methane (CH4). 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, NH3, 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.

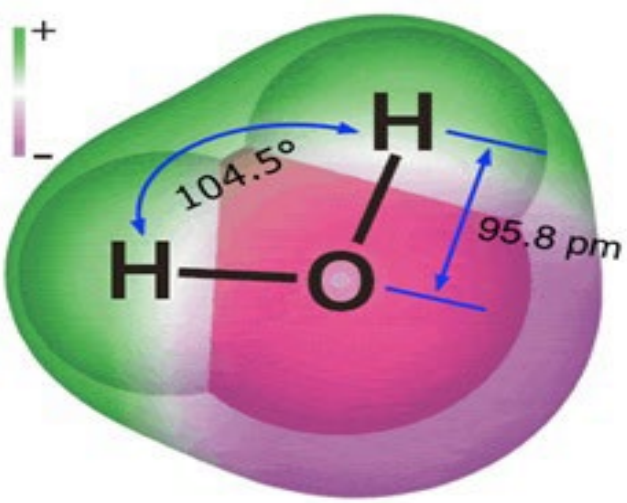


Figure 7.82 Electronic Geometry of NH_3: (a) tetrahedral electron-pair geometry with lone pair, (b) trigonal pyramidal molecular structure, (c) H-N-H bond angle of 106.8°

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

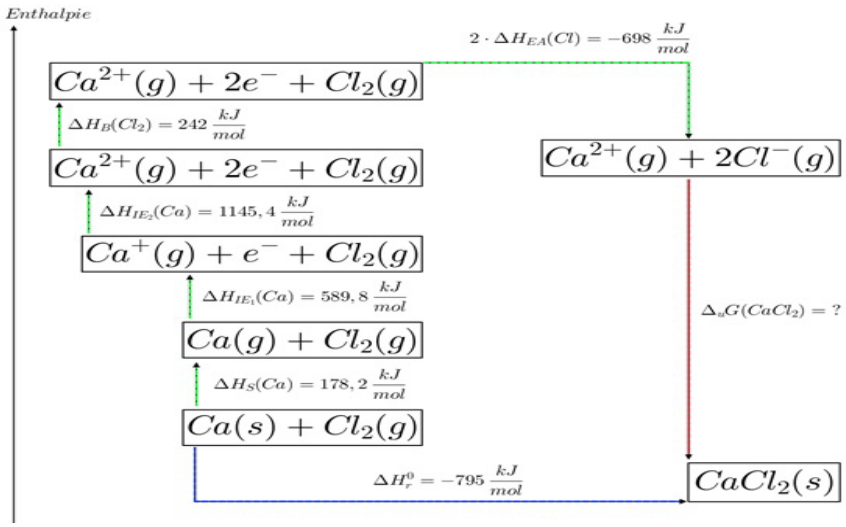


Figure 7.83 VSEPR Chart showing electron-pair geometries for 2-6 electron groups

Ref: www.openstax.org/

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).

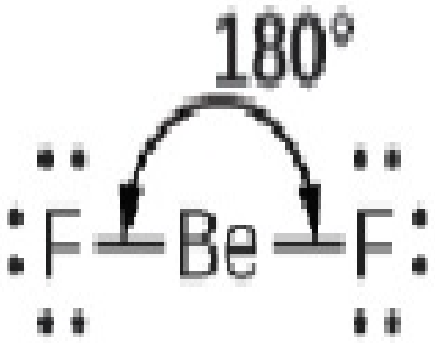


Figure 7.84 VSEPR Chart showing AXE notation with molecular geometries for different bonding and lone pair combinations

Ref: www.openstax.org/

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

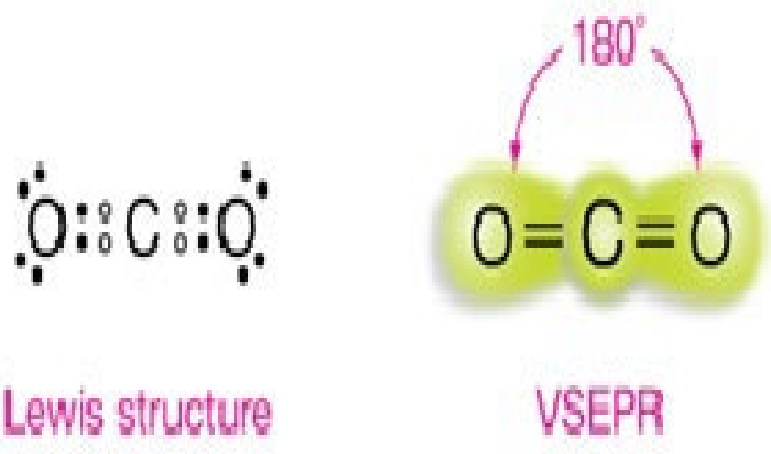
Thus, electron pairs will spread themselves as far from each other as possible to minimize repulsion. Using the VSEPR theory, the electron bond pairs and lone pairs on the center atom will help us predict the shape of a molecule. The shape of a molecule is determined by the location of the nuclei and its electrons.

The VSEPR theory is used 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.



Molecular models showing five VSEPR geometries: CO_2 (linear), SO_2 (bent), NH_3 (trigonal pyramidal), BCl_3 (trigonal planar), BrF_5 (square pyramidal)

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.

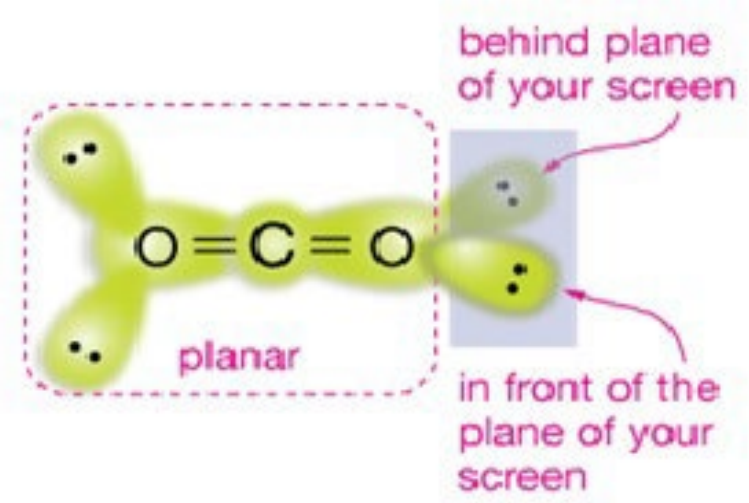


Figure-A and Figure-B: Common Electron-Pair Geometries for 2-6 Electron Groups with predicted bond angles

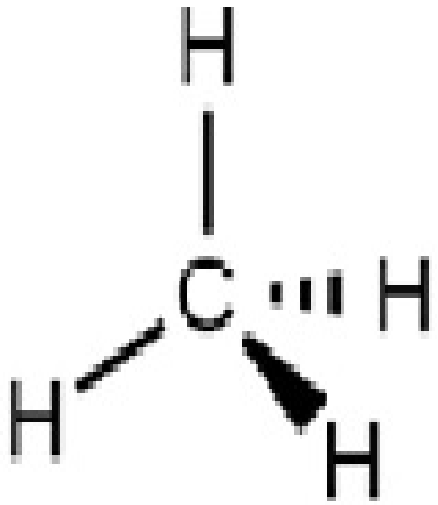


Figure 7.86 AXE Groups in VSEPR showing common molecular geometries and idealized bond angles

Ref: www.libretext.org/

The following we will illustrate 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.

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 AX3 molecule such as BF3, 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.

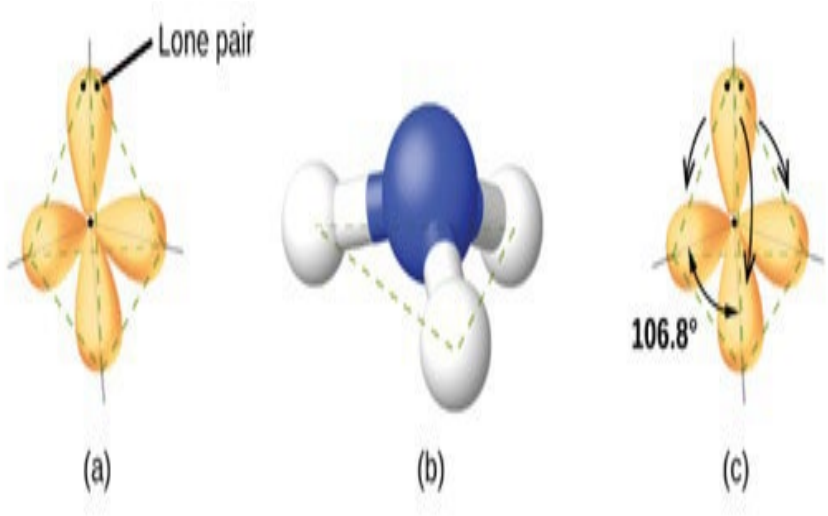


Figure 7.87 Trigonal Planar Shape of BF_3 Molecule with 120° bond angles

Tetrahedral coordination

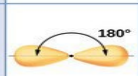
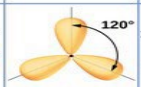
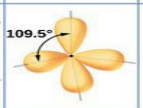
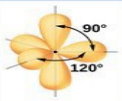
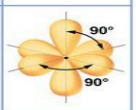
Number of regions	Two regions of high electron density (bonds and/or unshared pairs)	Three regions of high electron density (bonds and/or unshared pairs)	Four regions of high electron density (bonds and/or unshared pairs)	Five regions of high electron density (bonds and/or unshared pairs)	Six regions of high electron density (bonds and/or unshared pairs)
Spatial arrangement					
Line-dash-wedge notation					
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°

Figure 7.88 Tetrahedral CH_4 Molecule showing 109.5° bond angles and tetrahedral coordination

Methane, CH4, 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, CH2Cl2.

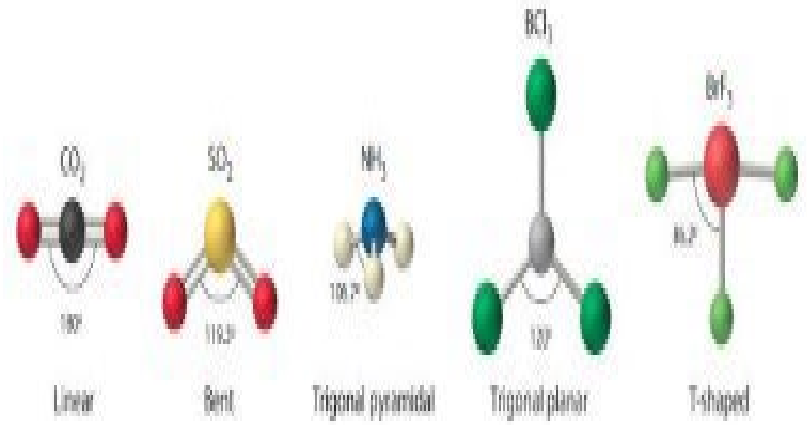


Figure 7.89 Shape of CH_2Cl_2 demonstrating that tetrahedral geometry means only one isomer exists

If the coordination around the carbon were square, then there would have to be two isomers of CH2Cl2, 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 that would allow the two isomers to be distinguished and separated.

The existence of only one kind of CH2Cl2 molecule means that all four positions surrounding the carbon atom are geometrically equivalent, which requires a tetrahedral coordination geometry.

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 CH3 tetrahedra joined

end-to-end. Similar alkane chains having the general formula H3C–(CH2)n–CH3 (or CnH2n+2) can be built up; a view of pentane, C5H12, is shown below.

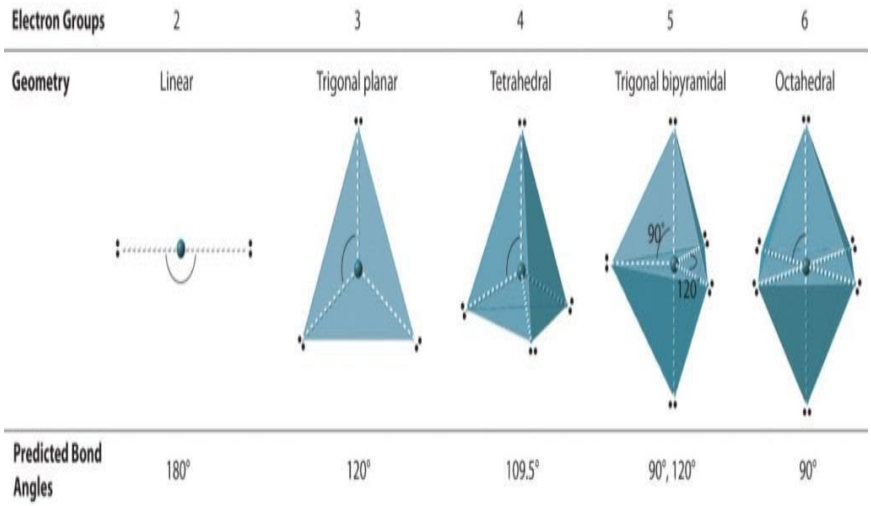


Figure 7.90 Tetrahedral Chain of Carbon Atoms in Pentane (C_5H_{12})

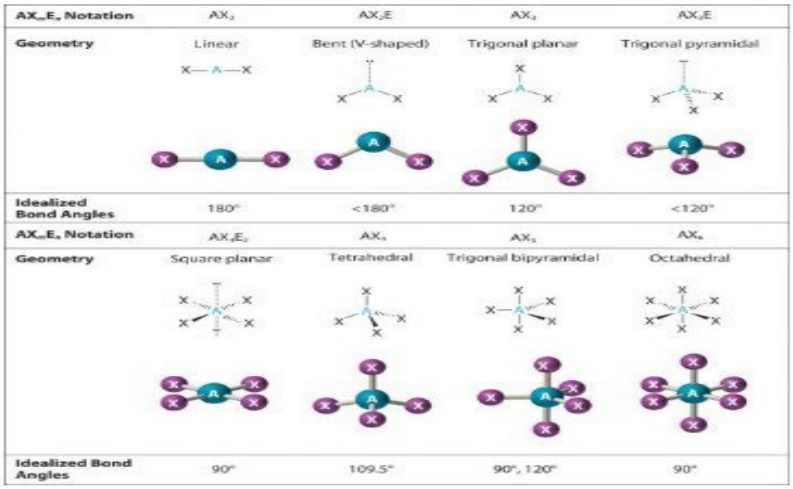


Figure 7.91 Shape of Long Chain Carbon Atoms showing zigzag backbone with free rotation around C-C bonds

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 AX4, AX2E2, 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: AX2E2

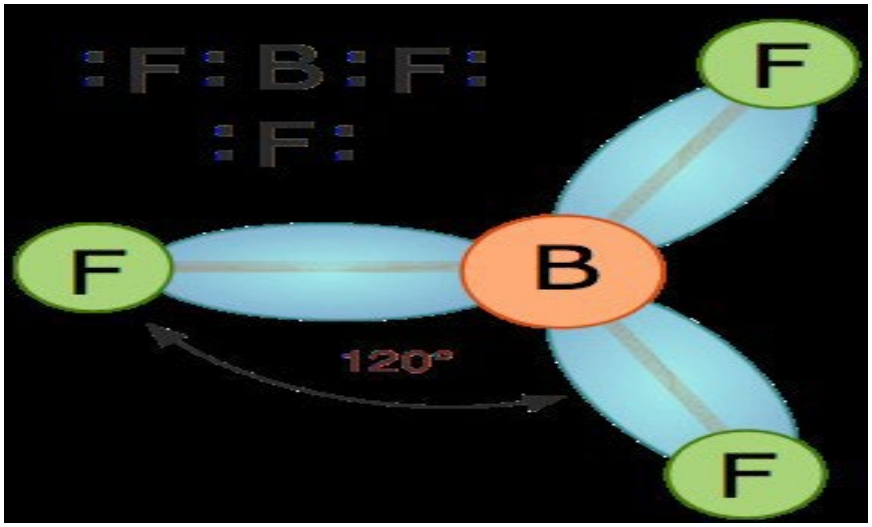


Figure 7.92 Water Molecule Shape: tetrahedral electron-pair geometry resulting in bent molecular geometry with 104.5° H-O-H angle

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 H2O molecule is described as bent.

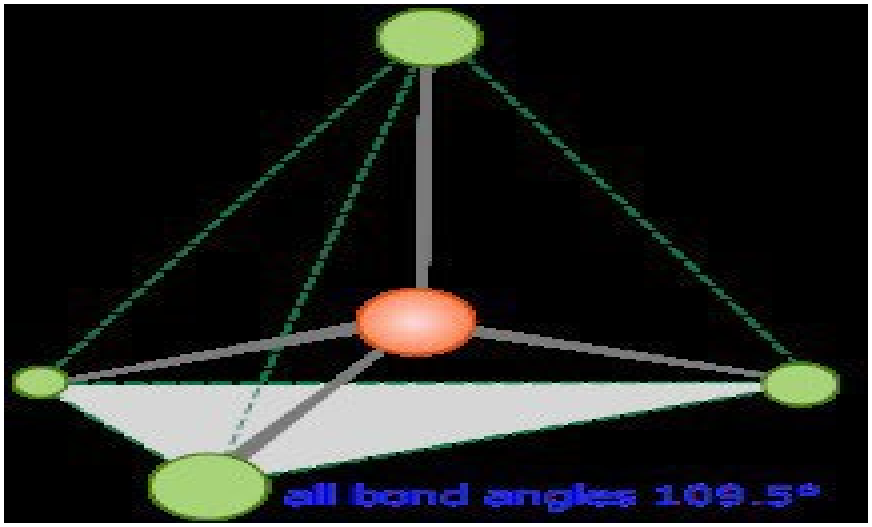


Figure 7.93 and 7.94 Bent shape of water and Tetrahedral Electronic Geometry of Water

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 H2O, 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.

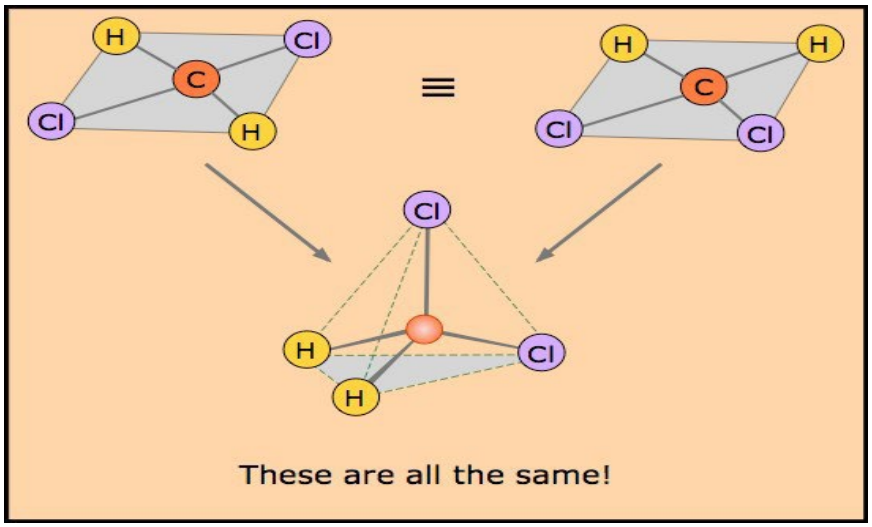


Figure 7.95 Charge Density of Water showing electrostatic potential map: blue = negative (oxygen end), red = positive (hydrogen ends)

Ammonia: AX3E

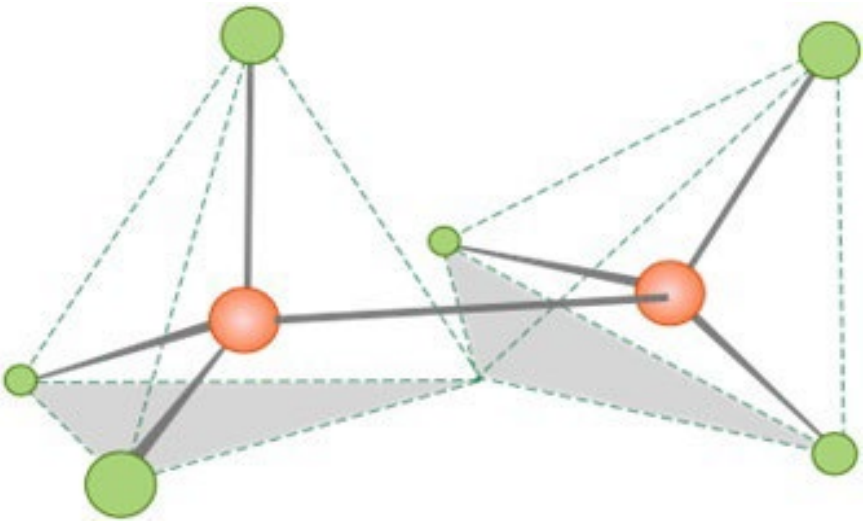


Figure 7.96 Shape of Ammonia NH_3 showing trigonal pyramidal geometry with 107° H-N-H bond angle

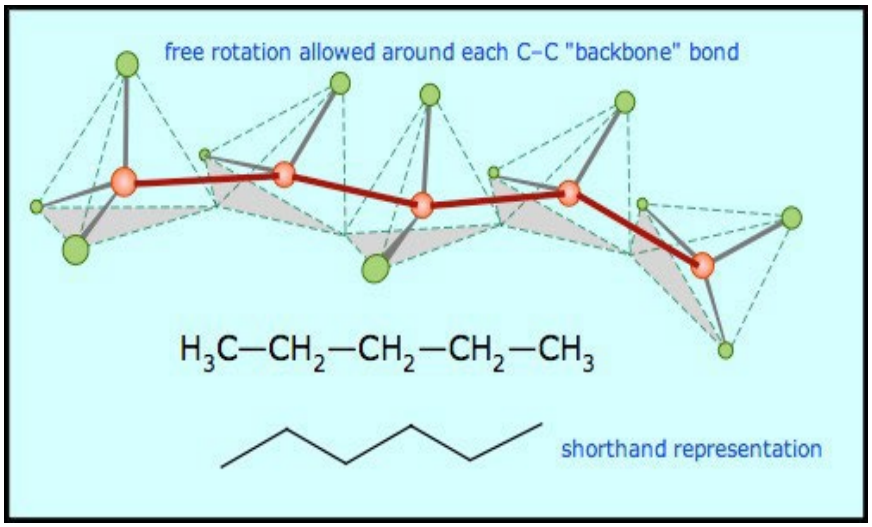


Figure 7.97 Computer-generated image of NH_3 molecule showing electrostatic potential (red = +, blue = −)

The electron-dot structure of NH3 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 H2O. 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 NH3 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. 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 AX5 are formed by some of the elements in Group 15 of the periodic table; PCl5 and AsF5 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 mathematician 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, LaC60 (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.

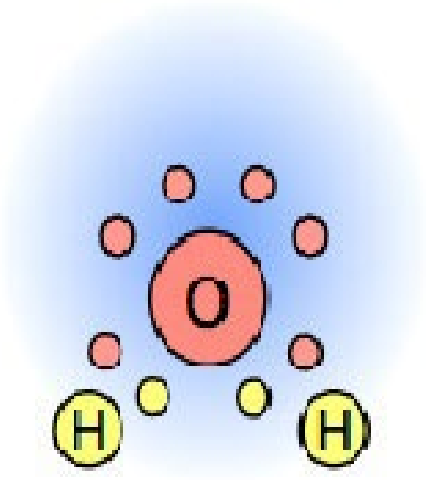


Figure 7.98 Electronic Geometry of Trigonal Bipyramidal showing axial and equatorial positions

The shape of PCl5 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.

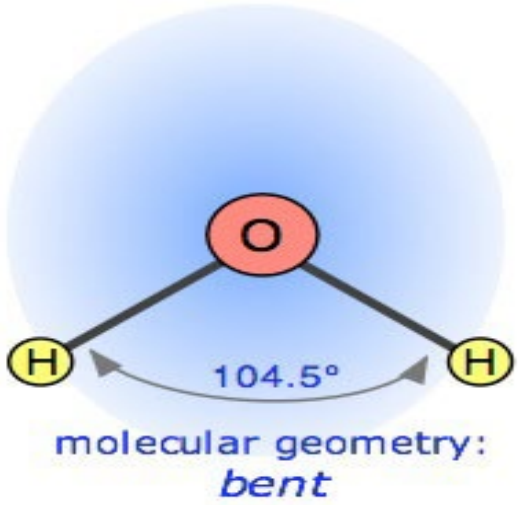


Figure 7.99 Ball and Stick Model of Trigonal Bipyramidal Geometry in PCl_5

Using this reasoning, we can predict that an AX4E 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 SF4 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.

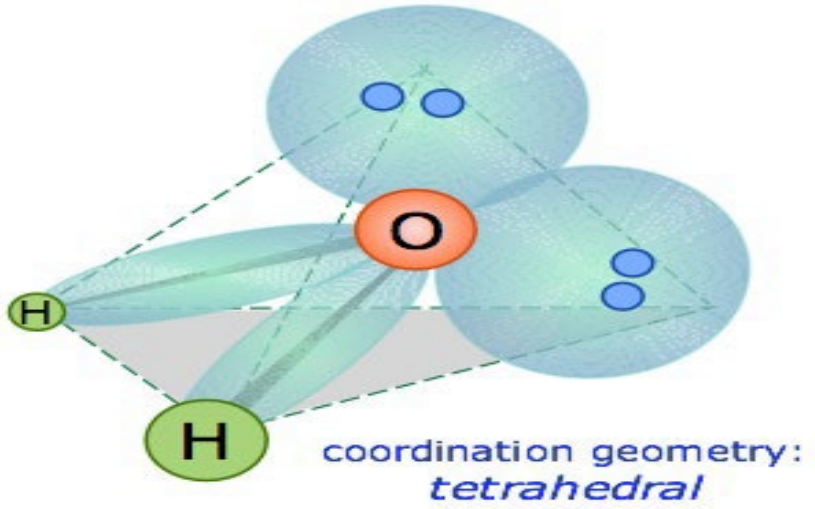


Figure 7.100 Effect of Lone Pairs in Trigonal Bipyramidal Geometry: SF_4 (see-saw), ICl_3 (T-shape), I_3^- (linear)

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.

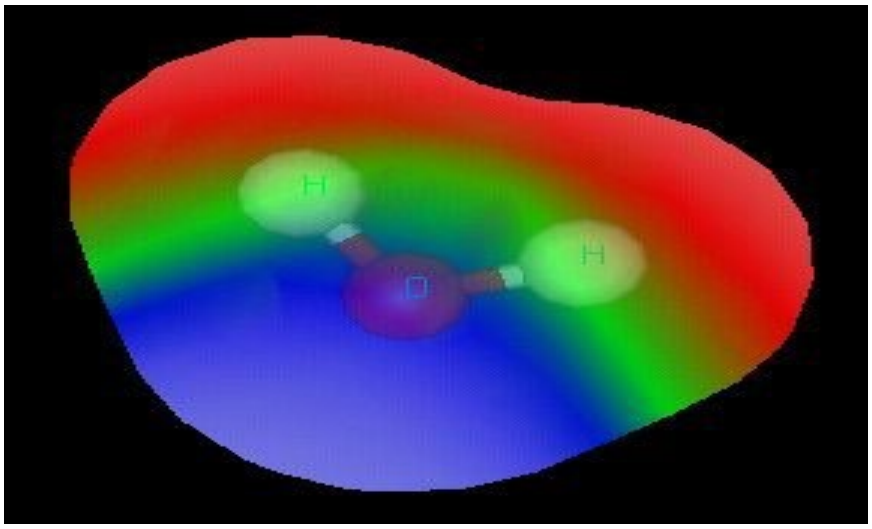


Figure 7.101 Electronic Geometry of Octahedral showing 90° bond angles between adjacent atoms

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 AX6 molecule.

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 (SF6 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 NH3) and O (in H2O). 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 $Fe(H2O)6^{3+}$.
- 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.

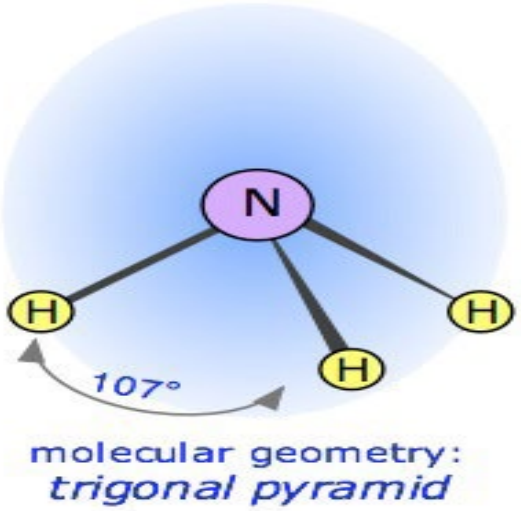


Figure 7.102 Lone Pairs of Octahedral Geometry: AX5E (ClF5, square pyramidal) and AX4E2 (XeF4, square planar)

Reference: https://www.youtube.com/watch?v=-pq2wum1uDc
Reference: https://www.youtube.com/watch?v=Moj85zwdULg
Reference: https://www.youtube.com/watch?v=umwN74a0A2g

Additional octahedral geometry structures and bond angle relationships

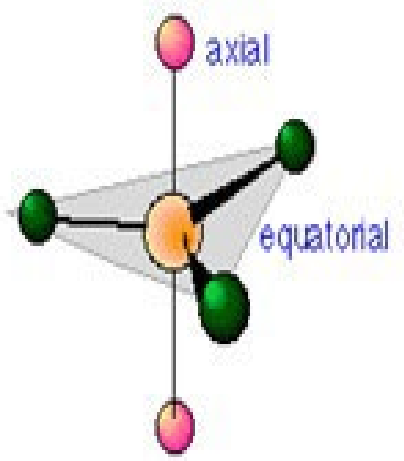
Following CLASSROOM ACTIVITY has been adapted from PhET simulation: https://phet.colorado.edu

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.

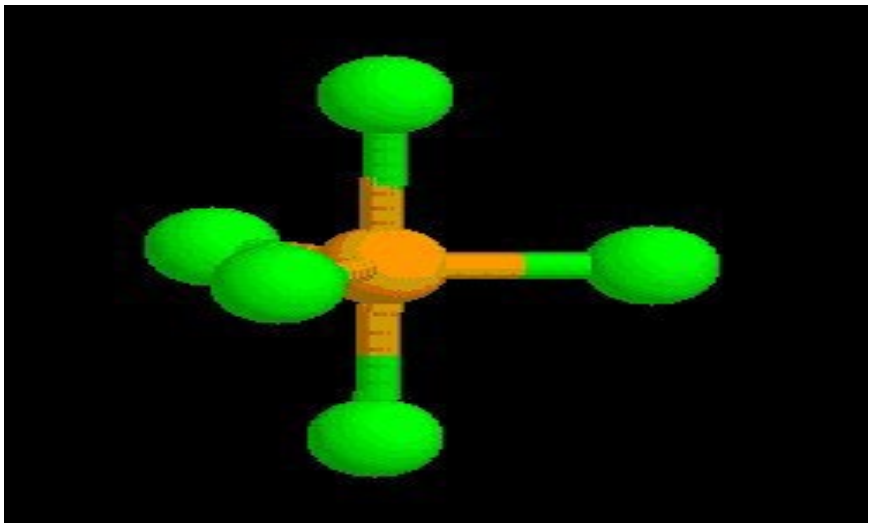
Predict the geometry for the three situations given in the table below. How do you think electron pairs will behave towards each other? This behavior will control how they arrange around a central atom depending on the number of electron pairs.



PhET Simulation: Molecule Shapes Basics interface showing central atom and bonding controls

20. Click the "Remove All" button.
21. Check the Show Bond Angles Option.
22. 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.



Student Activity Table for Recording VSEPR Geometries from PhET Simulation

Beware of molecular roadkill (flattened molecules)!!!

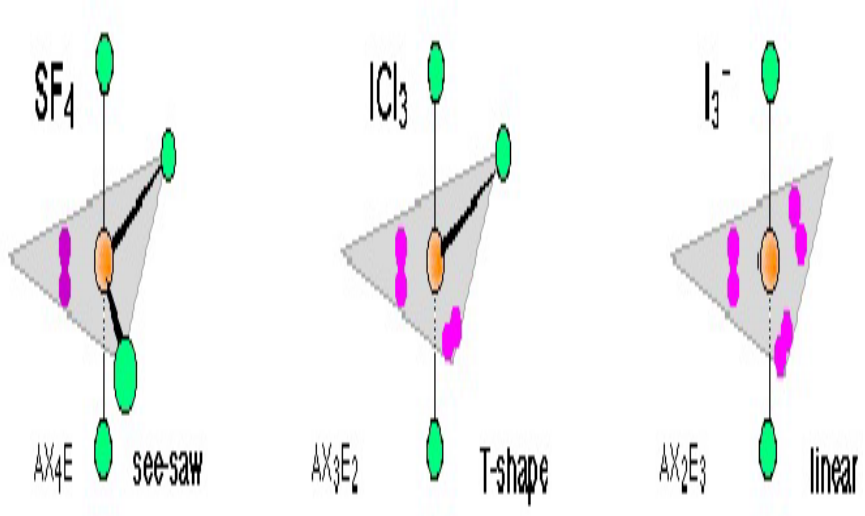
Now electron pairs are repulsive to each other; hence, they minimize repulsion by maximizing distance. They want to get away from each other! This is the basis of valence shell electron-pair repulsion theory or VSEPR. Let's see how well your predictions came out above and add two more geometries to the list. Go to the following PhET html5 simulation:

https://phet.colorado.edu/sims/html/molecule-shapes-basics/latest/molecule-shapes-basics_en.html

Draw the Lewis dot structures for the molecules below.
BeCl2 BF3 CH4 PCl5 SF6

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.

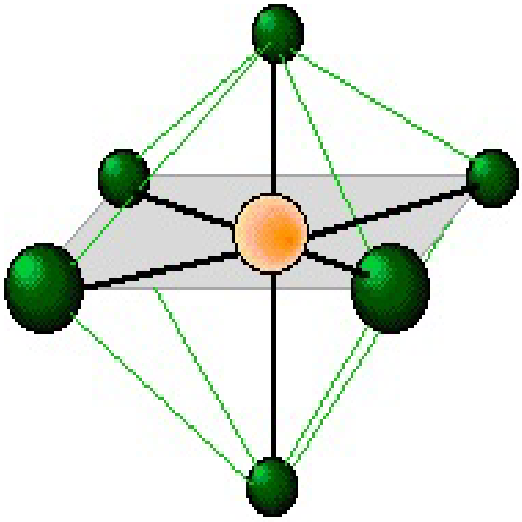
Click on the Real Molecules box at the bottom of the screen.



PhET Molecule Shapes: Basics simulation showing Model and Real Molecules selection options

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-Dimensional Geometries: Tetrahedral, Trigonal Bipyramidal, and 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.

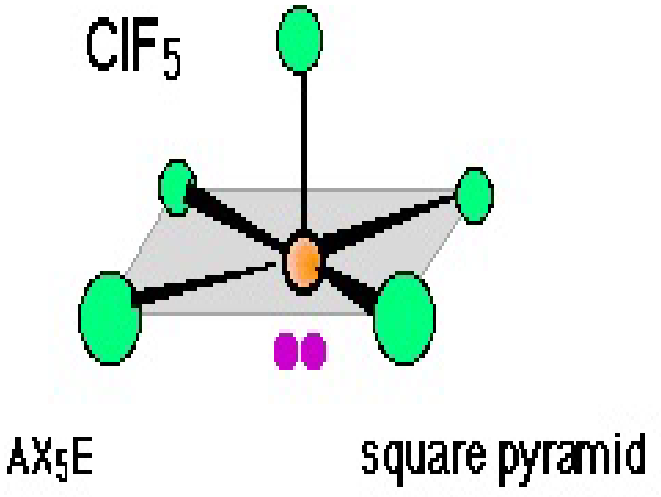
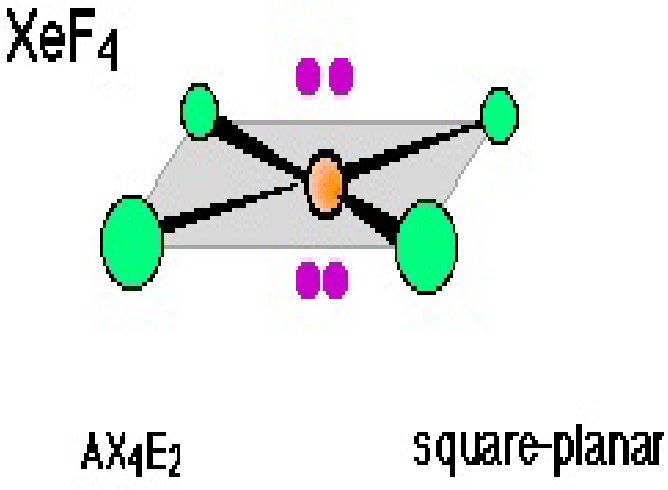


Diagram of Trigonal Bipyramidal Geometry showing axial positions (180° apart) and equatorial positions (120° apart)

Here are models of the ideal geometries that were just explored.
Source: https://www.indigoinstruments.com/molecular_models/molymod/



Physical molecular models showing tetrahedral, trigonal bipyramidal, and octahedral geometries

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.

SiH4 AlCl3 SeF6 AsF5

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.

CO2 H2CO H2C=CH2 HC≡CH CO

Draw the 3D structure of acetic acid, CH3COOH (first carbon is tetrahedral, second carbon is trigonal planar).

Determine the molecular geometry for the following three molecules:

CH4 NH3 H2O

What is different about ammonia and water compared to methane?

Chapter 8: ADVANCED THEORIES OF CHEMICAL BONDING

Key Concepts:

1. Valence Bond Theory
2. Hybridization
3. Orbital Overlaps & Types of Bonds
4. Molecular Orbital Theory
5. Magnetism & MO Theory

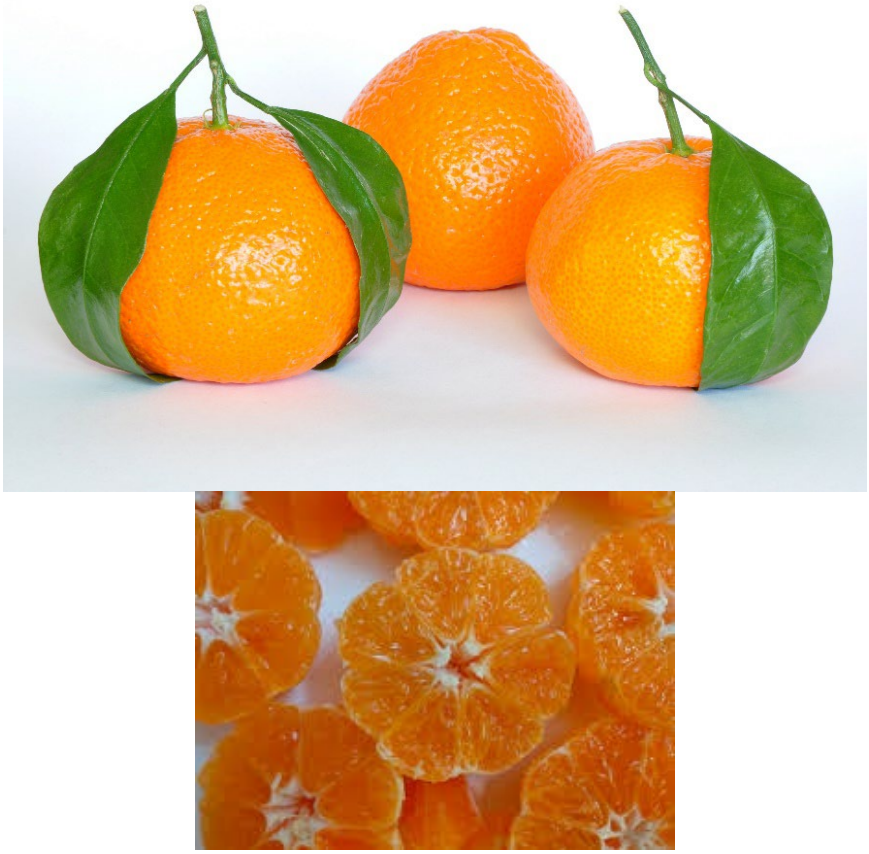


Figure: Mandarin oranges resembling orbital lobes — the rounded lobes of the fruit parallel the geometry of atomic p- and d-orbital lobes

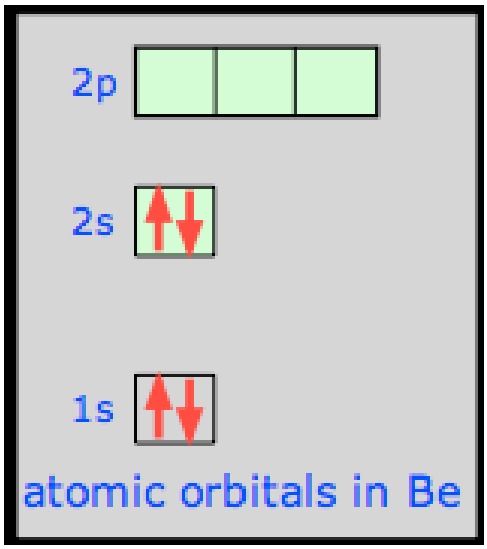
I. VALENCE BOND (VB) THEORY

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, this 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 $1s^2 2s^2$. 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.



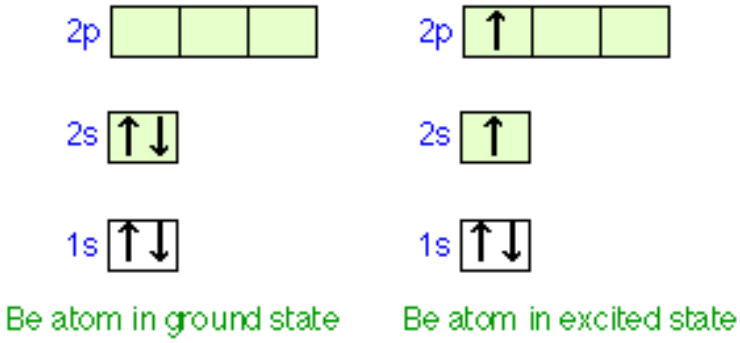


Figure: Beryllium electron configuration — ground state (left) and excited state (right) showing promotion of a 2s electron to the 2p level to allow bond formation

The only way that we can obtain two unpaired electrons for bonding in beryllium is to promote one of the 2s electrons to the 2p 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.

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 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: Linus Pauling (1901–1994), the principal developer of hybridization theory and author of The Nature of the Chemical Bond; winner of the 1954 Nobel Prize in Chemistry and the 1962 Nobel Peace Prize

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 2p and 2s 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.

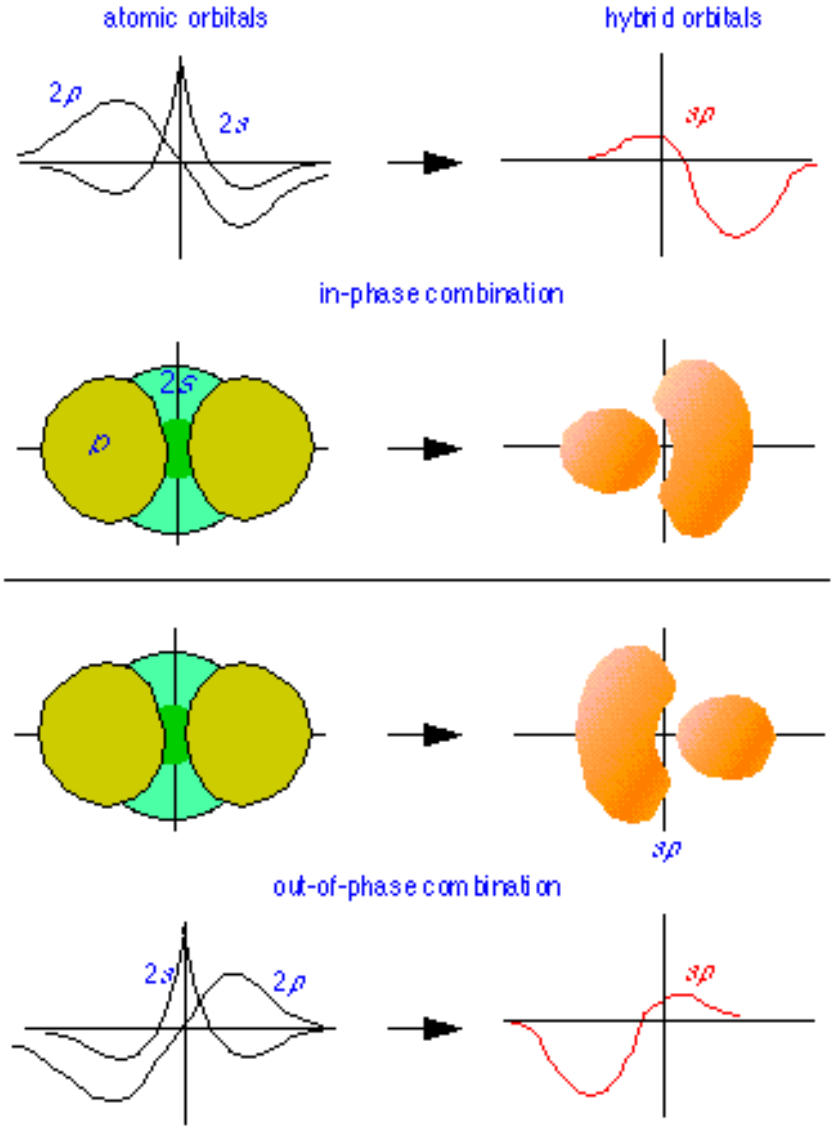


Figure: Construction of sp hybrid orbitals — in-phase (constructive) and out-of-phase (destructive) combinations of atomic s and p wave functions produce two equivalent sp hybrid orbitals pointing in opposite directions

Two central themes 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.

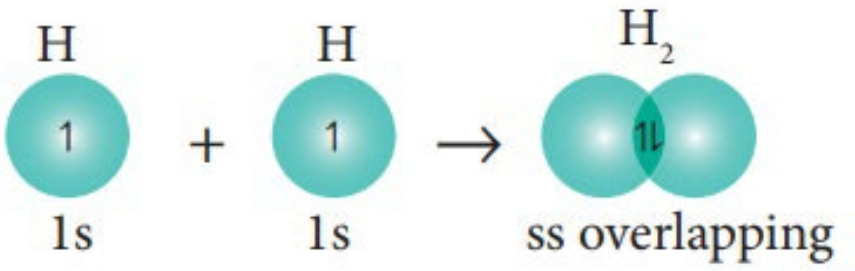


Fig 10. 18 Formation of hydrogen molecule

Figure: Fig 10.18 Formation of the hydrogen molecule (H_2) — two hydrogen 1s orbitals overlap to form a shared bonding region occupied by two electrons with opposite spins

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) sp^3 Hybridization

VB theory proposes that one s and all three p-orbitals of the central atom mix and form four sp^3 hybrid orbitals, which point toward the vertices of a tetrahedron. In methane CH_4, the central C atom is sp^3 hybridized. Its four valence electrons half-fill the four sp^3 hybrids, which overlap the half-filled 1s orbitals of the four H atoms and form four C-H bonds.

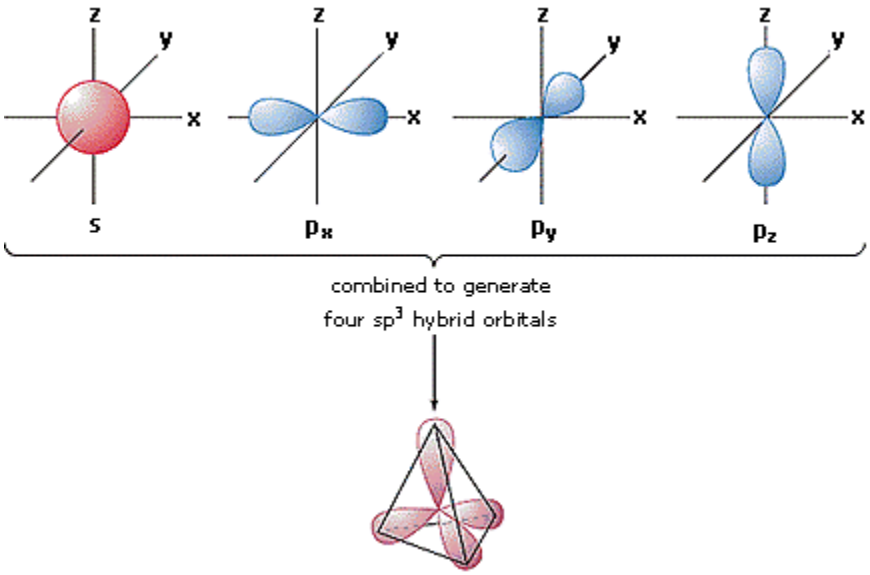


Figure: sp³ Hybrid Orbital Formation — the s, px, py, and pz atomic orbitals of carbon combine to generate four equivalent sp³ hybrid orbitals directed toward the vertices of a tetrahedron

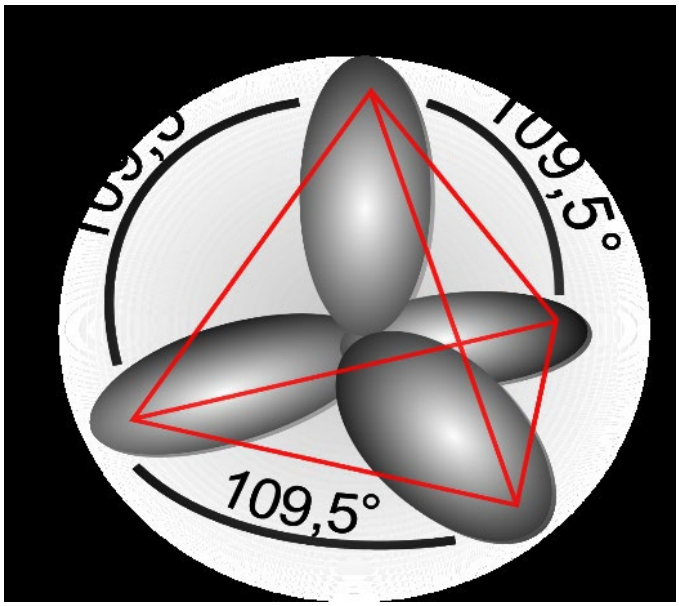


Figure: Tetrahedral geometry of sp³ hybrid orbitals — each of the four lobes is separated by 109.5° from its neighbors, consistent with the geometry of methane and other tetrahedral molecules

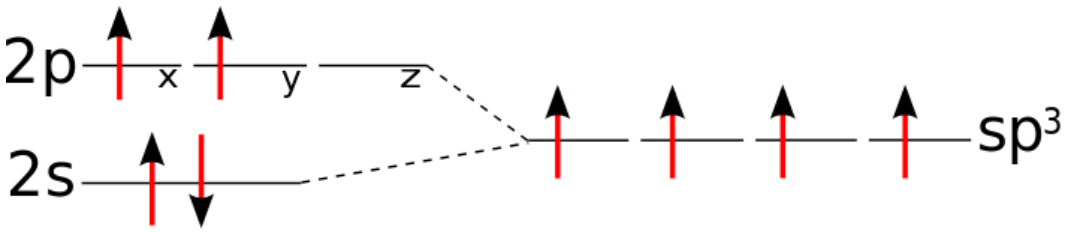


Figure: Orbital box diagram for sp³ hybridization of carbon — the 2s and three 2p atomic orbitals reorganize into four equivalent sp³ hybrid orbitals, each half-filled with one electron

CH_4 hybridization:

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 2p orbitals. In order to form four bonds (tetravalence), need four unpaired electrons in four separate but equivalent orbitals. We assume that the single 2s, and the three 2p 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.

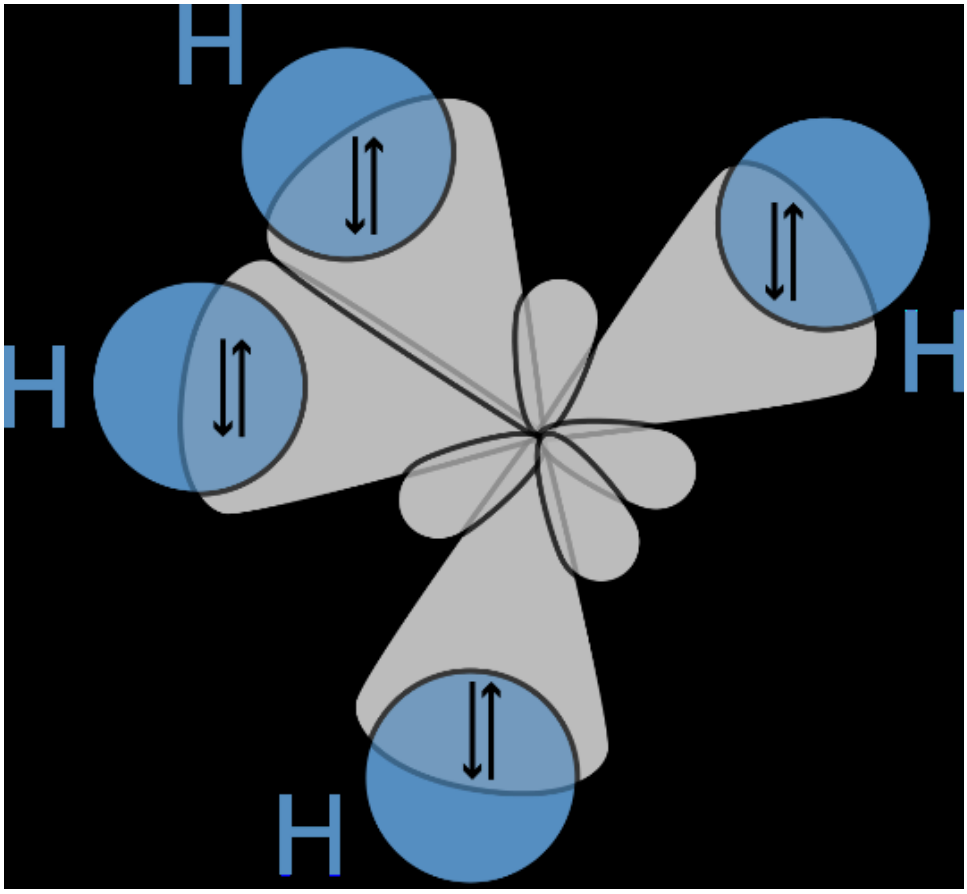


Figure: sp^3 hybridization in methane (CH_4) — carbon's four sp^3 hybrid orbitals overlap with the four hydrogen 1s orbitals to form four equivalent tetrahedral C–H bonds

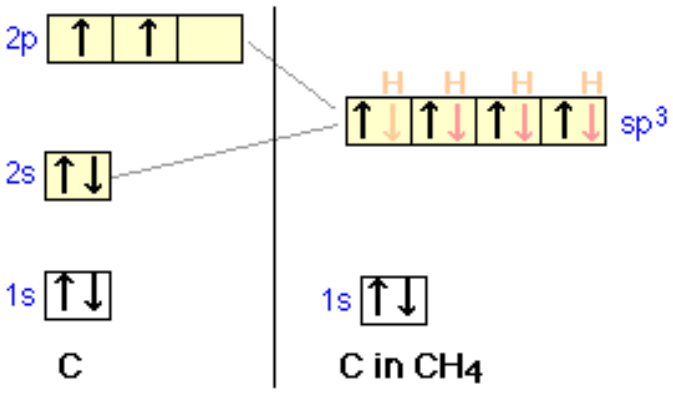


Figure: Orbital energy diagram for carbon in methane — sp^3 hybridization produces four degenerate hybrid orbitals at an intermediate energy between the original 2s and 2p levels

Methane is the simplest hydrocarbon; the molecule is approximately spherical, as is shown in the space-filling model:

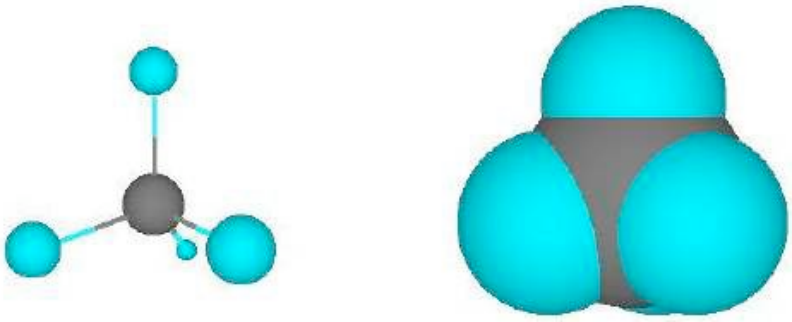


Figure: Space-filling (CPK) and ball-and-stick models of methane (CH_4) — the nearly spherical shape reflects the equal length and tetrahedral geometry of the four C–H bonds

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:

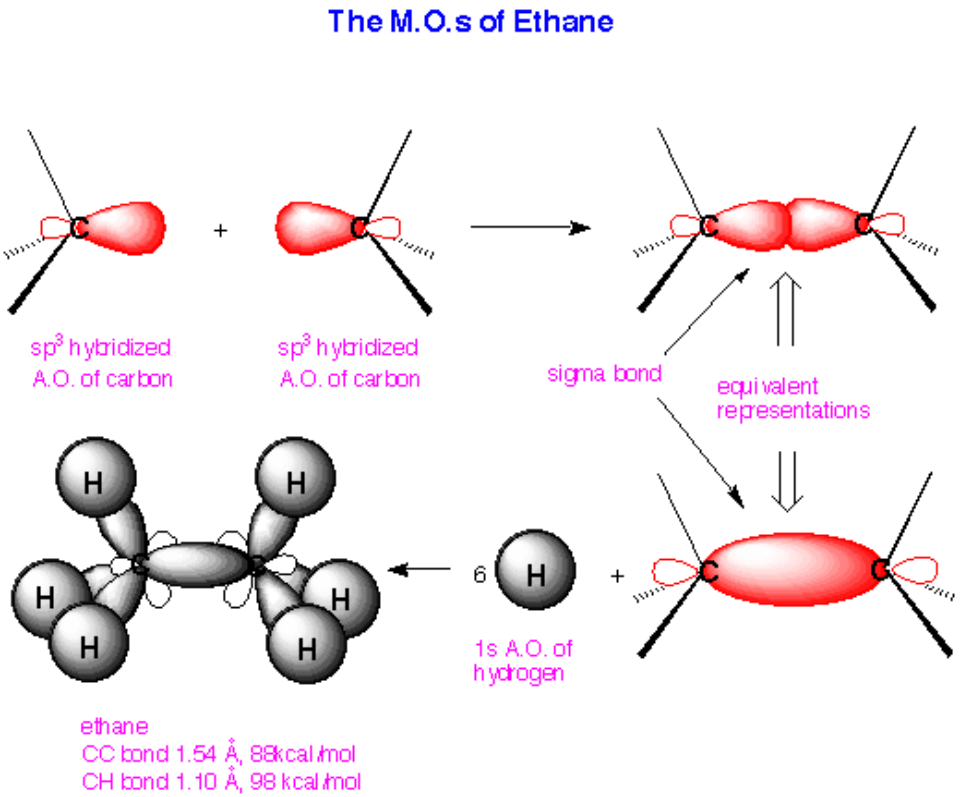


Figure: Molecular orbitals of ethane (C_2H_6) — two sp^3 carbon orbitals overlap end-to-end to form the C–C sigma bond; the remaining six sp^3 orbitals each overlap with a hydrogen 1s orbital to form the six C–H sigma bonds

This shows how an sp^3 orbital on each of 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.

4 Lone pair electrons in hybrid orbitals

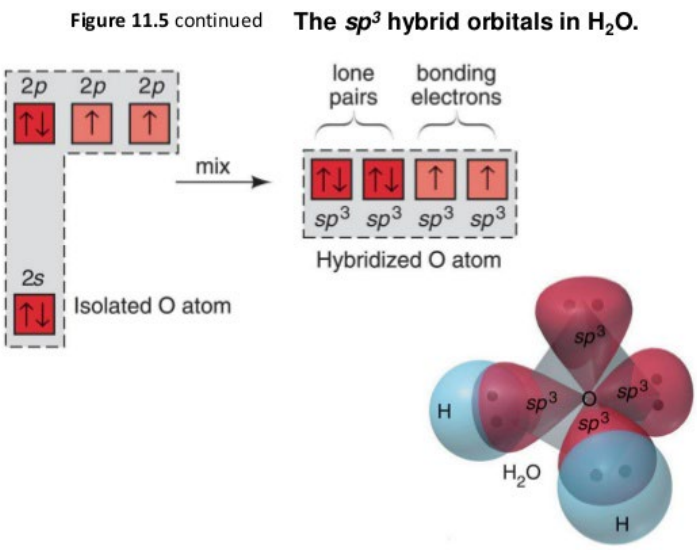


Figure: sp³ hybridization in ammonia (NH_3) — three of nitrogen's four sp³ hybrid orbitals form bonds with hydrogen atoms; the fourth contains the non-bonding lone pair, giving the molecule a trigonal pyramidal shape

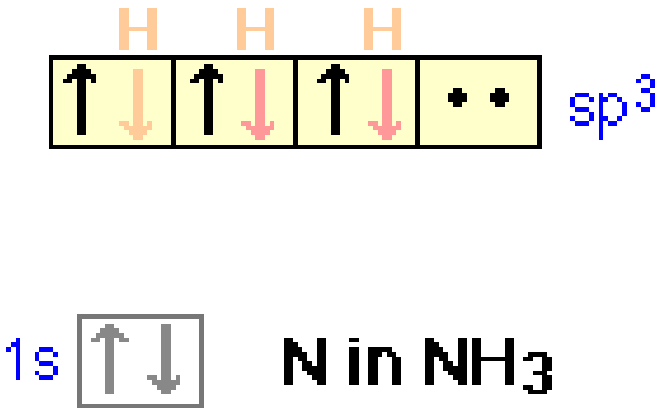


Figure: Electron configuration of nitrogen in NH_3 — the lone pair occupies one sp³ orbital while three bonding pairs occupy the remaining three sp³ orbitals

If lone pair electrons are present on the central atom, these can occupy one or more of the sp³ 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 2s and 2p orbitals, we can create four sp³-hybrid orbitals just as in carbon. Three of these can form shared-electron bonds with hydrogen, resulting in ammonia, NH_3. The fourth of the sp³ 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^+.

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.

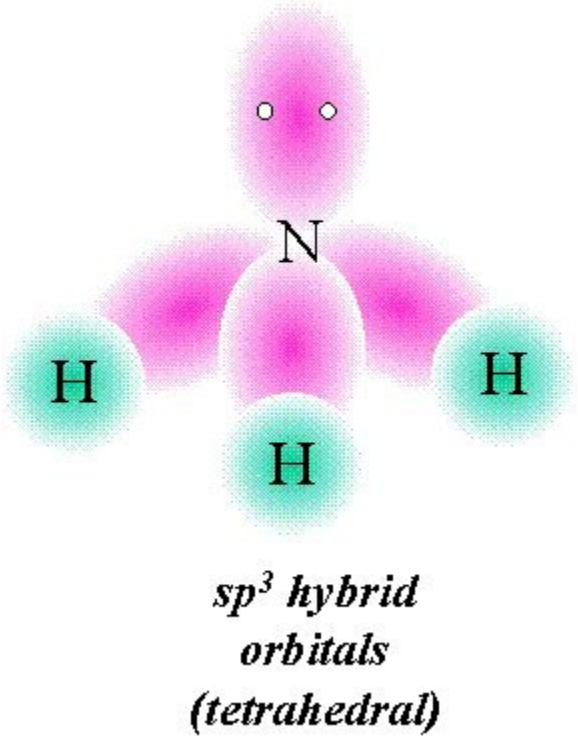
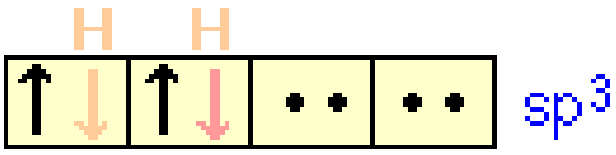


Figure: sp^3 hybridization in water (H_2O) — two sp^3 orbitals form O–H bonds while two sp^3 orbitals hold lone pairs; lone pair repulsion compresses the H–O–H angle from the ideal 109.5° to 104.5°



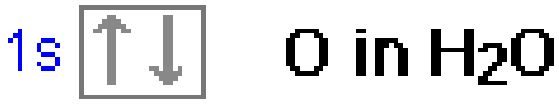


Figure: Orbital energy diagram for oxygen in water (H_2O) — sp^3 hybridization produces four orbitals; two hold lone pairs (dark boxes) and two form bonds with hydrogen atoms

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.

B) sp² Hybridization

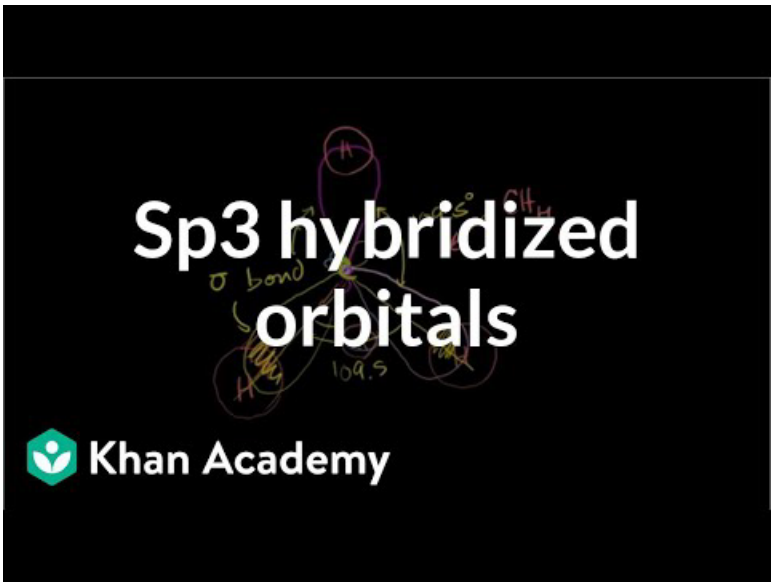


Figure: Khan Academy supplementary video: sp³ hybridized orbitals

From an energy standpoint, we can represent the transition from atomic s- and p-orbitals to an sp hybrid orbital in this way:

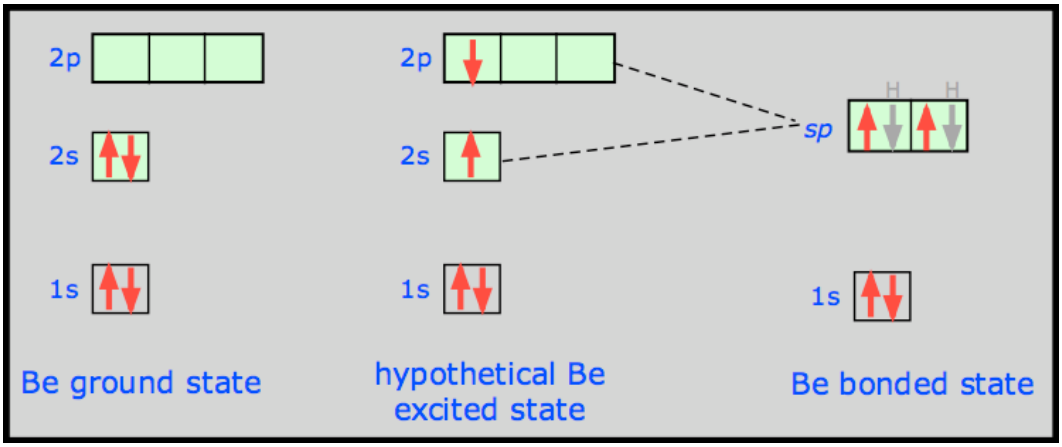


Figure: Energy diagram for sp hybridization of beryllium — the 2s and one 2p atomic orbital mix to form two sp hybrid orbitals (bonded state, right) at intermediate energy

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:

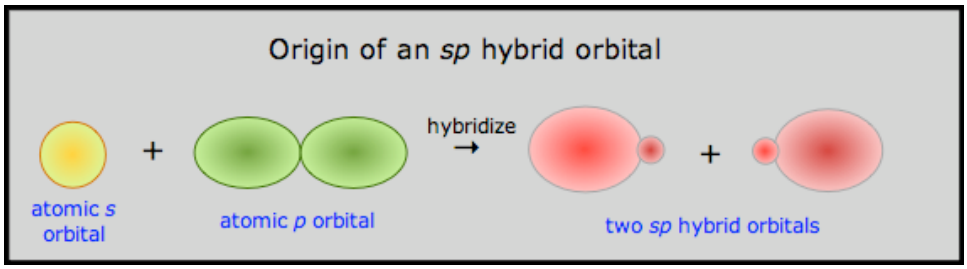


Figure: Origin of sp hybrid orbitals — an atomic s orbital and an atomic p orbital combine to produce two sp hybrid orbitals that point in opposite directions (180° apart)

The probability of finding the electron at any location is given not by ψ, but by ψ², 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, when one s-orbital mixes with two of three p-orbitals, three sp^2 hybrid orbitals are produced and one p orbital remains un-hybridized.

Figure: Formation of three sp^2 hybrid orbitals — one s orbital combines with two p orbitals to produce three equivalent sp^2 hybrids arranged at 120° in a plane, with one unhybridized p orbital remaining perpendicular

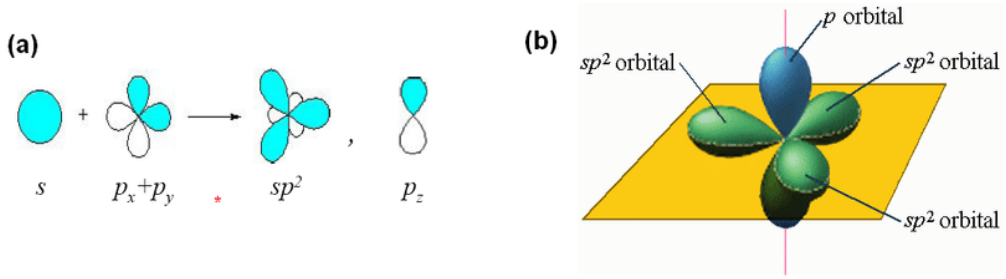


Figure: sp^2 hybridization geometry — (a) orbital combination equation and (b) three-dimensional arrangement showing three planar sp^2 hybrid orbitals and one perpendicular unhybridized pz orbital

Example: BF_3

VB Theory proposes that the central B atom in BF_3 molecule is sp^2 hybridized. The figure below shows three sp^2 hybrid orbitals in the trigonal plane, with the 3rd 2p orbital unhybridized and perpendicular to the plane. Each sp^2 hybrid orbital overlaps with 2p orbital of F atom. There are total six valence electrons present in three sp^2 orbitals, 3 from B atom and one from each F atom.

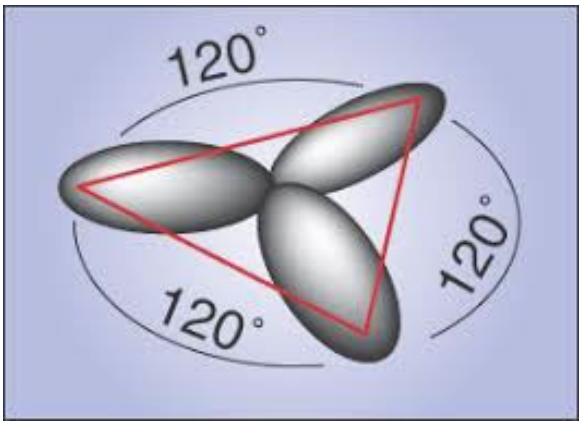


Figure: sp² hybridization in BF_3 — three sp² orbitals of boron form sigma bonds with fluorine atoms in a trigonal planar arrangement with 120° bond angles

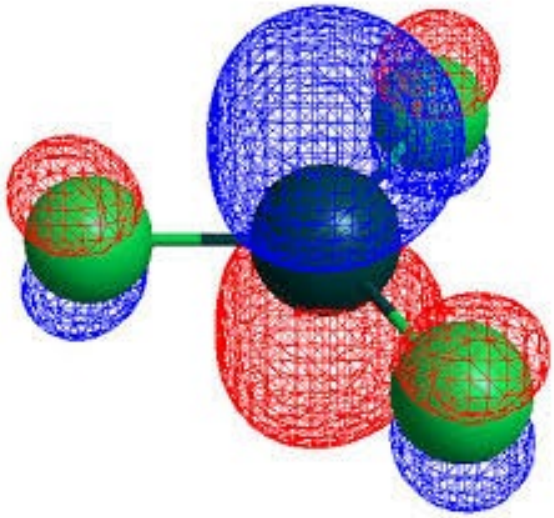


Figure: Electron density surface of BF_3 — the trigonal planar geometry and the unhybridized p orbital above and below the plane are visible in this molecular orbital representation

Ethylene (C_2H_4) is the example of a molecule where sp² hybridization can be observed. 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 lie perpendicular to the sp² plane. Two sp² orbitals from each C forms C-H sigma bond by overlapping 1s orbital of H atom.

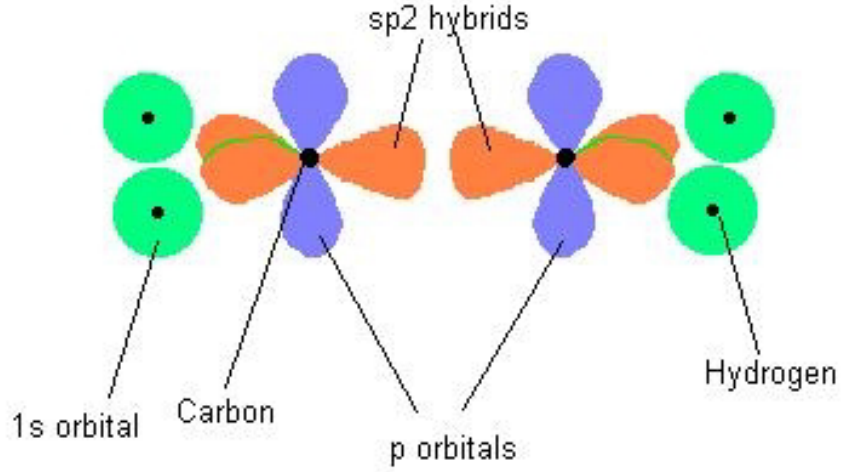


Figure: sp² orbital arrangement in ethylene (C_2H_4) — sigma bonds form from sp² hybrid overlaps; the remaining unhybridized p orbitals on each carbon are parallel and form the pi bond

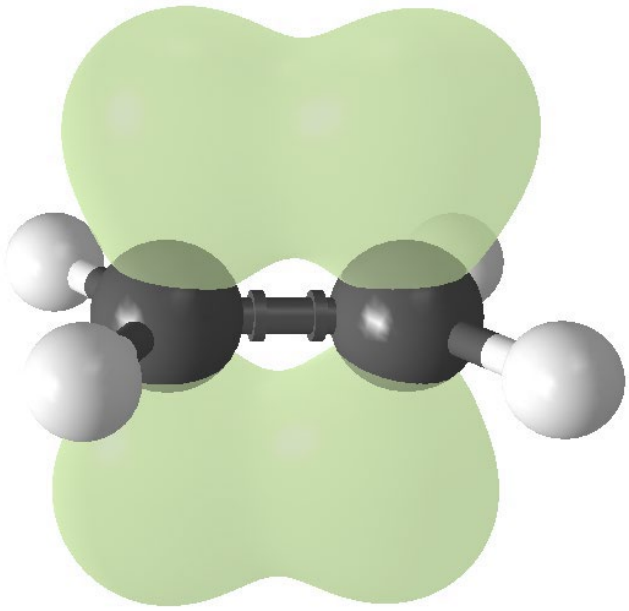


Figure: Pi electron cloud in ethylene (C_2H_4) — the delocalized pi bonding orbital (green) forms above and below the molecular plane from side-to-side overlap of the unhybridized p orbitals on each carbon

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.

Trigonal (sp^2) hybridization

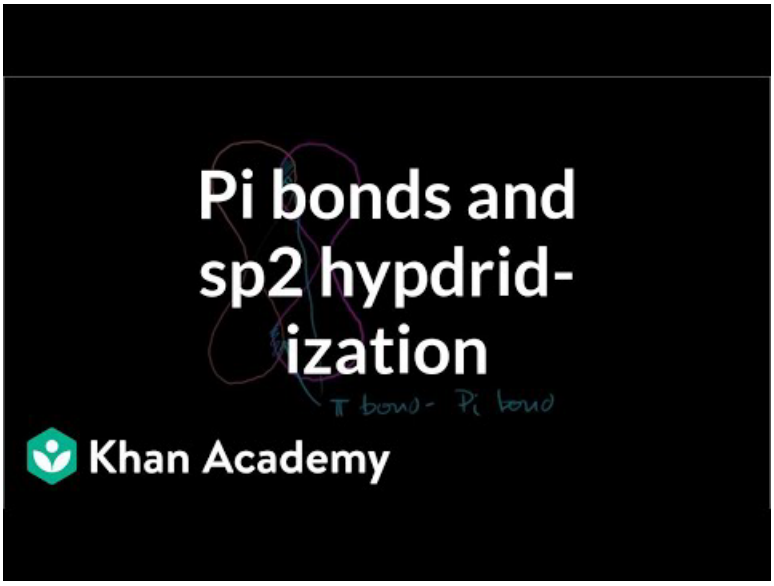


Figure: Khan Academy supplementary video: Pi bonds and sp^2 hybridization

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.

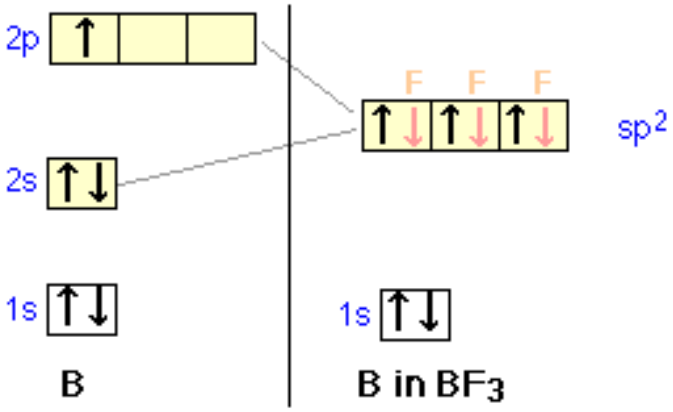


Figure: Orbital configuration of boron: ground state (left) versus sp^2 hybridized state in BF_3 (right) — hybridization produces three equivalent half-filled sp^2 orbitals

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.

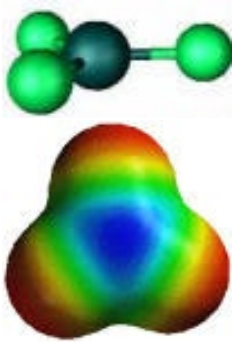


Figure: BF_3 molecular models — (left) ball-and-stick model showing trigonal planar geometry; (right) electrostatic potential map showing electron density distribution

C) sp Hybridization

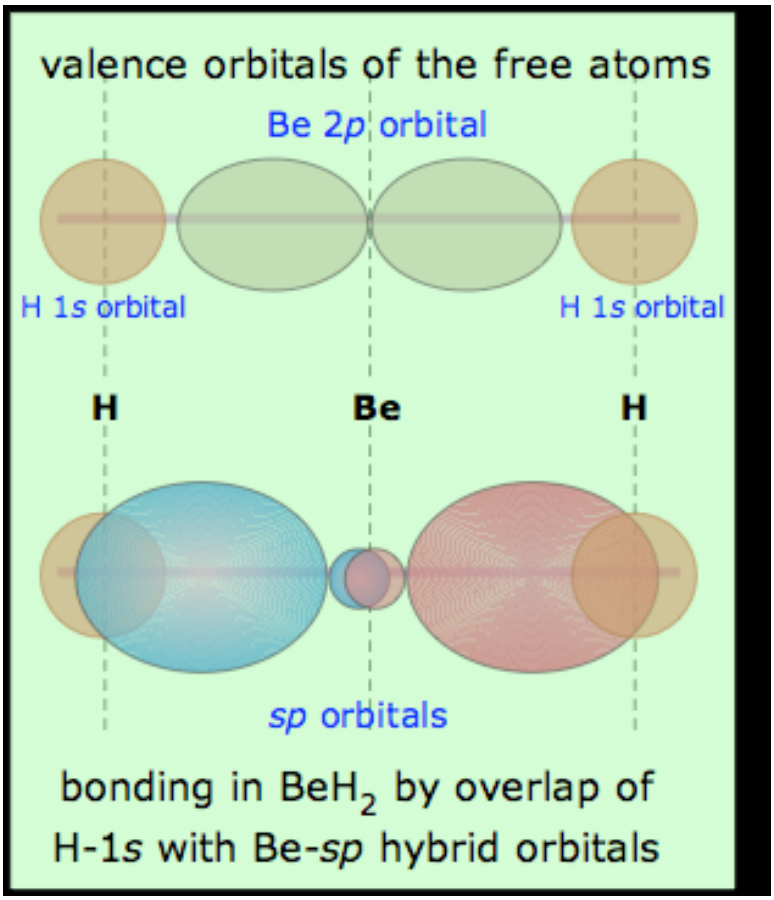


Figure: sp Hybridization in BeH_2 — the beryllium 2s and one 2p orbital combine to form two sp hybrid orbitals (180° apart) that overlap with hydrogen 1s orbitals, giving a linear molecule

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. As far as the shape of the molecule is concerned, the result is exactly the same as predicted by the VSEPR model. 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.

Beryllium chloride is one example of a molecule 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 bonds.

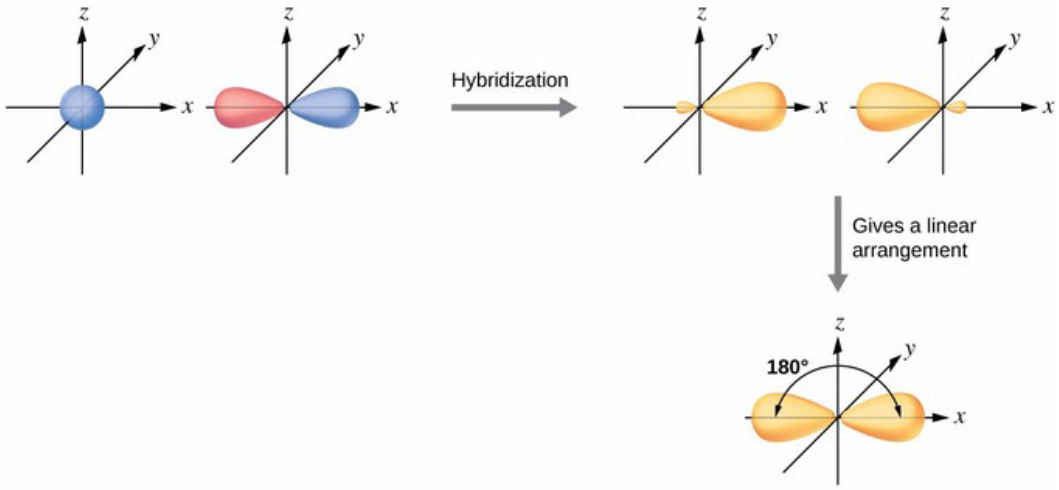


Figure: sp Hybridization in $BeCl_2$ — the 2s and one 2p orbital on beryllium hybridize to form two sp orbitals oriented 180° apart, producing the linear Cl–Be–Cl geometry

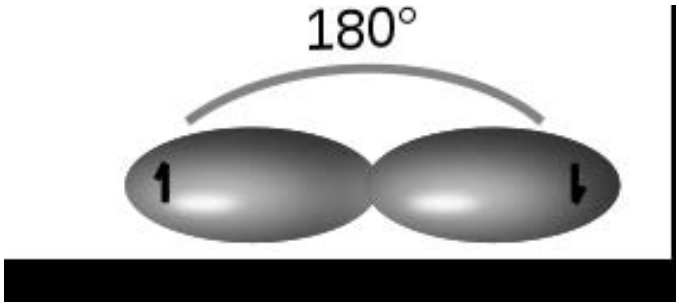


Figure: Ball-and-stick model of $BeCl_2$ (beryllium chloride) — linear geometry resulting from sp hybridization of beryllium

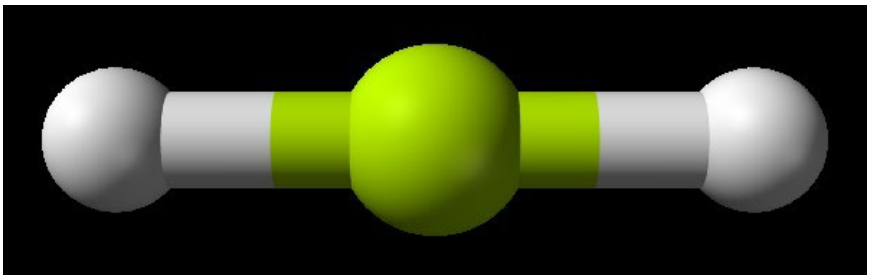


Figure: Orbital energy diagram for sp hybridization in $BeCl_2$ — isolated Be atom (left) versus hybridized Be (right) showing two sp hybrid orbitals at intermediate energy and two remaining unhybridized 2p orbitals

In case of acetylene (C_2H_2), each carbon has two unhybridized p orbitals.

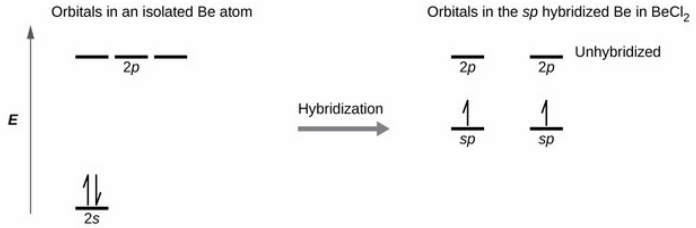


Figure: sp-Hybridized carbon in acetylene (C_2H_2) — two sp hybrid orbitals (gray, along the molecular axis) plus two unhybridized p orbitals (red and blue, mutually perpendicular) that will form two pi bonds

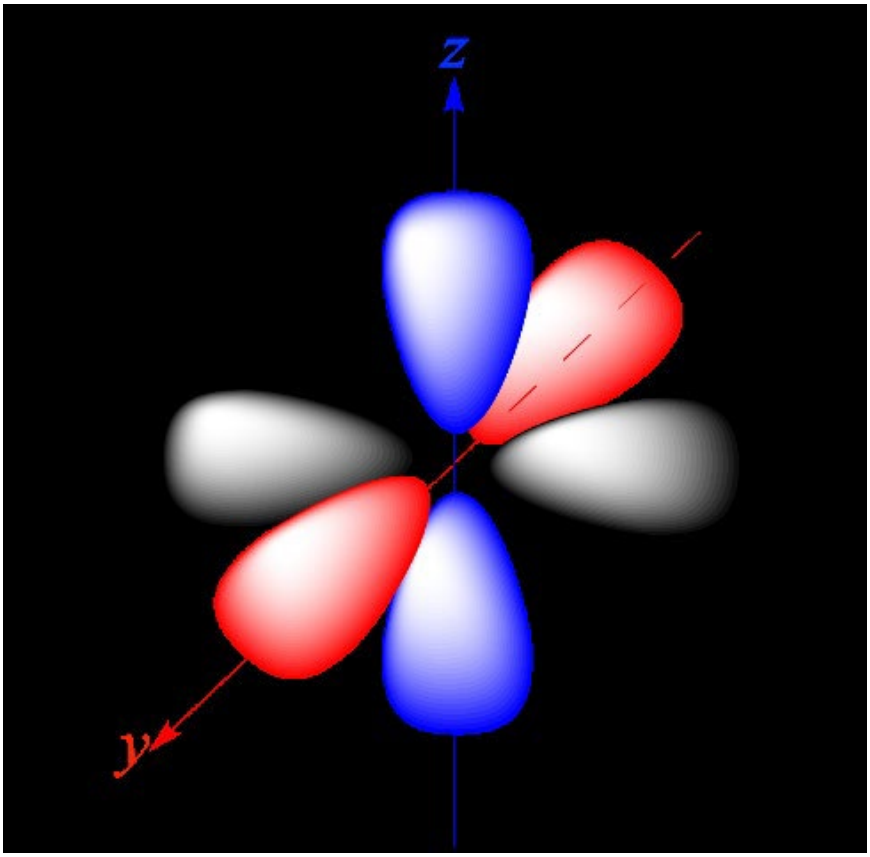


Figure: Orbital hybridization diagram for carbon in acetylene — 2s and 2pz combine to form two sp hybrid orbitals; 2px and 2py remain unhybridized and form two pi bonds

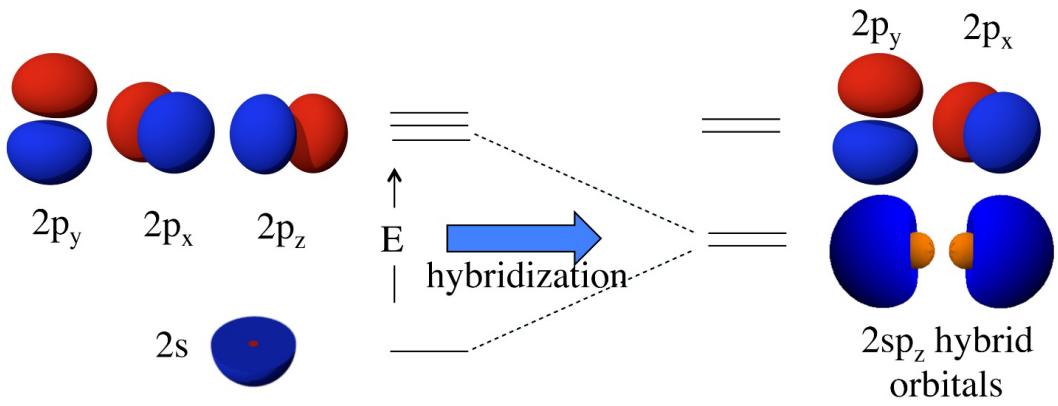


Figure: Energy level diagram for sp hybridization in acetylene — each carbon contributes one 2s and one 2p orbital to form two sp hybrids (50% s, 50% p character); the remaining two p orbitals form the two pi bonds of the C≡C triple bond

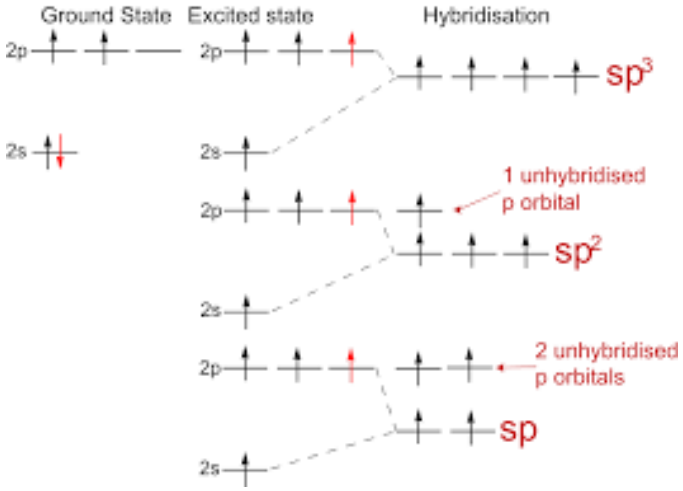


Figure: Summary orbital box diagram — progression from ground state through excited state to sp³, sp², and sp hybridized configurations, showing the number of unhybridized p orbitals remaining in each case

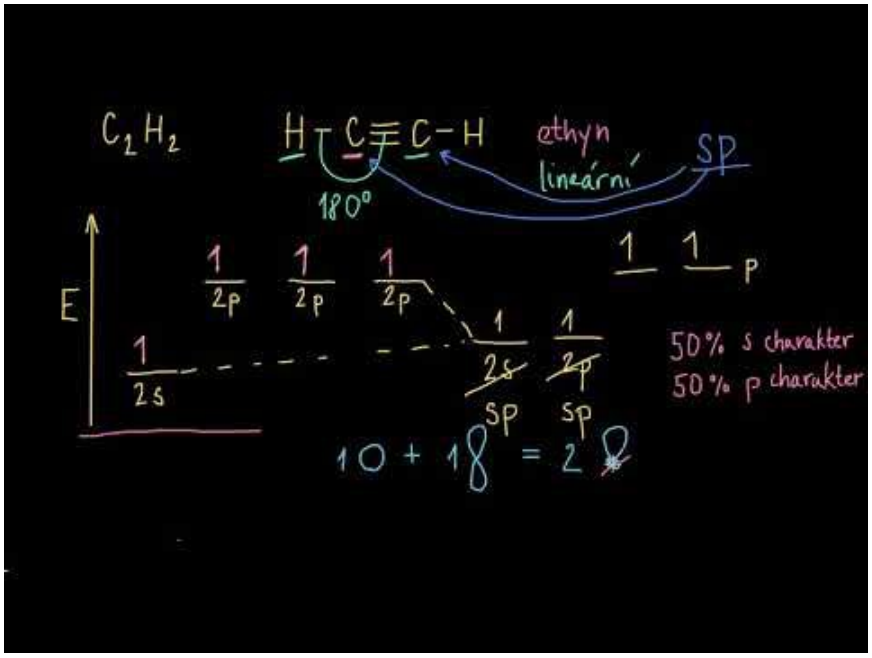


Figure: Khan Academy instructional diagram for sp hybridization in acetylene (C_2H_2) — showing the orbital energy levels, the linear geometry, and the 50% s / 50% p character of the sp hybrid orbitals

What you should be able to do:

3. Make sure you thoroughly understand the essential ideas which have been presented above.
4. Explain why the sharing of atomic orbitals (as implied in the Lewis model) cannot adequately account for the observed bonding patterns in simple molecules.
5. Sketch out a diagram illustrating how the plots of atomic s- and p- orbital wave functions give rise to a pair of hybrid orbitals.
6. 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.
7. 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^3d & sp^3d^2 Hybridization

There are five d orbitals that can also take part in hybridization:

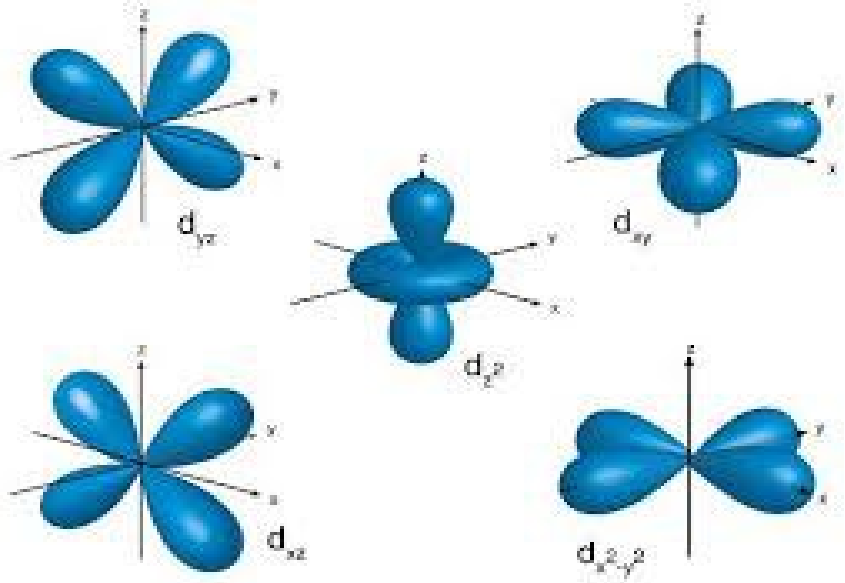


Figure: The five d atomic orbitals — dyz, dxy, dz², dxz, and dx²−y² — each has a distinct three-dimensional shape. These orbitals participate in sp³d and sp³d² hybridization schemes in molecules with expanded octets

sp³d Hybridization

Pentagonal bipyramidal molecules: sp³d hybridization

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 outermost 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 sp³d hybrid orbitals directed toward the corners of a trigonal bipyramid, as is predicted by VSEPR theory.

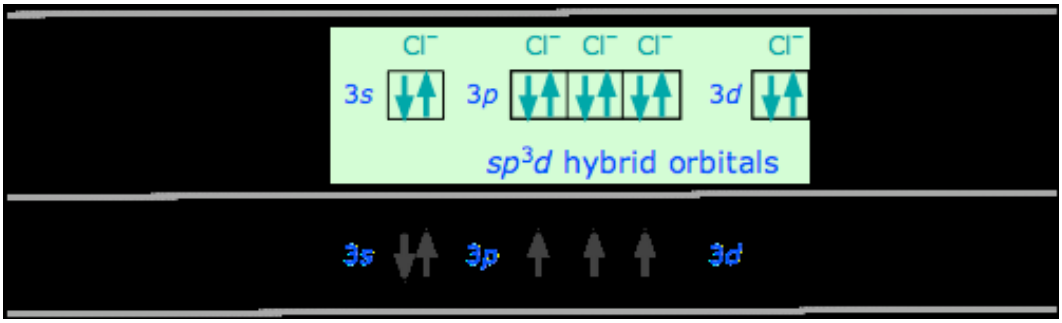


Figure: Orbital box diagram for sp³d hybridization in PCl_5 — the 3s, three 3p, and one 3d orbital of phosphorus each share an electron with a chlorine atom, producing five equivalent sp³d hybrid orbitals

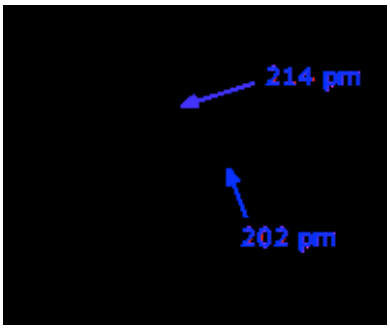


Figure: Structural diagram of PCl_5 — the five sp^3d hybrid orbitals produce a trigonal bipyramidal geometry with axial bond lengths of 214 pm and equatorial bond lengths of 202 pm

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 PCl_5, VB model proposes one 3s, three 3p and one of the five 3d orbitals of the central P atom mix and form five sp^3d hybrid orbitals.

E) sp^3d^2 Hybridization

To rationalize the shape of SF_6, 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 form sp^3d^2 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 atoms.

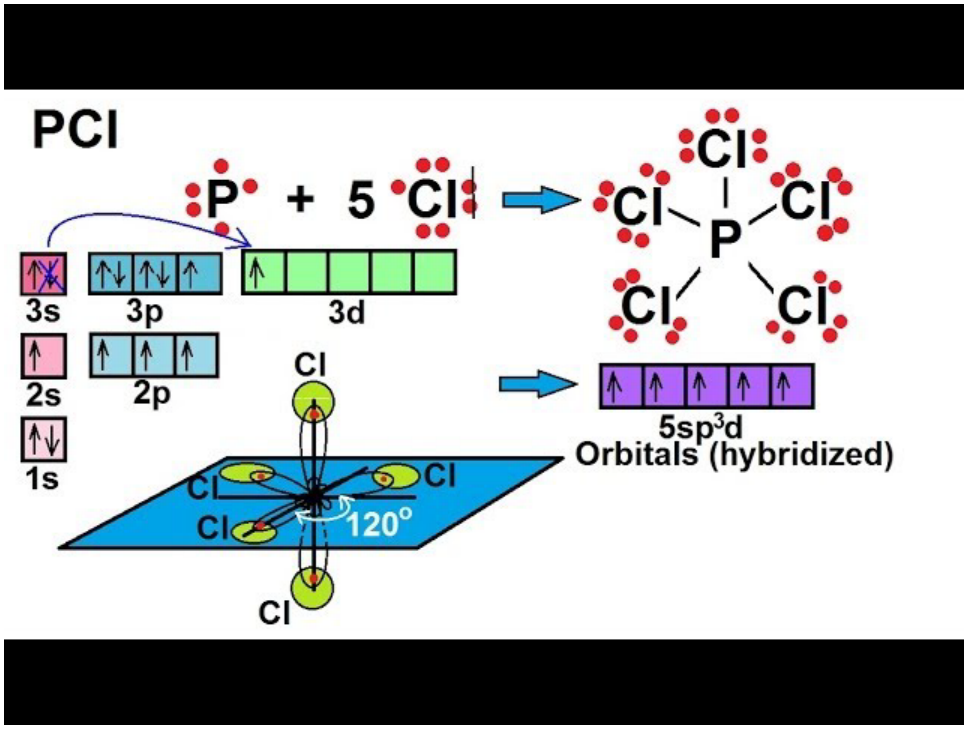


Figure: sp^3d hybridization diagram for PCl_5 — phosphorus combines one 3s, three 3p, and one 3d orbital to form five equivalent sp^3d hybrid orbitals in a trigonal bipyramidal arrangement; each orbital forms a bond with one chlorine atom

Octahedral coordination: sp^3d^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.

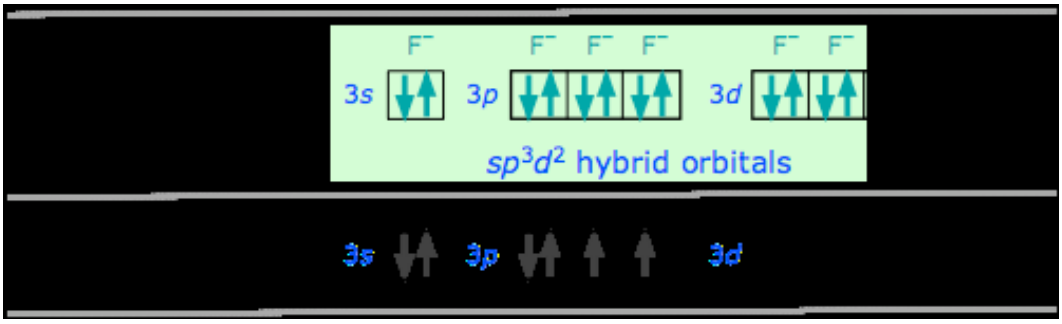


Figure: Orbital box diagram for sp^3d^2 hybridization in SF_6 — the 3s, three 3p, and two 3d orbitals of sulfur combine with six fluorine electrons to form six equivalent sp^3d^2 hybrid orbitals in an octahedral arrangement

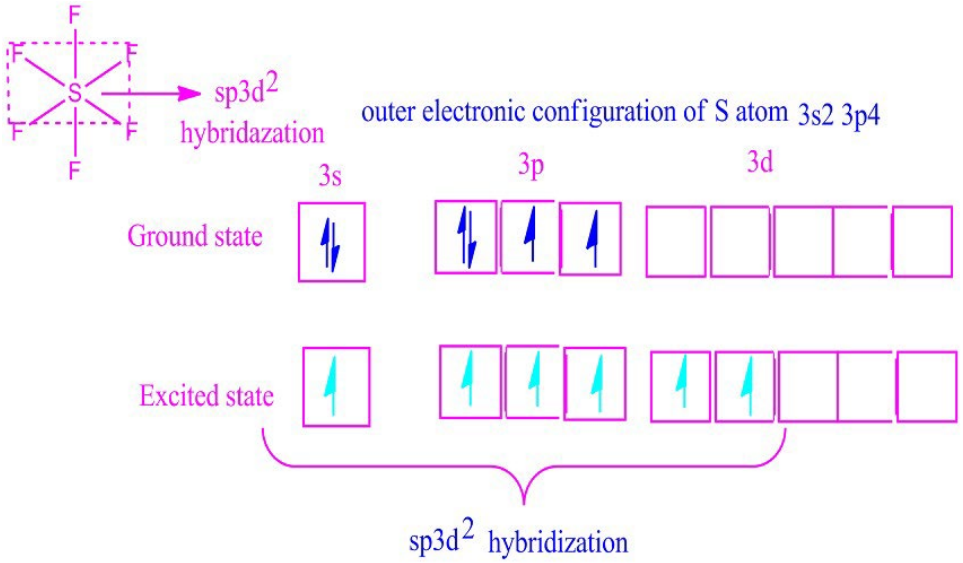


Figure: sp^3d^2 hybridization in SF_6 — (top) octahedral structure with six fluorine atoms at the vertices; (bottom) orbital diagrams showing the ground state and excited state configurations of sulfur, and the resulting sp^3d^2 hybrid set

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.

In summary:

- Six electron pairs (octahedral geometry): sp^3d^2
- Five electron pairs (trigonal bipyramidal): sp^3d
- Four electron pairs (tetrahedral): sp^3
- Three electron pairs (trigonal planar): sp^2

- Two electron pairs (linear): sp

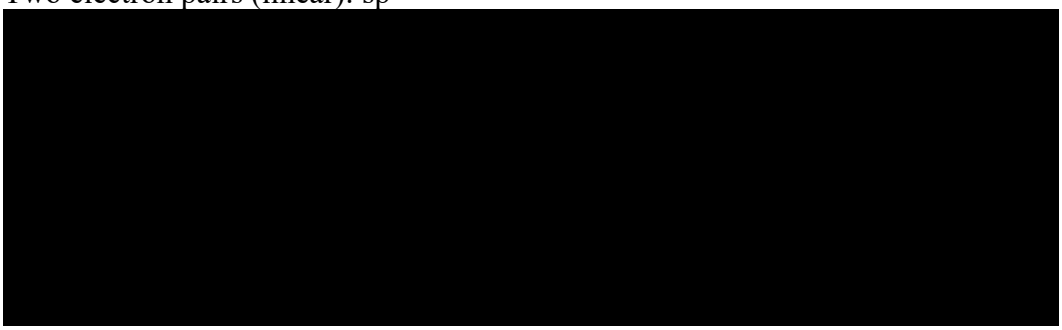


Figure: Comparison of sp^x, sd^x, and sp^x·d^y hybrid orbital shapes — the character of the hybrid orbital changes as the proportion of s, p, and d contributions varies, affecting both the shape and directionality of the resulting bond

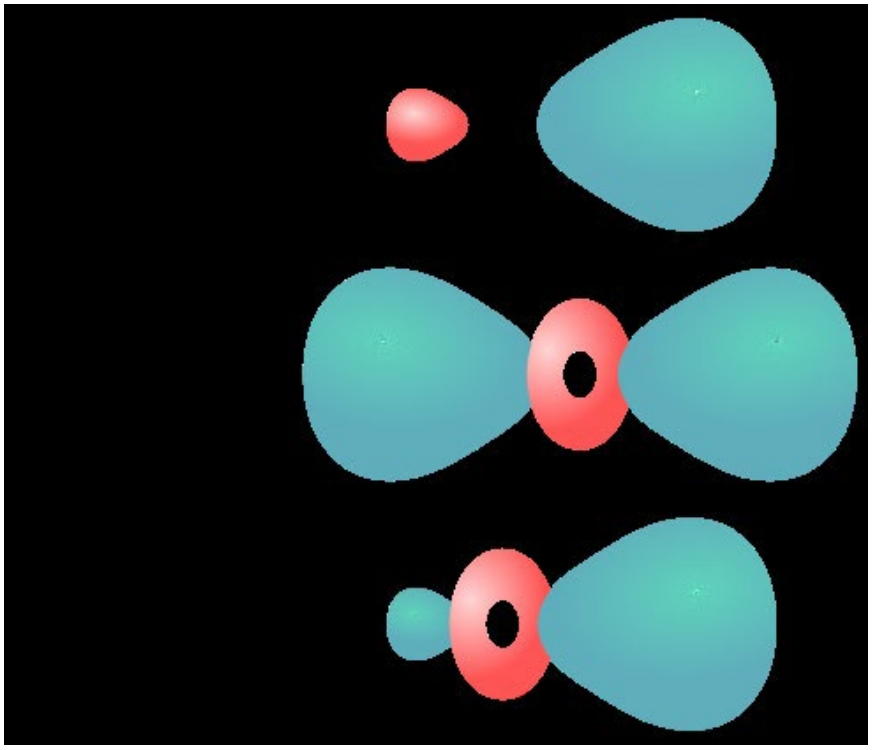


Figure: Resonance structures of SF_6 — the three equivalent Lewis structures (each ×12 or ×3 degenerate) converge to a resonance hybrid in which all six S–F bonds are equivalent, each with partial negative charge (−1/3) on fluorine

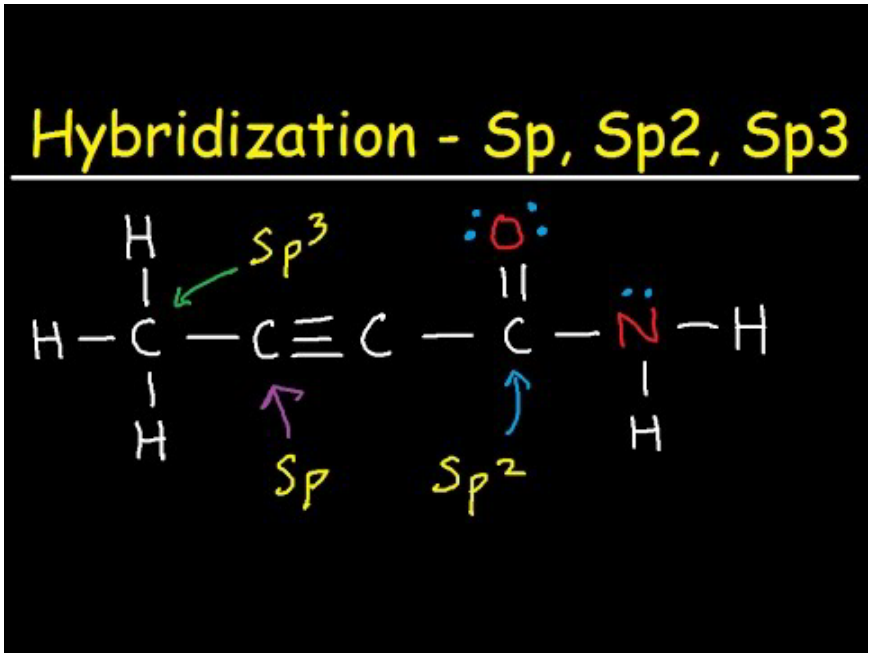


Figure: Khan Academy supplementary video: Hybridization — sp, sp², and sp³ hybridized carbon atoms illustrated on a single organic molecule

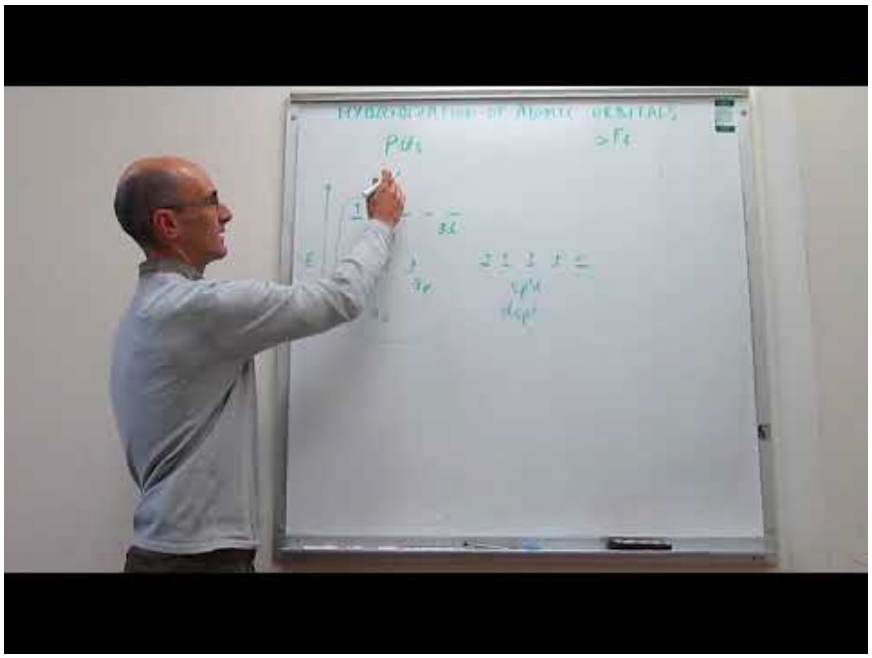


Figure: Supplementary instructional video on sp³d and sp³d² hybridization — an instructor at a whiteboard demonstrating orbital hybridization schemes for period 3 and beyond elements

*** 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.

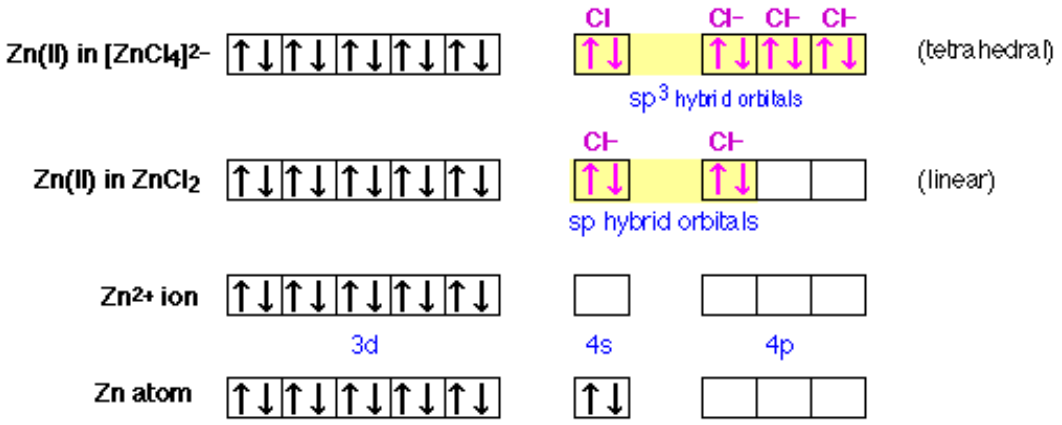


Figure: Electron configuration comparison for zinc species — Zn atom, Zn^{2+} ion, $ZnCl_2$ (linear, sp hybridization), and $[ZnCl_4]^{2-}$ (tetrahedral, sp^3 hybridization) showing how the hybrid type changes with coordination number

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 — each chloride ion possesses a complete octet of electrons. 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 $[PtCl_4]^{2-}$. The parent central ion (Pt^{2+} in this case) contains only eight electrons in its outmost d-subshell.

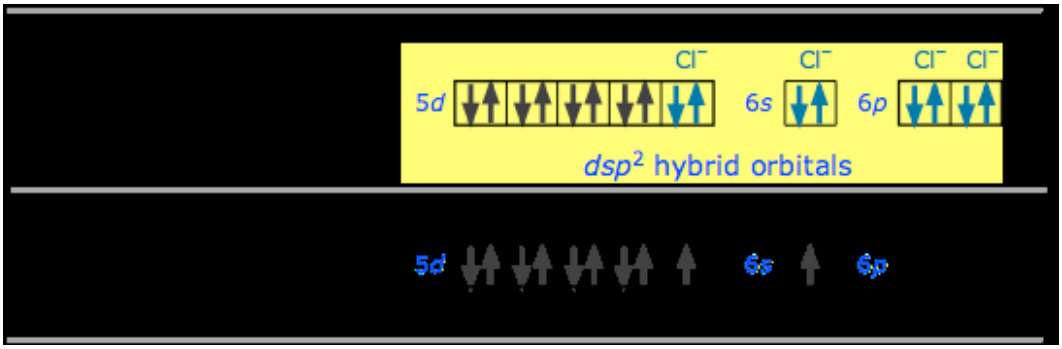


Figure: dsp² hybridization in $[PtCl_4]^{2-}$ — the 5d, 6s, and two 6p orbitals of platinum combine to form four equivalent dsp² hybrid orbitals that accept electron pairs from four chloride ligands in a square-planar arrangement

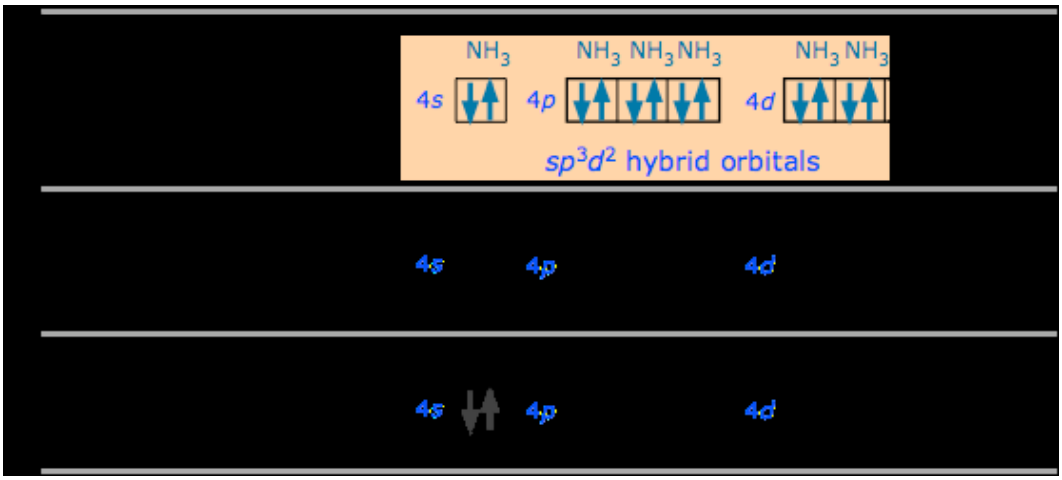


Figure: sp^3d^2 hybridization in the hexamminezinc(II) ion $[Zn(NH_3)_6]^{2+}$ — the 4s, 4p, and 4d orbitals combine to accept six NH_3 ligands in an octahedral coordination geometry

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 surprise, 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 outermost 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.

In sp^3d^2 hybridization the bonding orbitals are derived by mixing atomic orbitals having the same principal quantum number. A slightly different arrangement, known as d^2sp^3 hybridization, involves d orbitals of lower principal quantum number. Both arrangements produce octahedral coordination geometries.

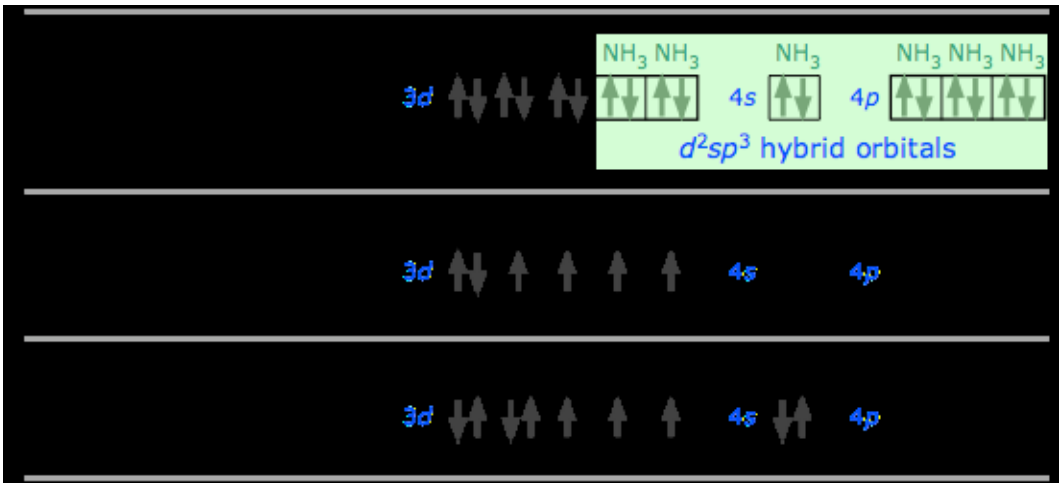


Figure: d^2sp^3 hybridization in hexamminecobalt(III) $[Co(NH_3)_6]^{3+}$ — cobalt uses two 3d, one 4s, and three 4p orbitals to form six d^2sp^3 hybrid orbitals that accept the six ammonia ligands in an octahedral arrangement

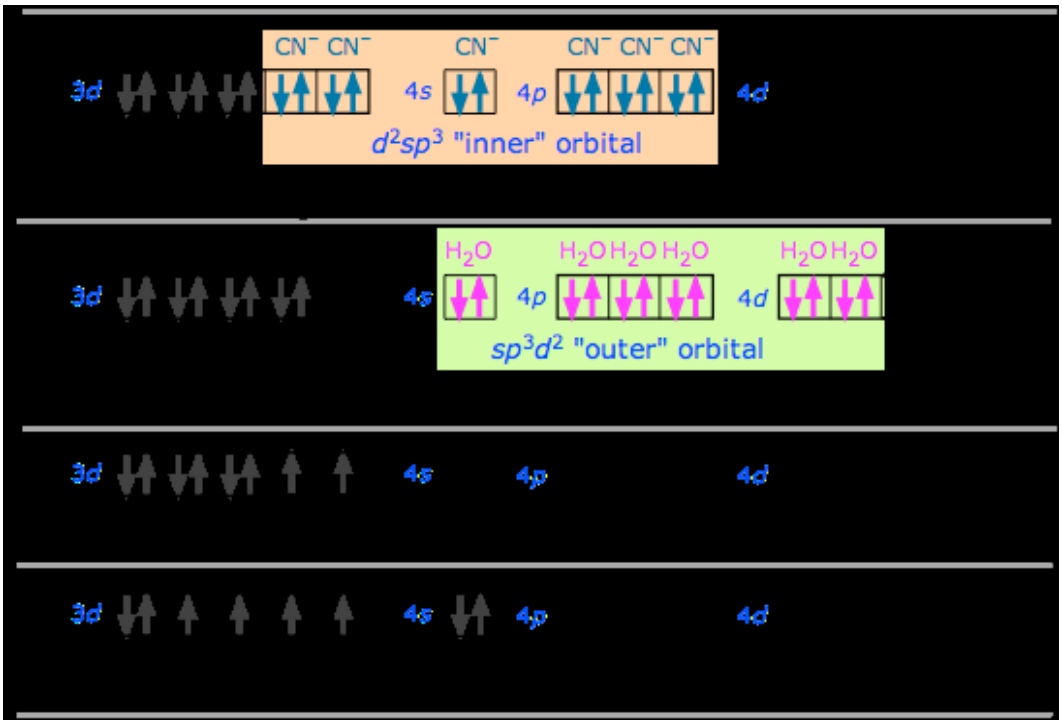


Figure: Inner-orbital d^2sp^3 versus outer-orbital sp^3d^2 octahedral complexes of iron(II) — $Fe(CN)_6^{4-}$ uses inner 3d orbitals (inner orbital complex) while $Fe(H_2O)_6^{2+}$ uses outer 4d orbitals (outer orbital complex)

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.

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 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.

Are hybrid orbitals 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. 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

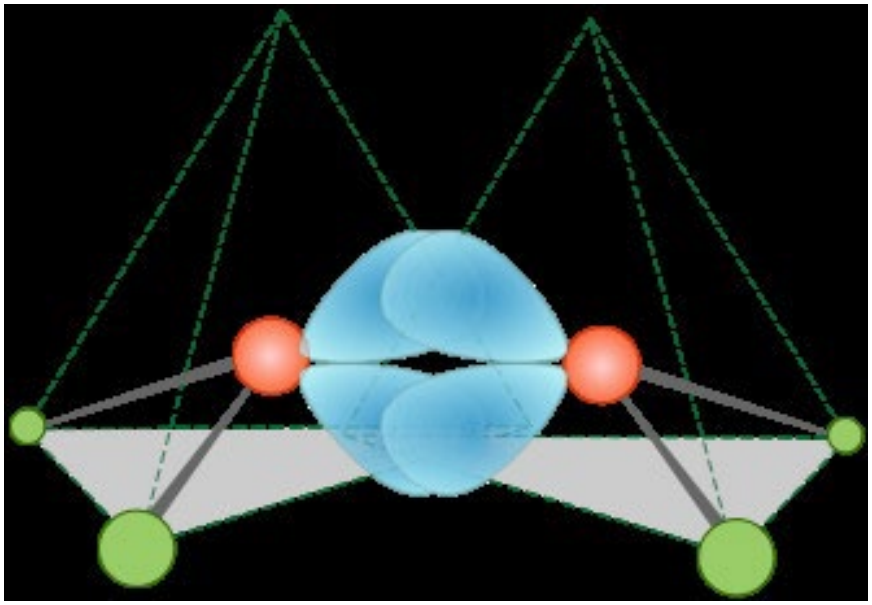


Figure: Bent-bond (banana bond) model of ethylene — an alternative to the sigma/pi description where the C=C double bond is represented by two equivalent curved ("banana") bonds rather than one sigma and one pi bond

Figure: Cyclopropane (C_3H_6) — the 60° C–C–C bond angles are far less than the tetrahedral 109.5°, requiring bent (banana) bonds rather than conventional sp^3 sigma bonds to describe the ring bonding

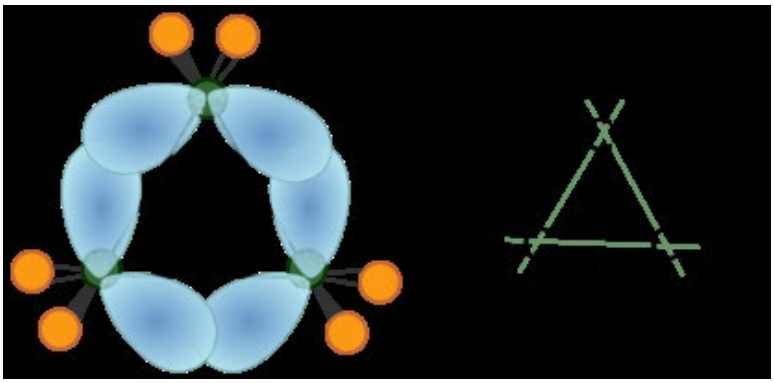


Figure: Three-dimensional bent-bond orbital model of cyclopropane — the orbital lobes arc outward along each C–C edge of the triangle rather than pointing directly between the nuclei, reflecting the ring strain from the compressed bond angles

What you should be able to do:

8. Make sure you thoroughly understand the following essential ideas which have been presented above.
9. Sketch out diagrams showing the hybridization and bonding in compounds containing single, double, and triple carbon-carbon bonds.
10. Define sigma and pi bonds.
11. 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 its 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 by 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.

Figure: Linus Pauling — the principal developer of hybridization theory and VB theory

HYBRIDIZATION WORKSHEET

Put your own molecule and fill out the table!

Molecule	Electronic Geometry	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

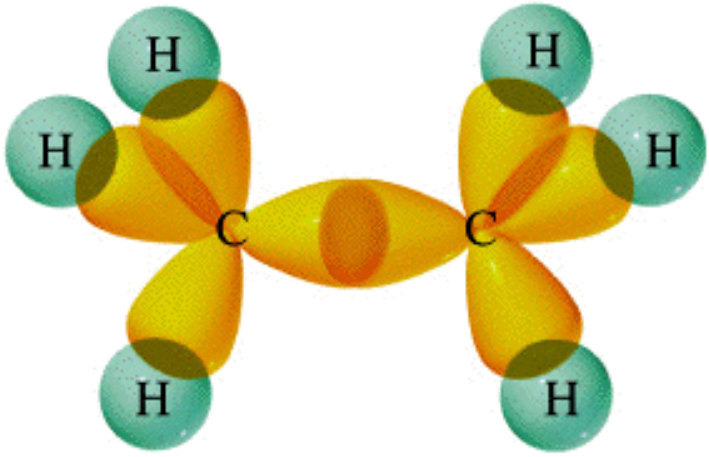


Figure: sp^3 hybridization and C–C sigma bond in ethane (C_2H_6) — each carbon forms four equivalent sp^3 hybrid orbitals; one overlaps end-to-end with the other carbon and three overlap with hydrogen atoms

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.

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.

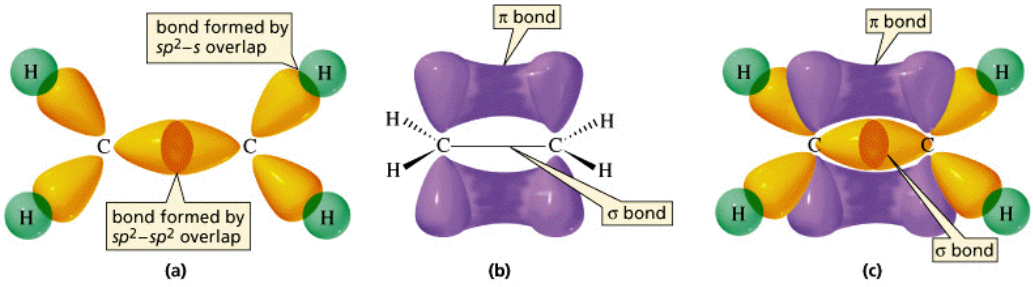


Figure: Three views of ethylene (C_2H_4): (a) sigma bond backbone from sp^2 hybrid overlaps, (b) pi bonding cloud from unhybridized pz orbital overlap, and (c) combined sigma + pi electron density

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. 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 pz 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.

More about sigma and pi bonds

The σ (sigma) bond has its maximum electron density along the line-of-centers joining the two atoms. 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. 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

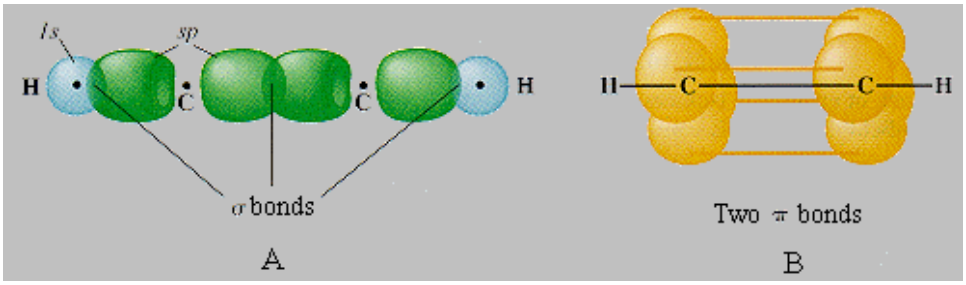


Figure: Triple bond in acetylene (C_2H_2) — (A) sigma bond framework from sp orbital overlaps; (B) complete triple bond showing one sigma bond plus two mutually perpendicular pi bonds formed by side-to-side overlap of the two unhybridized p orbitals on each carbon

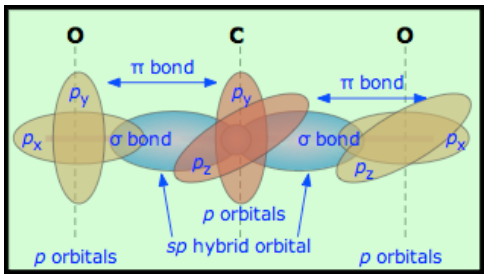


Figure: Orbital set for sp-hybridized carbon in acetylene — two sp hybrid orbitals and two unhybridized p orbitals that will form the two pi bonds of the triple bond

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.

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 sigma skeleton of the molecule is 180°.

Multiple bonds between unlike atoms

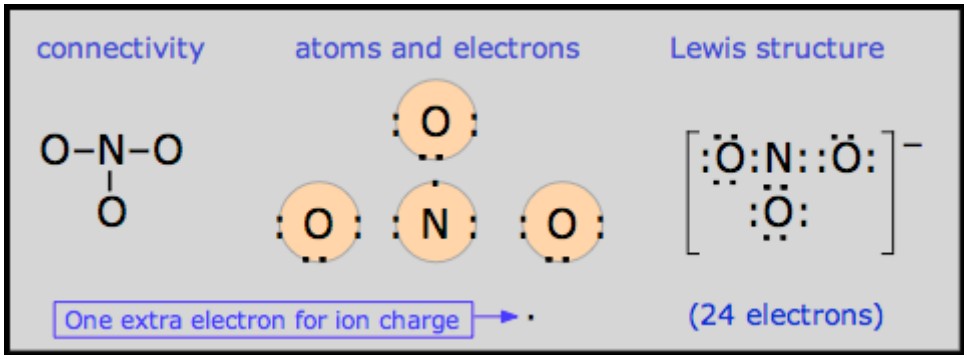


Figure: Bonding in carbon dioxide (CO_2) — sp hybridization at carbon produces two sigma bonds to oxygen; each oxygen contributes one p orbital to form two mutually perpendicular pi bonds with carbon's unhybridized p orbitals

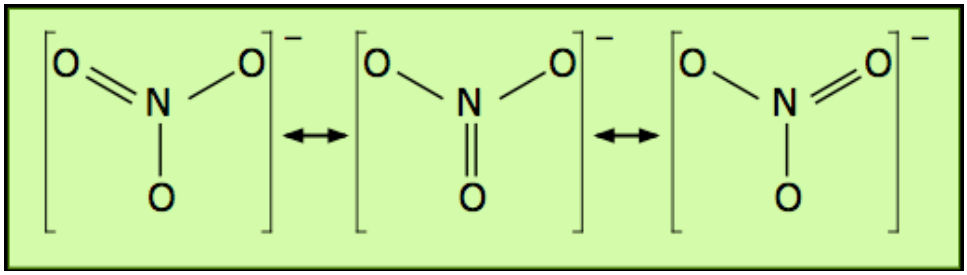


Figure: Sigma bond framework orbital diagram for CO_2 — sp hybridized carbon and oxygen orbitals forming the two C–O sigma bonds

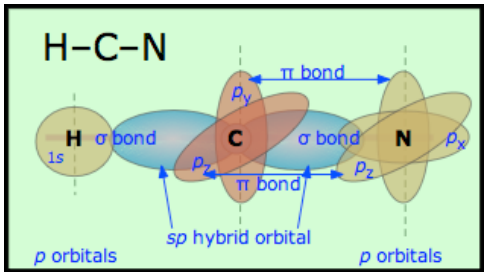


Figure: sp hybridization orbital set for carbon in CO_2

The nitrate ion

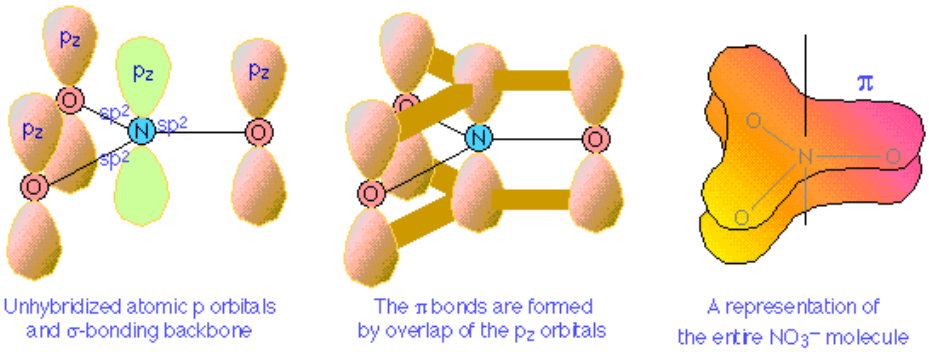


Figure: Bonding in the nitrate ion (NO_3^-) — (left) sp^2 sigma framework; (center) delocalized pi bonding from pz orbital overlap across all four atoms; (right) complete electron density representation of the ion

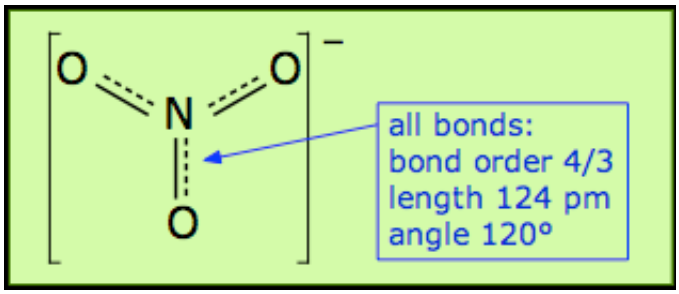


Figure: Resonance structures of NO_3^- — three equivalent Lewis structures are needed to represent the trigonal symmetry; the actual ion is a resonance hybrid with equal N–O bond order of 4/3

2 Conjugated double bonds

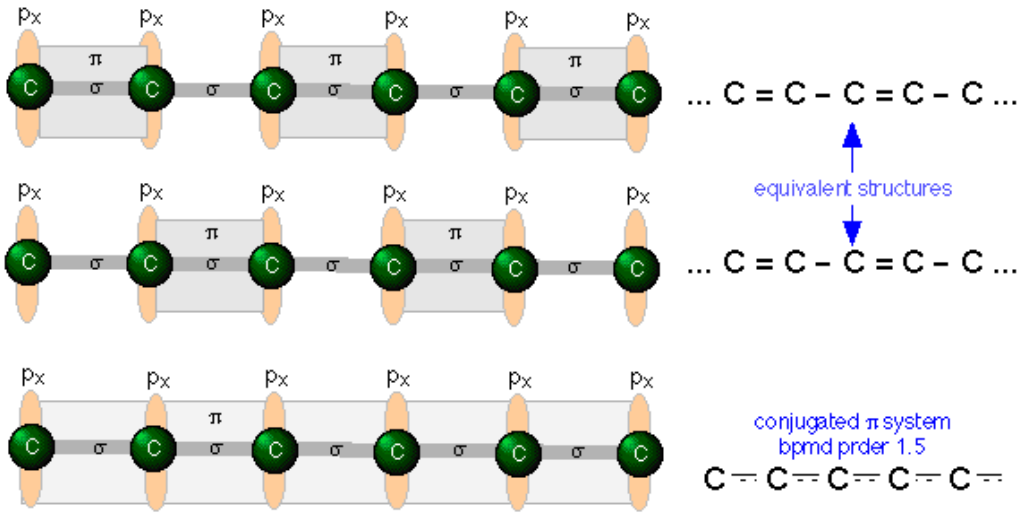
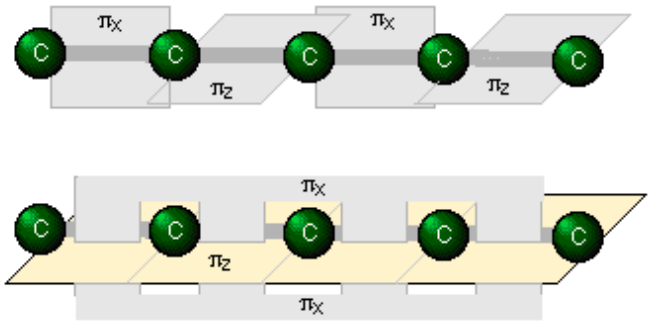


Figure: Conjugated pi bond delocalization in a carbon chain — the two equivalent resonance structures (rows 1 and 2) combine into a resonance hybrid (row 3) in which pi electron density is spread uniformly across all carbon atoms, giving each C–C bond an order of 1.5

Hybrid orbitals in benzene



... C = C = C = C ...

Figure: Sigma bond skeleton and unhybridized p orbitals of benzene — each carbon has three sp² sigma bonds (two C–C and one C–H); the unhybridized pz orbital on each carbon projects above and below the ring plane

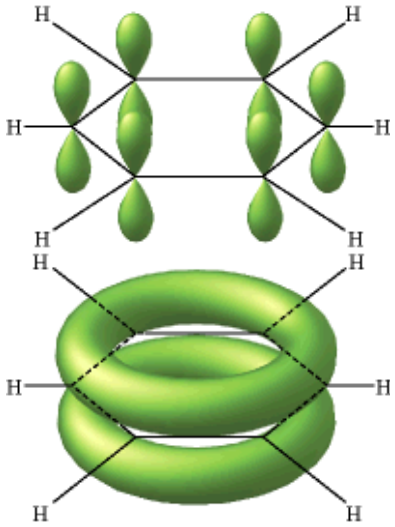


Figure: Delocalized pi electron cloud of benzene — the six pz orbitals merge into a continuous toroidal (donut-shaped) pi orbital above and below the ring plane, representing the aromatic delocalization

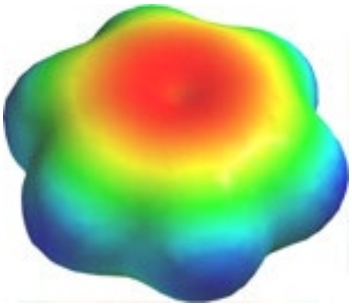


Figure: Computed electron density map of benzene — highest electron density (orange/red) appears at the outer periphery of the ring; the central hole (blue) has low electron density, consistent with the toroidal pi system

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 basic ring structure is composed of σ bonds formed from overlap of sp^2 hybrid orbitals on adjacent carbon atoms. The unhybridized carbon pz orbitals project above and below the plane of the ring. 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.

12. End to end overlap and sigma (σ) bonding. The bond resulting from such end-to-end overlap is called a sigma bond.
13. Side-to-side overlap and pi (π) bonding: When p orbitals overlap side by side, the resulting bond is a pi bond (π) and the electron density is above and below the internuclear axis.

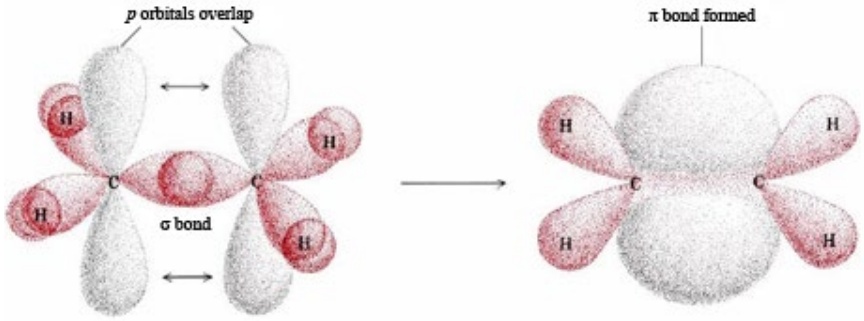


Figure: Formation of a pi (π) bond — side-to-side overlap of parallel p orbitals on adjacent carbon atoms creates a pi bond with electron density concentrated above and below the internuclear axis

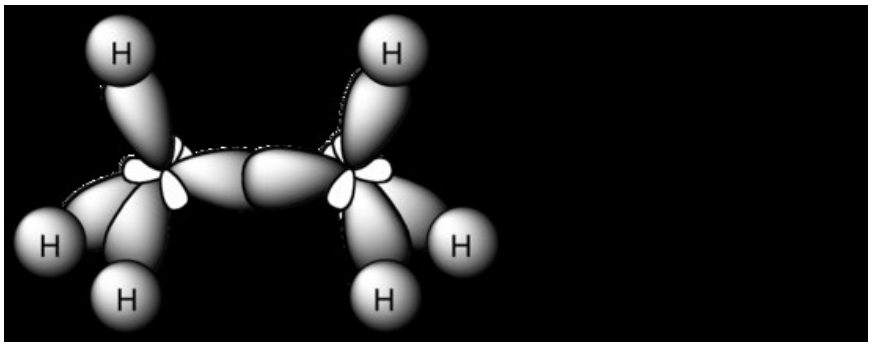


Figure: Sigma and pi bond orbital framework of ethylene — sp^2 hybrid orbitals form sigma bonds; parallel unhybridized p orbitals form the pi bond by side-to-side overlap

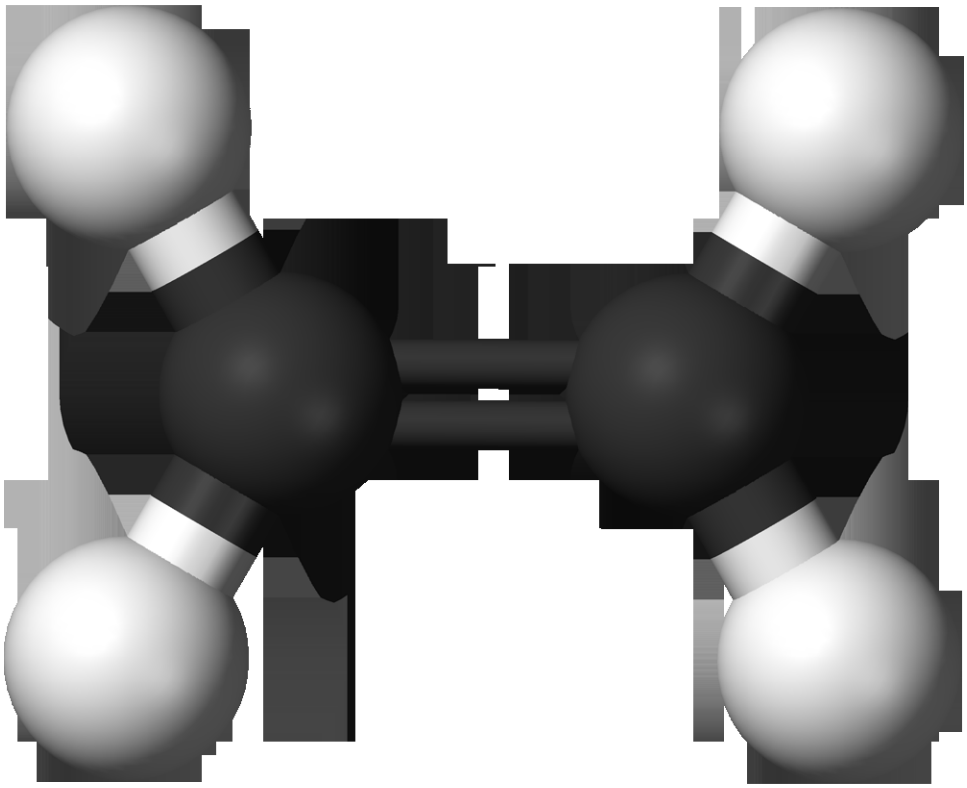


Figure: Complete orbital diagram of acetylene (H–C≡C–H) — two sp hybrid sigma bonds (C–H and C–C) plus four unhybridized p orbitals (two per carbon) oriented perpendicular to each other and to the molecular axis, forming two mutually perpendicular pi bonds

In case of acetylene, we see a triple bond C≡C consists of one sigma bond and two pi bonds. 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 to 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 result is a 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.

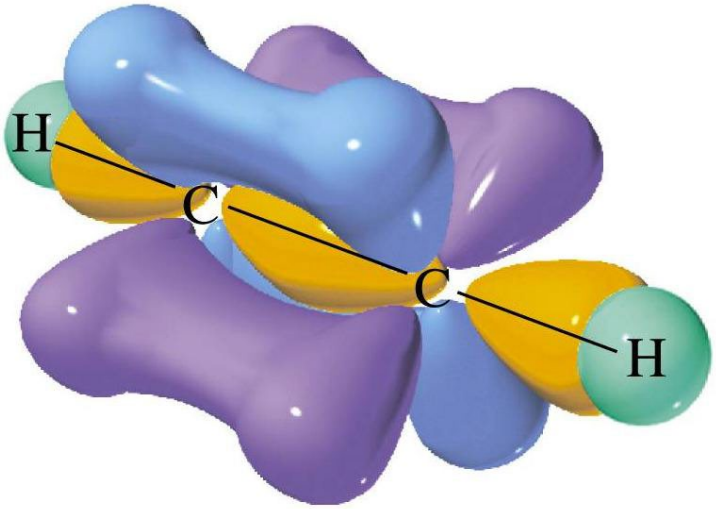


Figure: 1,2-Dichloroethane ($ClCH_2–CH_2Cl$) — the single C–C bond permits free rotation; the molecule is shown in a staggered conformation. Rotation is possible because only the sigma bond must be maintained

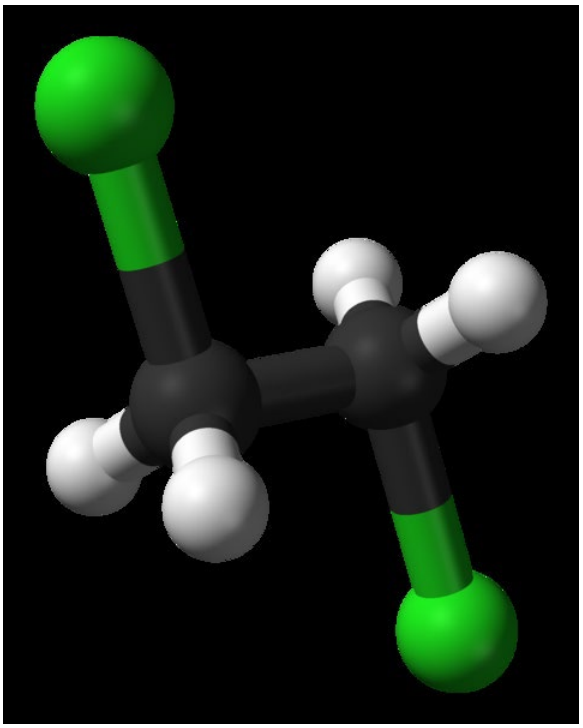


Figure: 1,2-Dichloroethene ($ClHC=CHCl$) — the C=C double bond restricts rotation because breaking the pi bond would be required; the molecule is locked in a planar geometry

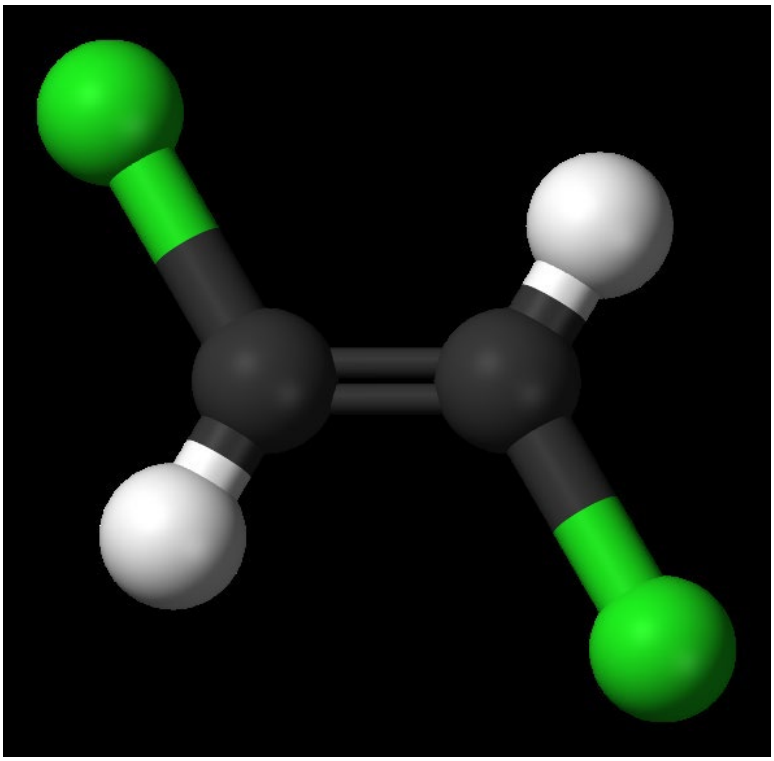


Figure: Sigma and pi bond electron density in the C=C double bond — sigma bond (yellow) along the bond axis; pi bond electron density (blue/purple) above and below the molecular plane

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, rotation around the single bond is possible.

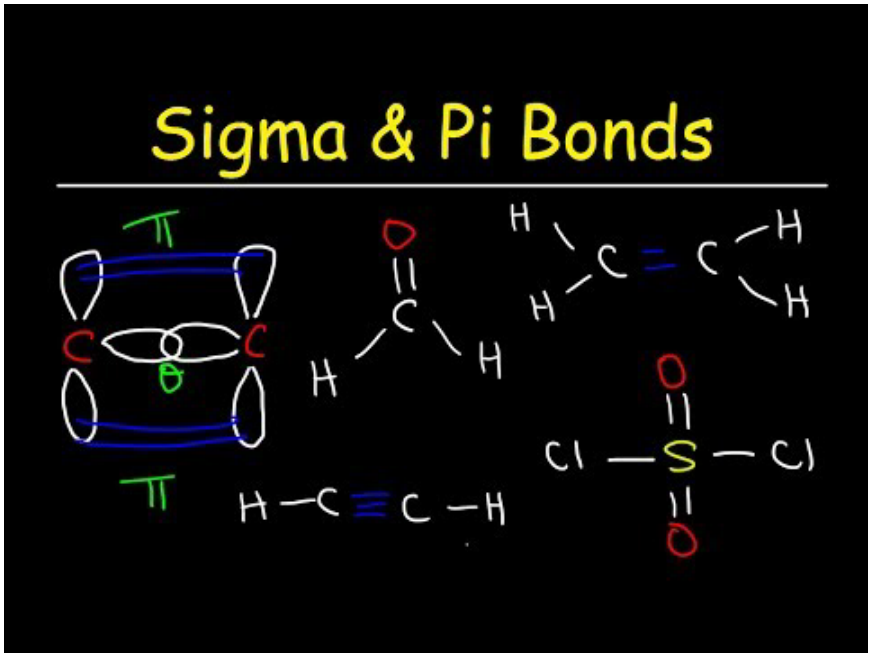


Figure: Khan Academy supplementary video: Sigma and Pi Bonds — illustrating sigma and pi bond types in various molecules including alkenes, alkynes, aldehydes, and sulfuryl compounds

What you should be able to do:

14. Make sure you thoroughly understand the following essential ideas which have been presented above.
15. Sketch out diagrams showing the hybridization and bonding in compounds containing single, double, and triple carbon-carbon bonds.
16. Define sigma and pi bonds.
17. Describe the hybridization and bonding in the benzene molecule.

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.

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 quantitative calculations. In its full development, molecular orbital theory involves a lot of complicated mathematics, but the fundamental ideas behind it are quite easily understood.

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 simplest molecule: hydrogen molecule ion

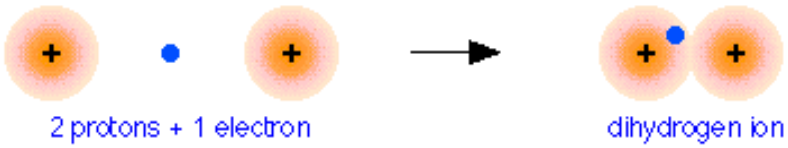


Figure: Formation of the hydrogen molecule ion (H_2^+) — a single electron shared between two protons is attracted to both nuclei simultaneously, creating a bonding molecular orbital and stabilizing the ion

As two H nuclei move toward each other, the 1s 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 1s 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. It turns out that when orbitals interact, they are free to change their forms, but there must always be the same number.

In-phase and out-of-phase wave combinations

How can we find the missing orbital? The "matter waves" corresponding to the two separate hydrogen 1s 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.

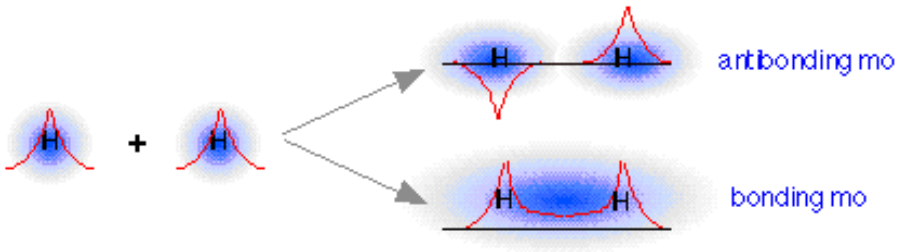


Figure: In-phase and out-of-phase combination of two hydrogen 1s orbitals — in-phase overlap (bottom) creates a bonding MO with electron density concentrated between the nuclei; out-of-phase overlap (top) creates an antibonding MO with a node between the nuclei

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.

The bonding orbital will have the lower potential energy, as the electron can simultaneously be close to two nuclei.

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.

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 is possible. Because the electron density–electron repulsions are reduced, the bonding MO is lower in energy than the isolated AOs.

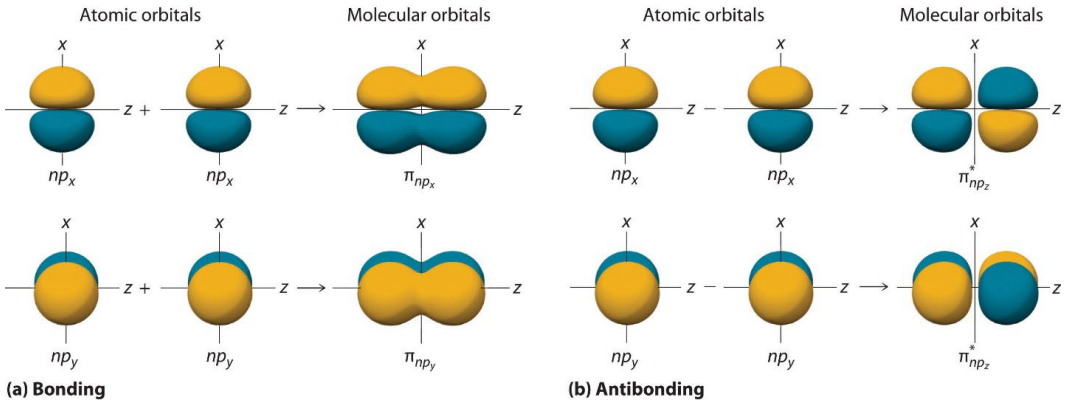


Figure: MO energy diagram for H_2 — two hydrogen 1s atomic orbitals combine to form a lower-energy bonding MO (σ1s, occupied by both electrons) and a higher-energy antibonding MO (σ1s, empty in ground state)*

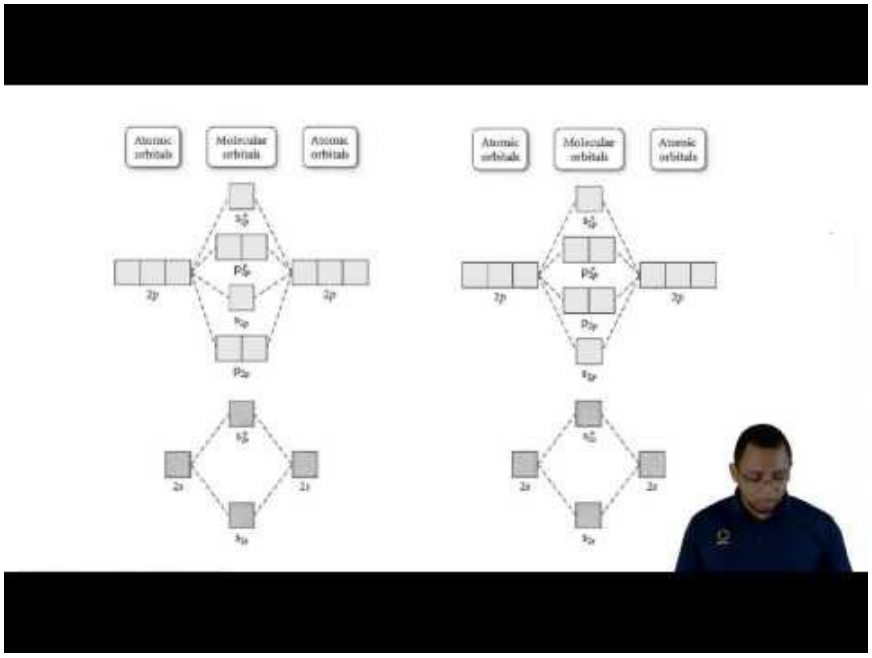


Figure: MO energy level diagram for H_2 — bonding MO (1σg) lies below the atomic orbital energy (stabilized); antibonding MO (1σu) lies above (destabilized); both electrons occupy the bonding MO, giving bond order = 1

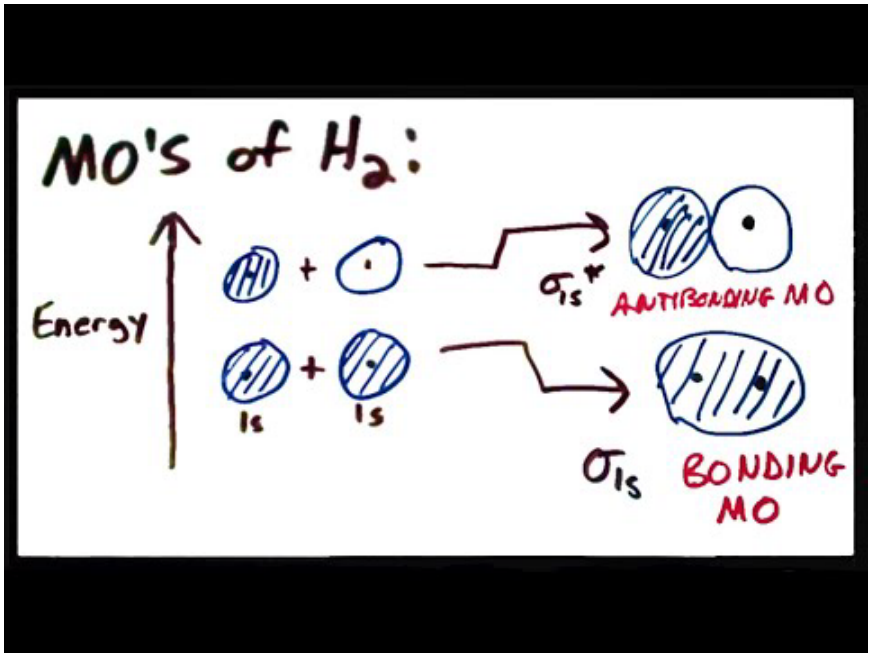


Figure: MO energy diagram for He_2 — four electrons fill both bonding and antibonding MOs equally, giving a bond order of 0 and predicting that dihelium (He_2) does not exist as a stable molecule

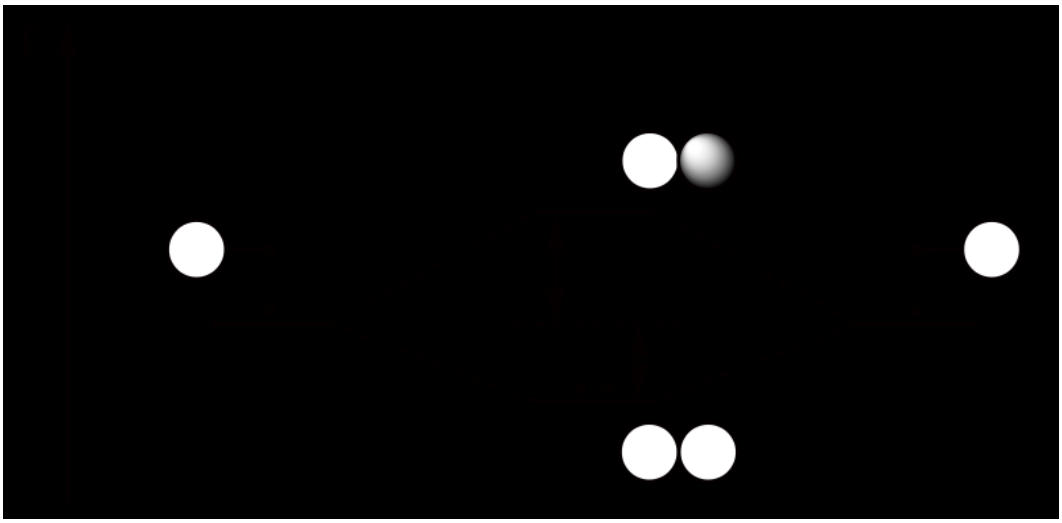


Figure: MO energy diagram for dioxygen (O_2) — twelve valence electrons fill bonding and antibonding MOs; the two highest-energy electrons occupy separate degenerate π antibonding orbitals (one each, spin-parallel), correctly predicting that O_2 is paramagnetic and has bond order 2*

The diagram below is for He_2 molecule. Bond order indicates that He_2 doesn't exist.

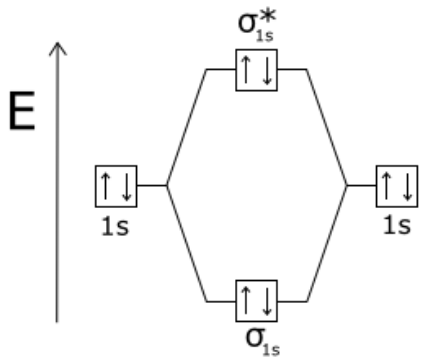


Figure: MO diagram for the dihydrogen cation (H_2^+) — one electron in the bonding MO gives bond order 0.5 and a bond energy of 270 kJ/mol

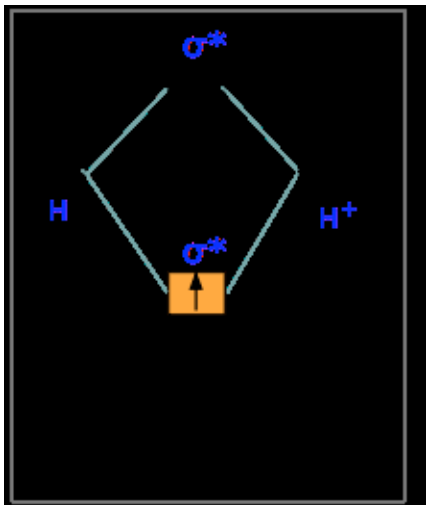


Figure: MO diagram for dihydrogen (H_2) — two electrons in the bonding MO give bond order 1 and a bond energy of 452 kJ/mol

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. 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."

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.

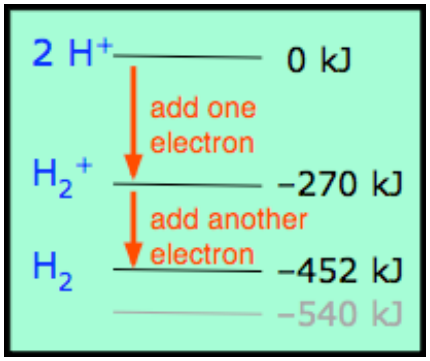


Figure: Energy diagram for H_2 formation — adding one electron to two protons stabilizes by 270 kJ/mol (H_2^+); adding a second electron provides less than double the stabilization (452 kJ/mol total) due to electron–electron repulsion

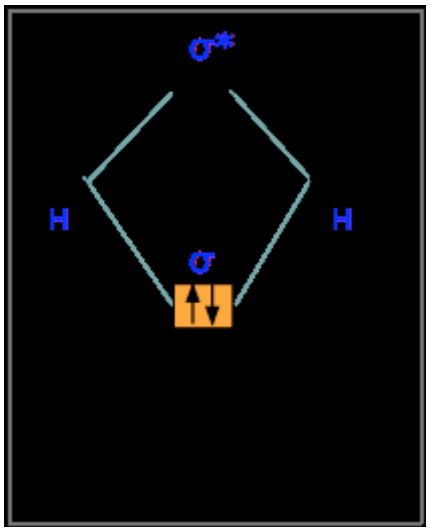


Figure: MO diagram for H_2 — bond order 1, bond energy 452 kJ/mol

*****MO's in dihelium**

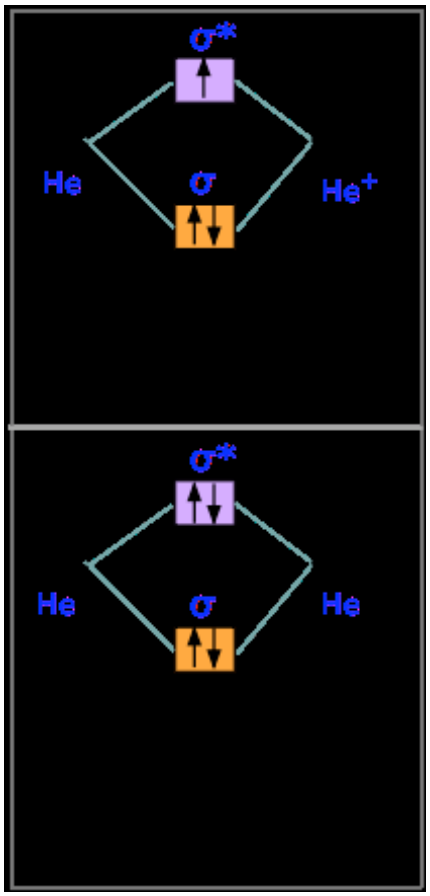


Figure: MO diagrams for He_2^+ (bond order 0.5, 301 kJ/mol) and He_2 (bond order 0, negligible bond energy) — He_2 is essentially non-existent because the antibonding orbital completely cancels the bonding orbital

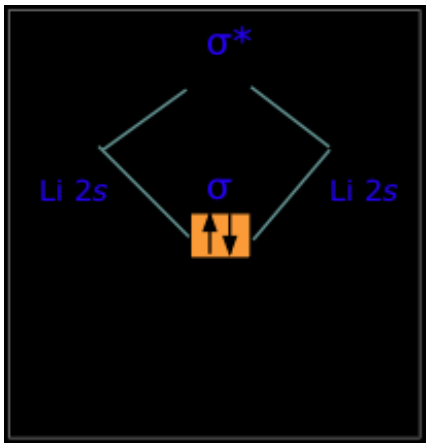


Figure: MO diagram for dilithium (Li_2) — only 2s valence orbitals are considered; bond order 1 and bond energy 110 kJ/mol; lower than H_2 because the 2s orbital is farther from the nucleus

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 1s 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.

Bonding of the Period 2 s-block Diatomic Molecules

Both Li and Be occur as metals under normal conditions, but MO theory predicts their stability as dilithium and diberyllium. Like the MOs formed from 1s AOs, those formed from 2s AOs are also σ orbitals, cylindrically symmetrical around the internuclear axis. Bond order in Li_2 = ½(2−0) = 1 and bond order for Be_2 = ½(2−2) = 0. Therefore, the 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. P orbitals 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 π MOs (π2p and π*2p).

- MOs 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 energy than anti-bonding MOs. Therefore σ2p is lower in energy than σ*2p and π2p is lower in energy than π*2p.
- p-orbitals can interact more extensively end to end than side to side. Thus σ2p is lower in energy than π2p. Similarly, the destabilizing effect of σ*2p MO is greater than that of the π*2p MO.

Energy order of MO derived from p orbital: σ2p < π2p < π*2p < σ*2p

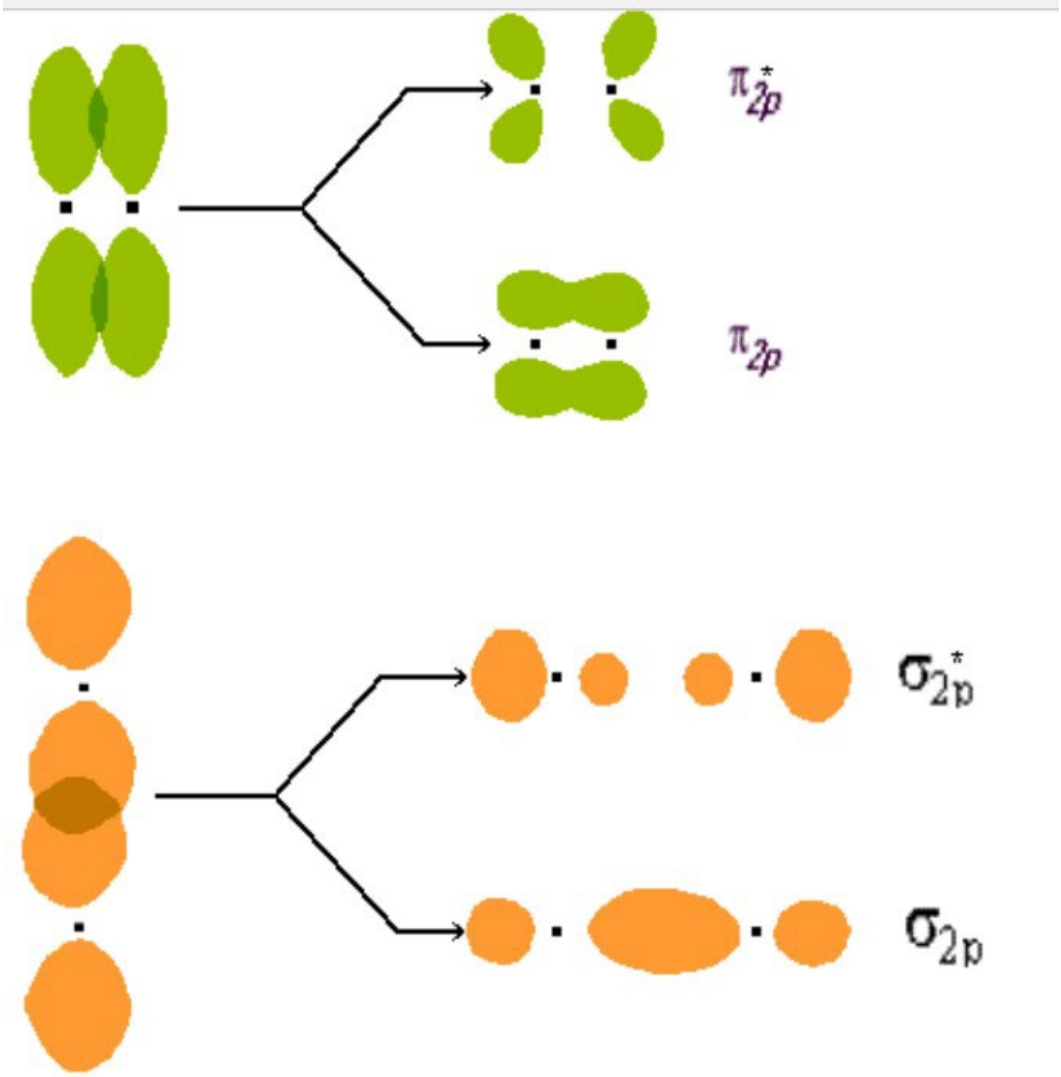


Figure: Formation of sigma and pi molecular orbitals from atomic p orbitals — (a) bonding: in-phase end-to-end and side-to-side overlaps; (b) antibonding: out-of-phase overlaps producing nodal surfaces between the nuclei

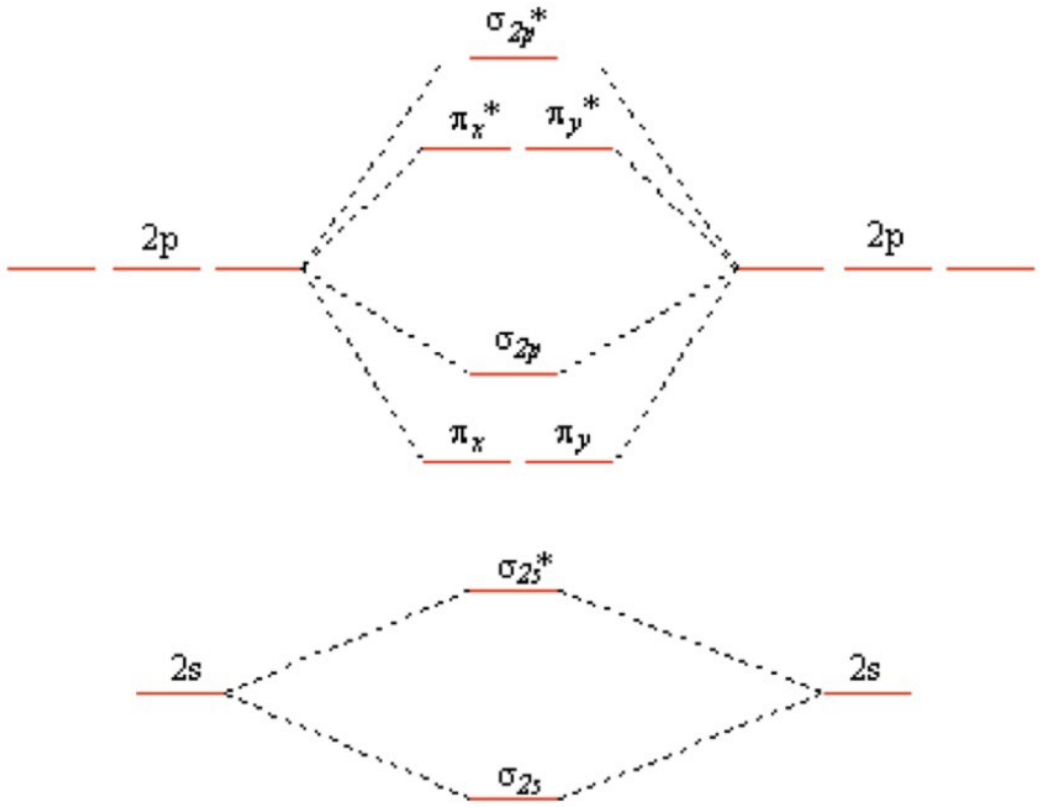


Figure: MO energy level diagram for B_2, C_2, and N_2 — in these molecules, the degenerate π2p bonding MOs lie below the σ2p bonding MO due to orbital mixing between 2s and 2p; this ordering reverses for O_2 and F_2

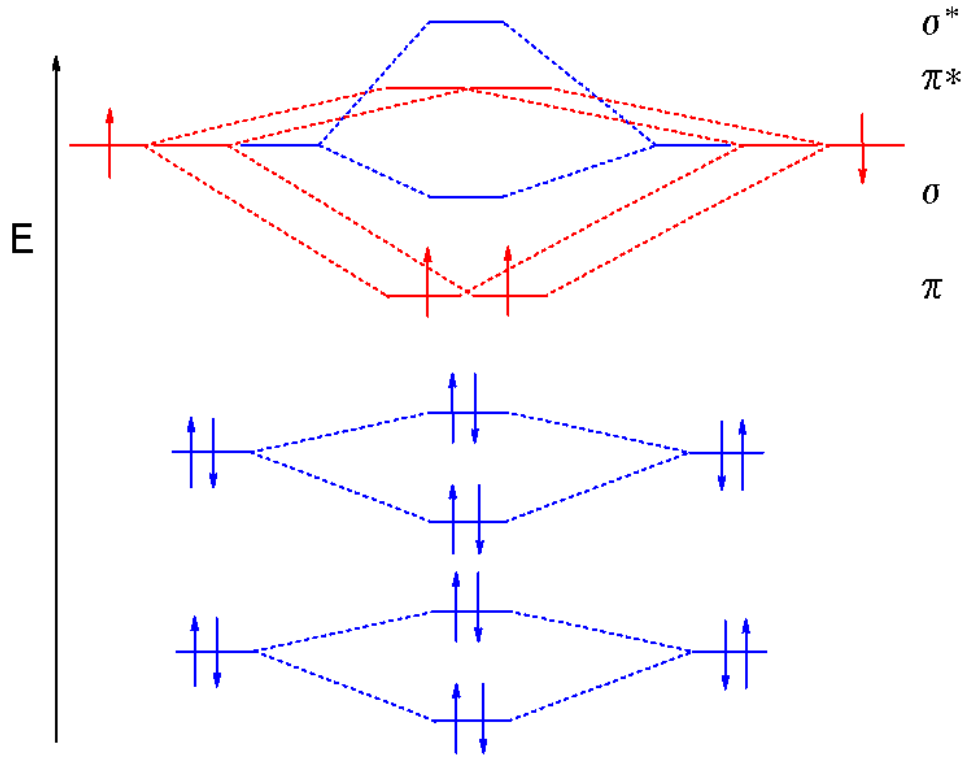


*Figure: MO energy diagram for B_2 — four electrons fill the σ2s and σ*2s MOs (net zero bond contribution); two more electrons occupy the degenerate π2p MOs one each (Hund's rule), giving bond order 1 and paramagnetism*

Bonding in the p-block homonuclear diatomic molecules

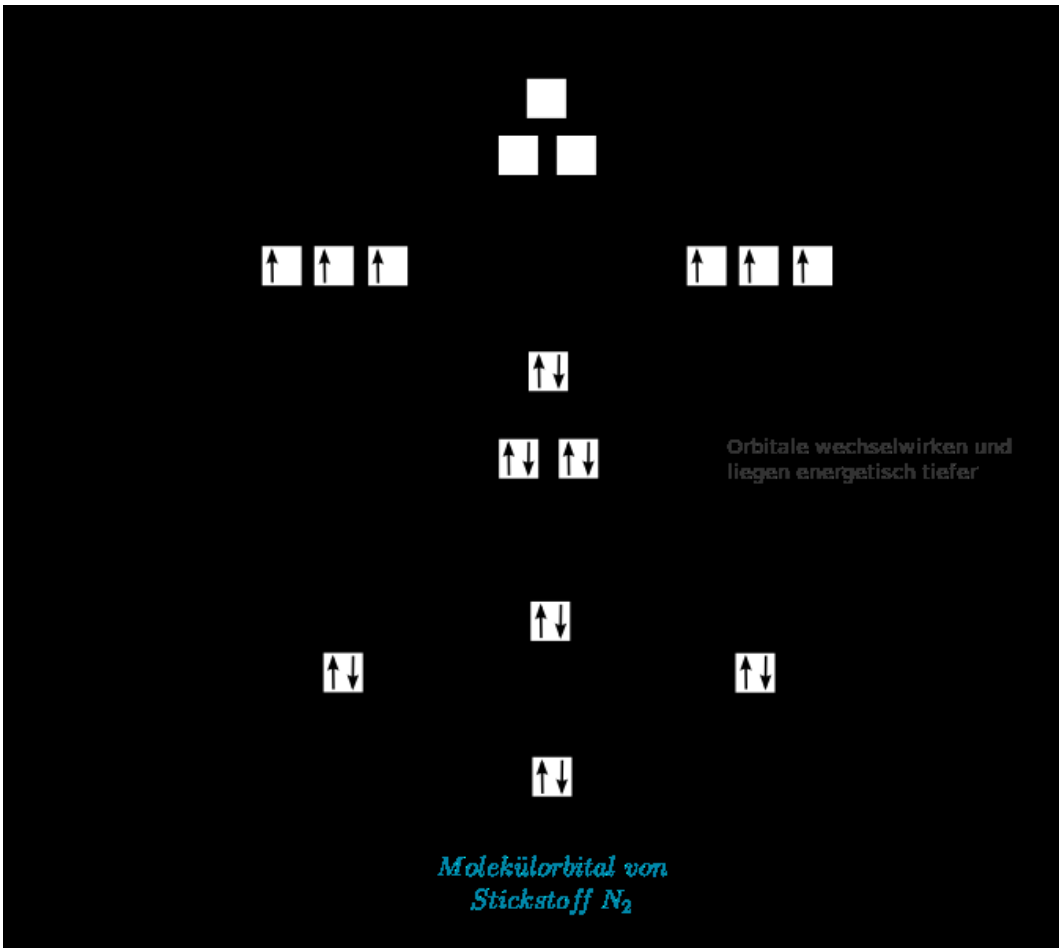


Figure: MO energy diagram for N_2 — six bonding electrons (σ2p + 2×π2p) minus zero antibonding electrons gives bond order 3, consistent with N_2's triple bond, high bond energy (945 kJ/mol), and diamagnetic character

The B_2 molecule has six outer electrons to place in its MOs. Four of these fill σ2s and σ*2s MOs. The remaining two electrons occupy the two π2p 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.

The two additional electrons present in C_2 will fill the π2p. 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.

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 be paramagnetic. According to VBT, O_2 should look like the Lewis structure which shows all the electrons paired. Therefore VBT predicts that O_2 should be diamagnetic.

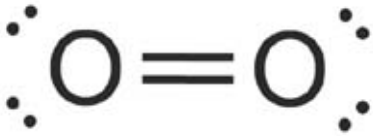


Figure: Lewis dot structure of O_2 — all electrons appear paired in this representation, which incorrectly predicts diamagnetic behavior; MO theory is needed to explain the observed paramagnetism

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 superposition of the wavefunctions of atomic orbitals.

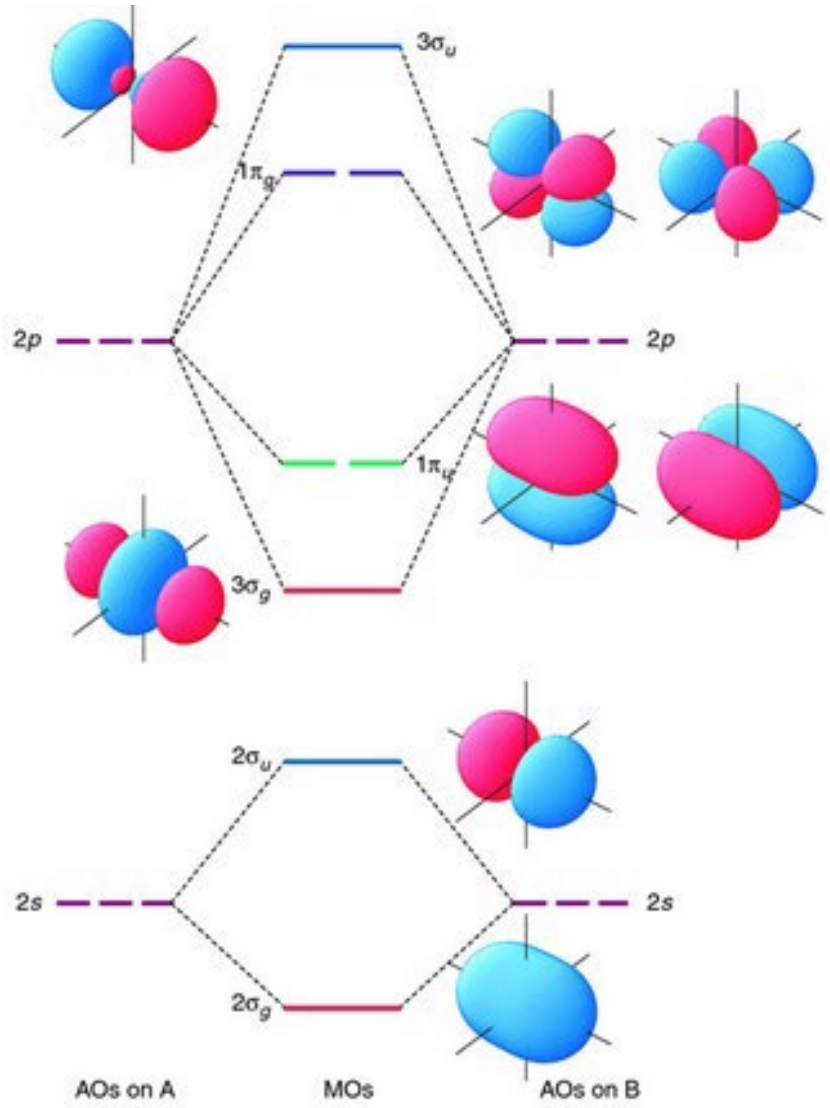


Figure: Complete MO diagram for O_2 with orbital shape images — the two highest-energy electrons singly occupy the degenerate 1πg antibonding orbitals (Hund's rule), correctly predicting that O_2 is paramagnetic with bond order 2*

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 O_2 should be paramagnetic, unlike VBT which predicts that O_2 is diamagnetic.

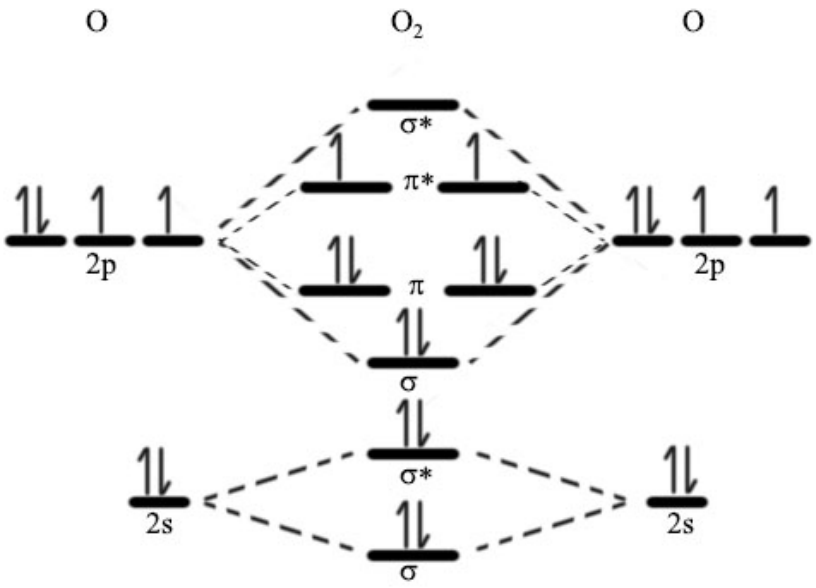


Figure: MO energy diagram for O_2 — twelve valence electrons fill eight bonding and four antibonding MOs; the two electrons in the degenerate π MOs are unpaired (highlighted), giving bond order 2 and predicting paramagnetism*

MO's in lithium hydride

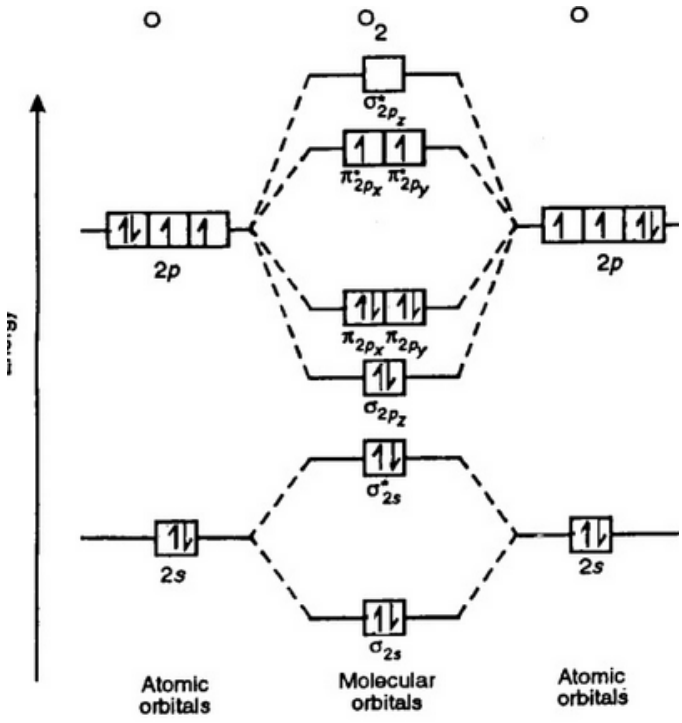


Figure: MO energy diagram for lithium hydride (LiH) — the Li 2s and H 1s orbitals combine to form one σ bonding MO; bond order 1, bond energy 243 kJ/mol; the electron density is skewed toward the more electronegative H, creating bond polarity

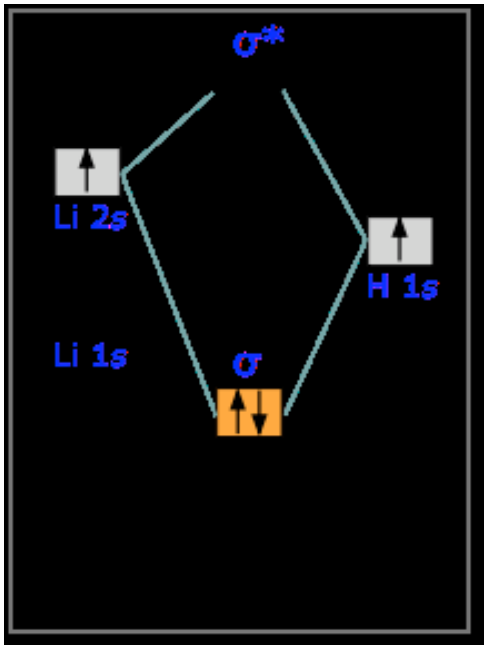


Figure: Electrostatic potential map of LiH — the color gradient shows electron density shifted toward hydrogen (blue, negative) and away from lithium (red, positive), visualizing the polar nature of the Li–H bond

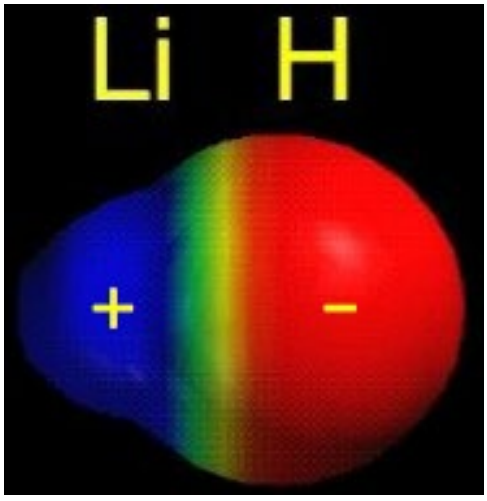


Figure: Detailed MO energy diagram for O_2 showing all valence molecular orbitals and their electron occupancy — the two π electrons are unpaired, confirming paramagnetism and bond order 2*

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.

The importance of direction

You will recall that there are three possible p orbitals for any value of the principal quantum number. These are frequently designated px, py, and pz, to indicate the axis along which the orbital is aligned.

These directional differences lead to the formation of two different classes of molecular orbitals.

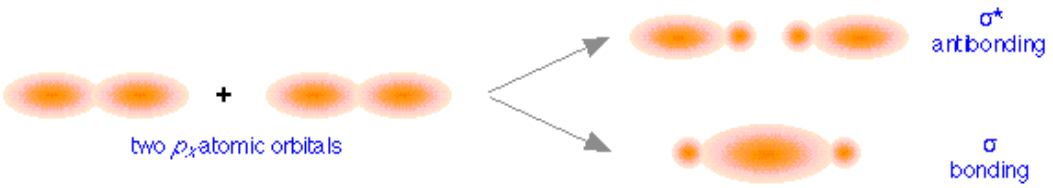


Figure: Formation of sigma (σ) molecular orbitals from px atomic orbitals — in-phase (bottom) produces a σ bonding MO with maximum electron density between the nuclei; out-of-phase (top) produces a σ antibonding MO with a nodal surface between the nuclei*

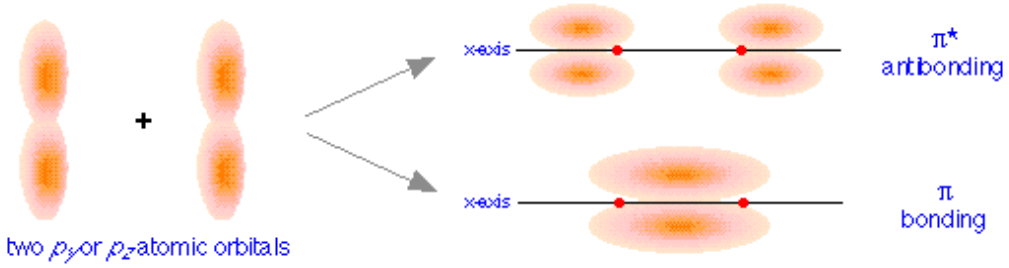


Figure: Formation of pi (π) molecular orbitals from py (or pz) atomic orbitals — in-phase side-to-side overlap (bottom) produces a π bonding MO with electron density above and below the bond axis; out-of-phase (top) produces a π antibonding MO with a node perpendicular to the bond*

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.

When we examine the results of the in- and out-of-phase combination of py and pz orbitals, we get the bonding and antibonding pairs that we would expect, but the resulting molecular orbitals have a different symmetry; these are called π (pi) orbitals. There are two of them, πy and πz differing only in orientation, but otherwise completely equivalent.

4 MO splitting patterns for second-row diatomics

If we combine the splitting schemes for the 2s and 2p 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.

Notice that the relative energies of the 2p-derived σ and π bonding molecular orbitals are reversed in O_2 and F_2. This is attributed to interactions between the 2s orbital each atom with the 2px orbital of the other, an effect similar to hybridization.

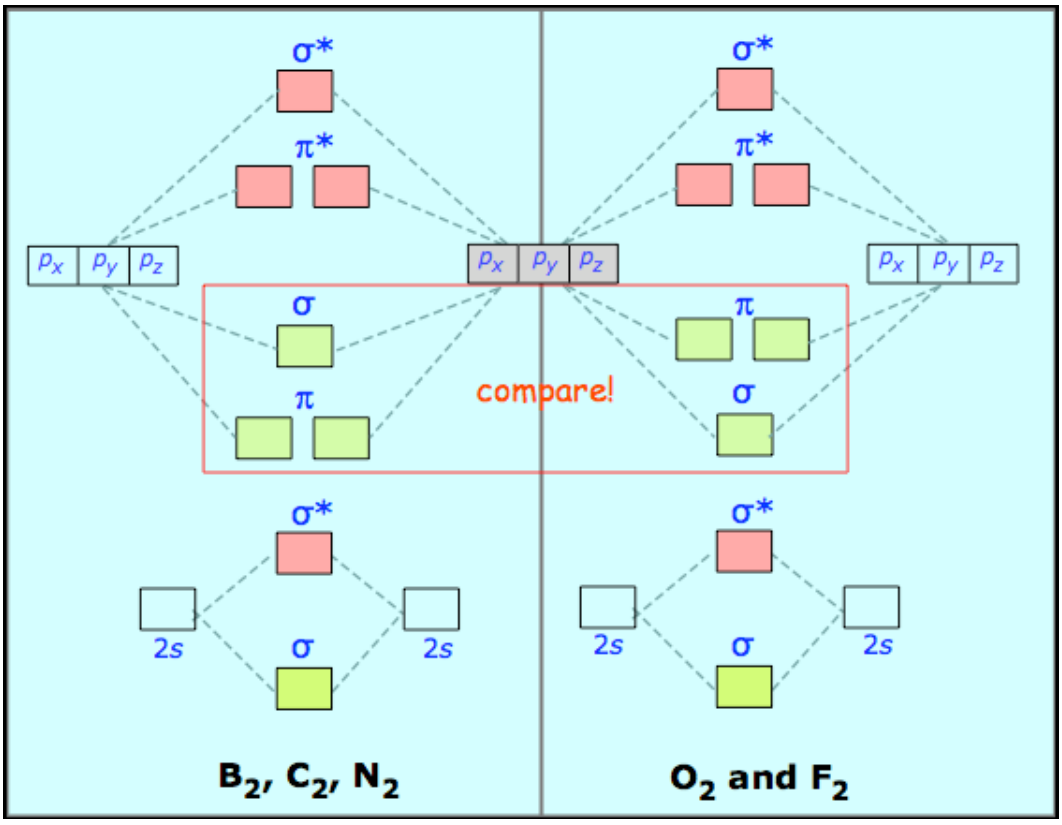


Figure: Comparison of MO splitting patterns — (left) B_2/C_2/N_2: π2p bonding MOs lie below σ2p due to 2s-2p orbital mixing; (right) O_2/F_2: σ2p lies below π2p as the mixing effect weakens with increasing nuclear charge

MO's in dicarbon

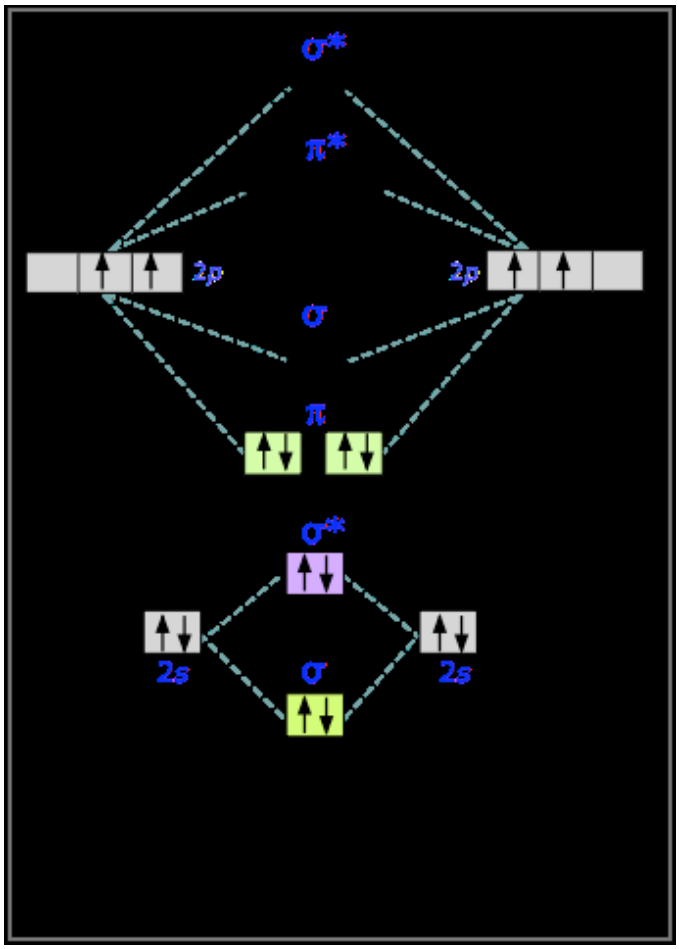


*Figure: MO energy diagram for dicarbon (C_2) — eight valence electrons fill σ2s, σ*2s, and both π2p bonding MOs; bond order 2, bond energy 301 kJ; C_2 is diamagnetic since all electrons are paired*

MO's in dioxygen

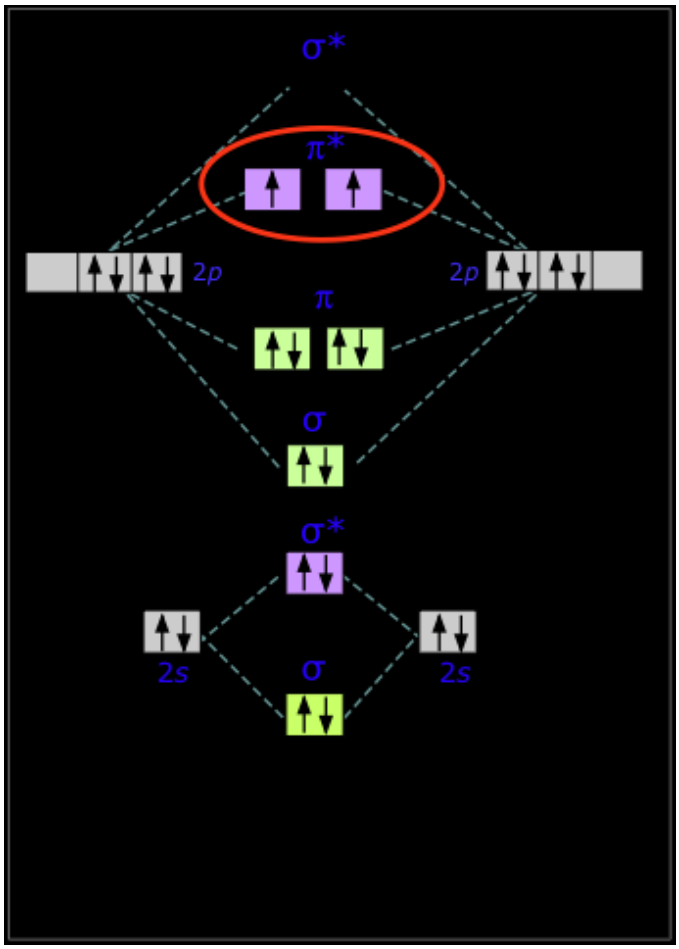


Figure: MO energy diagram for dioxygen (O_2) — twelve valence electrons fill eight bonding and four antibonding MOs; the two π electrons are unpaired (highlighted), giving bond order 2, bond energy 498 kJ, and paramagnetic behavior*

The electron configuration of oxygen is $1s^2 2s^2 2p^4$. In O_2, therefore, we need to accommodate twelve valence electrons (six from each oxygen atom) in molecular orbitals. 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 form, another variety, known as singlet oxygen, has a bond energy of only 402 kJ/mole. Singlet oxygen can be formed by the action of light and in certain chemical reactions.

Paramagnetism of O_2

The two unpaired electrons of the dioxygen molecule give this substance an unusual and distinctive property: O_2 is paramagnetic. 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.

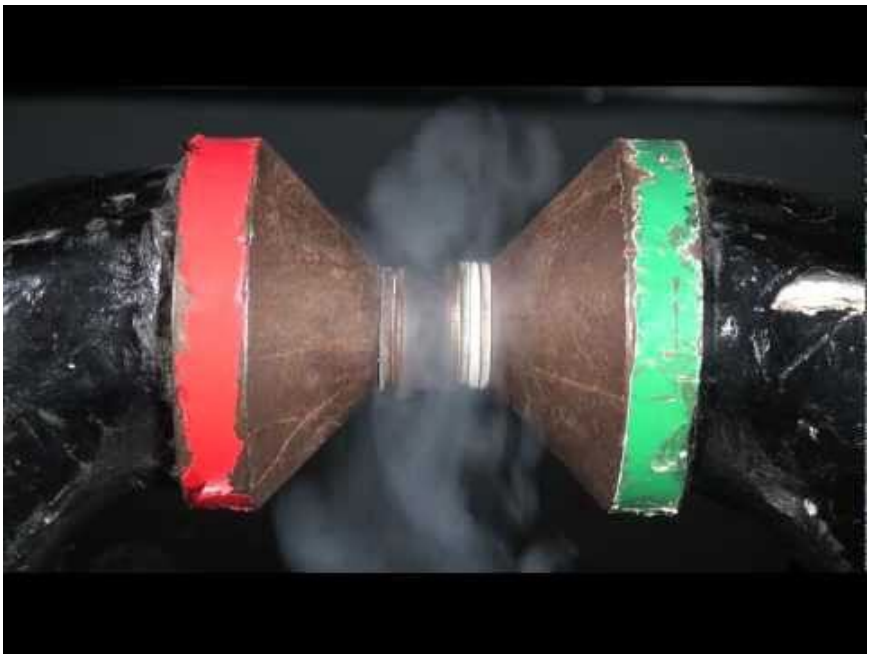


Figure: Demonstration of paramagnetism of liquid oxygen — liquid O_2 is attracted to the magnet and bridges between the N and S poles rather than flowing past, directly demonstrating the two unpaired electrons predicted by MO theory

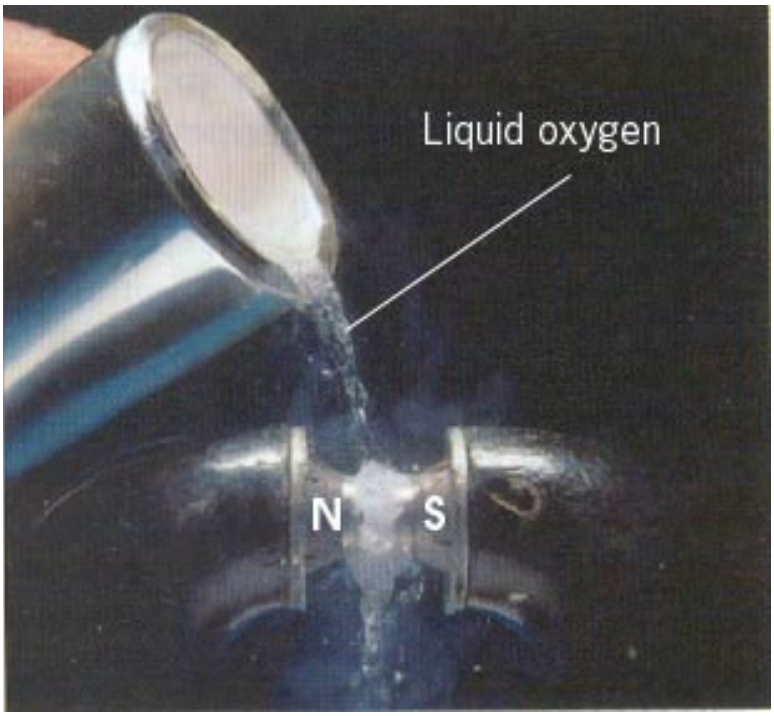


Figure: Liquid oxygen held between electromagnet poles — the paramagnetic liquid oxygen is attracted to the high-field region between the poles, providing a striking visual demonstration of MO theory's prediction of two unpaired electrons in O_2

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. Just as we would expect, O_2^+ has a bond energy higher than that of neutral dioxygen; removing the one electron actually gives us a more stable molecule.

MO's in lithium hydride (heteronuclear)

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. 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.

We need consider only the 2s orbital of lithium which combines with the 1s 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 1s 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. The bond polarity arises from the greater electron-attracting power of hydrogen — a consequence of the very small size of this atom.

Practice Questions: Sigma and Pi Bonds

What you should be able to do:

18. Make sure you thoroughly understand the following essential ideas which have been presented above.
19. In what fundamental way does the molecular orbital model differ from the other models of chemical bonding that have been described in these lessons?
20. Explain how bonding and antibonding orbitals arise from atomic orbitals, and how they differ physically.
21. Describe the essential difference between a sigma and a pi molecular orbital.
22. Define bond order, and state its significance.
23. 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

24. **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

25. **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

26. **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 orbitals

27. **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

28. **The sp^2 atomic hybrid orbital set accommodates _____ electron domains.**

A) 2 B) 3 C) 4 D) 5 E) 6

29. **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°

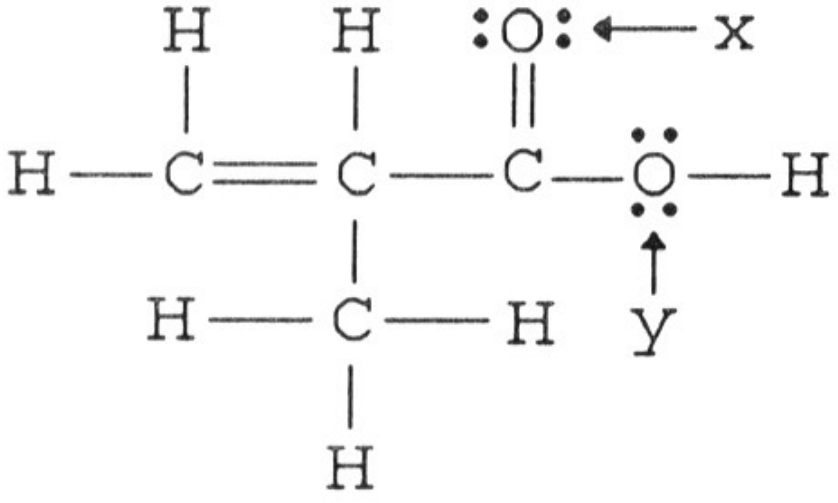


Figure: Structural formula for Question 6 — identify the hybridization of oxygen "x" and the C-O-H bond angle at oxygen "y"

30. **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 is pictured in the diagram:**

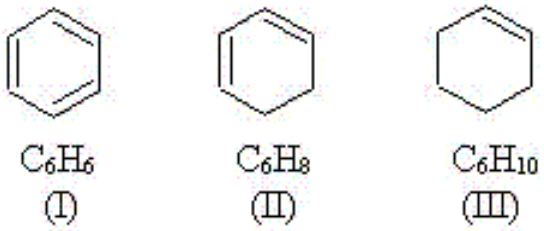


Figure: Orbital box diagram for Question 7 — silicon atom forming sp^3 hybrid orbitals; identify the hybridization change shown

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

31. **There are _____ σ bonds and _____ π bonds in $H_3C\text{-}CH_2\text{-}CH{=}CH\text{-}CH{=}CH_2$.**

A) 10, 3 B) 14, 2 C) 12, 2 D) 15, 2 E) 13, 2

32. **Molecular Orbital theory correctly predicts paramagnetism of oxygen gas, O_2. This is because _____.**

A) the energy of the π2p MOs is higher than that of the σ2p 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

33. **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

34. **A bonding or antibonding π orbital contains a maximum of _____ electrons.**

A) 1 B) 2 C) 4 D) 6 E) 8

35. **Use molecular orbital theory to predict which molecule or ion has the highest bond energy?**

C_2 a) C_2^+ b) C_2^-

36. **Use the molecules below to answer the next three questions.**

C_6H_6 (I) C_6H_8 (II) C_6H_{10} (III)

(Benzene, cyclohexadiene, and cyclohexene respectively)

37. **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

38. **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

39. **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

40. **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

41. **The hybridization of the B in BH_3 is sp^3.**

a. True b. False
ANSWER: False

42. **The hybridization of a molecule is measured to determine the shape of the molecule.**

a. True b. False
ANSWER: False

43. **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

44. **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

45. **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

46. **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

47. **What is the bond order of He_2^+?**

a. 0 b. 1/2 c. 1 d. 1½ e. 2
ANSWER: b

48. **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

49. **Larger bond order means greater bond strength.**

a. True b. False
ANSWER: True

50. **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

51. **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
ANSWER: c

52. **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 σ1s 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

53. **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

54. **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

Chapter 9-GASES

Key Concepts

I. Atmosphere
II. Characteristics of Gases
III. Gas Laws
IV. Combined Gas Law
V. Ideal Gas Law
VI. Molar Volume of A Gas
VII. Dalton's Law of Partial Pressure
VIII. Gas Stoichiometry
IX. Kinetic Molecular Theory
X. Diffusion & Effusion
XI. Real Gases

I. Atmosphere

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 1.1: City skyline viewed through Earth's atmosphere, showing the visible air layer that exerts pressure on all surfaces below.

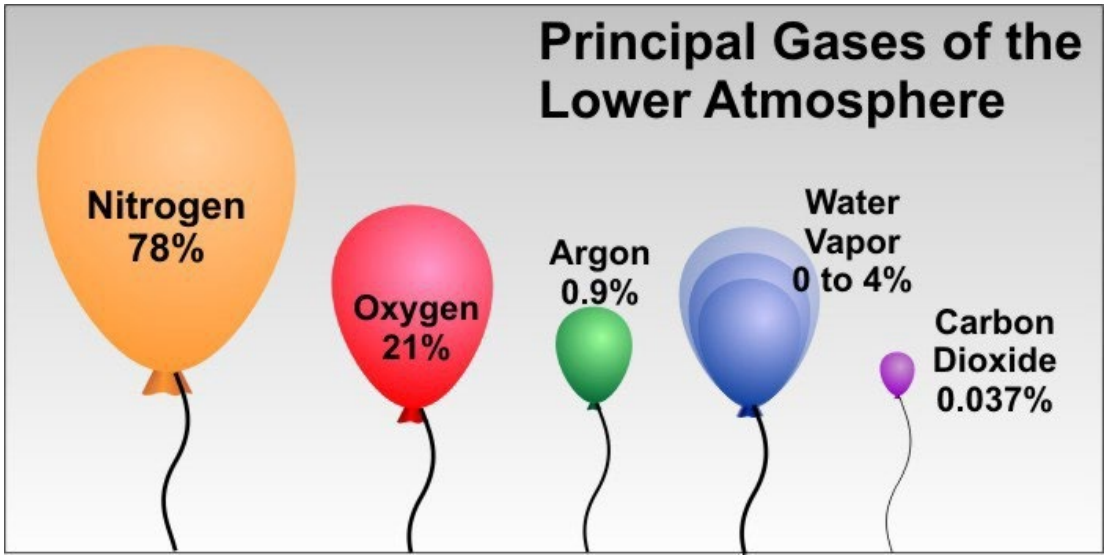


Figure 1.2: Principal gases of the lower atmosphere. Nitrogen makes up 78%, oxygen 21%, argon 0.9%, water vapor 0–4%, and carbon dioxide 0.037%.

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.

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. 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.

II. Characteristics of Gases

1. What's Special About Gases?

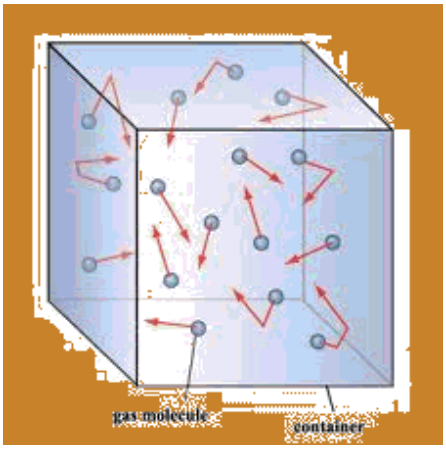


Figure 2.1: Comparison of gas and liquid volumes. The same substance occupies 1671 mL as a gas but only 1 mL as a liquid — illustrating how gases have much lower density than liquids.

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.

2. The Pressure of a Gas

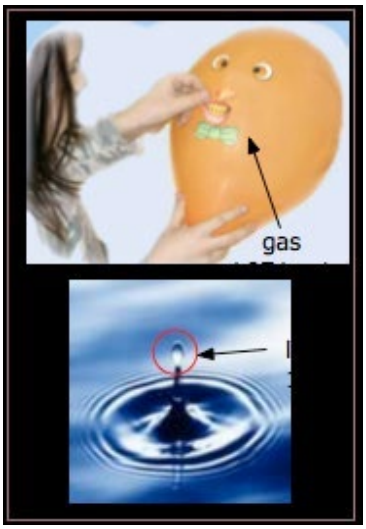


Figure 2.2: Gas molecules in constant random motion inside a container. Collisions of molecules with the container walls create gas pressure.

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.

Pressure Units

The unit of pressure in the SI system is the pascal (Pa), defined as a force of one newton per square metre ($1\ Nm^{-2} = 1\ kg\ m^{-1}\ s^{-2}$).

In chemistry, it is more common to express pressures in units of atmospheres or torr:

1 atm = 101325 Pa = 760 torr

The older unit millimetre of mercury (mm Hg) is almost the same as the torr. 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.

Figure 2.3: Logarithmic pressure scale showing the range of pressures encountered in nature and chemistry. The chemistry pressure range (highlighted) spans from approximately 10^{-4} to 10^{2} atm.

Atmospheric Pressure and the Barometer

The column of air above us exerts a force on each 1-cm² 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.

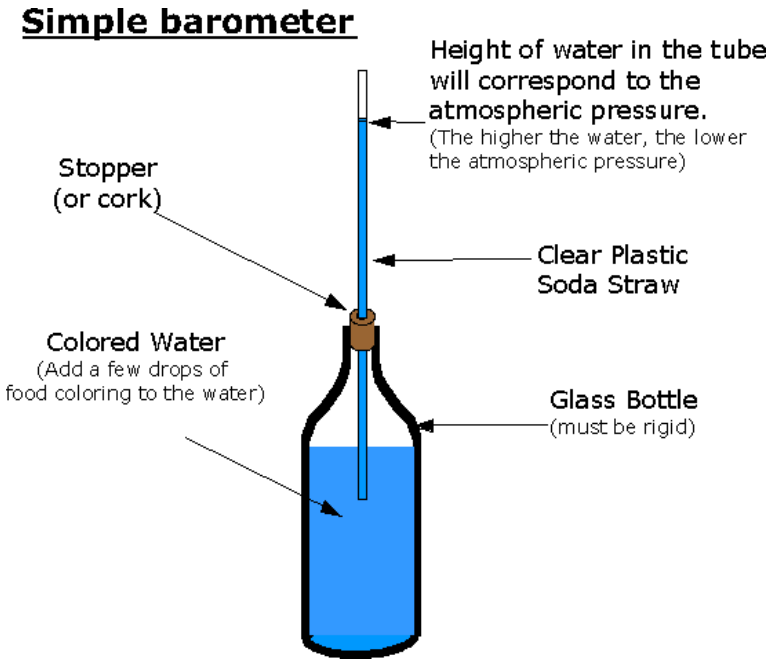


Figure 2.4: Relationship between altitude and atmospheric pressure. Pressure decreases from approximately 1000 mb at sea level to 100 mb at 12 km and 1 mb at 50 km altitude.

The Manometer

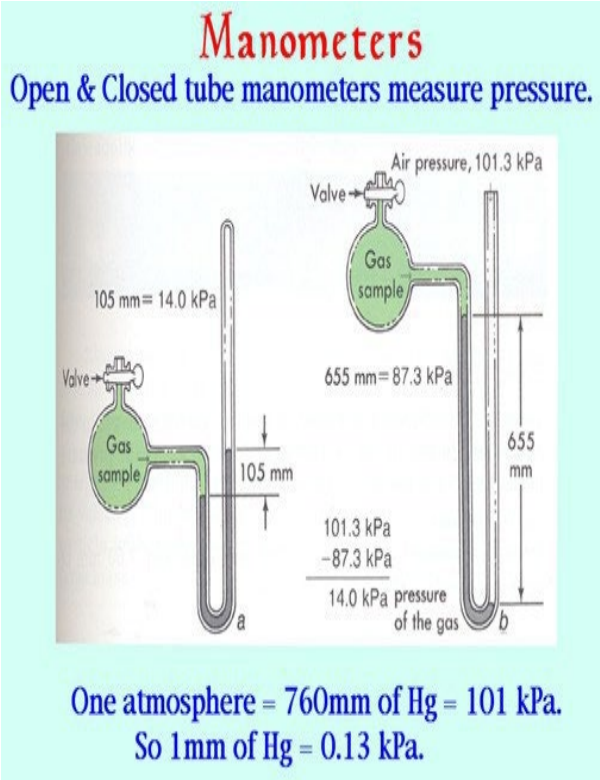


Figure 2.5: Simple water barometer. The height of colored water in the straw corresponds to atmospheric pressure — higher water level indicates lower atmospheric pressure.

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 a 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.

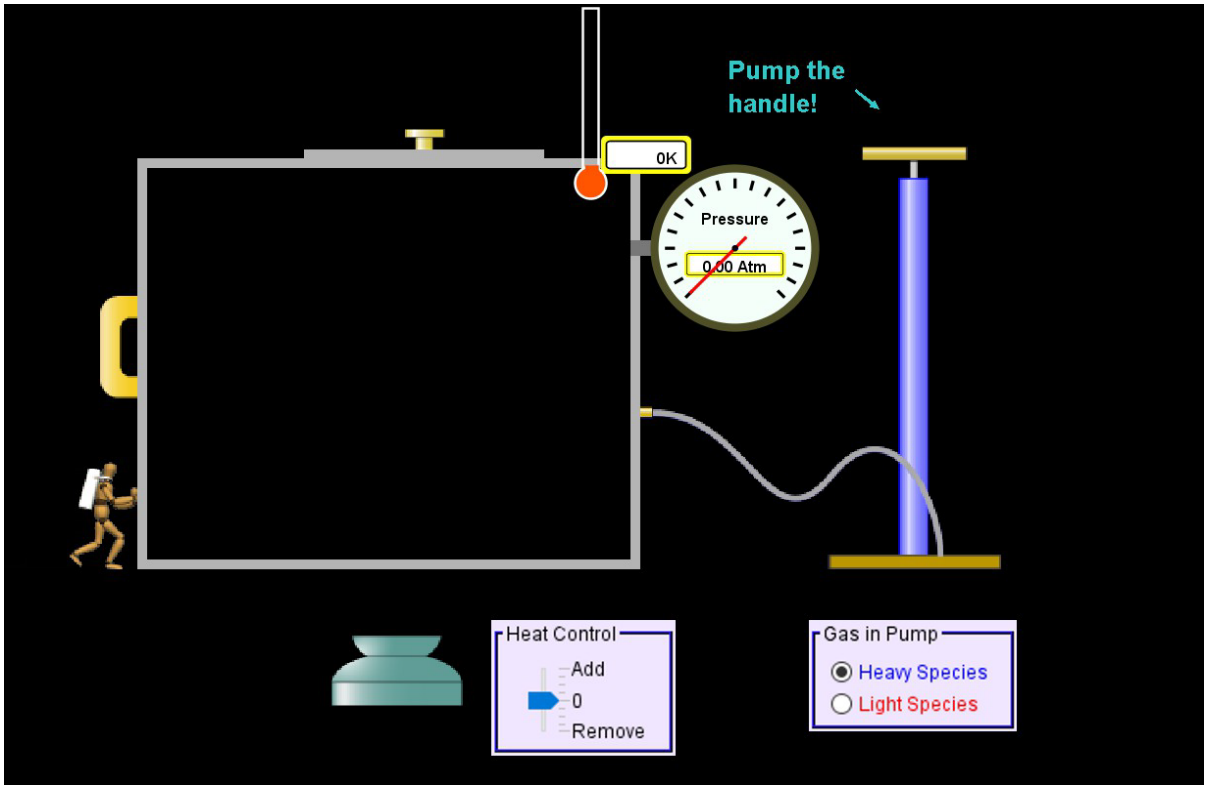


Figure 2.6: Open and closed tube manometers for measuring gas pressure. Left (closed-tube): the pressure difference is read directly in torr. Right (open-tube): atmospheric pressure must be subtracted to find gas pressure. 1 atm = 760 mmHg = 101 kPa.

The manometers ordinarily seen in the laboratory come in two types: closed-tube and open-tube. In the closed-tube unit, the longer limb of the J-tube is evacuated by filling it with mercury and then inverting it. In the open-tube manometer, the atmosphere pushes the mercury column down in the open side, and the pressure in torr is found from the difference in the levels.

Temperature Scales

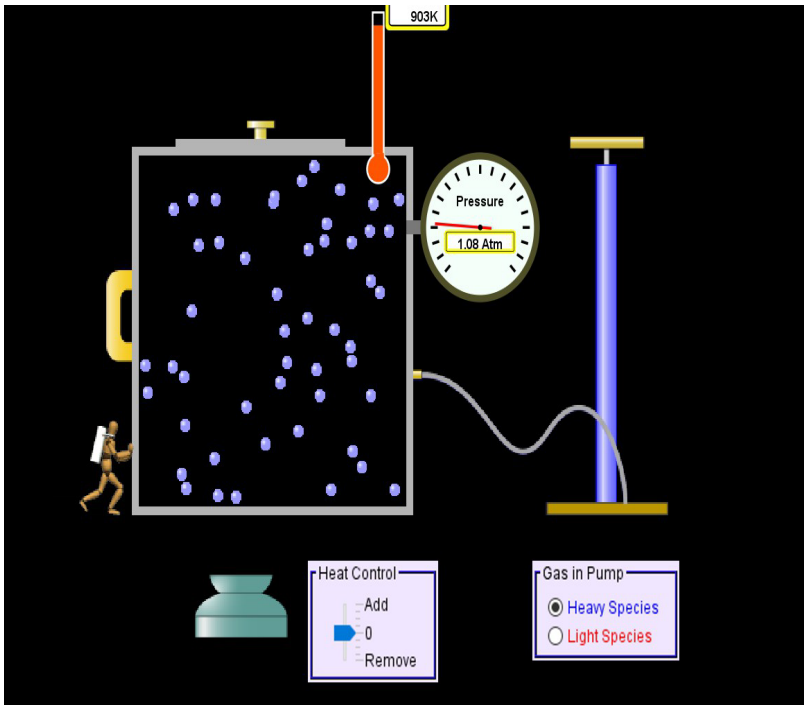


Figure 2.7: Comparison of Fahrenheit and Celsius temperature scales. Water freezes at 32°F (0°C) and boils at 212°F (100°C). The Fahrenheit scale has 180 degrees spanning the same range as 100 Celsius degrees.

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 Fahrenheit scale placed the zero point at the coldest temperature obtainable at the time (by mixing salt and ice). Water freezes at 32°F and boils at 212°F. The Fahrenheit scale is finer than the Celsius scale; 1F° = 5/9 C°.

Absolute Temperature

In 1802, 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. This temperature, –273°C, is called absolute zero.

The Kelvin scale, suggested by Lord Kelvin, places zero at –273.15°C. Since the Kelvin and Celsius degrees are the same size, room temperature (20°C) is about 293 K. Temperature in Kelvin = Temperature in Celsius + 273.

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. The SI unit of volume is the cubic metre, but in chemistry we more commonly use the litre and the millilitre (ml).

It's important to bear in mind 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.

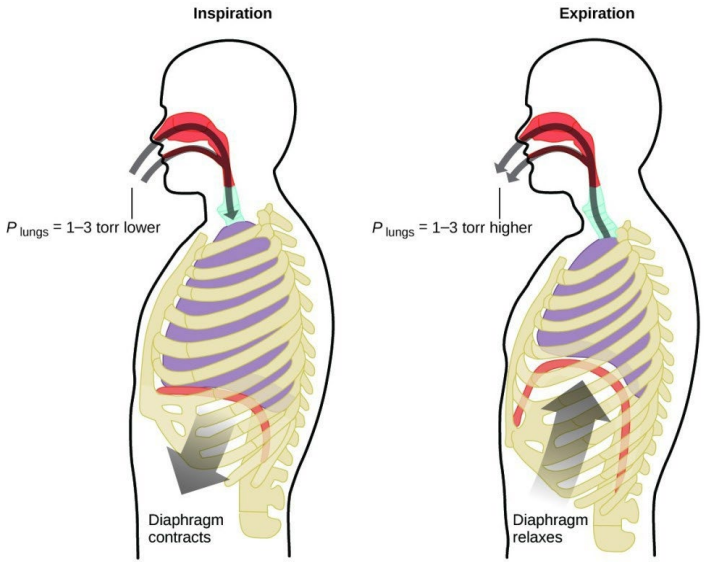


Figure 2.8: Gas burette for measuring gas volume. Gas is trapped above mercury in a calibrated tube; the volume is read from the scale. The mercury reservoir and flexible tubing allow pressure equalization.

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 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.

1 atm = 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.

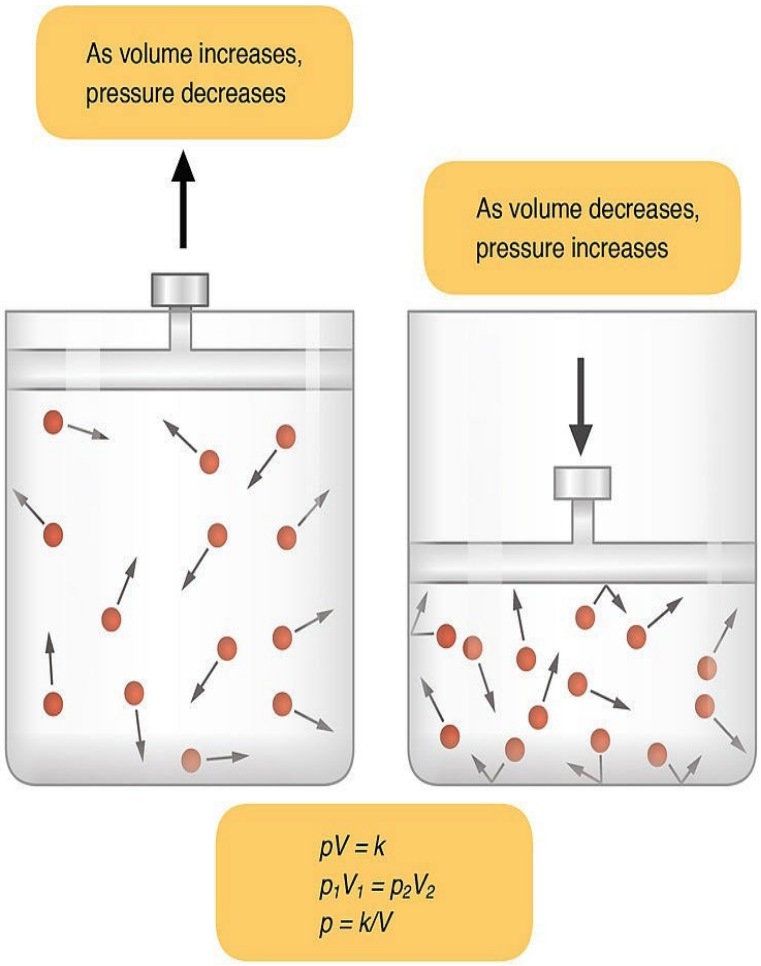


Figure 2.9: Mercury barometer. Atmospheric pressure supports a column of mercury 760 mm tall at sea level under standard conditions. The vacuum at the top ensures no gas pressure acts on the mercury from above.

Example: On a dry day, atmospheric pressure is 734 torr. What is the pressure in atmospheric units?

Answer: 734 torr × (1 atm / 760 torr) = 0.966 atm

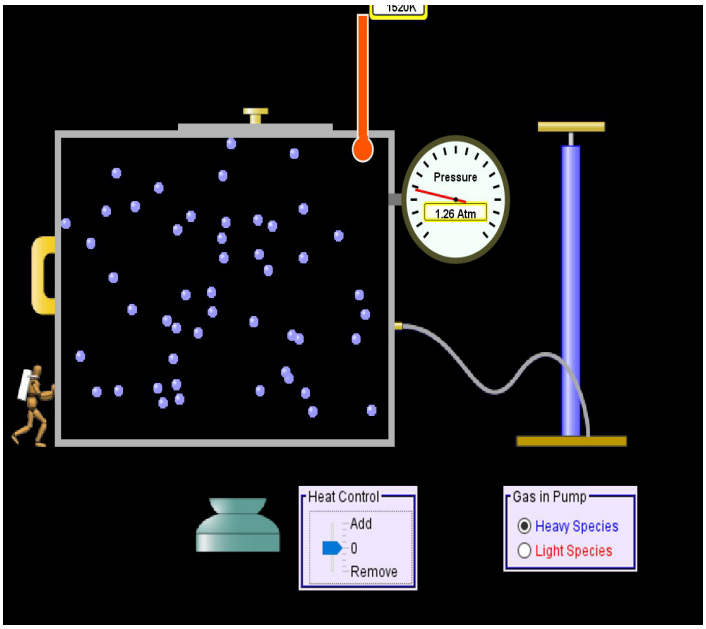


Figure 2.10: U-tube manometer. The difference in mercury levels between the two arms indicates the gas pressure. Used to measure pressures in practical laboratory applications.

Question: 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. 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.

Boyle's law states that the pressure of a gas, held at a constant temperature, varies inversely with its volume:

$PV = \text{constant}$ (at constant T)

$P_1V_1 = P_2V_2$

Figure 3.1: Boyle's J-tube apparatus. Air is trapped in the closed left arm; mercury in the open right arm exerts pressure. The difference in mercury levels (76 cm = 1 atm) gives pressure; the air column length gives volume.

Table 1: Boyle's Law Experimental Data — Pressure, Volume, and PV Product

Volume	Pressure	P × V
96.0	2.00	192
76.0	2.54	193
46.0	4.20	193
26.0	7.40	193

Table 1: Original data from Boyle's experiment showing the inverse relationship between pressure and volume. The product P × V remains approximately constant (≈193) at constant temperature, confirming Boyle's Law.

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.

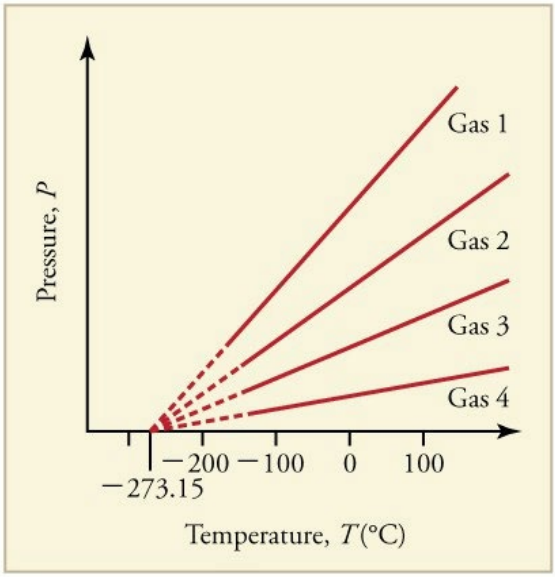


Figure 3.2: Boyle's Law illustrated. Left: increased volume → decreased pressure. Right: decreased volume → increased pressure. The product pV remains constant at constant temperature.

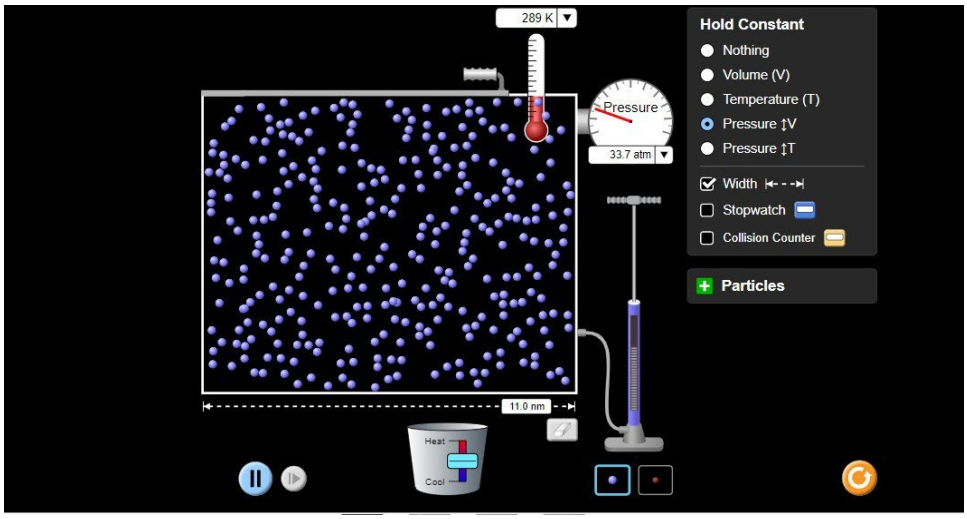


Figure 3.3: Pressure vs. Volume graph (Boyle's Law isotherm). The hyperbolic curve shows the inverse relationship between P and V at constant temperature. Each temperature produces a separate isotherm; the curve never reaches either axis.

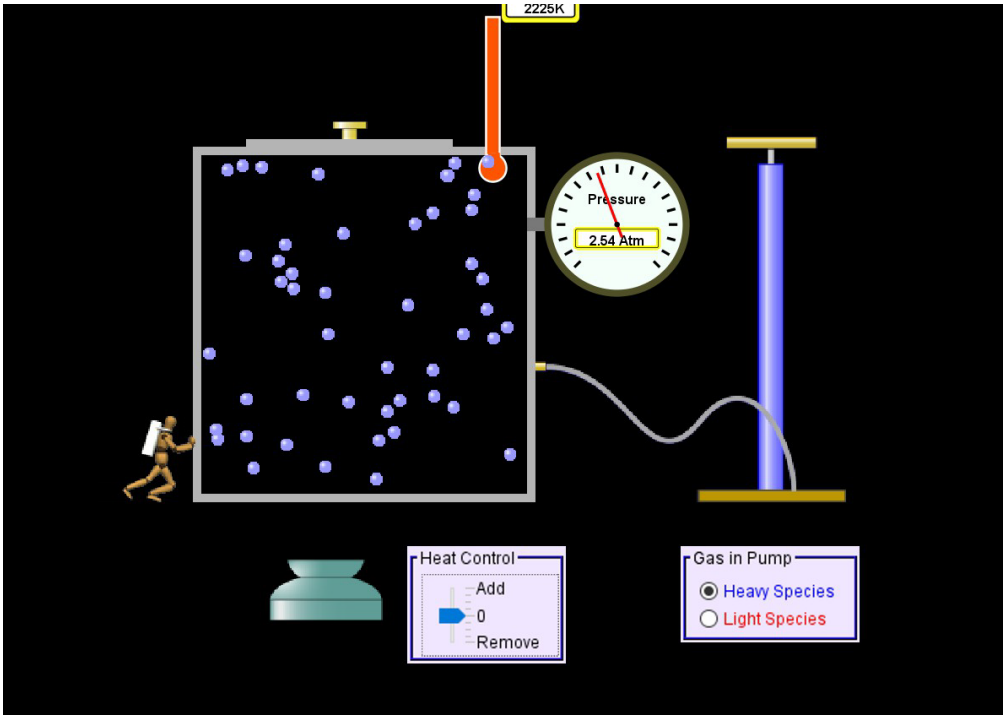


Figure 3.4: PhET Gas Properties simulation interface (https://phet.colorado.edu/en/simulation/legacy/gas-properties). Use this simulation to explore Boyle's, Charles's, and Avogadro's Laws interactively.

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 temperature is kept constant.

Boyle's law has wide application in various fields like scuba diving, human breathing technique.

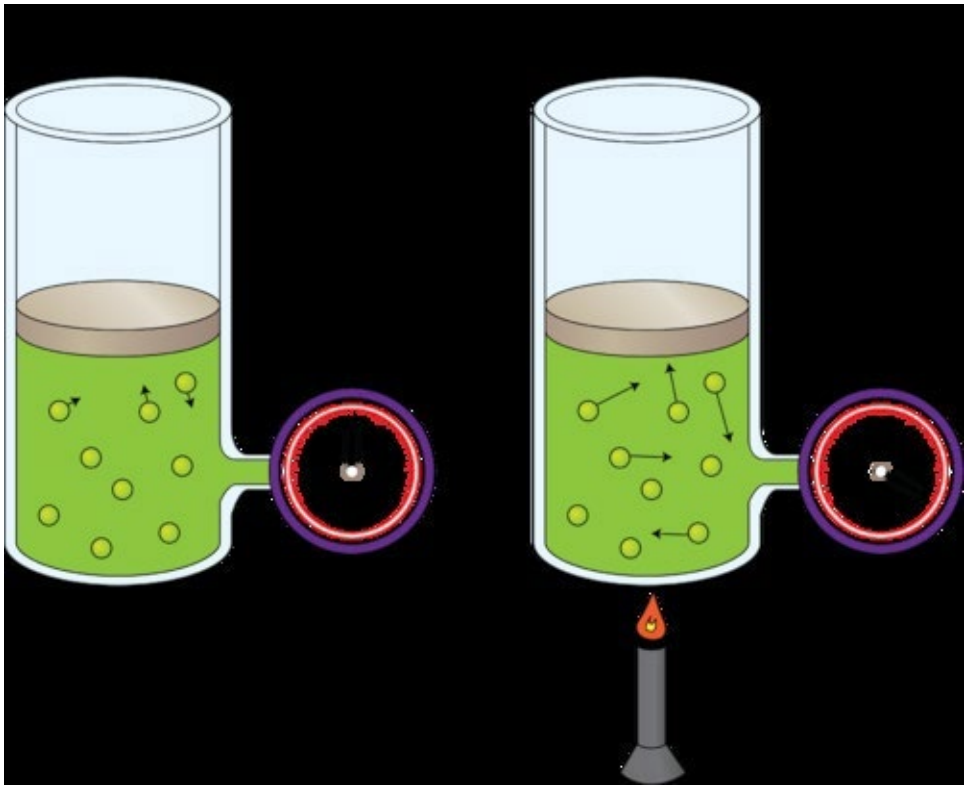


Figure 3.5: PhET simulation demonstrating Boyle's Law. At 903K with 50 molecules in a compressed volume, pressure reads 1.08 Atm. Compressing the volume increases molecular collision frequency with walls, raising pressure.

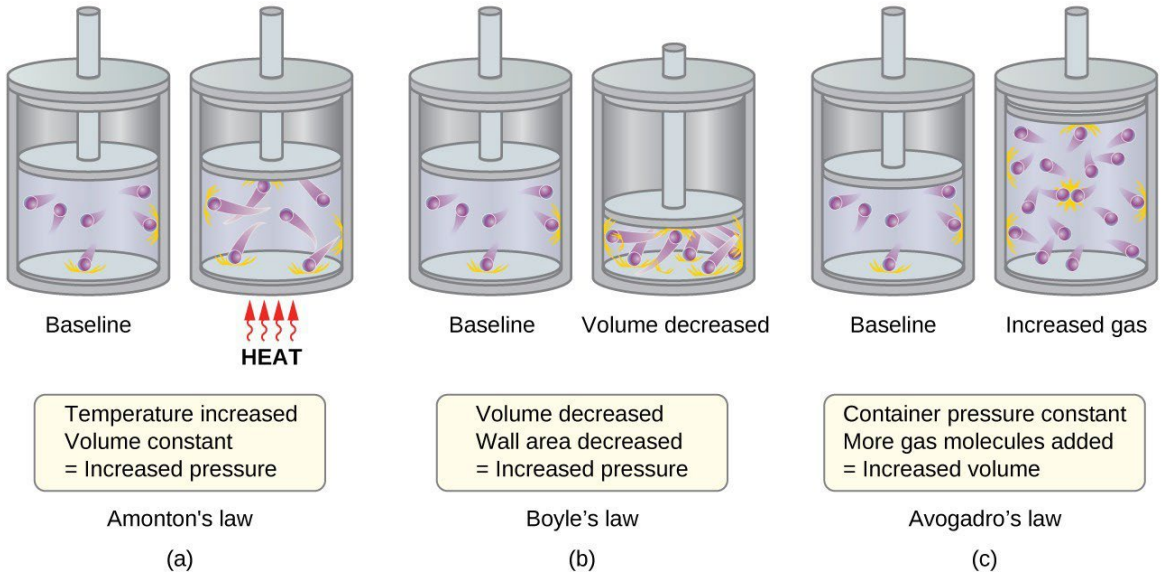


Figure 3.6: Boyle's Law applied to human breathing. Inspiration (left): diaphragm contracts → lung volume increases → pressure drops below atmospheric → air enters. Expiration (right): diaphragm relaxes → lung volume decreases → pressure rises above atmospheric → air exits.

When a person breathes in, the diaphragm contracts and volume of the lungs gets 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.

Mathematically: $P_1V_1 = P_2V_2$ (at constant T)

P_1 = initial pressure, P_2 = final pressure, T_1 = initial temperature in Kelvin, T_2 = final temperature in Kelvin

If we plot different Pressure vs. Volume for a gaseous system at a constant temperature, the curve will be parabolic in nature.

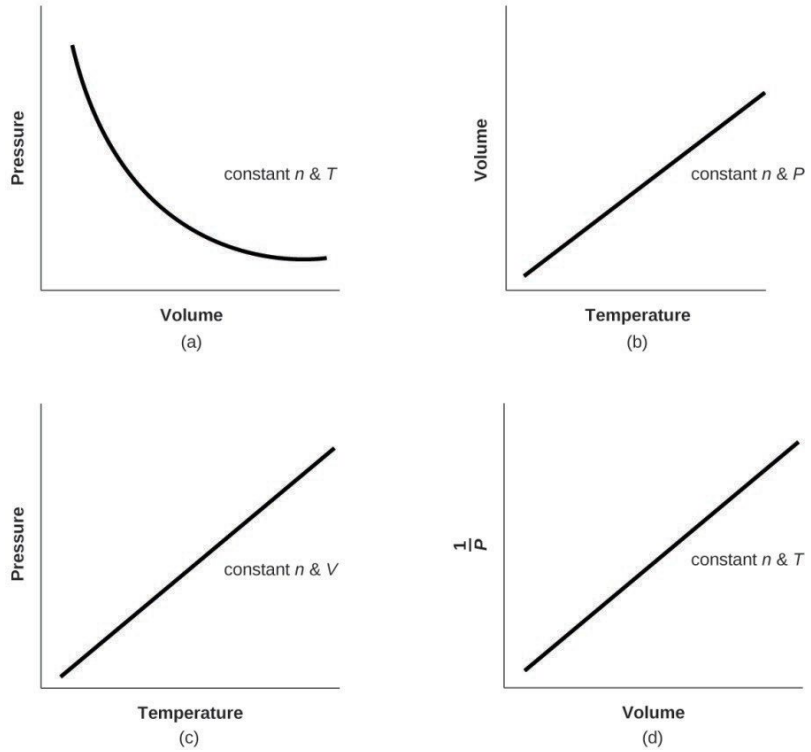


Figure 3.7: Pressure vs. Volume graph showing experimental data points following a hyperbolic curve consistent with Boyle's Law ($P_1V_1 = P_2V_2$ at constant T). Each curve represents a single temperature (isotherm).

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?

Answer: Since the volume is doubled, pressure must be half of the initial pressure. New pressure = 15.0/2 = 7.50 atm

2. Charles's Law (Volume-Temperature Relations)

Charles's Law: Volume of a fixed amount of gas is directly proportional to the kelvin temperature if the pressure is kept constant.

This concept is applied in hot air balloons, where the volume of the gas is expanded by applying heat and once it becomes less dense than air, it can float in air.

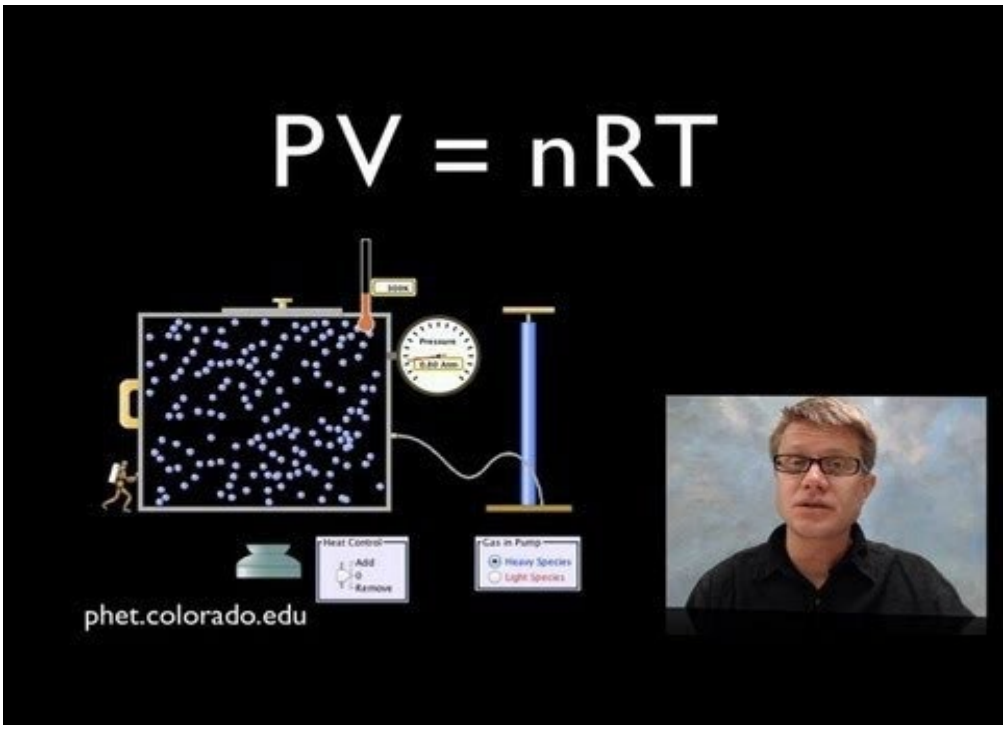


Figure 3.8: PhET simulation demonstrating Charles's Law. At 1520K (increased from 400K), the chamber volume has expanded while pressure remains approximately constant at 1.26 Atm. Higher temperature → greater volume at constant pressure.

Charles's Law: Volume of a fixed amount of gas is directly proportional to the kelvin temperature if the pressure is kept constant.

Mathematically: $V_1/T_1 = V_2/T_2$ (at constant P)

V_1 = initial volume, V_2 = final volume, T_1 = initial temperature in Kelvin, T_2 = final temperature in Kelvin

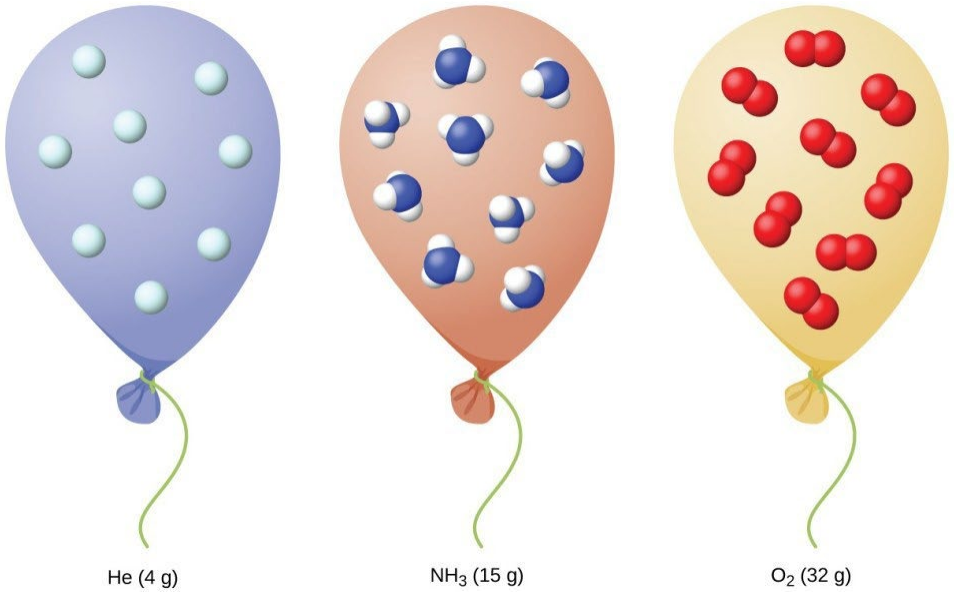


Figure 3.9: Hot air balloon illustrating Charles's Law. Heating the air inside the balloon increases its volume, making the air less dense than the surrounding atmosphere. The buoyant force then lifts the balloon.

We can understand the absolute zero temperature from Charles's Law. For a sample of gas, when temperature decreases, volume of the gas molecules decrease. Hypothetically if the absolute temperature of a gaseous system reaches zero i.e. –273°C, all the gas molecules' motion will cease and the volume of the gas molecule would be zero.

Figure 3.10: Pressure vs. Temperature plot for four different gases (Charles's Law). All lines extrapolate to –273.15°C (absolute zero) where pressure and volume would theoretically equal zero.

Equation: $V_1/T_1 = V_2/T_2$ (at constant P)

Example: A volume of 1.00 L of gas at 37°C is expelled from the lungs to cold outside at temperature –5°C. What is the volume of the air at that temperature?

Answer: V_2 is unknown.

$1.00/(37+273) = V_2/(–5+273)$, $1/310 = V_2/268$, $V_2 = 0.865$ L

3. Volume and the Number of Molecules: Avogadro's Law

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.

Avogadro's Law: Volume of a gas is directly proportional to the number of moles of gas if the pressure and temperature are kept constant.

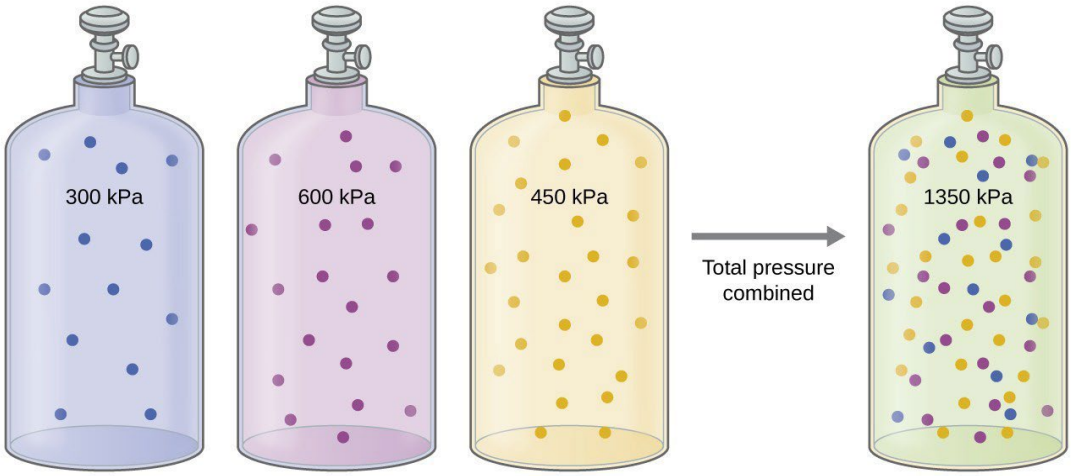


Figure 3.11: PhET simulation demonstrating Avogadro's Law. Doubling the number of molecules (from 50 to 100) at constant temperature and pressure causes the container volume to double. Equal volumes of gases contain equal numbers of molecules (E.V.E.N. principle).

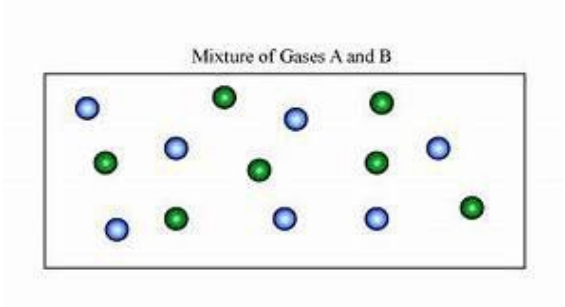


Figure 3.12: Avogadro's Law — Volume vs. Amount (moles) graph. The straight line through the origin shows that volume is directly proportional to the number of moles of gas at constant T and P ($V_1/n_1 = V_2/n_2$).

Mathematically: $V_1/n_1 = V_2/n_2$ (at constant P and T)

V_1 = initial volume, V_2 = final volume, n_1 = initial moles, n_2 = final moles

Example: The lungs of an average male hold 0.25 mol of air in a volume of 5.5 L. How many moles of air do the lungs of an average female hold if the volume is 4.5 L?

Answer: $5.5/0.25 = 4.5/n_2$, $22 = 4.5/n_2$, $n_2 = 0.205$ mol or 0.20 mols

4. Gay-Lussac's Law (Amonton's Law)

Gay-Lussac's Law: With volume remaining constant, the pressure of a gas molecule is directly proportional to its absolute temperature. When temperature increases, the gas molecules possess high kinetic energy and collide more frequently, increasing gas pressure.

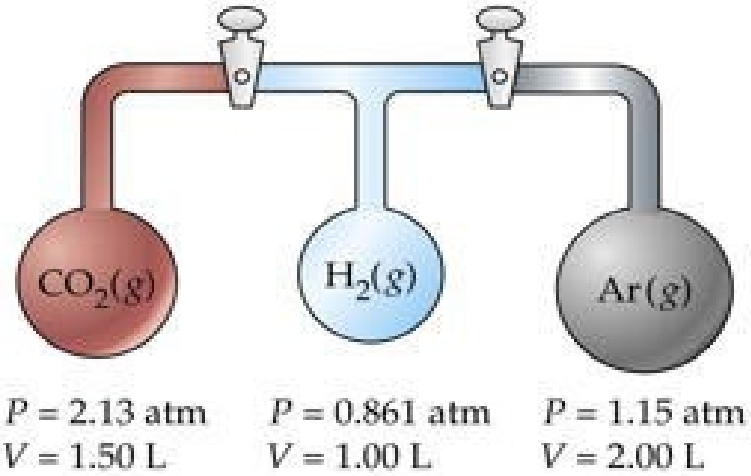


Figure 3.13: Gay-Lussac's Law. At constant volume, increasing temperature increases molecular speed and collision frequency, raising pressure. Left: lower T, lower P. Right: higher T (heated), higher P.

Figure 3.14: PhET simulation of Gay-Lussac's Law at 2225K showing increased pressure (2.54 Atm) at constant volume. Higher temperature → faster molecules → more frequent wall collisions → higher pressure.

Mathematically: $P_1/T_1 = P_2/T_2$ (at constant V and n)

P_1 = initial pressure, P_2 = final pressure, T_1 = initial temperature, T_2 = final temperature

Example: The tire on a bicycle in a cool garage is stored at 20°C and 80 psi. What is the pressure inside the tire after riding the bike at 43°C?

Answer: $80/(20+273) = P_2/(43+273)$, $0.273 = P_2/316$, $P_2 = 0.273 \times 316 = 86.3$ psi or 86 psi.

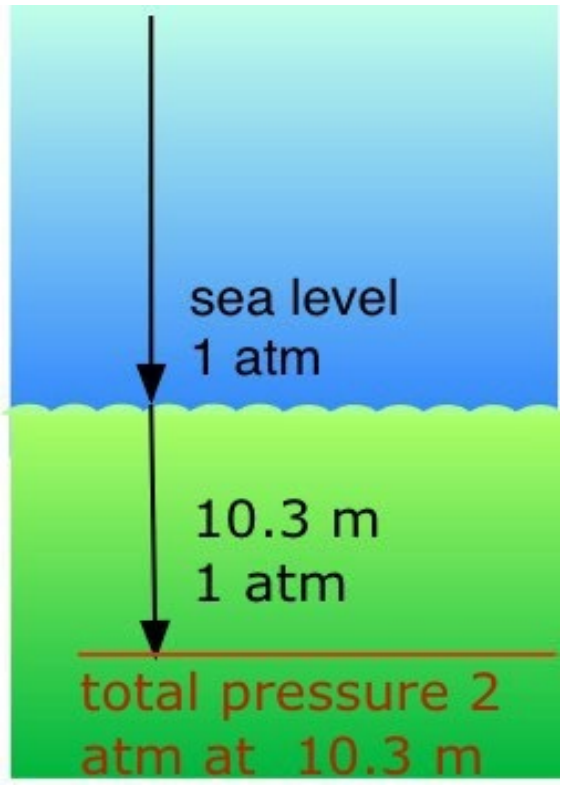


Figure 3.15: Summary of the three basic gas laws. Boyle's Law (constant T): $P_1V_1 = P_2V_2$. Charles' Law (constant P): $V_1/T_1 = V_2/T_2$. Gay-Lussac's Law (constant V): $P_1/T_1 = P_2/T_2$.

Checking Comprehension:

1. Calculate the temperature of a gas when it is expanded to 5.25 L. The gas originally occupies 3.45 L of space at 282 K.

2. The temperature of a gas is increased from 125°C to 182°C inside of a rigid container. The original pressure of the gas was 1.22 atm, what will the pressure of the gas be after the temperature change?

3. The volume of gas in a container was originally 3.24 L, while at standard pressure, 1.00 atm. What will the volume be if the pressure is increased to 1.20 atm?

IV. Combined Gas Law

The combined gas law is an expression obtained mathematically combining Boyle's and Charles'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.

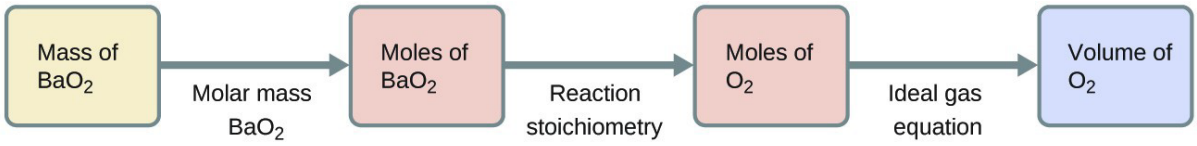


Figure 4.1: Visual summary of three gas laws. (a) Amonton's Law: heating at constant volume increases pressure. (b) Boyle's Law: decreasing volume at constant temperature increases pressure. (c) Avogadro's Law: adding gas at constant pressure increases volume.

Mathematically, when amount of gas (n) is constant:

$(P_1V_1)/T_1 = (P_2V_2)/T_2$

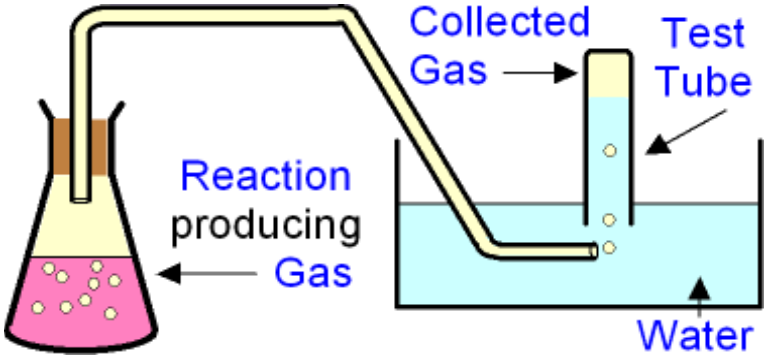


Figure 4.2: Graphical relationships between gas properties. (a) P vs V: inverse relationship (Boyle's Law). (b) V vs T: direct relationship (Charles's Law). (c) P vs T: direct relationship (Gay-Lussac's Law). (d) 1/P vs V: linear relationship confirming inverse proportionality.

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°C and the pressure is 540 mm of Hg?

Answer: V_2 is unknown.

$222\times760/(25+273) = V_2\times540/(-40+273)$, $V_2 = 244.3$ L or 244 L.

Question: The pressure inside a 1.0 L balloon at 25°C was 750 mm of Hg. What is the pressure inside the balloon when it is cooled to –40°C and expands to 5.0 L volume?

V. Ideal Gas Law

The ideal gas law holds for all ideal gases at any temperature, pressure, and volume. Real gases behave most like ideal gases at low pressures (atm or less) and high temperatures (K or higher). It combines all the gas law variables into one equation.

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 the universal gas constant.

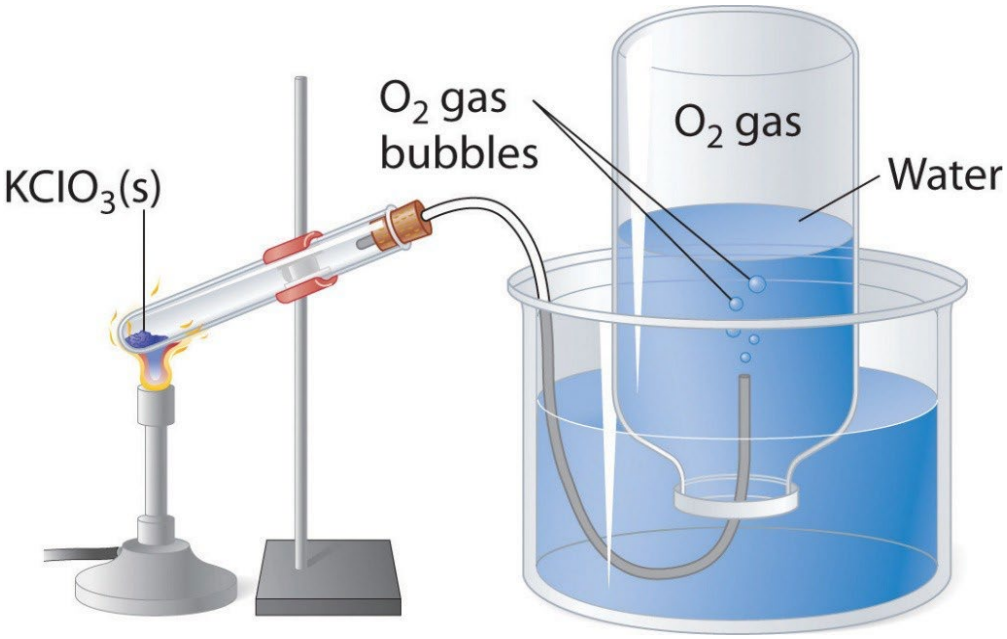


Figure 5.1: The Ideal Gas Law (PV = nRT) is derived by combining Boyle's Law ($P \propto 1/V$), Charles's Law ($V \propto T$), and Avogadro's Law ($V \propto n$) into a single unified equation.

PV = nRT (Must know this!)

Where R = Ideal Gas Constant = 0.08206 L·atm/mol·K = 8.314 J/mol·K

With this equation, any one of the characteristics gas properties (P, V, T or n) can be calculated given the other three.

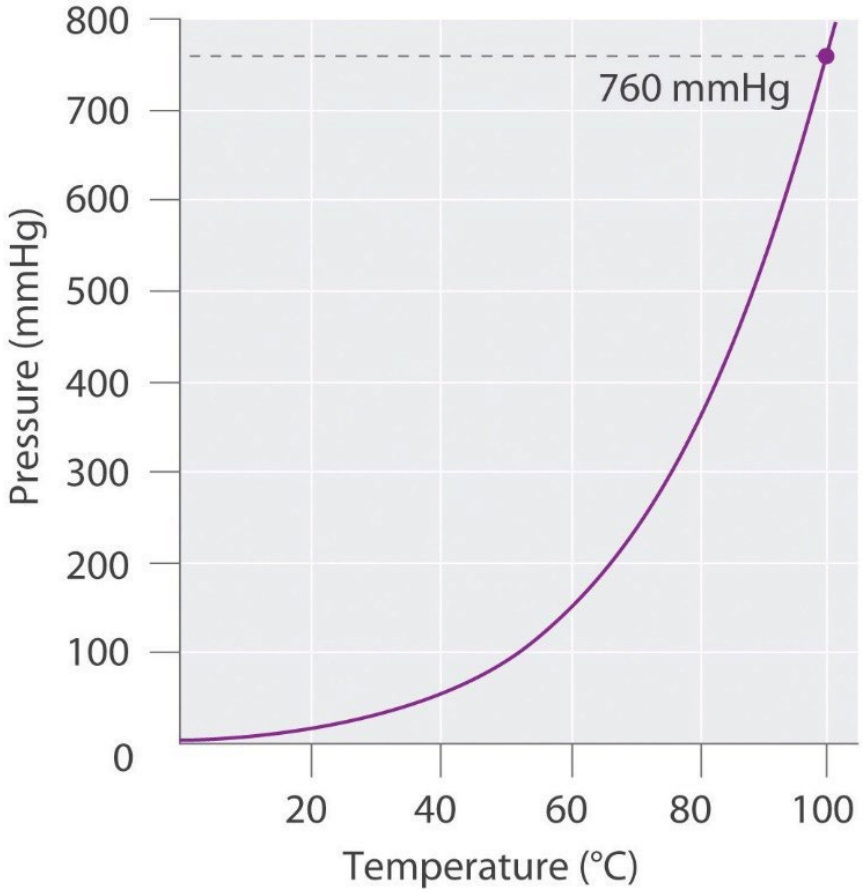


Figure 5.2: Universal gas constant R expressed in multiple unit systems. Use R = 0.0821 L·atm/(mol·K) when pressure is in atm and volume in liters; use R = 8.314 J/(mol·K) for energy calculations.

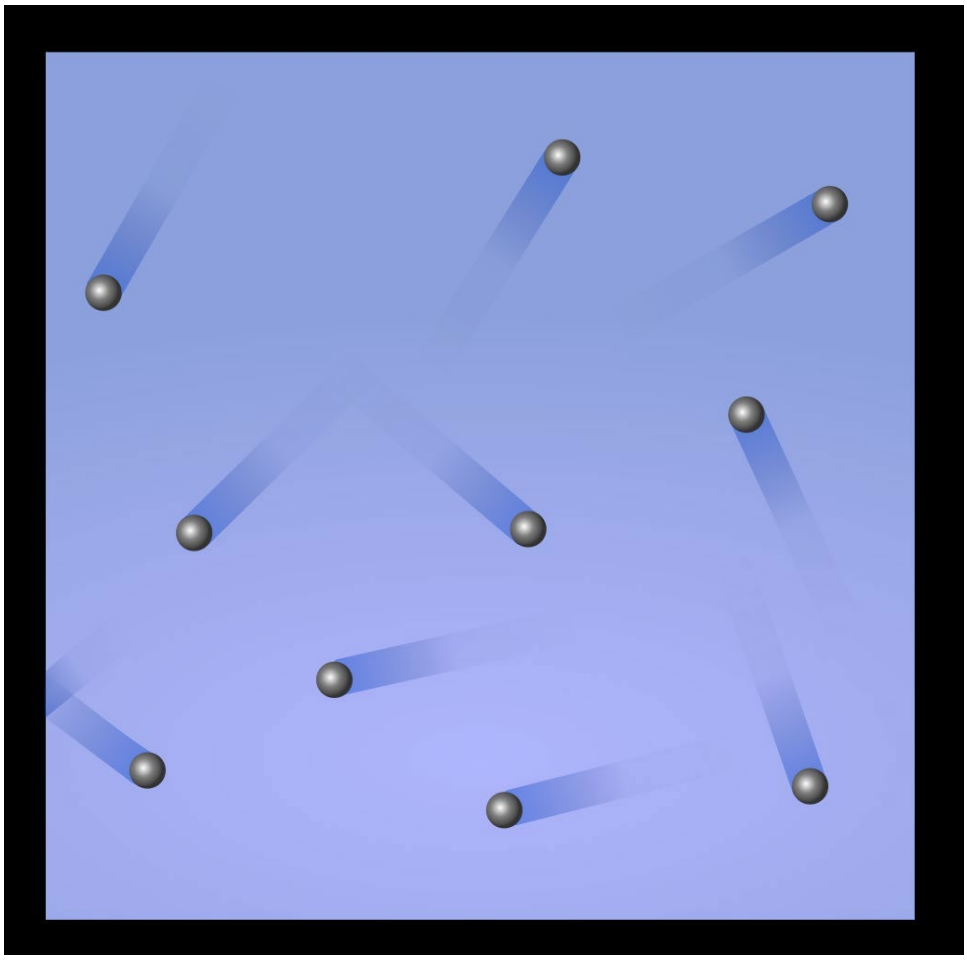


Figure 5.3: PV = nRT — the Ideal Gas Law. This simulation at phet.colorado.edu demonstrates how all four gas properties (P, V, n, T) are interrelated. Changing any one variable affects the others according to this equation.

Ideal gas law follows all the assumptions of kinetic molecular theory. Real molecules only behave ideally at low pressure and high temperature.

4. 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. The ideal gas equation of state is: PV = nRT

An ideal gas is defined as a hypothetical substance that obeys the ideal gas equation of state.

Solution example: Use the ideal gas equation to find the number of moles of CO_2 gas: n = PV/RT

Example: How many moles of gas are in a typical human breath that takes in 0.50 L of air at 1.0 atm pressure and 35°C?

Number of moles n is unknown. T = 35+273 = 308 K

n = PV/RT = (1.0×0.50)/(0.0821×308) = 0.0198 mol or 0.020 mol

VI. Molar Volume of a Gas

Further application of Ideal Gas Law: Density and Molar Mass

1. The Molar Volume of a Gas

The molar mass of a pure substance is the mass of 6.02×10^{23} (Avogadro's number) of particles or molecular units of that substance.

STP (Standard Temperature and Pressure)

STP conditions are: 1 atm (760 mm of pressure) and 273 K (0°C)

At STP, one mole of any gas has the same volume: 22.4 L — called the standard molar volume.

Example: 1 mol = 22.4 L. How many moles are present in 5.00 L of O_2 at STP?

(1 mol / 22.4 L) = (x mol / 5.00 L), x = 0.223 mols

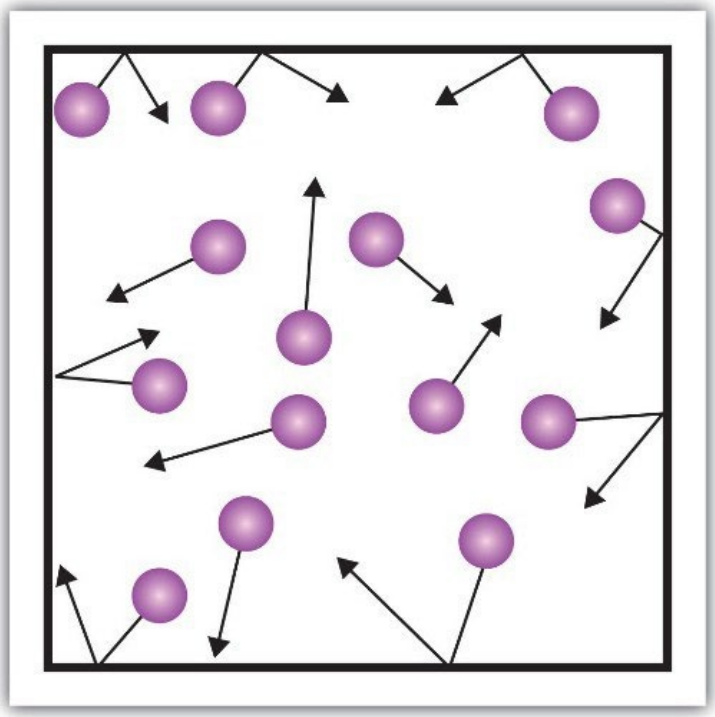


Figure 6.1: At STP, all different gases occupy the same volume (22.4 L per mole). Left: 1 mol He (4 g). Center: 1 mol NH_3 (17 g). Right: 1 mol O_2 (32 g). Despite different masses, all three balloons are the same size — demonstrating the E.V.E.N. principle.

Questions:

1. Burning 1 mol 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: 273 K, 1 atm

The magnitude of this volume depends on the temperature and pressure. At STP (T = 273 K and P = 1 atm), 1 mole of any gas occupies 22.414 litres.

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.

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.

Average molar mass formula: $\bar{m} = \Sigma\, x_i m_i$ (sum of mole fractions times individual molar masses)

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: m = (0.21×32) + (0.78×28) + (0.01×40) = 29 g/mol

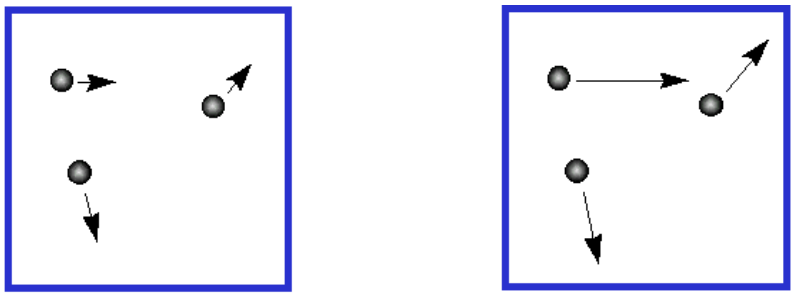
Problem Example 4: Uranium hexafluoride UF_6 gas (MW = 352) density at STP:

(352 g mol^{-1}) ÷ (22.4 L mol^{-1}) = 15.7 g L^{-1}

Problem Example 5: Molar mass of a gas with density 3.33 g/L at 30°C and 780 torr = 80 g mol^{-1}

Problem Example 6: Composition of a CO_2/CH_4 mixture with STP density 1.214 g/L: mole fraction of CO_2 = 0.40, CH_4 = 0.60

3. Expressing the Composition of a Gas Mixture



Lower average kinetic energy
Lower absolute temperature

Higher average kinetic energy
Higher absolute temperature

Figure 6.2: Volume fractions in gas mixtures. When partitioned Gas A (2/3 volume) and Gas B (1/3 volume) are allowed to mix, total volume is unchanged (Avogadro's Law). Volume fractions equal mole fractions for ideal gases.

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.

Volume fractions are often called partial volumes. For oxygen in air: mole fraction = 0.21/1.00 = 0.21

The mathematical form of the Ideal Gas Law extended: PV = nRT and n = m/MW and d = m/V

Problem Example 7: O_2/N_2O mixture with density 1.482 g/L at 25°C and 0.980 atm. N_2O mole fraction = 5/12 = 0.42

Problem Example 8: CO_2 (MW=44) and Neon (MW=20.2) equal masses: mole fraction of Ne = 0.32

Density of an ideal gas: d = (M × P) / (R × T)

Question: What is the density of an ideal gas with molecular mass of 50 g/mol at 2 atm and 27°C?

Solution: T = 27+273 = 300 K; R = 0.0821 L·atm/mol·K

d = (50×2)/(0.0821×300) = 4.06 g/L

VII. Dalton's Law of Partial Pressure

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.

Dalton's Law of Partial Pressures states that the total pressure exerted by a mixture of gases is the sum of the partial pressures of the individual gases.

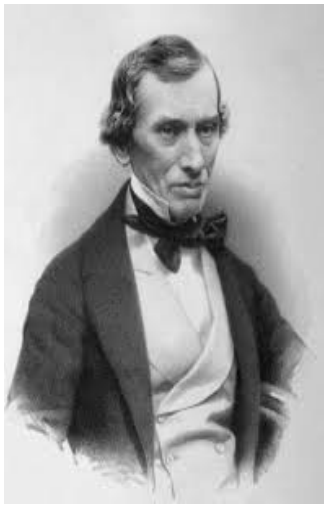


Figure 7.1: Dalton's Law of Partial Pressures. Three separate gas cylinders at 300 kPa, 600 kPa, and 450 kPa are combined into one container. The total pressure equals the sum: 300 + 600 + 450 = 1350 kPa.

Mathematically: $P_total = P_1 + P_2 + P_3 + ... + P_n = \Sigma P_i$

Partial pressure of a gas can be calculated using the mole fraction of a gas in a gas mixture and total pressure: $P_a = X_a \times P_total$

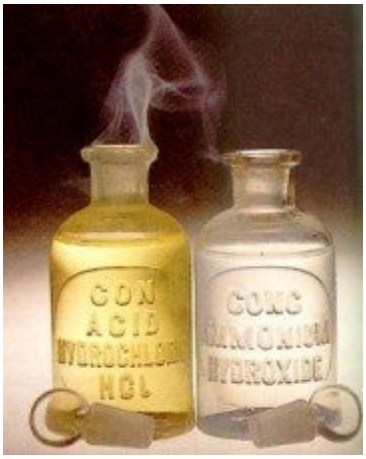


Figure 7.2: Mixture of Gas A (blue) and Gas B (green). With 7 molecules of each type out of 14 total, each has a mole fraction of 0.5. If total pressure = 1 atm, each gas exerts a partial pressure of 0.5 atm.

Example: In the diagram above, total molecules = 14. Gas A (blue) = 7, Gas B (green) = 7.

Mole fraction of A = 7/14 = 0.5; Mole fraction of B = 7/14 = 0.5

If total pressure = 1 atm: Partial pressure of A = 0.5×1 = 0.5 atm; Partial pressure of B = 0.5×1 = 0.5 atm

Mole Fractions of Gas Mixtures

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: $X_i = n_i / n_total$

The mole fraction is a dimensionless quantity between 0 and 1. The sum of all mole fractions equals 1.

The relationship between partial pressure and mole fraction: $P_a = X_a \times P_total$

Earth's atmosphere: 78% N_2, 21% O_2, 0.9% Ar, with trace amounts of CO_2, H_2O, and others.

Partial pressure of N_2 = 0.78 × 760 mmHg = 593 mmHg

Partial pressure of O_2 = 0.21 × 760 mmHg = 160 mmHg

Problem Example 9: Fluorine and xenon (MW 131.3) in 2.0-L flask. Partial pressure of Xe = 350 torr, total = 724 torr. Mass of Xe = 4.9 g

Problem Example 10: Three connected flasks — CO_2(g) at 2.13 atm/1.50 L, H_2(g) at 0.861 atm/1.00 L, Ar(g) at 1.15 atm/2.00 L. After opening stopcocks: final pressure = 1.41 atm; CO_2 is most abundant.

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. This arrangement is called a pneumatic trough.

When the gas enters the bottle it displaces the water and becomes trapped in the upper part. The partial pressure of H_2O is known as the vapor pressure of water.

$P_gas = P_total – P_H_2O$

Problem Example 11: O_2 collected over water: atmospheric pressure = 754 torr, temperature = 22°C, volume = 155 mL. Vapor pressure of water at 22°C = 19.8 torr.

$P_O_2 = 754 – 19.8 = 734$ torr = 0.966 atm

$n = PV/RT = (0.966 \times 0.155)/(0.082 \times 295) = 0.00619$ mol

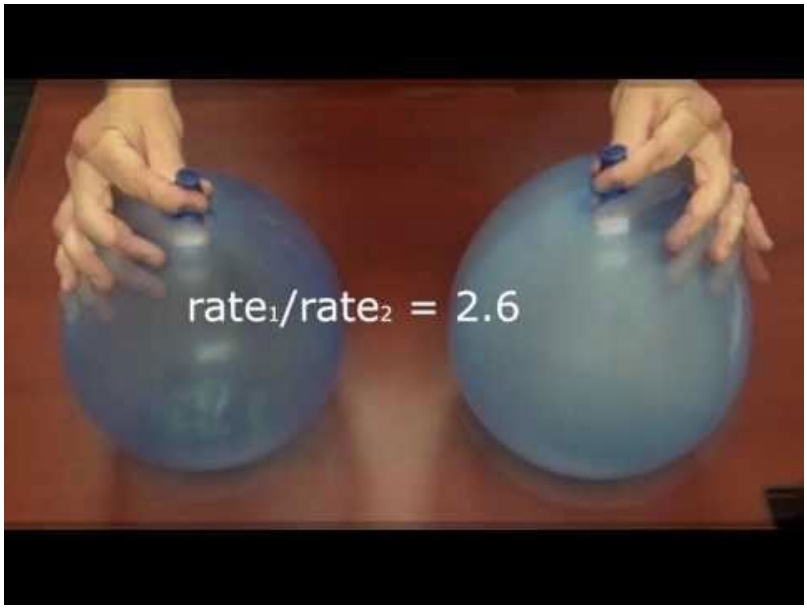


Figure 7.3: Scuba diving and Dalton's Law. At depth, total pressure increases (1 atm per 10.3 m). Without adjusting gas mixtures, partial pressure of O_2 would become toxic. Divers' tanks use helium-enriched mixtures to maintain safe partial pressures of each gas.

Scuba Diving and Dalton's Law: Below the water surface, pressure increases by 1 atm for each 10.3 m increase in depth. At 100 ft (~30 m), the O_2 partial pressure of 0.8 atm would be high enough to cause oxygen toxicity. The preferred diluting agent for deep diving is helium.

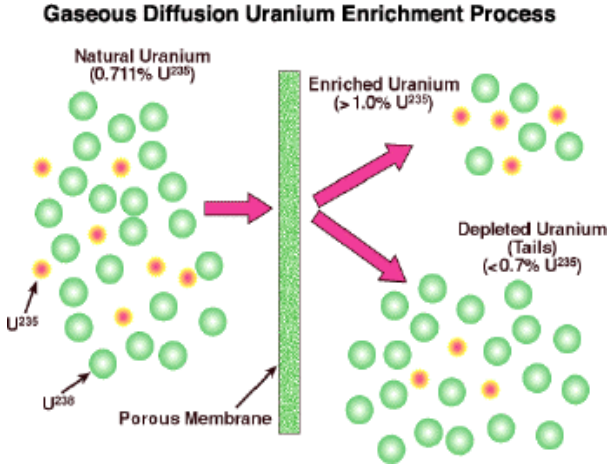


Figure 7.4: Pressure-depth relationship in water. Pressure increases by 1 atm for every 10.3 m of depth. At 10.3 m, a diver experiences 2 atm total pressure (1 atm atmospheric + 1 atm water pressure).

Table 2: Vapor Pressure of Water at Various Temperatures (T in °C, P in mmHg)

T (°C)	P (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

T (°C)	P (mmHg)	T	P	T	P	T	P
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
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

Table 2: Vapor pressure of water (in mmHg) as a function of temperature (°C). To find the pressure of a gas collected over water, subtract the appropriate vapor pressure from total pressure: P_gas = P_total − P_H₂O.

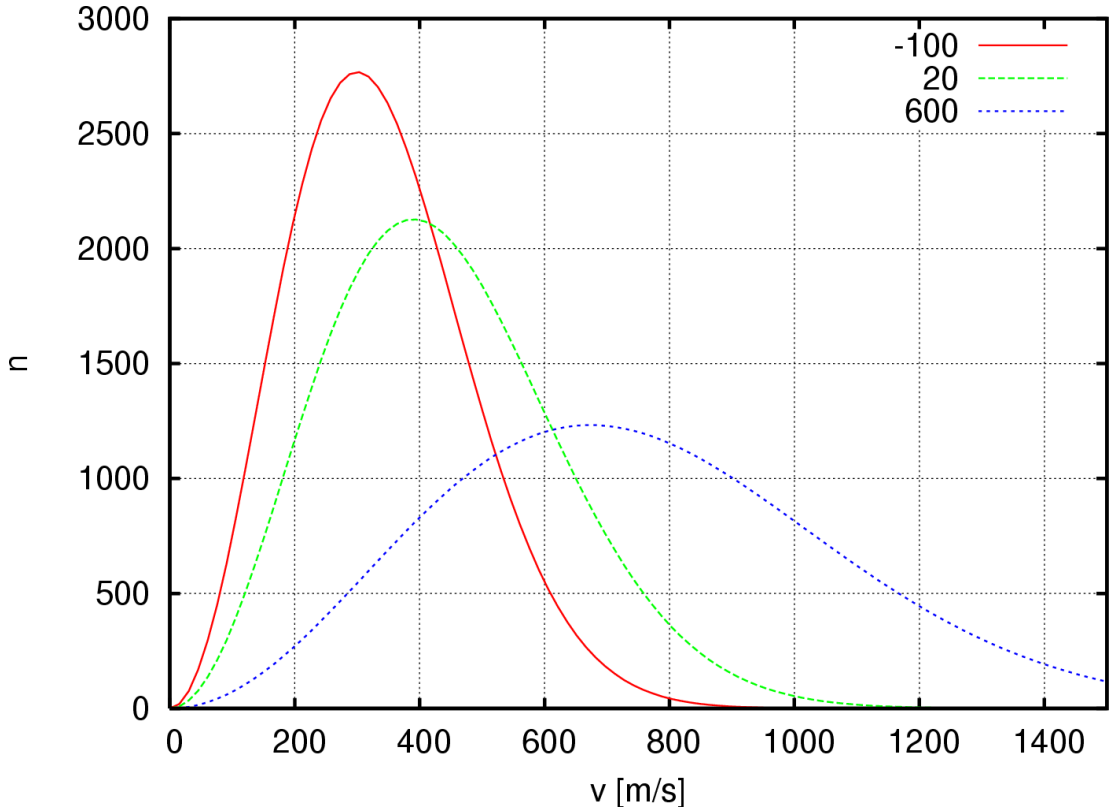


Figure 7.5: Vapor pressure of water as a function of temperature. The curve rises steeply near the boiling point (100°C = 760 mmHg). When collecting gases over water, this vapor pressure must be subtracted from total pressure to find the pressure of the collected gas.

Practice Questions:

1. CO_2 is added to a container containing 2.5 atm of O_2 to give total pressure 4.0 atm. What is the partial pressure of CO_2?

2. Blast furnace gases: total pressure 0.99 atm, CO_2 partial = 0.05 atm, H_2S partial = 0.02 atm. What is the remaining air partial pressure?

3. O_2 at 401 mmHg and Cl_2 at 0.639 atm. Total pressure in atm?

4. 3 mol N_2 and 4 mol O_2 in 35 L at 25°C. Total pressure in atm?

5. 5 mol CO_2, 3 mol N_2, 1 mol H_2; total pressure 1.05 atm. Partial pressure of CO_2?

6. He/Ar mixture, 30% He by volume, total pressure 4.00 atm. Partial pressures of He and Ar?

7. Flask A: 4.0 L N_2 at 2.0 atm. Flask B: 10.0 L CO at 1.4 atm. Final pressure after connecting?

8. Container A (1.23 L, 3.24 atm), B (0.93 L, 2.82 atm), C (1.42 L, 1.21 atm). Combined into D (1.51 L). Pressure in D?

Practice Problems (Density and Molar Mass):

1. Density of N_2O at 325 K and 113.0 kPa?

2. Density of Freon 12 (CF_2Cl_2) at 30.0°C and 0.954 atm?

3. Which is denser at same T and P: dry air or water-saturated air? Explain.

4. O_2 cylinder: 3.00 L at 10.0 atm, 28.0°C. Mass of oxygen?

5. Molar mass of gas: 0.0494 g in 0.100 L at 26°C and 307 torr?

6. Molar mass: 0.281 g in 125 mL at 126°C and 777 torr?

7. How could you show propene is C_3H_6 not CH_2?

8. Gaseous phosphorus fluoride: density 3.93 g/L at STP. Molar mass and molecular formula?

9. Compound: 39% C, 45% N, 16% H. 0.157 g in 125 mL at 99.5 kPa and 22°C. Molecular formula?

VIII. Gas Stoichiometry

In reactions involving gaseous reactants and products we often report quantities in volumes at specific pressures and temperatures. We can convert these quantities to amounts (in moles) using the ideal gas law.

General form: Volume A → amount of A (in moles) → amount of B (in moles) → volume or mass of B

At STP: use molar volume 22.4 L = 1 mol to convert between volume and moles.

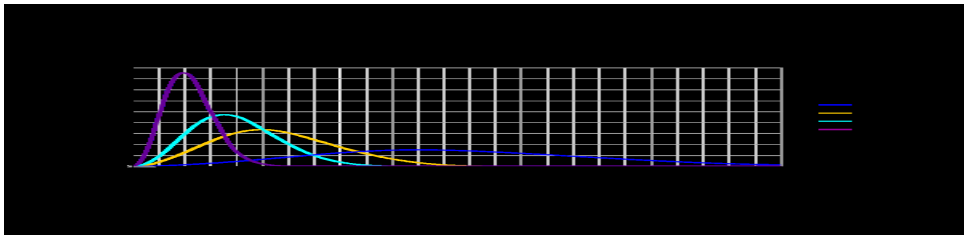


Figure 8.1: Gas stoichiometry roadmap. To find the volume of O_2 produced from BaO_2: convert mass to moles (using molar mass), convert moles of BaO_2 to moles of O_2 (using stoichiometric ratio), then convert moles of O_2 to volume (using ideal gas law).

Question: In laboratory, 25.0 g of BaO_2 was heated to produce gaseous oxygen. Oxygen gas was collected over water at 738 mm Hg and 23°C. Vapor pressure of water is 21 torr at 23°C. How many Liters of oxygen was produced?

Molar mass of BaO_2 = 169.3 g/mol

Reaction: $2\ BaO_2 \rightarrow 2\ BaO + O_2$ (note: actually $2\ BaO_2 \rightarrow 2\ BaO + O_2$, ratio 2:1 for O_2)

Moles of BaO_2 = 25.0g / 169.3 g/mol = 0.1477 mol

Moles of O_2 = 0.1477 mol × (2 mol O_2 / 2 mol BaO_2) = 0.1477 mol

Pressure of O_2 = 738–21 = 717 torr = 717×(1 atm/760) = 0.943 atm

Temperature = 23+273 = 296 K

V = nRT/P = (0.1477×0.0821×296) / 0.943 = 3.81 L

Gas Collected Over Water

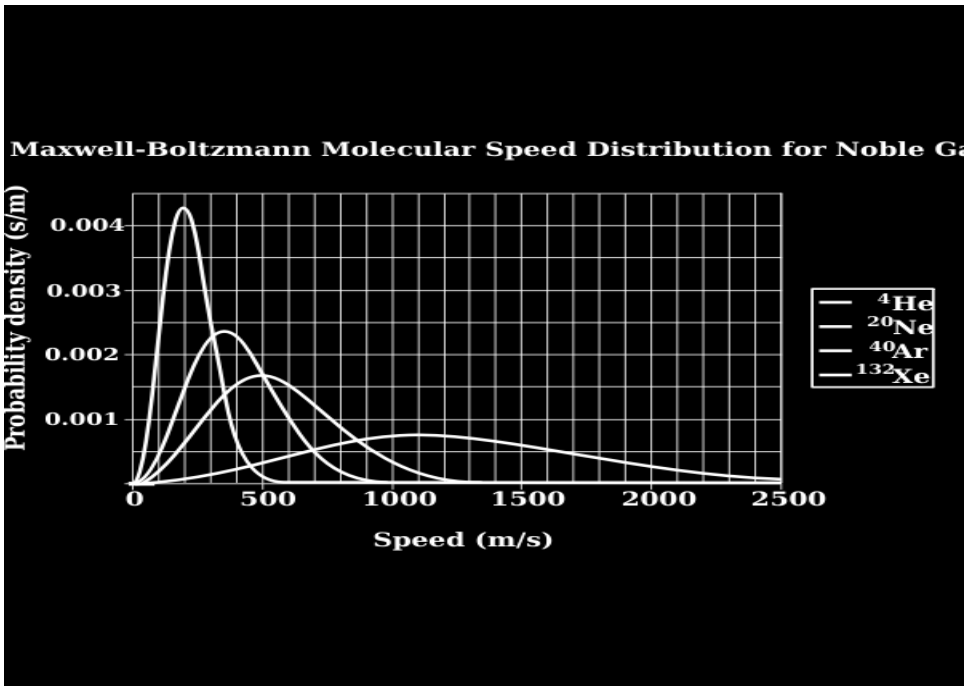


Figure 8.2: Apparatus for collecting gas over water. Gas produced in the reaction flask bubbles through water and is trapped in the inverted collection tube. The collected gas is a mixture of the product gas and water vapor, so vapor pressure of water must be subtracted: P_gas = P_total − P_H₂O.

The law of partial pressure is frequently used to determine the yield of a water-insoluble gas formed in a reaction:

$P_{total} - P_{H_2O} = P_{gas}$

Apply PV = nRT to find the moles. Knowing the molar mass, find the mass of the gas.

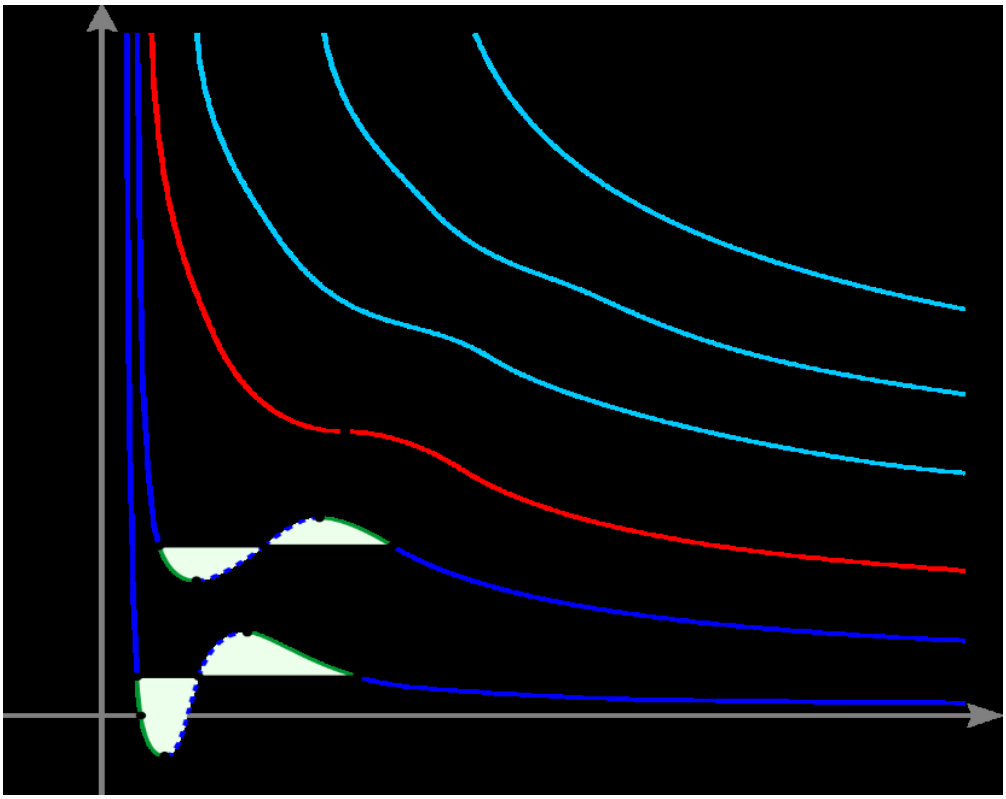


Figure 8.3: Collection of O_2 gas from thermal decomposition of $KClO_3$. $2\ KClO_3(s) \rightarrow 2\ KCl(s) + 3\ O_2(g)$. Oxygen displaces water in the inverted bottle. Note: the collected gas contains both O_2 and water vapor, so the water vapor pressure must be subtracted.

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: the gas collected inside the bottle is a mixture of the product gas and water vapor, not pure product.

IX. Kinetic Molecular Theory

The properties such as temperature, pressure, and volume are known as macroscopic properties of matter. The kinetic molecular theory of gases relates these macroscopic properties to the behavior of the individual molecules.

The kinetic molecular theory applies strictly to an ideal gas, but under many conditions it describes the behavior of real gases quite accurately.

1. The Basic Ideas of Kinetic Molecular Theory

The basic tenets of the kinetic-molecular theory are as follows:

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.

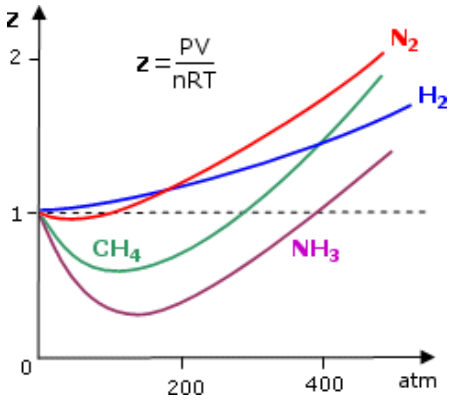


Figure 9.1: Kinetic Molecular Theory assumption A — Gas molecules are widely separated. The space between molecules is much larger than the molecules themselves, so molecular volume is negligible compared to container volume.

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 the molecules move in straight lines until they collide with each other or with the walls of the container.

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".

Figure 9.2: KMT assumption E — Average kinetic energy is proportional to absolute temperature. Left: lower temperature → slower molecules → lower kinetic energy. Right: higher temperature → faster molecules → higher kinetic energy. KE_avg = (3/2)RT/N_A.

E) The average kinetic energy of the gas molecules is directly proportional to the absolute temperature. This implies that all molecular motion would cease if the temperature were reduced to absolute zero.

According to this model, most of the volume occupied by a gas is empty space. Gas molecules at ordinary temperatures and pressures have velocities of the order of 0.1–1 km/sec and each molecule experiences approximately 10^{10} collisions with other molecules every second.

Kinetic explanation of Boyle's Law: 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's Law: 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 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.

Kinetic explanation of Dalton's Law: "Every gas is a vacuum to every other gas." Each gas present in a mixture acts independently of the others, contributing its own pressure to the total pressure in proportion to its mole fraction.

Kinetic energy formula: $KE = \frac{1}{2}mv^2$

X. Diffusion & Effusion

The process by which gas molecules spread out in response to a concentration gradient is diffusion. Heavier molecules diffuse more slowly than lighter molecules.

Effusion is the process by which a gas escapes from its container through a tiny hole into an evacuated space.

Graham's Law of Effusion (1846): The effusion rate is inversely proportional to the square root of the molar mass.

$R_1/R_2 = \sqrt{(M_2/M_1)}$

Diffusion: random motion with direction. Diffusion refers to the transport of matter through a concentration gradient; substances move from regions of higher concentration to those of lower concentration.

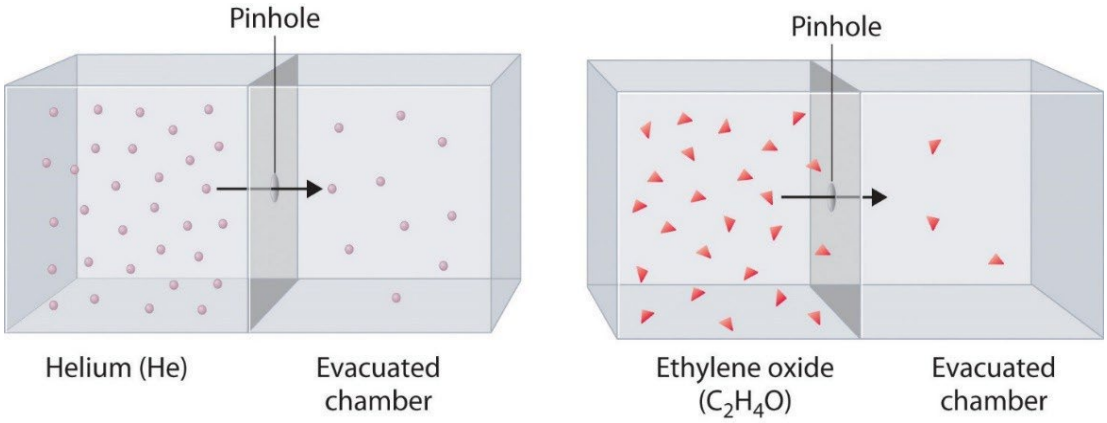


Figure 10.1: Diffusion demonstration. HCl gas from the left bottle and NH_3 gas from the right bottle diffuse through air and react where they meet: $HCl(g) + NH_3(g) \rightarrow NH_4Cl(s)$. The white smoke of solid ammonium chloride marks the meeting point.

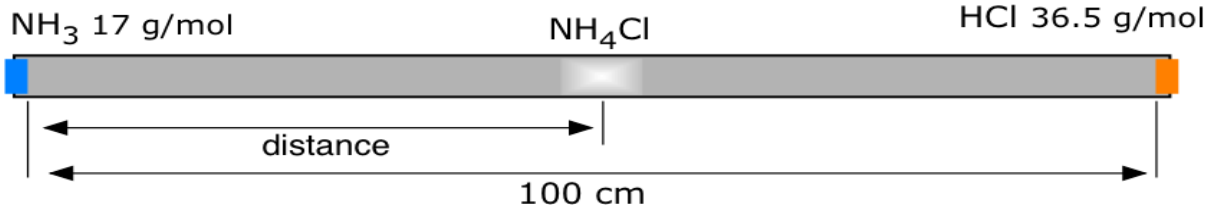


Figure 10.2: Diffusion of N_2 and O_2 between connected flasks. Top: Before mixing, N_2 (green) and O_2 (blue/orange) are separate. Bottom: After opening the stopcock, both gases distribute evenly, each at half its original pressure in both flasks.

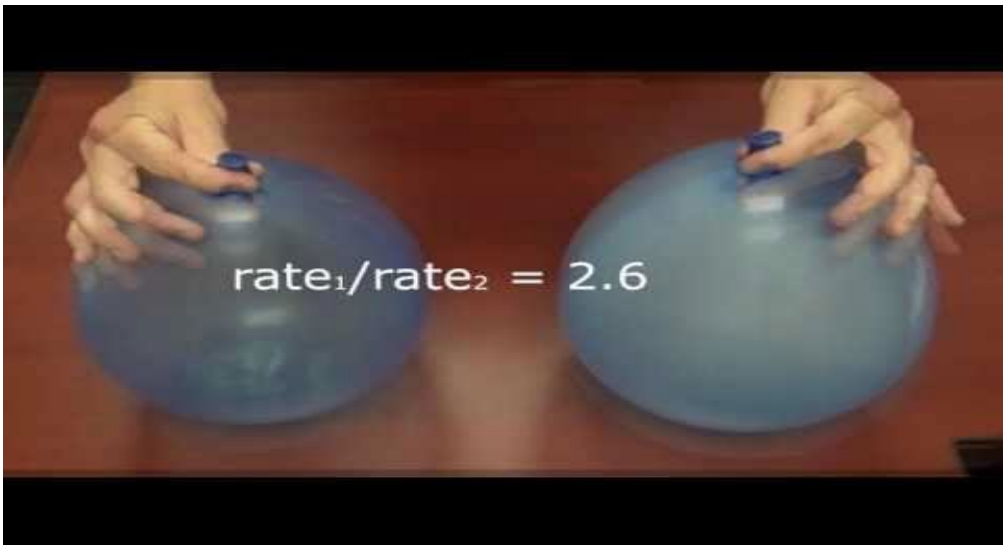


Figure 10.3: Effusion of gases through a pinhole. Left: Helium (He, MW = 4 g/mol) effuses rapidly due to its low molar mass. Right: Ethylene oxide (C_2H_4O, MW = 44 g/mol) effuses more slowly. According to Graham's Law, rate of effusion $\propto 1/\sqrt{M}$.

Around 1830, Thomas Graham 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.

Graham's Law: $v_1/v_2 = \sqrt{(M_2/M_1)}$

This means the average velocity of the lighter molecules must be greater than those of the heavier molecules.

Because of the presence of many other gas molecules, diffusion rates are much lower than effusion rates.

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 (C_2H_6) to effuse?

Uranium Enrichment (Graham's Law Application):

Natural uranium (mostly U^{238}, only 0.7% fissionable U^{235}) reacts with fluorine to form gaseous UF_6. In the gaseous diffusion process, UF_6 diffuses repeatedly through a porous wall. The lighter $U^{235}F_6$ isotope passes through slightly more rapidly, enriching the mixture in U^{235}. This process must be repeated over a thousand times to achieve the desired enrichment.

Distribution of Molecular Speed

In a sample of gas, several different molecules are moving at different speeds. Root Mean Square Velocity: $u = \sqrt{(3RT/M)}$

Q: What is the root-mean-square speed for a sample of oxygen gas at 298 K?

$u = \sqrt{(3RT/M)} = \sqrt{(3 \times 8.314 \times 298 / 0.032)} = 484$ m/s

XI. Behavior of Real Gases

Real Gases differ from ideal gases to the extent that they do not always fit the assumptions of kinetic molecular theory.

The assumptions tend to break at high pressure where the volume is higher than predicted for an ideal gas — because molecular volumes are no longer negligible compared to the space between molecules.

The assumptions also break at low temperature where the pressure is lower than predicted — because attractions between molecules combined with low kinetic energy cause partially inelastic collisions.

At moderately high pressure, values of PV/RT less than 1 are mainly due to intermolecular attractions. At very high pressure, values of PV/RT greater than 1 are mainly due to molecular volume.

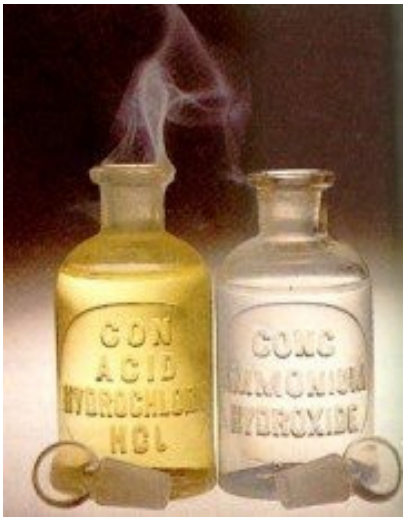


Figure 11.1: Johannes Diderik van der Waals (1837–1923), Nobel Prize-winning physicist who developed the Van der Waals equation to describe the behavior of real gases by accounting for intermolecular attractions and molecular volume.

Van der Waals Equation (The Ideal Gas Law redesigned):

$[P + (an^2/V^2)](V - nb) = nRT$

P = observed pressure, V = observed volume, T = temperature, n = moles

"a" = Van der Waals constant related to intermolecular attractions (strength and complexity of molecules)

"b" = Van der Waals constant related to molecular volume

At ordinary conditions, Van der Waals equation becomes the ideal gas equation (a and b ≈ 0 for ideal gases).

*** Adapted from Chem I Virtual textbook:
http://www.chem1.com/acad/webtext/virtualtextbook.html

Practice Questions: Chapter 9

5. What temperature scale should be used if we wish to express Charles's Law as a simple direct proportionality? c. Kelvin

6. Which law relates the volume and pressure of a gas under conditions of constant temperature? b. Boyle's law

12. Which of the following is a mathematical statement of the combined gas law? c. $P_1V_1T_2 = P_2V_2T_1$

13. Which law relates the volume and number of molecules of a gas under conditions of constant temperature and pressure? a. Avogadro's law

15. A quantity of neon gas is under 1.05 atm pressure at 303 K in a 10.0 L vessel. How many moles? c. 0.422 mol

16. Temperature of gas increased from 20°C to 40°C at constant pressure: d. The volume will increase slightly.

17. Temperature decreased from 60°C to 30°C at constant pressure: c. The volume will decrease slightly.

18. Which increases as temperature increases? a. kinetic energy

19. Constant temperature, 10.0 L at 1140 torr changed to 1.00 atm. New volume: c. 15.0 L

20. Volume of 8.00 g O_2 at STP: a. 5.60 L

21. Instrument for measuring atmospheric pressure: b. a barometer

22. CO_2 occupies 22.4 L at STP: b. Contains 6.02×10^{23} molecules.

23. Chloroform boiling point 61.7°C: b. Chloroform is more volatile than water.

24. London dispersion forces: a. They increase as the number of electrons in a molecule increases.

25. Pairs that do NOT engage in hydrogen bonding: d. None — they all engage in hydrogen bonding.

26. Mathematical statement of ideal gas law: b. $PV = nRT$

27. Molecule that can engage in hydrogen bonding: a. HF

28. Ideal gas law rearranged for n: b. $PV/RT = n$

29. Mathematical statement of Boyle's Law: b. $P_1V_1 = P_2V_2$

30. Balloon: 2.00 L at 1.10 atm and 300 K rises to 418 mmHg and 200 K. New volume: b. 2.67 L

31. Which is NOT true per kinetic molecular theory: c. When gas molecules collide they stick together.

32. Phase change not involving a liquid: c. sublimation

33. N_2 partial pressure in dry air at 760.0 torr: c. 593.4 torr

34. Law that applies only to mixtures of gases: 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