

## CHM 111 GENERAL CHEMISTRY I

Course Synopsis: Atoms, molecules and chemical reactions. Modern electronic theory of atoms. Electronic configuration, periodicity and building up of the periodic table. Hybridization and shapes of simple molecules. Valence Forces; Structure of solids. Chemical equations and stoichiometry; Chemical bonding and intermolecular forces, kinetic theory of matter. Elementary thermochemistry; rates of reaction, equilibrium and thermodynamics. Acids, bases and salts. Properties of gases. Redox reactions and introduction to electrochemistry. Radioactivity.

Required Lecture Hours: 3hrs/week X 15 weeks = 45 hours

Number of Units = 3

Course Lecturer: Professor Tunde Odesanya

### Atoms

Most of the Universe consists of matter and energy. Energy is the capacity to do work. Matter has mass and occupies space. All matter is composed of basic elements that cannot be broken down to substances with different chemical or physical properties.

Elements are substances consisting of one type of atom, for example Carbon atoms make up diamond, and also graphite. Pure (24K) gold is composed of only one type of atom, gold atoms. Atoms are the smallest particle into which an element can be divided. The ancient Greek philosophers developed the concept of the atom, although they considered it the fundamental particle that could not be broken down.

Since the work of Enrico Fermi and his colleagues, we now know that the atom **is** divisible, often releasing tremendous energies as in nuclear explosions or (in a controlled fashion in) thermonuclear power plants.

Subatomic particles were discovered during the 1800s. For our purposes we will concentrate only on three of them, summarized in Table 1. The proton is located in the center (or nucleus) of an atom, each atom has at least one proton. Protons have a charge of +1, and a mass of approximately 1 atomic mass unit (amu). Elements differ from each other in the number of protons they have, e.g. Hydrogen has 1 proton; Helium has 2.

The neutron also is located in the atomic nucleus (except in Hydrogen). The neutron has no charge, and a mass of slightly over 1 amu. Some scientists propose the neutron is made up of a proton and electron-like particle.

The electron is a very small particle located outside the nucleus. Because they move at speeds near the speed of light the precise location of electrons is hard to pin down. Electrons occupy orbitals, or areas where they have a high statistical probability of occurring. The charge on an

electron is -1. Its mass is negligible (approximately 1800 electrons are needed to equal the mass of one proton).

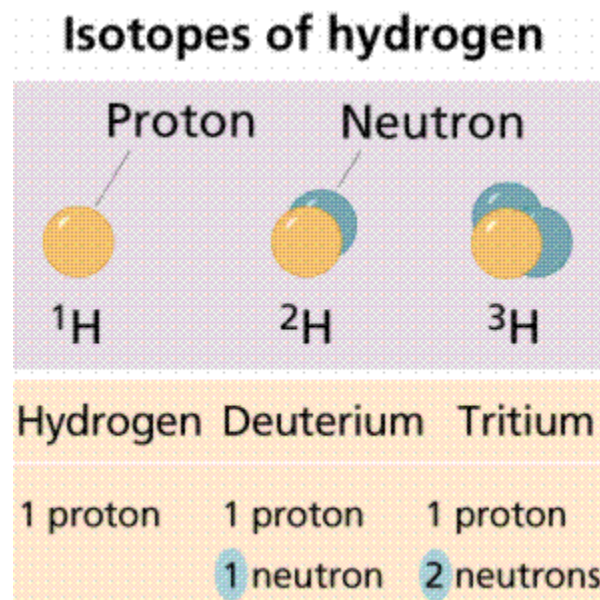
Table 1. Subatomic particles of use in biology.

Name	Charge	Location	Mass
Proton	+1	atomic nucleus	$1.6726 \times 10^{-27}$ kg
Neutron	0	atomic nucleus	$1.6750 \times 10^{-27}$ kg
Electron	-1	electron orbital	$9.1095 \times 10^{-31}$ kg

The atomic number is the number of protons an atom has. It is characteristic and unique for each element. The atomic mass (also referred to as the atomic weight) is the number of protons and neutrons in an atom. Atoms of an element that have differing numbers of neutrons (but a constant atomic number) are termed isotopes. Isotopes, shown in Figure 1 and Figure 2, can be used to determine the diet of ancient peoples by determining proportions of isotopes in mummified or fossilized human tissues. Biochemical pathways can be deciphered by using isotopic tracers. The age of fossils and artifacts can be determined by using radioactive isotopes, either directly on the fossil (if it is young enough) or on the rocks that surround the fossil (for older fossils like dinosaurs). Isotopes are also the source of radiation used in medical diagnostic and treatment procedures.

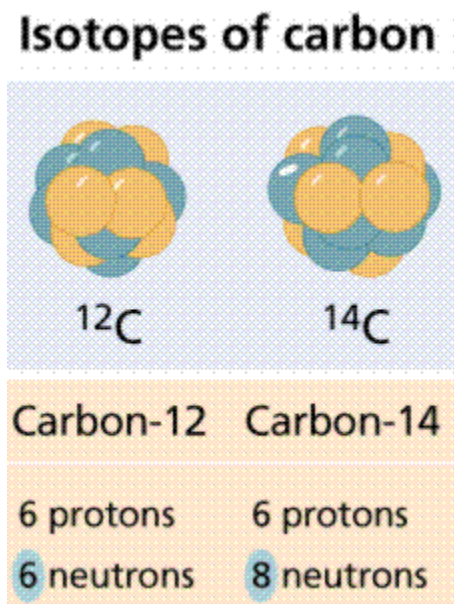
Each of these isotopes of hydrogen has only one proton (Figure 1). Isotopes differ from each other in the number of neutrons, not in the number of protons.

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Some isotopes are radioisotopes, which spontaneously decay, releasing radioactivity. Other isotopes are stable. Examples of radioisotopes are Carbon-14 (symbol  $^{14}\text{C}$ ), and deuterium (also known as Hydrogen-2;  $^2\text{H}$ ). Stable isotopes are  $^{12}\text{C}$  and  $^1\text{H}$ .

Figure 2. Carbon has three isotopes, of which carbon-12 and carbon-14 are the most well known. Image from Purves et al., *Life: The Science of Biology*, 4th Edition, by Sinauer Associates ([www.sinauer.com](http://www.sinauer.com)) and WH Freeman ([www.whfreeman.com](http://www.whfreeman.com)), used with permission.



The Periodic Table of the Elements, a version of which is shown in Figure 3, provides a great deal of information about various elements.

Figure 3. The Periodic Table of the Elements.

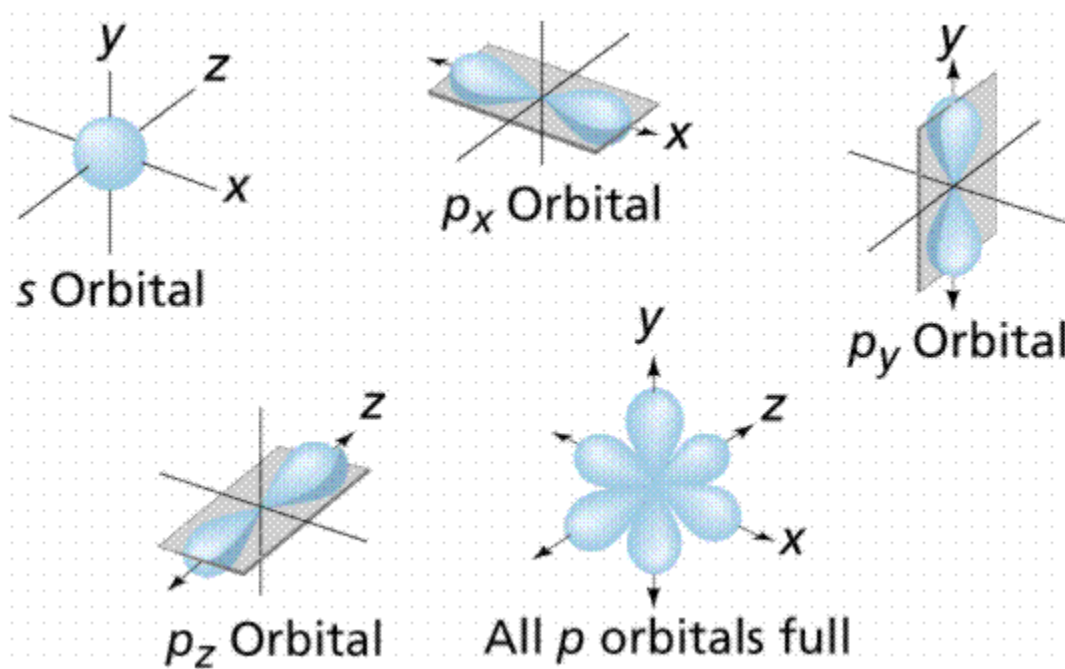
Each Roman numerated column on the label (at least the ones ending in A) tells us how many electrons are in the outer shell of the atom. Each numbered row on the table tells us how many electron shells an atom has. Thus, Hydrogen, in column IA, row 1 has one electron in one shell. Phosphorous in column VA, row 3 has 5 electrons in its outer shell, and has three shells in total.



An orbital is also an area of space in which an electron will be found 90% of the time. Orbitals have a variety of shapes. Each orbital has a characteristic energy state and a characteristic shape. The *s* orbital is spherical. Since each orbital can hold a maximum of two electrons, atomic numbers above 2 must fill the other orbitals. The *p<sub>x</sub>*, *p<sub>y</sub>*, and *p<sub>z</sub>* orbitals are dumbbell shaped, along the x, y, and z axes respectively. These orbital shapes are shown in Figure 5.

Energy levels (also referred to as electron shells) are located a certain "distance" from the nucleus. The major energy levels into which electrons fit, are (from the nucleus outward) K, L, M, and N. Sometimes these are numbered, with electron configurations being:  $1s^2 2s^2 2p^1$ , (where the first shell K is indicated with the number 1, the second shell L with the number 2, etc.). This nomenclature tells us that for the atom mentioned in this paragraph, the first energy level (shell) has two electrons in its *s* orbital (the only orbital it can have), and second energy level has a maximum of two electrons in its *s* orbital, plus one electron in its *p* orbital.

Figure 5. Geometry of orbitals. S-orbitals are spherical, p-orbitals are shaped like a dumbbell or figure 8. Image from Purves et al., Life: The Science of Biology, 4th Edition, by Sinauer Associates ([www.sinauer.com](http://www.sinauer.com)) and WH Freeman ([www.whfreeman.com](http://www.whfreeman.com)), used with permission.

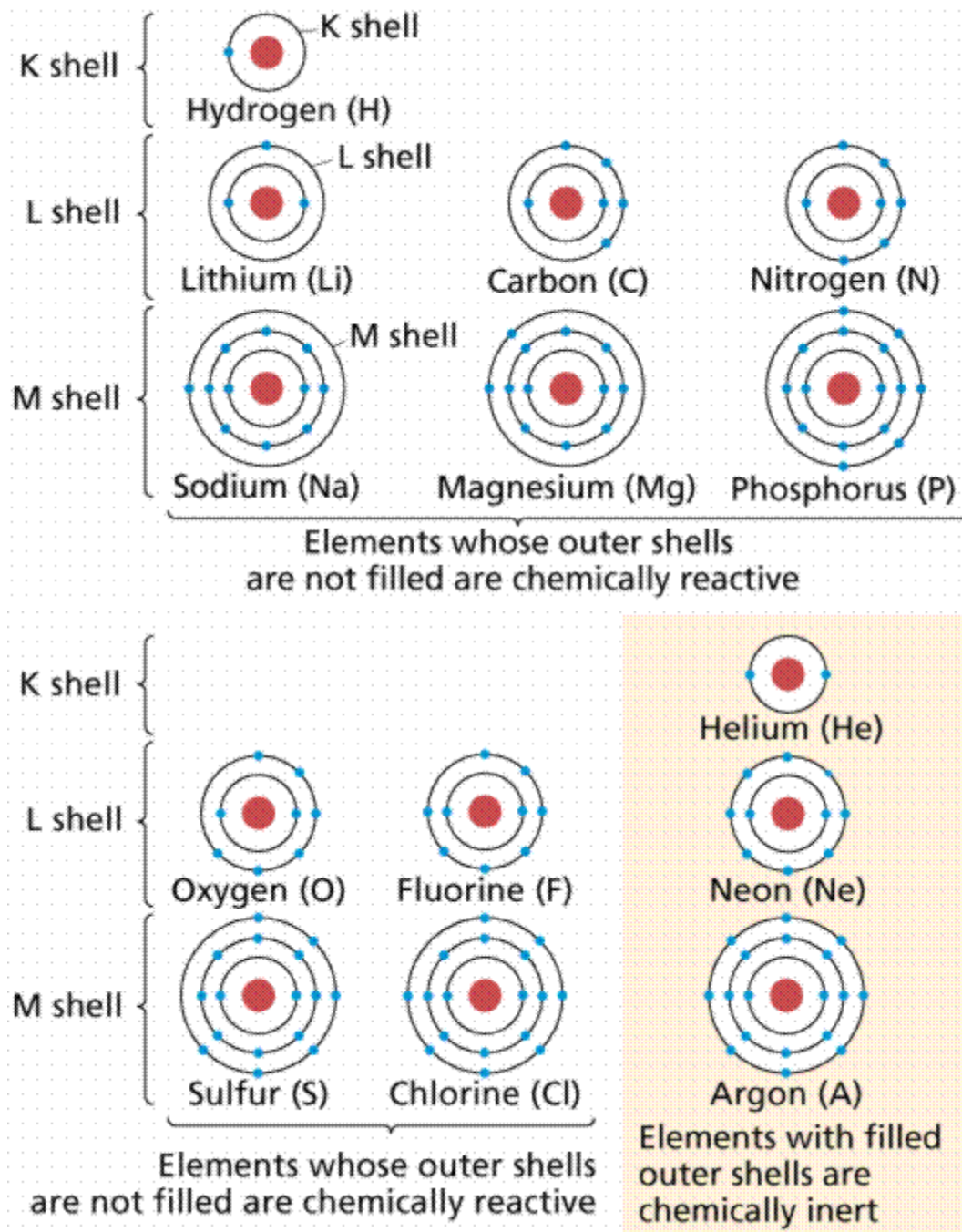


## Chemical Bonding |

During the nineteenth century, chemists arranged the then-known elements according to chemical bonding, recognizing that one group (the furthestmost right column on the Periodic Table, referred to as the Inert Gases or Noble Gases) tended to occur in elemental form (in other words, not in a molecule with other elements). It was later determined that this group had outer electron shells containing two (as in the case of Helium) or eight (Neon, Xenon, Radon, Krypton, etc.) electrons.

As a general rule, for the atoms we are likely to encounter in biological systems, atoms tend to gain or lose their outer electrons to achieve a Noble Gas outer electron shell configuration of two or eight electrons. The number of electrons that are gained or lost is characteristic for each element, and ultimately determines the number and types of chemical bonds atoms of that element can form. Atomic diagrams for several atoms are shown in Figure 6.

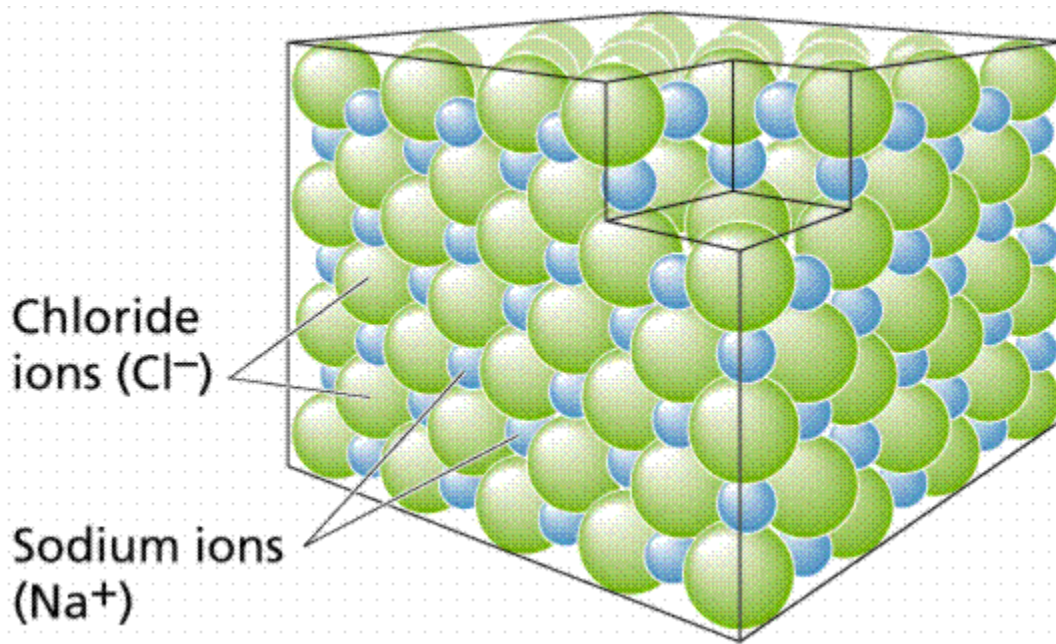
Figure 6. Atomic diagrams illustrating the filling of the outer electron shells. Images from Purves et al., *Life: The Science of Biology*, 4th Edition, by Sinauer Associates (www.sinauer.com) and WH Freeman (www.whfreeman.com), used with permission.



Ionic bonds are formed when atoms become ions by gaining or losing electrons. Chlorine is in a group of elements having seven electrons in their outer shells (see Figure 6). Members of

this group tend to gain one electron, acquiring a charge of -1. Sodium is in another group with elements having one electron in their outer shells. Members of this group tend to lose that outer electron, acquiring a charge of +1. Oppositely charged ions are attracted to each other, thus  $\text{Cl}^-$  (the symbolic representation of the chloride ion) and  $\text{Na}^+$  (the symbol for the sodium ion, using the Greek word *natrium*) form an ionic bond, becoming the molecule sodium chloride, shown in Figure 7. Ionic bonds generally form between elements in Group I (having one electron in their outer shell) and Group VIIa (having seven electrons in their outer shell). Such bonds are relatively weak, and tend to disassociate in water, producing solutions that have both Na and Cl ions.

Figure 7. TOP: Formation of a crystal of sodium chloride. Each positively charged sodium ion is surrounded by six negatively charged chloride ions; likewise each negatively charged chloride ion is surrounded by six positively charged sodium ions. The overall effect is electrical neutrality. Image from Purves et al., *Life: The Science of Biology*, 4th Edition, by Sinauer Associates ([www.sinauer.com](http://www.sinauer.com)) and WH Freeman ([www.whfreeman.com](http://www.whfreeman.com)), used with permission. BOTTOM: Table Salt Crystal (SEM x625). This image is copyright Dennis Kunkel at [www.DennisKunkel.com](http://www.DennisKunkel.com), used with permission.

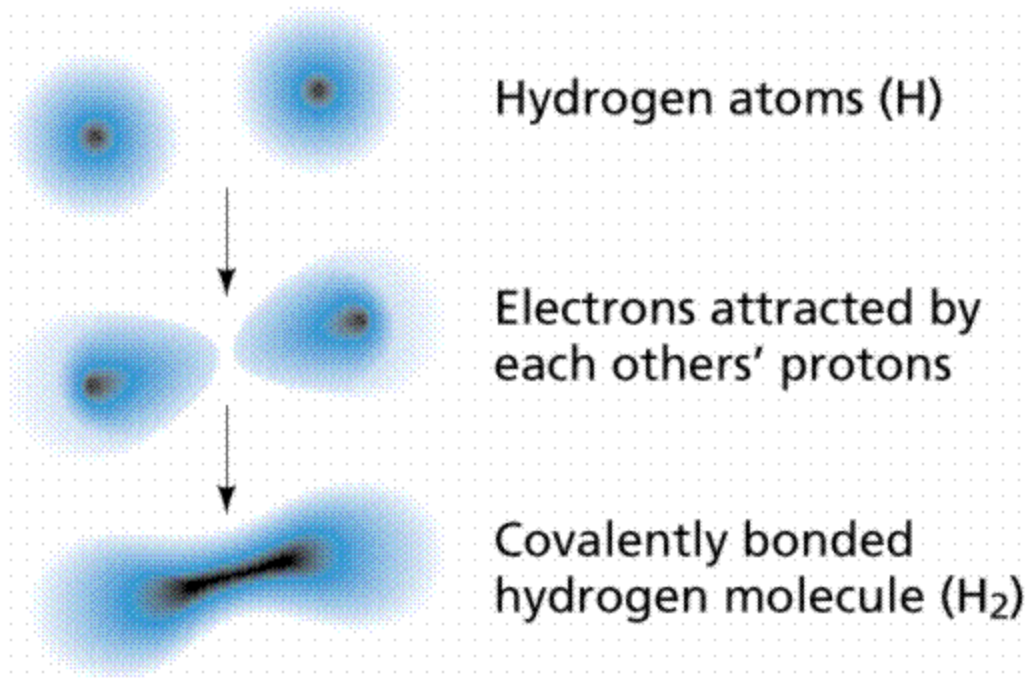




Covalent bonds form when atoms share electrons. Since electrons move very fast they can be shared, effectively filling or emptying the outer shells of the atoms involved in the bond. Such bonds are referred to as electron-sharing bonds. An analogy can be made to child custody: the children are like electrons, and tend to spend some time with one parent and the rest of their time with the other parent. In a covalent bond, the electron clouds surrounding the atomic nuclei overlap, as shown in Figure 8.

Figure 8. Formation of a covalent bond between two Hydrogen atoms. Image from Purves et al., *Life: The Science of Biology*, 4th Edition, by Sinauer Associates ([www.sinauer.com](http://www.sinauer.com)) and WH Freeman ([www.whfreeman.com](http://www.whfreeman.com)), used with permission.

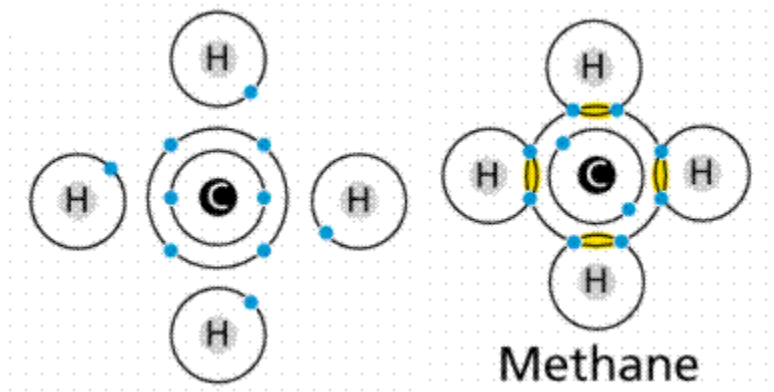




Carbon (C) is in Group IVa, meaning it has four electrons in its outer shell. Thus to become a "happy atom", Carbon can either gain **or** lose four electrons. By sharing the electrons with other atoms, Carbon can become a happy atom, alternately filling and emptying its outer shell, as with the four hydrogens shown in Figure 9.

Figure 9. Formation of covalent bonds in methane. Carbon needs to share four electrons, in effect it has four slots. Each hydrogen provides an electron to each of these slots. At the same time each hydrogen needs to fill one slot, which is done by sharing an electron with the carbon.

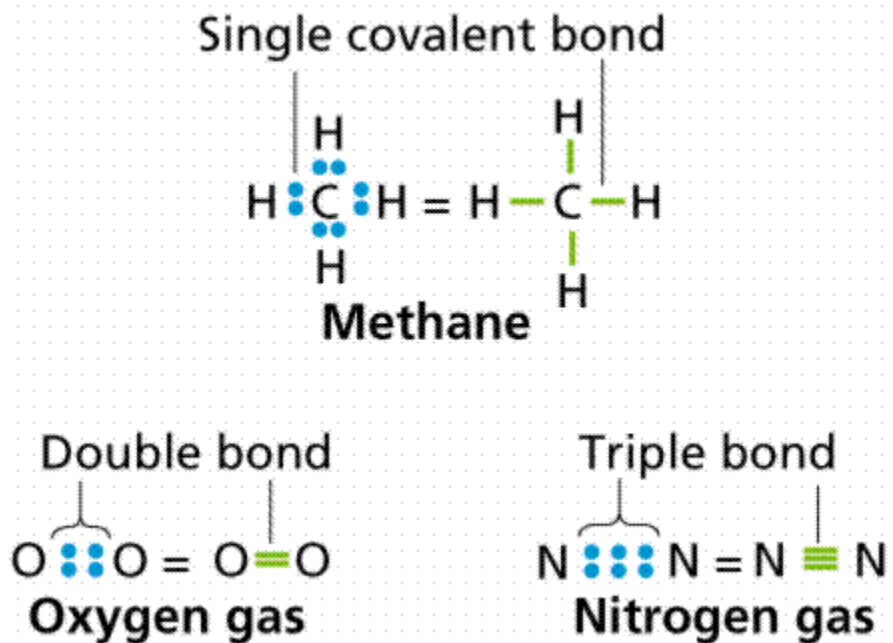
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The molecule methane (chemical formula CH<sub>4</sub>) has four covalent bonds, one between Carbon and each of the four Hydrogens. Carbon contributes an electron, and Hydrogen contributes an electron. The sharing of a single electron pair is termed a single bond. When two pairs of electrons are shared, a double bond results, as in carbon dioxide. Triple bonds are known,

wherein three pairs (six electrons total) are shared as in acetylene gas or nitrogen gas. The types of covalent bonds are shown in Figure 10.

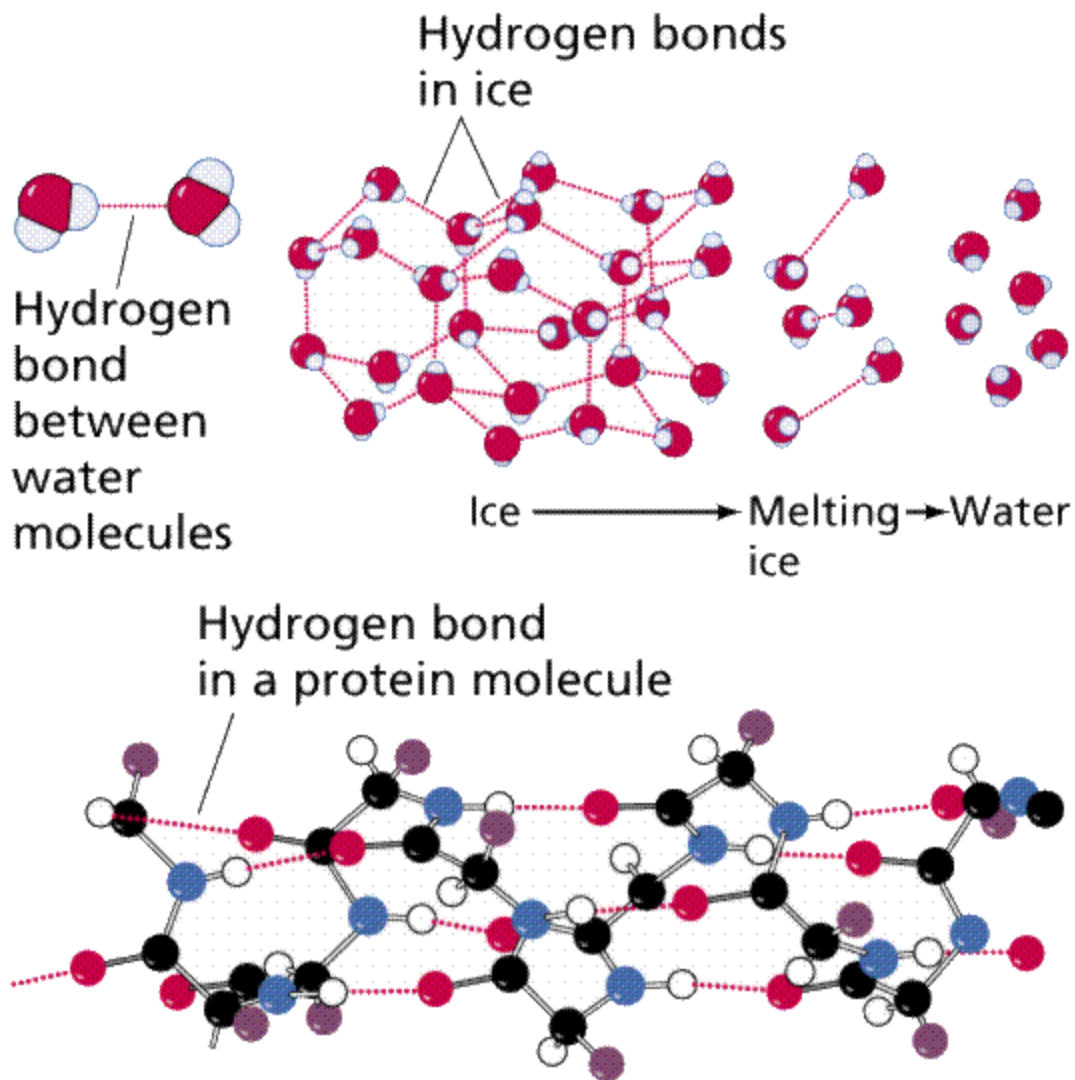
Figure 10. Ways of representing covalent bonds. Image from Purves et al., *Life: The Science of Biology*, 4th Edition, by Sinauer Associates ([www.sinauer.com](http://www.sinauer.com)) and WH Freeman ([www.whfreeman.com](http://www.whfreeman.com)), used with permission.



Sometimes electrons tend to spend more time with one atom in the bond than with the other. In such cases a polar covalent bond develops. Water ( $\text{H}_2\text{O}$ ) is an example. Since the electrons spend so much time with the oxygen (oxygen having a greater electronegativity, or electron affinity) that end of the molecule acquires a slightly negative charge. Conversely, the loss of the electrons from the hydrogen end leaves a slightly positive charge. The water molecule is thus polar, having positive and negative sides.

Hydrogen bonds, as shown in Figure 11, result from the weak electrical attraction between the positive end of one molecule and the negative end of another. Individually these bonds are very weak, although taken in a large enough quantity, the result is strong enough to hold molecules together or in a three-dimensional shape.





Figure 11. TOP: Formation of a hydrogen bond between the hydrogen side of one water molecule and the oxygen side of another water molecule. BOTTOM: The presence of polar areas in the amino acids that makeup a protein allows for hydrogen bonds to form, giving the molecule a three-dimensional shape that is often vital to that protein's proper functioning. Images from Purves et al., *Life: The Science of Biology*, 4th Edition, by Sinauer Associates ([www.sinauer.com](http://www.sinauer.com)) and WH Freeman ([www.whfreeman.com](http://www.whfreeman.com)), used with permission.

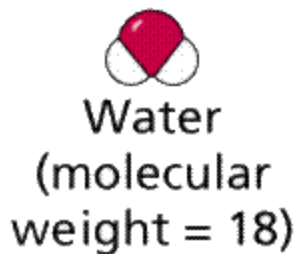
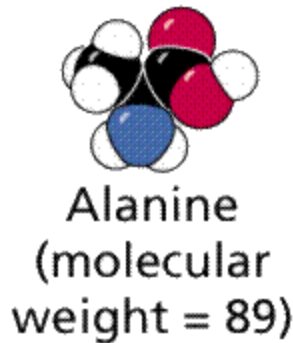
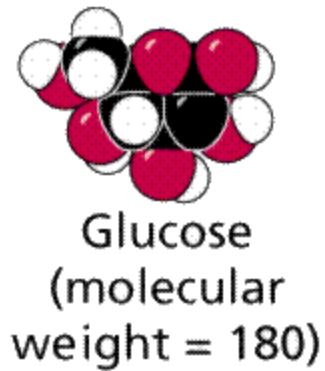


## Chemical reactions and molecules |

Molecules are compounds in which the elements are in definite, fixed ratios, as seen in Figure 12. Those atoms are held together usually by one of the three types of chemical bonds discussed above. For example: water, glucose, ATP. Mixtures are compounds with variable formulas/ratios of their components. For example: soil. Molecular formulas are an expression in the simplest whole-number terms of the composition of a substance. For example, the sugar glucose has 6 Carbons, 12 hydrogens, and 6 oxygens per repeating structural unit. The formula is written  $C_6H_{12}O_6$ .

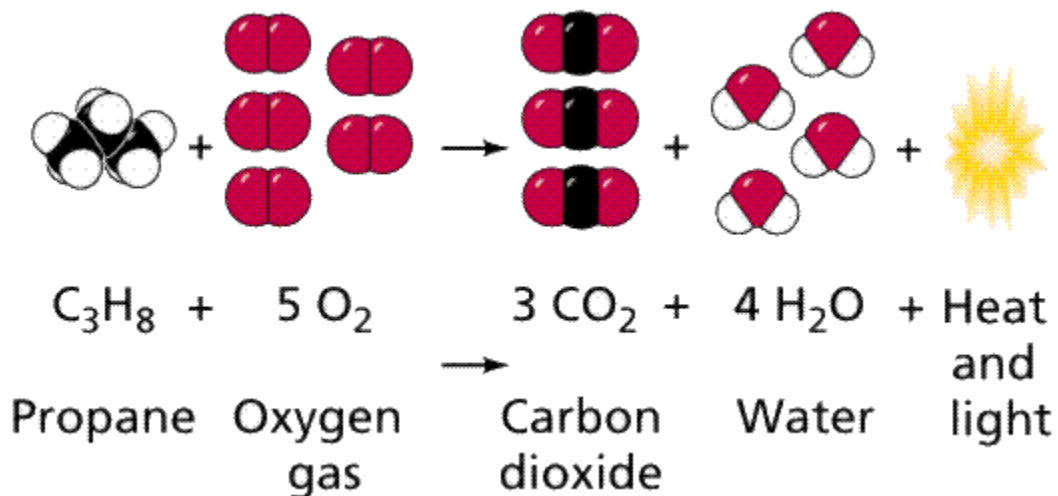
Figure 12. Determination of molecular weights by addition of the weights of the atoms that make up the molecule. Image from Purves et al., *Life: The Science of Biology*, 4th Edition, by Sinauer Associates ([www.sinauer.com](http://www.sinauer.com)) and WH Freeman ([www.whfreeman.com](http://www.whfreeman.com)), used with permission.

- 14  Nitrogen (N)
- 16  Oxygen (O)
- 12  Carbon (C)
- 1  Hydrogen (H)



Chemical reactions occur in nature, and some also can be performed in a laboratory setting. One such reaction is diagrammed in Figure 13. Chemical equations are linear representations of how these reactions occur. Combination reactions occur when two separate reactants are bonded together, e.g.  $A + B \rightarrow AB$ . Disassociation reactions occur when a compound is broken into two products, e.g.  $AB \rightarrow A + B$ .

Figure 13. Diagram of a chemical reaction: the combustion of propane with oxygen, resulting in carbon dioxide, water, and energy (as heat and light). This chemical reaction takes place in a camping stove as well as in certain welding torches. Image from Purves et al., *Life: The Science of Biology*, 4th Edition, by Sinauer Associates ([www.sinauer.com](http://www.sinauer.com)) and WH Freeman ([www.whfreeman.com](http://www.whfreeman.com)), used with permission.



Biological systems, while unique to each species, are based on the chemical bonding properties of carbon. Major organic chemicals (those associated with or formed by the actions of living things) usually include some ratios of the following elements: C, H, N, O, P, S.

## Assignments |

- All forms of matter are composed of one or more elements. Be able to list the major elements in living things.
- Describe how protons, electrons, and neutrons are arranged into atoms and ions.
- Define the terms atomic number and atomic mass and be able to describe their significance.
- Atoms with the same atomic number but a different mass number are isotopes. List the isotopes of hydrogen and of carbon.
- Be able to describe radioisotopes and list three ways they are used in biology.
- The union between the electron structures of atoms is known as the chemical bond. Be able to list and describe the three types of chemical bonds found in living things.
- Be able to describe the distribution of electrons in the space around the nucleus of an atom.
- An atom tends to react with other atoms when its outermost shell is only partly filled with electrons. Be able to discuss why this happens.
- Be able to define the two types of ions and describe how ionic bonds form between positive and negative ions.
- In a covalent bond, atoms share electrons. List several elements that tend to form covalent bonds.
- Distinguish between a nonpolar covalent bond and a polar covalent bond and give an example of each.
- Define hydrogen bond and describe conditions under which hydrogen bonds form and cite one example.
- Explain what is meant by the polarity of the water molecule, and how the polarity of water molecules allows them to interact with one another.

In chemistry, **valence bond (VB) theory** is one of the two basic theories, along with molecular orbital (MO) theory, that were developed to use the methods of quantum mechanics to explain chemical bonding. It focuses on how the atomic orbitals of the dissociated atoms combine to give individual chemical bonds when a molecule is formed. In contrast, molecular orbital theory has orbitals that cover the whole molecule.<sup>[1]</sup>

According to this theory a **covalent bond** is formed between two atoms by the overlap of *half filled valence* atomic orbitals of each atom containing one unpaired electron. A valence bond structure is similar to a Lewis structure, but where a single Lewis structure cannot be written, several valence bond structures are used. Each of these VB structures represents a specific Lewis structure. This combination of valence bond structures is the main point of resonance theory. Valence bond theory considers that the overlapping atomic orbitals of the participating atoms form a chemical bond. Because of the overlapping, it is most probable that electrons should be in the bond region. Valence bond theory views bonds as weakly coupled orbitals (small overlap). Valence bond theory is typically easier to employ in ground state molecules. The core orbitals and electrons remain essentially unchanged during the formation of bonds.

$\sigma$  bond between two atoms: localization of electron density

Two p-orbitals forming a  $\pi$ -bond.

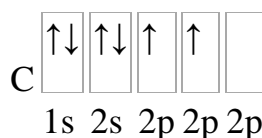
The overlapping atomic orbitals can differ. The two types of overlapping orbitals are sigma and pi. Sigma bonds occur when the orbitals of two shared electrons overlap head-to-head. Pi bonds occur when two orbitals overlap when they are parallel. For example, a bond between two s-orbital electrons is a sigma bond, because two spheres are always coaxial. In terms of bond order, single bonds have one sigma bond, double bonds consist of one sigma bond and one pi bond, and triple bonds contain one sigma bond and two pi bonds. However, the atomic orbitals for bonding may be hybrids. Often, the bonding atomic orbitals have a character of several possible types of orbitals. The methods to get an atomic orbital with the proper character for the bonding is called hybridization.

### Types of hybridisation

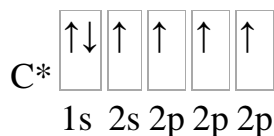
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Hybridisation describes the bonding of atoms from an atom's point of view. For a tetrahedrally coordinated carbon (e.g., methane  $\text{CH}_4$ ), the carbon should have 4 orbitals with the correct symmetry to bond to the 4 hydrogen atoms.

Carbon's ground state configuration is  $1s^2 2s^2 2p^2$  or more easily read:

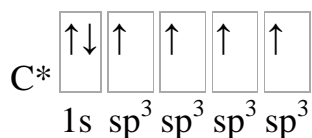


The carbon atom can use its two singly occupied p-type orbitals, to form two covalent bonds with two hydrogen atoms, yielding the singlet methylene  $\text{CH}_2$ , the simplest carbene. The carbon atom can also bond to four hydrogen atoms by an excitation (or promotion) of an electron from the doubly occupied 2s orbital to the empty 2p orbital, producing four singly occupied orbitals.



The energy released by the formation of two additional bonds more than compensates for the excitation energy required, energetically favoring the formation of four C-H bonds.

Quantum mechanically, the lowest energy is obtained if the four bonds are equivalent, which requires that they are formed from equivalent orbitals on the carbon. A set of four equivalent orbitals can be obtained that are linear combinations of the valence-shell (core orbitals are almost never involved in bonding) s and p wave functions,<sup>[9]</sup> which are the four  $sp^3$  hybrids.



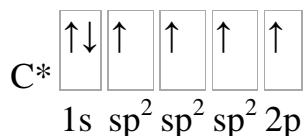
In  $\text{CH}_4$ , four  $\text{sp}^3$  hybrid orbitals are overlapped by hydrogen 1s orbitals, yielding four  $\sigma$  (sigma) bonds (that is, four single covalent bonds) of equal length and strength.

## Ethene structure

*See also: trigonal planar molecular geometry*

Other carbon compounds and other molecules may be explained in a similar way. For example, ethene ( $\text{C}_2\text{H}_4$ ) has a double bond between the carbons.

For this molecule, carbon  $\text{sp}^2$  hybridises, because one  $\pi$  (pi) bond is required for the double bond between the carbons and only three  $\sigma$  bonds are formed per carbon atom. In  $\text{sp}^2$  hybridisation the 2s orbital is mixed with only two of the three available 2p orbitals, usually denoted  $2p_x$  and  $2p_y$ . The third 2p orbital ( $2p_z$ ) remains unhybridised.



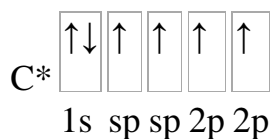
forming a total of three  $\text{sp}^2$  orbitals with one remaining p orbital. In ethylene (ethene) the two carbon atoms form a  $\sigma$  bond by overlapping one  $\text{sp}^2$  orbital from each carbon atom. The  $\pi$  bond between the carbon atoms perpendicular to the molecular plane is formed by 2p–2p overlap. Each carbon atom forms covalent C–H bonds with two hydrogens by s– $\text{sp}^2$  overlap, all with  $120^\circ$  bond angles. The hydrogen–carbon bonds are all of equal strength and length, in agreement with experimental data.

## sp

### Two sp orbitals

*See also: linear molecular geometry*

The chemical bonding in compounds such as alkynes with triple bonds is explained by sp hybridization. In this model, the 2s orbital is mixed with only one of the three p orbitals,



resulting in two sp orbitals and two remaining p orbitals. The chemical bonding in acetylene (ethyne) (C<sub>2</sub>H<sub>2</sub>) consists of sp–sp overlap between the two carbon atoms forming a σ bond and two additional π bonds formed by p–p overlap. Each carbon also bonds to hydrogen in a σ s–sp overlap at 180° angles

## CHEMICAL EQUATIONS AND STOICHIOMETRY

Chemical equations are symbolic representations of chemical reactions. The reacting materials (reactants) are given on the left, and the products are displayed on the right, usually separated by an arrow showing the direction of the reaction. The numerical coefficients next to each chemical entity denote the proportion of that chemical entity before and after the reaction. The law of conservation of mass dictates that the quantity of each element must remain unchanged in a chemical reaction. Therefore, in a balanced equation each side of the chemical equation must have the same quantity of each element.

**Chemical equations:** A chemical equation shows what reactants are needed to make specific products. Reactions are balanced by adding coefficients so that there are the same number of atoms of each element on both sides of the reaction. So the left side of the equation, 2H<sub>2</sub>+O<sub>2</sub>→2H<sub>2</sub>O, has four hydrogen atoms and two oxygen atoms, as does the right side of the equation, 2H<sub>2</sub>O.

### Stoichiometry

Stoichiometry is the field of chemistry that is concerned with the relative quantities of reactants and products in chemical reactions. For any balanced chemical reaction, whole numbers (coefficients) are used to show the quantities (generally in moles ) of both the reactants and products. For example, when oxygen and hydrogen react to produce water, one mole of oxygen reacts with two moles of hydrogen to produce two moles of water.

In addition, stoichiometry can be used to find quantities such as the amount of products that can be produced with a given amount of reactants and percent yield. Upcoming concepts will explain how to calculate the amount of products that can be produced given certain information.

The relationship between the products and reactants in a balanced chemical equation is very important in understanding the nature of the reaction. This relationship tells us what materials and how much of them are needed for a reaction to proceed. Reaction stoichiometry describes the quantitative relationship among substances as they participate in various chemical reactions.



In a balanced chemical equation, the coefficients can be used to determine the relative amount of molecules, formula units, or moles of compounds that participate in the reaction. The coefficients in a balanced equation can be used as molar ratios, which can act as conversion factors to relate the reactants to the products. These conversion factors state the *ratio* of reactants that react but do not tell *exactly how much* of each substance is actually involved in the reaction.

### Determining Molar Ratios

The molar ratios identify how many moles of product are formed from a certain amount of reactant, as well as the number of moles of a reactant needed to completely react with a certain amount of another reactant. For example, look at this equation:



From this reaction equation, it is possible to deduce the following molar ratios:

- 1 mol CH<sub>4</sub>: 1 mol CO<sub>2</sub>
- 1 mol CH<sub>4</sub>: 2 mol H<sub>2</sub>O
- 1 mol CH<sub>4</sub>: 2 mol O<sub>2</sub>
- 2 mol O<sub>2</sub>: 1 mol CO<sub>2</sub>
- 2 mol O<sub>2</sub>: 2 mol H<sub>2</sub>O

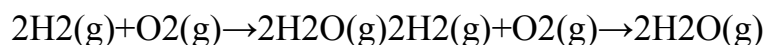
In other words, 1 mol of methane will produce 1 mole of carbon dioxide (as long as the reaction goes to completion and there is plenty of oxygen present). These molar ratios can also be expressed as fractions. For example, 1 mol CH<sub>4</sub>: 1 mol CO<sub>2</sub> can be expressed as  $\frac{1 \text{ mol CH}_4}{1 \text{ mol CO}_2}$ . These molar ratios will be very important for quantitative chemistry calculations that will be discussed later.

### Using Stoichiometry to Calculate Moles

The next step is to inspect the coefficients of each element of the equation. The coefficients can be thought of as the amount of moles used in the reaction. The key is reaction stoichiometry, which describes the quantitative relationship among the substances as they participate in the chemical reaction. The relationship between two of the reaction's participants (reactant or product) can be viewed as conversion factors and can be used to facilitate mole-to-mole conversions within the reaction.

#### EXAMPLE 1

For example, to determine the number of moles of water produced from 2 mol O<sub>2</sub>, the balanced chemical reaction should be written out:



There is a clear relationship between  $O_2$  and  $H_2O$ : for every one mole of  $O_2$ , two moles of  $H_2O$  are produced. Therefore, the ratio is one mole of  $O_2$  to two moles of  $H_2O$ , or 1 mol  $O_2$  = 2 moles  $H_2O$ . Assume abundant hydrogen and *two* moles of  $O_2$ , then one can calculate:

2 moles  $O_2$  · 2 mol  $H_2O$  / 1 mol  $O_2$  = 4 moles  $H_2O$

Therefore, 4 moles of  $H_2O$  were produced by reacting 2 moles of  $O_2$  in excess hydrogen. Each stoichiometric conversion factor is reaction-specific and requires that the reaction be balanced. Therefore, each reaction must be balanced before starting calculations.

# Kinetic Molecular Theory of Gases

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## Learning Objectives

1. State the major concepts behind the kinetic molecular theory of gases.
2. Demonstrate the relationship between kinetic energy and molecular speed.
3. Apply the kinetic molecular theory to explain and predict the gas laws.

Gases were among the first substances studied using the modern scientific method, which was developed in the 1600s. It did not take long to recognize that gases all shared certain physical behaviours, suggesting that gases could be described by one all-encompassing theory. The kinetic molecular theory of gases is a model that helps us understand the physical properties of gases at the molecular level. It is based on the following concepts:

1. Gases consist of particles (molecules or atoms) that are in constant random motion.
2. Gas particles are constantly colliding with each other and the walls of their container. These collisions are elastic; that is, there is no net loss of energy from the collisions.
3. Gas particles are small and the total volume occupied by gas molecules is negligible relative to the total volume of their container.
4. There are no interactive forces (i.e., attraction or repulsion) between the particles of a gas.
5. The average kinetic energy of gas particles is proportional to the absolute temperature of the gas, and all gases at the same temperature have the same average kinetic energy.

The kinetic molecular theory of gases describes this state of matter as composed of tiny particles in constant motion with a lot of distance between the particles. Because most of the volume occupied by a gas is empty space, a gas has a low density and can expand or contract under the appropriate influence. The fact that gas particles are in constant motion means that two or more gases will always mix as the particles from the individual gases move and collide with each other. The number of collisions the gas particles make with the walls of their container and the force with which they collide determine the magnitude of the gas pressure.

## Kinetic Energy and Molecular Speed

Gas particles are in constant motion, and any object in motion has kinetic energy ( $E_k$ ). Kinetic energy, for an individual atom, can be calculated by the following equation where  $m$  is the mass, and  $u$  is the speed.

$$E_k = 1/2 mu^2$$

Overall the molecules in a sample of a gas share an average kinetic energy; however, individual molecules exhibit a distribution of kinetic energies because of having a distribution of speeds. This distribution of speeds arises from the collisions that occur between molecules in the gas phase. Although these collisions are elastic (there is no net loss of energy), the individual speeds of each molecule involved in the collision may change. For example, in the collision of two molecules, one molecule may be deflected at a slightly higher speed and the other at a slightly lower speed, but the average kinetic energy does not change.

speed distribution

When analyzing a diagram of the distribution of molecular speeds, there are several commonly used terms to be familiar with. The most probable speed ( $u_{mp}$ ) is the speed of the largest number of molecules, and corresponds to the peak of the distribution. The average speed ( $u_{av}$ ) is the mean speed of all gas molecules in the sample. The root-mean-square (rms) speed ( $u_{rms}$ ) corresponds to the speed of molecules having exactly the same kinetic energy as the average kinetic energy of the sample.

According to the kinetic molecular theory, the average kinetic energy of gas particles is proportional to the absolute temperature of the gas. This can be expressed with the following equation where  $k$  represents the Boltzmann constant. The Boltzmann constant is simply the gas constant  $R$  divided by the Avogadro's constant ( $N_A$ ). The bar above certain terms indicates they are average values.

$$\overline{E_k} = \frac{3}{2}kT \quad \overline{E_k} = \frac{3}{2}kT$$

Since average kinetic energy is related both to the absolute temperature and the molecular speed, we can combine the equation above with the previous one to determine the rms speed.

$$\overline{E_k} = \frac{1}{2}m\overline{u^2} = \frac{3}{2}kT \quad \overline{E_k} = \frac{1}{2}m\overline{u^2} = \frac{3}{2}kT$$

$$\sqrt{\overline{u^2}} = \sqrt{\frac{3kT}{m}} \quad \sqrt{\overline{u^2}} = \sqrt{\frac{3kT}{m}}$$

This demonstrates that the rms speed is related to the temperature. We can further manipulate this equation by multiplying the numerator and denominator by Avogadro's constant ( $N_A$ ) to give us a form using the gas constant ( $R$ ) and molar mass ( $M$ ).

$$\sqrt{\overline{u^2}} = \sqrt{\frac{3RT}{M}} \quad \sqrt{\overline{u^2}} = \sqrt{\frac{3RT}{M}}$$

This form of the equation demonstrates that the rms speed of gas molecules is also related to the molar mass of the substance. Comparing two gases of different molar mass at the same temperature, we see that despite having the same average kinetic energy, the gas with the smaller molar mass will have a higher rms speed.

### Example

Calculate the rms speed of nitrogen molecules at 25°C. Solution  $\sqrt{u^2} = \sqrt{3RTM} = \square \square$

$$\square \sqrt{3(8.3145 \text{ J K}^{-1} \text{ mol}^{-1})(298.15 \text{ K})28.02 \times 10^{-3} \text{ kg mol}^{-1}} \sqrt{u^2} = 3RTM = 3(8.3145 \text{ J K}^{-1} \text{ mol}^{-1})(298.15 \text{ K})28.02 \times 10^{-3} \text{ kg mol}^{-1} \sqrt{u^2} = \sqrt{2.654 \times 10^5 \text{ J kg}^{-1}} \sqrt{u^2} = 2.654 \times 10^5 \text{ J kg}^{-1}$$

Knowing that  $1 \text{ J} = 1 \text{ kg m}^2 \text{ s}^{-2}$  we can convert to metres per

second:  $\sqrt{u^2} = \sqrt{2.654 \times 10^5 \text{ J kg}^{-1} \times 1 \text{ kg m}^2 \text{ s}^{-2} \text{ J}^{-1}} \sqrt{u^2} = \sqrt{2.654 \times 10^5 \text{ m}^2 \text{ s}^{-2}}$

$$\square = 515.2 \text{ m s}^{-1} \sqrt{u^2} = 2.654 \times 10^5 \text{ J kg}^{-1} \times 1 \text{ kg m}^2 \text{ s}^{-2} \text{ J}^{-1} \sqrt{u^2} = 2.654 \times 10^5 \text{ m}^2 \text{ s}^{-2} = 515.2 \text{ m s}^{-1}$$

### Applying the Kinetic Molecular Theory to the Gas Laws

The kinetic molecular theory can be used to explain or predict the experimental trends that were used to generate the gas laws. Let's work through a few scenarios to demonstrate this point.

#### What will happen to the pressure of a system where the volume is decreased at constant temperature?

This problem can be approached in two ways:

1. The ideal gas law can be rearranged to solve for pressure and estimate the change in pressure:

$$PV = nRT \quad PV = nRT$$

$$P = \frac{nRT}{V} \quad P = \frac{nRT}{V}$$

Volume is located in the denominator of the equation, and it is being decreased. This means the rest of the equation is being divided by a smaller number, so that should make the pressure larger.

2. The kinetic molecular theory can be used. Since the temperature is remaining constant, the average kinetic energy and the rms speed remain the same as well. The volume of the container has decreased, which means that the gas molecules have to move a shorter distance to have a collision. There will therefore be more collisions per second, causing an increase in pressure.

#### What will happen to the pressure of a system where the temperature is increased and the volume remains constant?

Again, this type of problem can be approached in two ways:

1. The ideal gas law can be rearranged to solve for pressure and estimate the change in pressure.

$$p = \frac{nRT}{V} \quad p = \frac{nRT}{V}$$

Temperature is located in the numerator; there is a direct relationship between temperature and pressure. Therefore an increase in temperature should cause an increase in pressure.

2. The kinetic molecular theory can be used. Temperature is increased, so the average kinetic energy and the rms speed should also increase. This means that the gas molecules will hit the container walls more frequently and with greater force because they are all moving faster. This should increase the pressure.

## Key Takeaways

- The physical behaviour of gases is explained by the kinetic molecular theory of gases.
- The number of collisions that gas particles make with the walls of their container and the force at which they collide determine the magnitude of the gas pressure.
- Temperature is proportional to average kinetic energy.

## Exercises

1. State the ideas of the kinetic molecular theory of gases.
2. Calculate the rms speed of  $\text{CO}_2$  at  $40^\circ\text{C}$ .
3. Using the kinetic molecular theory, explain how an increase in the number of moles of gas at constant volume and temperature affects the pressure.

## Answers

1. Gases consist of tiny particles of matter that are in constant motion. Gas particles are constantly colliding with each other and the walls of a container. These collisions are elastic; that is, there is no net loss of energy from the collisions. Gas particles are separated by large distances. The size of gas particles is tiny compared to the distances that separate them and the volume of the container. There are no interactive forces (i.e., attraction or repulsion) between the particles of a gas. The average kinetic energy of gas particles is dependent on the temperature of the gas.
2. 421 m/s
3. Temperature remains the same, so the average kinetic energy and the rms speed should remain the same. Increasing the number of moles of gas means there are more molecules of gas available to collide with the walls of the container at any given time. Therefore pressure should increase.

## Properties of gases

Gas is a state of matter that has no fixed shape and no fixed volume. Gases have lower density than other states of matter, such as solids and liquids. There is a great deal of empty space between particles, which have a lot of kinetic energy. The particles move very fast and collide into one another, causing them to diffuse, or spread out, until they are evenly distributed throughout the volume of the container.

When more gas particles enter a container, there is less space for the particles to spread out, and they become compressed. The particles exert more force on the interior volume of the container. This force is called pressure. There are several units used to express pressure. Some of the most common are atmospheres (atm), pounds per square inch (psi), millimeters of mercury (mmHg) and pascals (Pa). The units relate to one another this way:  $1 \text{ atm} = 14.7 \text{ psi} = 760 \text{ mmHg} = 101.3 \text{ kPa}$  (1,000 pascals).

Besides pressure, denoted in equations as P, gases have other measurable properties: temperature (T), volume (V) and number of particles, which is expressed in a mole number (n or mol). In work involving gas temperature, the Kelvin scale is often used.

Because temperature and pressure vary from place to place, scientists use a standard reference point, called **standard temperature and pressure (STP)**, in calculations and equations.

Standard temperature is the freezing point of water — 32 degrees Fahrenheit (0 degrees Celsius, or 273.15 Kelvin). Standard pressure is one atmosphere (atm) — the pressure exerted by the atmosphere on Earth at sea level.

## Redox Reactions and Introduction to Electrochemistry

**Redox reactions** are **oxidation-reduction** chemical **reactions** in which the reactants undergo a change in their oxidation states. ... The substance getting reduced in a chemical **reaction** is known as the oxidizing agent, while a substance that is getting oxidized is known as the reducing agent.

Every chemical **reaction** in which the **oxidation** number of a participating chemical species varies is called an **oxidation-reduction reaction**, also called a **redox reaction**. ...

An **example** of a **redox reaction** is the formation of hydrogen fluoride.

An **oxidation-reduction reaction** is any chemical **reaction** in which the oxidation number of a molecule, atom, or ion changes by gaining or losing an electron. **Redox reactions** are common and vital to some of the basic functions of life, including photosynthesis, respiration, combustion, and corrosion or rusting.

Electrochemistry is the branch of physical chemistry that studies the relationship between electricity, as a measurable and quantitative phenomenon, and identifiable chemical change, with either electricity considered an outcome of a particular chemical change or vice versa. Wikipedia

**Electrochemistry** is the study of **chemical** processes that cause electrons to move. This movement of electrons is called electricity, which can be generated by movements of

electrons from one element to another in a reaction known as an oxidation-reduction ("redox") reaction

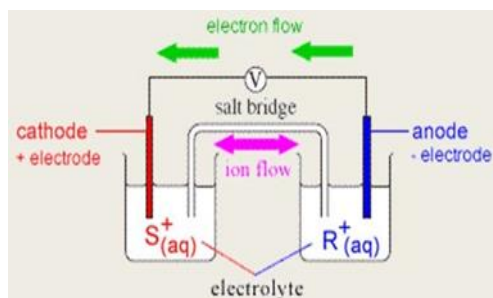
### Principle

The movement of the ions is therefore responsible for the transfer of charge in solution from one electrode to the other. In practice the charge will be carried by several ions, both cations (positively charged) and anions (negatively charged).

There are two types of **electrochemical cells**: **galvanic**, also called Voltaic, and electrolytic. Electrochemical Cell

An electrochemical cell typically consists of

- Two electronic conductors (also called electrodes)
- An ionic conductor (called an electrolyte)
- the electron conductor used to link the electrodes is often a metal wire, such as copper wiring



## ACIDS, BASES AND SALTS

Before we discuss the ways in which chemists manage to classify all of the various substances in the universe, we should spend some time looking at three words which cover a lot of substances. These words are used in everyday speech but we need to define them clearly so that everybody uses them to mean the same thing.

An **ACID** is a substance that:-

- a) Reacts with a base to make a salt and water only.
- b) Reacts with many metals to produce a salt and hydrogen gas only.



- c) Reacts with a carbonate to make a salt, water and carbon dioxide only.
- d) Turns litmus indicator red.
- e) Has a low pH number (0 to 6).

A **BASE** is a substance that:-

- a) Reacts with an acid to make a salt and water only.
- b) Turns litmus indicator blue.
- c) Has a high pH number (8 to 14).

A **SALT**:-

- a) Is the product, together with water, of a reaction between a base and an acid.
- b) Has a pH number of 7.

These definitions may not seem particularly helpful at this stage but it does give us some foothold in a topic that we shall pay several visits to. The pH scale, as you can see, is just a guide to how acidic or basic a substance is - very strong acids are pH 1, weak acids are pH 4 or 5, a neutral substance has a pH of 7, a weak base pH 9 or 10 and a strong base is pH

14. If you know, for instance, that the pH of gastric juice from the human stomach is pH 1, it immediately tells you that this is a very acidic substance, and that blood at pH 7.4 is very slightly basic

Some substances, like the litmus mentioned above, are indicators. An indicator is a substance that changes its color if it goes from an acidic to a basic environment and vice versa. A few indicators have a whole range of colors (the universal indicator follows the colors of the spectrum), but others have just two. In the case of litmus, it is reddish under acidic conditions and blueish under basic conditions, whereas neutral litmus is midway between blue and red.

Many substances from nature are indicators, such as red cabbage, beetroot and many colored flowers.

You may like to learn these following 'word equations' that summarize the reactions of

acids. In equation 2, we use the word **ALKALI**. This is just a word that describes bases which are soluble in water; so all alkalis are bases but only some bases are alkalis,

1) Acid + Base  $\implies$  Salt + Water

2) Acid + Alkali  $\implies$  Salt + Water

3) Acid + Carbonate  $\implies$  Salt + Water + Carbon Dioxide

4) Acid + Metal  $\implies$  Salt + Hydrogen

Now for the names and formulas of three very well known acids;

SULPHURIC ACID is  $\text{H}_2\text{SO}_4$ , NITRIC ACID is  $\text{HNO}_3$ , HYDROCHLORIC

ACID is  $\text{HCl}$ . And three common bases (all of which are alkalis);SODIUM

HYDROXIDE is  $\text{NaOH}$ , POTASSIUM HYDROXIDE is  $\text{KOH}$ , and

LITHIUM HYDROXIDE is  $\text{LiOH}$ . Salts are named after the acid they are

made from, therefore; Sulphuric acid produces- SULPHATES, Nitric acid

produces NITRATES

and Hydrochloric acid produces CHLORIDES.

Using equation 1 (from above) we can substitute a few

specific names:- sulphuric acid + sodium hydroxide  $\implies$

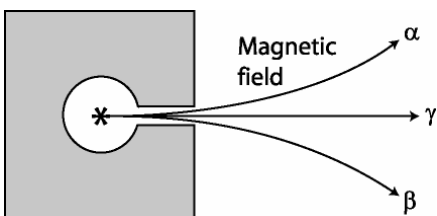
sodium sulphate + water.

Note - if you were reading this equation out loud, you would say 'sulphuric

acid plus sodium hydroxide gives sodium sulphate plus water'. Note that the "=>" should never be written as simply "=", nor should it be referred to as "equals", but always "gives".

## Radioactivity

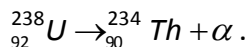
Nuclei can break up in several ways. Typically, the breakup occurs with the emission of



one or more particles, called  $\alpha$  particles,  $\beta$  particles, and  $\gamma$  rays.  $\beta$  particles we have already seen: they are negatively charged (or sometimes positively charged) electrons.  $\alpha$  particles are helium nuclei (two protons plus two neutrons).  $\gamma$  rays are particles of light. They are very energetic particles of light, but they are electromagnetic waves, or rays, nevertheless.

These three types of emitted particles ( $\alpha$ ,  $\beta$ , and  $\gamma$ ) have obvious differences, but can easily be distinguished by the way they are (or are not) deflected by a magnetic field.

**Alpha decay** occurs in nuclei that have too many protons. The protons repel one another, and the result is that an  $\alpha$  particle is thrown off. For example, uranium spontaneously decays by emission of an alpha particle to form thorium:



Level																		
n=1	H																	He
n=2	Li	Be											B	C	N	O	F	Ne
n=3	Na	Mg											Al	Si	P	S	Cl	Ar
etc.	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
	Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
	Fr	Ra	Ac															
			Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu		
			Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr		

atom jumps to the left two spaces.

Since alpha particles have a positive charge, their trajectory is bent by a magnetic field as shown above. Typically, alpha particles move relatively slowly, since they are relatively heavy compared with electrons. When they collide with other nuclei in the air and in solid or liquid materials, they lose most of their energy very quickly. Thus, alpha particles are said to have a short "range." They don't go very

far, typically a few millimeters in air, or less in condensed materials. A sheet of paper is enough to stop alpha particles.

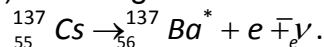
**Beta decay** occurs when a neutron in the nucleus decays into a proton, an electron (a  $\beta$  particle), and an antineutrino. But this increases the number of protons in the nucleus

Since two protons are thrown off, the atomic number  $Z$  decreases by two to 90. But the change in  $Z$  means that the number of electrons around the nucleus must also decrease by two, so the chemical properties change and the atom becomes a new chemical element. In this example, the new element corresponding to 90 electrons is thorium. On the periodic table the

(the atomic number  $Z$ ) by one, so, the atom jumps to the right one space on the periodic

Level																		
n=1	H																	He
n=2	Li	Be											B	C	N	O	F	Ne
n=3	Na	Mg											Al	Si	P	S	Cl	Ar
etc.	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
	Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
	Fr	Ra	Ac															
			Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu		
			Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr		

table. Radioactive cesium ( $^{137}\text{Cs}$ ) decays in this way, and forms barium ( $^{137}\text{Ba}$ ) (actually excited barium  $^{137}\text{Ba}^*$ , as we see in a minute) following the reaction

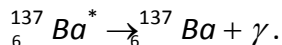


Because it is radioactive,  $^{137}\text{Cs}$  is a pernicious but also useful radioactive

species that illustrates many properties of radioactivity that Curie, Hahn, and Meitner, and others investigated.  $^{137}\text{Cs}$  is formed in nuclear explosions, so it is found in fallout from atmospheric explosions. It is also formed in nuclear reactors. It is a threat from terrorists who would mix it with conventional explosives to distribute it over some area to make that area radioactive. This is the concept of a "dirty bomb." It is also used industrially for sterilizing food and other applications.

Beta particles move much faster than alpha particles, typically a good fraction of the speed of light. As they move through liquids like water, they can give off a blue glow called Cherenkov radiation because the particles are actually moving faster than the speed of light in the water. This is why nuclear reactors glow blue. Since beta particles (electrons) have a negative charge, their trajectories are bent in a magnetic field opposite that of the alpha particles. This is indicated in the figure shown above. They can also be separated from alpha particles by a sheet of paper that absorbs the alphas, but not the betas. However, betas can be stopped by a thin sheet of aluminum.

**Gamma decay** occurs in nuclear isomers that have too much energy, for example:



The asterisk indicates carbon with excess energy. Gamma rays are actually particles of light – very energetic light. Even more energetic than x-rays. We all know that x-rays can go right through you, and gamma rays can go even farther, even through sheets of lead. Since light isn't bent by a magnetic field, gamma rays go straight in the figure above. Note that the chemical element (Ba) doesn't change in this reaction. The nucleus changes from excited  $\text{Ba}^*$  to normal Ba, but the chemistry is unaffected.