Fundamentals of Chemistry

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TABLE OF CONTENTS

TABLE OF CONTENTS (Cont.)

REFERENCES

- Donald H. Andrews and Richard J. Kokes, <u>Fundamental Chemistry</u>, John Wiley & Sons, Inc., 1963

- Compressed Gas Association, Inc., <u>Handbook of Compressed Gases</u>, 2nd Edition, Reinhold Publishing Corporation, 1981.

- R. A. Day, Jr. and R. C. Johnson, <u>General Chemistry</u>, Prentice Hall, Inc., 1974.

- Dickerson, Gray, Darensbourg and Darensbourg, <u>Chemical Principles</u>, 4th Edition, The Benjamin Cummings Publishing Company, 1984.

- Academic Program for Nuclear Plant Personnel, Volume II, <u>Chemistry</u>, Columbia, MD, General Physics Corporation, Library of Congress Card #A 326517, 1972.

- General Physics Corporation, <u>Fundamentals of Chemistry</u>, General Physics Corporation, 1982.

- Glasstone and Sesonske, <u>Nuclear Reactor Engineering</u>, 3rd Edition, Van Nostrand Reinhold Company, 1981.

- McElroy, <u>Accident Prevention Manual for Industrial Operations Engineering and Technology</u>, Volume 2, 8th Edition, National Safety Council, 1980.

- Sienko and Plane, <u>Chemical Principles and Properties</u>, 2nd Edition, McGraw and Hill, 1974.

- Underwood, <u>Chemistry for Colleges and Schools</u>, 2nd Edition, Edward Arnold, Ltd., 1967.

- Norman V. Steere and Associates, <u>CRC Handbook of Laboratory Safety</u>, 2nd Edition, CRC Press, Inc., 1971.

CHARACTERISTICS OF ATOMS

Chemistry is defined as the systematic investigation of the properties, structure, and behavior of matter and the changes matter undergoes. This general definition raises many questions. These questions are answered in the study of chemistry. Terms and basic concepts that help in understanding chemistry will be discussed in this chapter.

EO 1.1   **DEFINE the following terms:**

a.	**States of matter**	d.	**Mole**
b.	**Atomic weight**	e.	**Gram atomic weight**
c.	**Molecular weight**	f.	**Gram molecular weight**

EO 1.2   **LIST the components of an atom, their relative sizes, and charges.**

EO 1.3   **STATE the criterion used to classify an atom chemically.**

Characteristics of Matter

The term *states of matter* refers to the physical forms in which matter exists: solid, liquid, and gas. Solids are characterized as having both a definite shape and a definite volume. In a solid, the forces that keep the molecules or atoms together are strong. Therefore, a solid does not require outside support to maintain its shape.

Liquids have definite volumes but indefinite shapes and are slightly compressible. Liquids take the shape of their containers. The forces that keep a liquid's molecules or atoms together are weaker than in the solids.

Gases are readily compressible and capable of infinite expansion. They have indefinite shape and indefinite volume. Of the three states, gases have the weakest forces holding their molecules or atoms together.

The different states of matter have one thing in common; they can all be broken down into fundamental units called atoms.

The Atom Structure

All matter is composed of atoms, existing individually or in combination with each other. An atom is an extremely small electrically-neutral particle. It is the smallest unit involved in the chemical change of matter. Atoms can be treated as distinct particles because they behave as such chemically, but atoms themselves are composed of even smaller subparts. Understanding these atomic subparticles is important in understanding chemistry.

An atom is composed of a positively-charged nucleus orbited by one or more negatively-charged particles called electrons. A simplified schematic representation of this arrangement is illustrated in Figure 1. The nucleus is the core of an atom. It has a positive charge because it usually consists of two particles, the neutron and the proton (hydrogen is the exception with only a proton in the nucleus). The neutrons are electrically neutral, and the protons are electrically positive. A nucleus with one proton has a charge of +1 (or simply 1), and a nucleus with two protons has a +2 charge. Together the neutrons and protons give the nucleus its mass, but the proton alone gives the nucleus its positive charge.

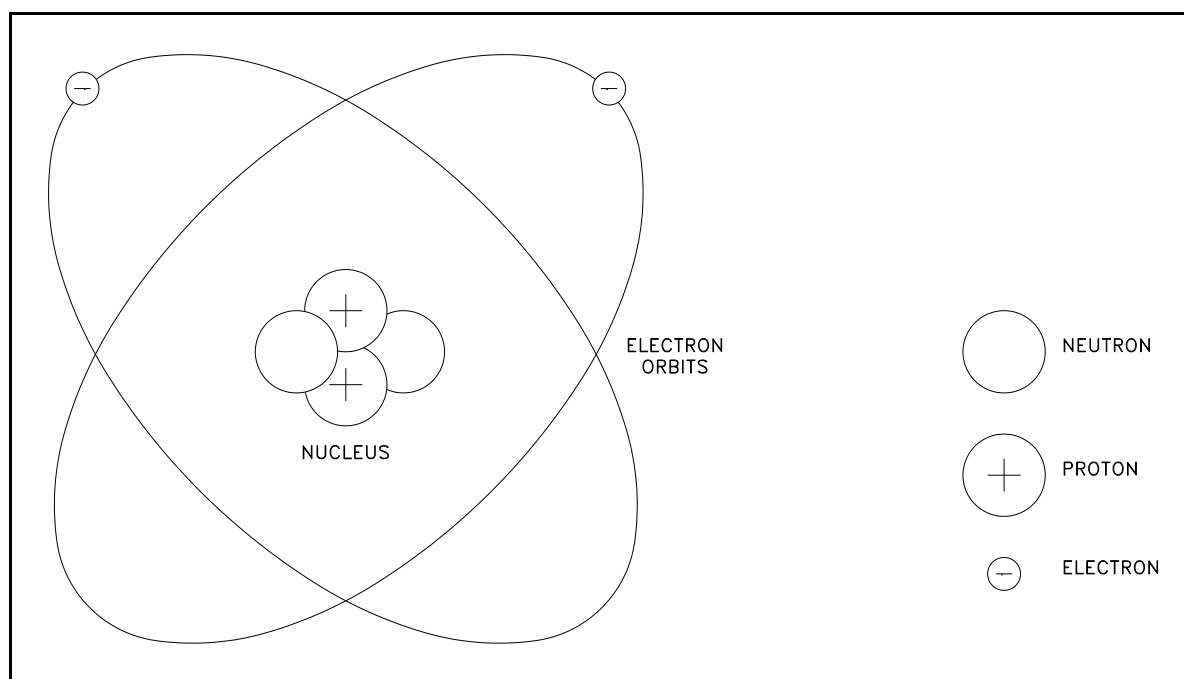Neutrons and protons are relatively massive and are essentially equal in mass.

Figure 1 Schematic of a Simple Atom (Helium)

The particles that orbit the nucleus are electrons. They are very small, with a mass only 1/1835 the mass of a proton or neutron. Each electron is negatively charged, and the charge of one electron is equal in magnitude (but opposite in sign) to the charge of one proton. The number of electrons orbiting a nucleus is exactly equal to the number of protons contained in that nucleus. The equal and opposite charges cancel each other, and the atom as a whole is neutral. The electrons are bound in the atom by electrostatic attraction. The atom remains neutral unless some external force causes a change in the number of electrons.

The diameter of the atom is determined by the range of the electrons in their travels around the nucleus and is approximately 10^{-8} cm. The diameter of the nucleus is roughly 10,000 times smaller, approximately 10^{-13} to 10^{12} cm. Because the nucleus is composed of neutrons and protons that are about 1835 times heavier than an electron, the nucleus contains practically all the mass of the atom, but constitutes a very small fraction of the volume. Although electrons are individually very small, the space in which they orbit the nucleus constitutes the largest part of the atomic volume.

Figure 1 illustrates these size relationships, but not to scale. If the nucleus were the size shown, the electrons would be several hundred feet away.

Some of the properties of the atom and its component parts are summarized in Table 1. The masses listed in Table 1 are measured in atomic mass units (amu), which is a relative scale in which the mass of a proton is about 1.0.

TABLE 1 Properties of the Atom and its Fundamental Particles		
Particle Name	Relative Mass (amu)	Relative Charge (based on charge of proton)
Electron	0.00055 or 1/1835	-1
Proton	1.0	1
Neutron	1.0	0

Chemical Elements

An atom is classified chemically by the number of protons in its nucleus. Atoms that have the same number of protons in their nuclei have the same chemical behavior. Atoms that have the same number of protons are grouped together and constitute a chemical element.

Chemical Symbols

At one time chemists used various symbols, similar to shorthand, for the atoms of the different elements. These symbols were very cumbersome and were replaced by abbreviations of the names of the elements. Each element has been assigned a specific one or two letter symbol based on the first letter of its chemical name. Because there are several elements with the same first letter, it is often necessary to add the second letter to the symbol. In some cases the symbol comes from an abbreviation for the old latin name of the element. For example, Fe stands for iron (ferrum) and Cu for copper (cuprum). The first letter of the chemical symbol is always capitalized. If the symbol has two letters, the second letter is always lowercase.

Atomic Number

The number of protons in the nucleus plays such an important role in identifying the atom that it is given a special name, the *atomic number*. The symbol Z is often used for atomic number (or number of protons). Hydrogen has an atomic number of 1 and lawrencium has an atomic number of 103. The atomic number is also equal to the number of electrons.

Atomic Mass Number

The sum of the total number of protons, Z, and the total number of neutrons, N, is called the *atomic mass number*. The symbol is A. Not all atoms of the same element have the same atomic mass number, because, although the Z is the same, the N and thus the A are different. Atoms of the same element with different atomic mass numbers are called *isotopes*.

Atomic Weight

In Table 1, the masses of atomic particles are given in atomic mass units (amu). These units represent a relative scale in which the mass of the isotope carbon-12 is used as the standard and all others are related to it. Specifically, 1 amu is defined as 1/12 the mass of the carbon-12 atom. Since the mass of a proton or a neutron is approximately 1 amu, the mass of a particular atom will be approximately equal to its atomic mass number, Z.

The atomic weight of an element is generally more useful than isotopic masses. The *atomic weight* of an element is defined as the weighted average of the masses of all of its natural occurring isotopes. The atomic weight of the elements are listed in Table 2. The elements that have their atomic weights in parentheses are unstable. For these elements, the atomic weight of the longest living isotope is used rather than the average of the masses of all occurring isotopes.

| | | | **TABLE 2** | | | |
| | | | **Table of Elements** | | | |
Name and Symbol		Atomic Number	Atomic Weight (amu)	Name		Atomic Number	Atomic Weight (amu)
Actinium	Ac	89	(227)	Curium	Cm	96	(247)
Aluminum	Al	13	26.981	Dysprosium	Dy	66	162.50
Americium	Am	95	(243)	Einsteinium	Es	99	(252)
Antimony	Sb	51	121.75	Erbium	Er	68	167.26
Argon	Ar	18	39.948	Europium	Eu	63	151.96
Arsenic	As	33	74.921	Fermium	Fm	100	(257)
Astatine	At	85	(210)	Fluorine	F	9	18.998
Barium	Ba	56	137.34	Francium	Fr	87	(223)
Berkelium	Bk	97	(247)	Gadolinium	Gd	64	157.25
Beryllium	Be	4	9.012	Gallium	Ga	31	69.72
Bismuth	Bi	83	208.980	Germanium	Ge	32	72.59
Boron	B	5	10.811	Gold	Au	79	196.967
Bromine	Br	35	79.909	Hafnium	Hf	72	178.49
Cadmium	Cd	48	112.40	Helium	He	2	4.0026
Calcium	Ca	20	40.08	Holmium	Ho	67	164.930
Californium	Cf	98	(251)	Hydrogen	H	1	1.0079
Carbon	C	6	12.011	Indium	In	49	114.82
Cerium	Ce	58	140.12	Iodine	I	53	126.904
Cesium	Cs	55	132.905	Iridium	Ir	77	192.2
Chlorine	Cl	17	35.453	Iron	Fe	26	55.874
Chromium	Cr	24	51.996	Krypton	Kr	36	83.80
Cobalt	Co	27	58.933	Lanthanum	La	57	138.91
Copper	Cu	29	63.546	Lawrencium	Lw	103	(260)

TABLE 2 (Cont.) Table of Elements						
Name and Symbol		Atomic Number	Atomic Weight (amu)	Name		Atomic Number	Atomic Weight (amu)
Lead	Pb	82	207.19	Potassium	K	19	39.102
Lithium	Li	3	6.939	Praseodymium	Pr	59	140.90
Lutetium	Lu	71	174.97	Protactinium	Pa	91	231.03
Magnesium	Mg	12	24.312	Promethium	Pm	61	(145)
Manganese	Mn	25	54.938	Radium	Ra	88	226.02
Mendelevium	Md	101	(258)	Radon	Rn	86	(222)
Mercury	Hg	80	200.59	Rhenium	Re	75	186.2
Molybdenum	Mo	42	95.94	Rhodium	Rh	45	102.90
Neodymium	Nd	60	144.24	Rubidium	Rb	37	85.47
Neon	Ne	10	20.183	Ruthenium	Ru	44	101.07
Neptunium	Np	93	237.05	Samarium	Sm	62	150.35
Nickel	Ni	28	58.71	Scandium	Sc	21	44.956
Niobium	Nb	41	92.906	Selenium	Se	34	78.96
Nitrogen	N	7	14.006	Silicon	Si	34	78.96
Nobelium	No	102	(259)	Silver	Ag	47	107.87
Osmium	Os	76	190.2	Sodium	Na	11	22.989
Oxygen	O	8	15.999	Strontium	Sr	38	87.62
Palladium	Pd	46	106.41	Sulfur	S	16	32.064
Phosphorus	P	15	30.973	Tantalum	Ta	73	180.94
Platinum	Pt	78	195.09	Technetium	Tc	43	(98)
Plutonium	Pu	94	(244)	Tellurium	Te	52	127.60
Polonium	Po	84	(209)	Terbium	Tb	65	158.92

<table>
<tr><td colspan="6">TABLE 2 (Cont.)
Table of Elements</td></tr>
</table>

Name and Symbol		Atomic Number	Atomic Weight (amu)	Name		Atomic Number	Atomic Weight (amu)
Thallium	Tl	81	204.37	Vanadium	V	23	50.942
Thorium	Th	90	232.03	Xenon	Xe	54	131.30
Thulium	Tm	69	168.93	Ytterbium	Yb	70	173.04
Tin	Sn	50	118.69	Yttrium	Y	39	88.905
Titanium	Ti	22	47.90	Zinc	Zn	30	65.37
Tungsten	W	74	183.85	Zirconium	Zr	40	91.22
Uranium	U	92	238.03				

Molecules

Molecules are groups or clusters of atoms held together by means of chemical bonding. There are two types of molecule; molecules of an element and molecules of a compound.

Molecules of an Element

In certain cases, two single atoms of an element can be attracted to one another by a bond to form a molecule. Examples of this are hydrogen, oxygen, and bromine. The molecular formulas for these are H_2, O_2, and Br_2. Most gaseous elements exist as molecules of two atoms.

Molecules of a Compound

Two atoms of different elements held together by a bond form a compound. The molecule is the primary particle of a chemical compound. Some examples of this type of molecule include hydrogen chloride (HCl), water (H_2O), methane (CH_4), and ammonia (NH_3).

Molecular Weight

The weight of a molecule, the *molecular weight,* is the total mass of the individual atoms. Therefore, it is fairly simple to calculate the mass of any molecule if its formula is known (that is, the elements and the number of each that make up the molecule). Note that the terms mass and weight are used interchangeably in chemistry.

Example 1:

The compound water has a formula of H_2O. This means there is one atom of oxygen and two atoms of hydrogen. Calculate the molecular weight.

Solution:

The molecular weight is calculated as follows:

1 atom $\times$ 16.000 (the atomic weight of oxygen) = 16.000 amu
2 atoms $\times$ 1.008 (the atomic weight of hydrogen) = 2.016 amu
molecular weight of water = 18.016 amu

Example 2:

Calculate the molecular weight of H_2SO_4.

Solution:

hydrogen	2 atoms $\times$ 1.008 amu = 2.016 amu
sulfur	1 atom $\times$ 32.064 amu = 32.064 amu
oxygen	4 atoms $\times$ 15.999 amu = 63.996 amu
	molecular weight = 98.076 amu

Example 3:

Calculate the molecular weight of HCl.

Solution:

hydrogen	1 atom $\times$ 1.008 amu = 1.008 amu
chlorine	1 atom $\times$ 35.453 amu = 35.453 amu
	molecular weight = 36.461 amu

Avogadro's Number

Consider one atom of oxygen and one atom of sulfur, and compare their atomic weights.

Oxygen's atomic weight = 15.999 amu

Sulfur's atomic weight = 32.06 amu

The sulfur atom weighs approximately twice as much as the oxygen atom.
$(32.06 \div 15.99 \approx 2)$

Because the sulfur atom weighs twice as much as an oxygen atom, a one gram sample of oxygen contains twice as many atoms as a one gram sample of sulfur. Thus, a two gram sample of sulfur contains the same number of atoms as a one gram sample of oxygen.

From this previous example, one might suggest that a relationship exists between the weight of a sample and the number of atoms in the sample. In fact, scientists have determined that there is a definite relationship between the number of atoms in a sample and the sample's weight. Experimentation has shown that, for any element, a sample containing the atomic weight in grams contains 6.022×10^{23} atoms. Thus 15.999 grams of oxygen contains 6.022×10^{23} atoms, and 32.06 grams of sulfur contains 6.022×10^{23} atoms. This number (6.022×10^{23}) is known as *Avogadro's number*. The importance of Avogadro's number to chemistry should be clear. It represents the number of atoms in X grams of <u>any</u> element, where X is the atomic weight of the element. It permits chemists to predict and use exact amounts of elements needed to cause desired chemical reactions to occur.

The Mole

A single atom or a few atoms are rarely encountered. Instead, larger, macroscopic quantities are used to quantify or measure collections of atoms or molecules, such as a glass of water, a gallon of alcohol, or two aspirin. Chemists have introduced a large unit of matter, the mole, to deal with macroscopic samples of matter.

One mole represents a definite number of objects, substances, or particles. (For example, a mole of atoms, a mole of ions, a mole of molecules, and even, theoretically, a mole of elephants.) A *mole* is defined as the quantity of a pure substance that contains 6.022×10^{23} units (atoms, ions, molecules, or elephants) of that substance. In other words, a mole is Avogadro's number of anything.

For any element, the mass of a mole of that element's atoms is the atomic mass expressed in units of grams. For example, to calculate the mass of a mole of copper atoms, simply express the atomic mass of copper in units of grams. Because the atomic mass of copper is 63.546 amu, a mole of copper has a mass of 63.546 grams. The value for the atomic mass of gold is 196.967 amu. Therefore, a mole of gold has a mass of 196.967 grams. The mass of a mole of atoms is called the *gram atomic weight* (GAW). The mole concept allows the conversion of grams of a substance to moles and vice versa.

GOLD   COPPER

1.060"   0.938"

196.967g   63.546g

EACH SPHERE CONTAINS
6.022×10^{23} ATOMS

Figure 2 A Mole of Gold Compared to a Mole of Copper

Figure 2 contains a ball of gold and a ball of copper. The two balls are of different masses and different sizes, but each contains an identical number of atoms.
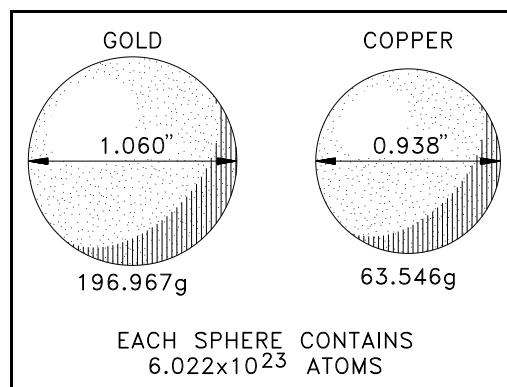
Example 1:

A silver bar has a mass of 1870 grams. How many moles of silver are in the bar?

Solution:

Since the atomic mass of silver (Ag) is 107.87 amu, one mole of silver has a mass of 107.87 grams. Therefore, there is one mole of Ag per 107.87 grams of Ag or $\dfrac{1 \ \text{mole Ag}}{107.87 \ \text{grams Ag}}$. There are 1870 grams of silver.

$$\frac{1870 \ \text{grams Ag}}{1} \times \frac{1 \ \text{mole Ag}}{107.87 \ \text{grams Ag}} = 17.3 \ \text{mole Ag}$$

Example 2:

Mercury (Hg) is the only metal that exists as a liquid at room temperature. It is used in thermometers. A thermometer contains 0.004 moles of mercury. How many grams of mercury are in the thermometer?

Solution:

Since the atomic mass of Hg is 201 amu, one mole of Hg has a mass of 201 grams of Hg or $\dfrac{201 \ \text{grams Hg}}{1 \ \text{mole Hg}}$. There are 0.004 moles of Hg.

$$\frac{0.004 \ \text{moles Hg}}{1} \times \frac{201 \ \text{grams Hg}}{1 \ \text{mole Hg}} = 0.8 \ \text{grams Hg}$$

Mole of Molecules

The mass of a mole of molecules of a substance is the molecular mass expressed in grams. For example, an oxygen molecule (O_2) has a molecular mass equivalent to 32.0 grams because each oxygen atom has a molecular mass of 16.0 grams. (Recall that to obtain the molecular mass, the atomic masses of all atoms that appear in the formula are added.) If the atomic masses of the carbon and four hydrogen atoms in methane, CH_4, are added, the total is 16 amu. Therefore, one mole of CH_4 has a mass of 16 grams. The mass of a mole of molecules is called the molar mass or *gram molecular weight* (GMW).

Summary

The important information found in this chapter is summarized below.

Characteristics of Atoms Summary

• The following terms are defined:

States of matter is a term which refers to the physical forms in which matter exists; solid, liquid and gas. Solids are characterized as having both a definite shape and a definite volume. Liquids have definite volumes but indefinite shapes and are slightly compressible. Gases are readily compressible and capable of infinite expansion.

Atomic weight is defined as the weighted average of the masses of all its natural occurring isotopes.

Molecular weight will be the total weight of the individual atoms of a molecule.

A mole is Avogadro's number of any substance.

Gram atomic weight is the mass of a mole of atoms.

Gram molecular weight is the mass of a mole of molecules, (GMW).

• The components of an atom are protons, neutrons, and electrons. A proton has a mass of 1.0 amu and a positive charge (+1). The neutron also has a mass of 1.0 amu but is neutral in charge. The electron has a mass of .00055 or 1/1835 amu and a negative charge (-1).

• An atom is classified chemically by the number of protons in its nucleus.

THE PERIODIC TABLE

All known elements fall into a pattern when placed in a periodic table, and the position in this pattern is decided by the element's atomic number. This chapter will discuss the significance of this fact.

EO 1.4 **DEFINE the following subdivisions of the periodic table:**

    a. **Periods of the periodic table**
    b. **Groups of the periodic table**
    c. **Classes of the periodic table**

EO 1.5 **Given a periodic table, IDENTIFY the following subdivisions:**

    a. **Periods of the periodic table**
    b. **Groups of the periodic table**
    c. **Classes of the periodic table**

EO 1.6 **LIST the characteristics that elements in the same group on the periodic table share.**

EO 1.7 **DEFINE the term valence.**

Periodic Table

Over many years of chemical investigation, scientists have discovered a remarkable feature of the elements. If the elements are arranged in the order of their atomic numbers, the chemical properties of the elements are repeated somewhat regularly. To a lesser extent, the physical properties are also repeated periodically. This periodic repetition can be seen in Table 3. Compare the properties of lithium (Li), sodium (Na), and potassium (K), and also those of beryllium (Be), magnesium (Mg), and calcium (Ca). In the list of elements shown in Table 3 the properties are repeated every eighth element.

<table>
<tr><td colspan="5">TABLE 3
Description of the Properties of the First Twenty Elements</td></tr>
<tr><td>Element</td><td>Symbol</td><td>Atomic Number</td><td>Atomic Weight</td><td>Description of Properties</td></tr>
<tr><td>Hydrogen</td><td>H</td><td>1</td><td>1.008</td><td>Colorless gas, reacts readily with oxygen to form H_2O; forms HCl with chlorine.</td></tr>
<tr><td>Helium</td><td>He</td><td>2</td><td>4.003</td><td>Colorless gas, very non-reactive chemically.</td></tr>
</table>

TABLE 3 (Cont.)
Description of the Properties of the First Twenty Elements

Lithium	Li	3	6.939	Silvery white, soft metal, very reactive chemically, forms Li_2O and LiCl readily.
Beryllium	Be	4	9.012	Grey metal, much harder than lithium, fairly reactive chemically, forms BeO and $BeCl_2$ easily.
Boron	B	5	10.811	Yellow or brown non-metal, very hard element, not very reactive, but will form B_2O_3, and BCl_3
Carbon	C	6	12.011	Black non-metal, brittle, non-reactive at room temperature. Forms CO_2 and CCl_4.
Nitrogen	N	7	14.007	Colorless gas, not very reactive, will form N_2O_5 and NH_3.
Oxygen	O	8	15.999	Colorless gas, moderately reactive,will combine with most elements, forms CO_2, MgO, etc.
Fluorine	F	9	18.998	Green-yellow gas, extremely reactive, irritating to smell, forms NaF, MgF_2.
Neon	Ne	10	20.183	Colorless gas, very non-reactive chemically.
Sodium	Na	11	22.990	Silvery soft metal, very reactive chemically, forms Na_2O and NaCl.
Magnesium	Mg	12	24.312	Silvery white metal, much harder than sodium. Fairly reactive, forms MgO and $MgCl_2$.
Aluminum	Al	13	26.982	Silvery white metal, like magnesium but not as reactive. Forms Al_2O_3 and $AlCl_3$.
Silicon	Si	14	28.086	Gray, non-metallic, non-reactive at room temperature, forms SiO_2 and $SiCl_4$.
Phosphorus	P	15	30.974	Black, red, violet, or yellow solid, low melting point, quite reactive, forms P_2O_5 and PCl_3.
Sulfur	S	16	32.064	Yellow solid with low melting point. Moderately reactive, combines with most elements, forms SO_2, MgS, etc.
Chlorine	Cl	17	35.453	Greenish-yellow gas, extremely reactive, irritating to smell, forms NaCl, $MgCl_2$.
Argon	Ar	18	39.948	Colorless gas, very non-reactive chemically.
Potassium	K	19	39.102	Silver soft metal, very reactive chemically, forms K_2O and KCl.
Calcium	Ca	20	40.080	Silver-white metal, much harder than potassium, fairly reactive, forms CaO and $CaCl_2$.

A table in which elements with similar chemical properties are grouped together is called a periodic table. One of the most common versions is shown in Figure 3. In this table, elements are arranged in order of increasing atomic number in succeeding rows. Each horizontal row is called a *period.* Note that some periods are longer than others. Elements with similar chemical properties appear in vertical columns called *groups*. Each group is designated by a Roman numeral and a capital letter, except the one on the extreme right-hand side, Group 0 (the inert gases). At the bottom of the periodic table are two long rows of elements identified as the lanthanide series and the actinide series. They are separated from the table primarily to keep it from becoming too wide. Also, the elements within each of these two series show similar chemical properties.

The number directly below each element is its atomic number, and the number above each element is its atomic weight. In several cases the atomic weights are in parentheses. This indicates that these elements have no stable isotopes; that is, they are radioactive. The value enclosed in parentheses and used for the atomic weight is the atomic mass number of the most stable known isotope, as indicated by the longest half-life.

Figure 3   Periodic Table of the Elements

Classes of the Periodic Table

There are three broad *classes* of elements. These are the metals, the non-metals, and the semi-metals. These three classes are grouped together on the periodic table as shown on Figure 4.
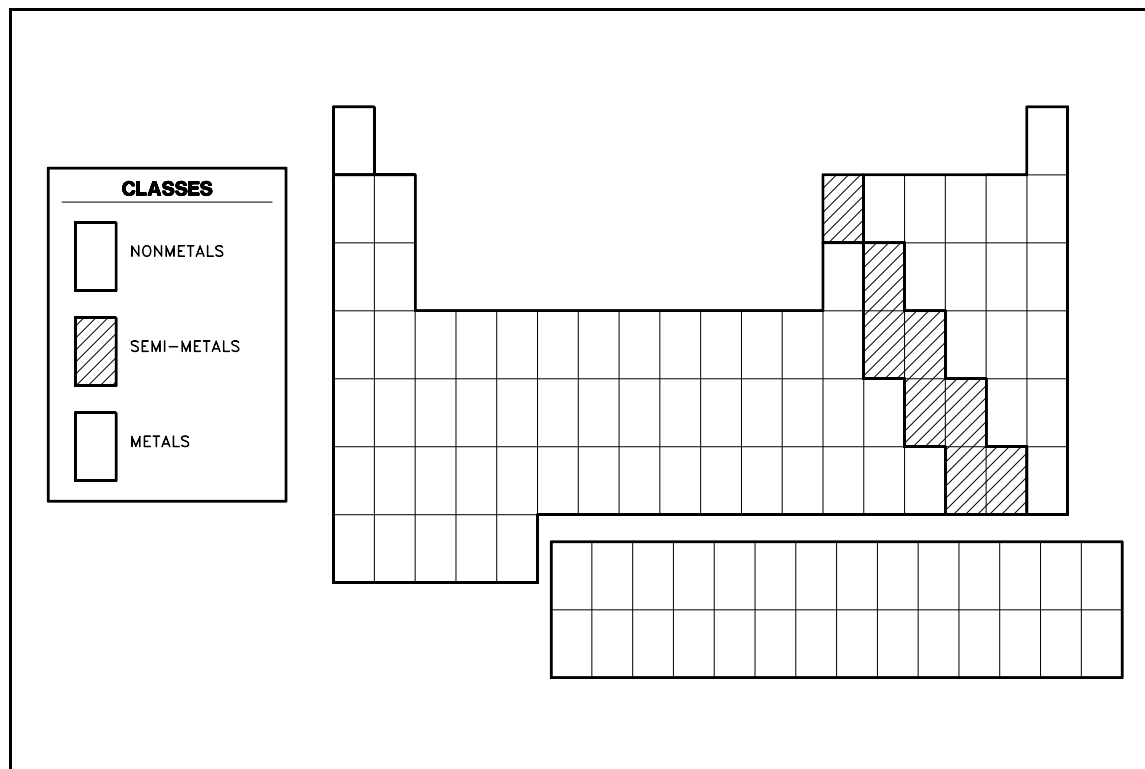

Figure 4   Regional Schematic of Periodic Table

Metals

The metals constitute the largest class of elements and are located on the left and toward the center of the periodic table as shown in Figure 4. In Figure 3, the heavy line running step-wise from boron (B) to astatine (At) generally separates the metals from the rest of the elements (elements in the actinide and lanthanide series are metals). Metals tend to lose electrons to form positive ions rather than to gain electrons and become negative ions.

Most people are familiar with metals' physical properties. They are usually hard and strong, capable of being shaped mechanically (malleable and ductile), and good conductors of heat and electricity, and they have lustrous surfaces when clean. More important for chemical classification are the chemical properties of metals because the physical properties are not common to all metals. For example, mercury (Hg) is a metal, although it is a liquid at room temperature, and sodium is a metal although it is not at all hard or strong. Metals can be involved in a wide range of chemical reactions. Their reactions with water range from violent with sodium and potassium to imperceptible with gold and platinum. Metals are divided into the following two categories.

1.   The light metals, which are soft, have a low density, are very reactive chemically, and are unsatisfactory as structural materials.

2.   The transition metals, which are hard, have a high density, do not react readily, and are useful structural materials.

The metals in Category 1 are located at the far left of the table (Groups IA and IIA). The metals in Category 2 are located in the middle of the table (the B groups).

Nonmetals

The nonmetals occupy the part of the periodic table to the right of the heavy, step-like line. (refer to Figure 3 and Figure 4)

In general, the physical properties of the nonmetals are the opposite of those attributed to metals. Nonmetals are often gases at room temperature. The nonmetals that are solids are not lustrous, are not malleable or ductile, and are poor conductors of heat and electricity. Some nonmetals are very reactive, but the nature of the reactions is different from that of metals. Nonmetals tend to gain electrons to form negative ions rather than to lose electrons to form positive ions.

The six elements in Group 0 represent a special subclass of nonmetals. They are all very unreactive gases, so they are called the inert gases. For many years it was believed that the inert gases would not and could not participate in chemical reactions. In 1962, the first true compounds of an inert gas, XeF_4 and $XePtF_6$, were positively identified.

Since that time, several other compounds have been prepared. The preparation of these compounds requires special conditions; under ordinary conditions, the inert gases may be considered nonreactive.

Semi-Metals

The obvious trend in the periodic table is that from left to right, across any period, the elements change from distinctly metallic (Group IA) to distinctly nonmetallic (Group VIIA). This change in character is not sharply defined, but is gradual. Generally, elements well to the left of the heavy diagonal line are metals, and those well to the right are nonmetals. Some of the elements near the line, however, exhibit properties of metals under some conditions and properties of nonmetals under other conditions. These elements are called the semi-metals and include boron (B), silicon (Si), germanium (Ge), arsenic (As), and tellurium (Te). They are usually classified as semi-conductors of electricity and are widely used in electrical components.

Group Characteristics

Each set of elements appearing in the vertical column of a periodic table is called a Group and represents a family of elements that have similar physical and chemical properties. Group IA is the Alkali Family; Group IIA is the Alkaline Earth Family; Group VIA is the Oxygen Family; Group VIIA is the Halogen Family. On the left side of the table are Group IA elements (except hydrogen), which are soft metals that undergo similar chemical reactions. The elements in Group IIA form similar compounds and are much harder than their neighbors in Group IA.

As shown in the previous section, there are some exceptions to the generalizations concerning chemical properties and the periodic table. The most accurate observation is that all elements within a particular group have similar physical and chemical properties.

This observation is most accurate at the extreme sides of the table. All elements in Group 0 are unreactive gases, and all elements in Group VIIA have similar chemical properties, although there is a gradual change in physical properties. For example, fluorine (F) is a gas while iodine (I) is a solid at room temperature.

Groups with a B designation (IB through VIIB) and Group VIII are called transition groups. In this region of the table, exceptions begin to appear. Within any group in this region, all the elements are metals, but their chemical properties may differ. In some cases, an element may be more similar to neighbors within its period than it is to elements in its group. For example, iron (Fe) is more similar to cobalt (Co) and nickel (Ni) than it is to ruthenium (Ru) and osmium (Os). Most of these elements have several charges, and their ions in solution are colored (ions of all other elements are colorless).

The line separating metals from nonmetals cuts across several groups. In this region of the table, the rule of group similarities loses much of its usefulness. In Group IVA, for example, carbon (C) is a nonmetal; silicon (Si) and germanium (Ge) are semi-metals; and tin (Sn) and lead (Pb) are metals.

Chemical activity can also be determined from position in the periodic table. The most active metals are the members of the Alkali Family, e.g., cesium (Cs) and francium (Fr). The most active nonmetals are the members of the Halogen Family, e.g., fluorine (F) and chlorine (Cl). The Noble Gases in Group 0 are inert. The activity of metals decreases when proceeding to the right in the periodic table; the activity of nonmetals decreases when proceeding to the left.

Atomic Structure of Electrons

Based on experimental data, it is known that chemical reactions involve only the electrons in atoms. In fact, only some of the electrons are involved. Because chemical properties are periodic, there must also be a periodic characteristic about electrons. This characteristic is the manner in which electrons are arranged in the atom. Electrons are in constant motion around the nucleus. They have both kinetic and potential energy, and their total energy is the sum of the two. The total energy is quantized; that is, there are definite, discrete values of total energy that atomic electrons can possess. These energy states can be visualized as spherical shells around the nucleus separated by forbidden areas where electrons cannot exist in a stable state. This sort of arrangement is illustrated in Figure 5.

FLUORINE

CHLORINE

BROMINE

IODINE

IN THE DIAGRAM ABOVE, THE DARK AREAS REPRESENT THE ELECTRON CLOUDS OR SHELLS. THE NUCLEI
OF THE ATOMS HAVE NOT BEEN SHOWN. THE DARK AREAS IN THE CENTER REPRESENT THE INNERMOST SHELL.
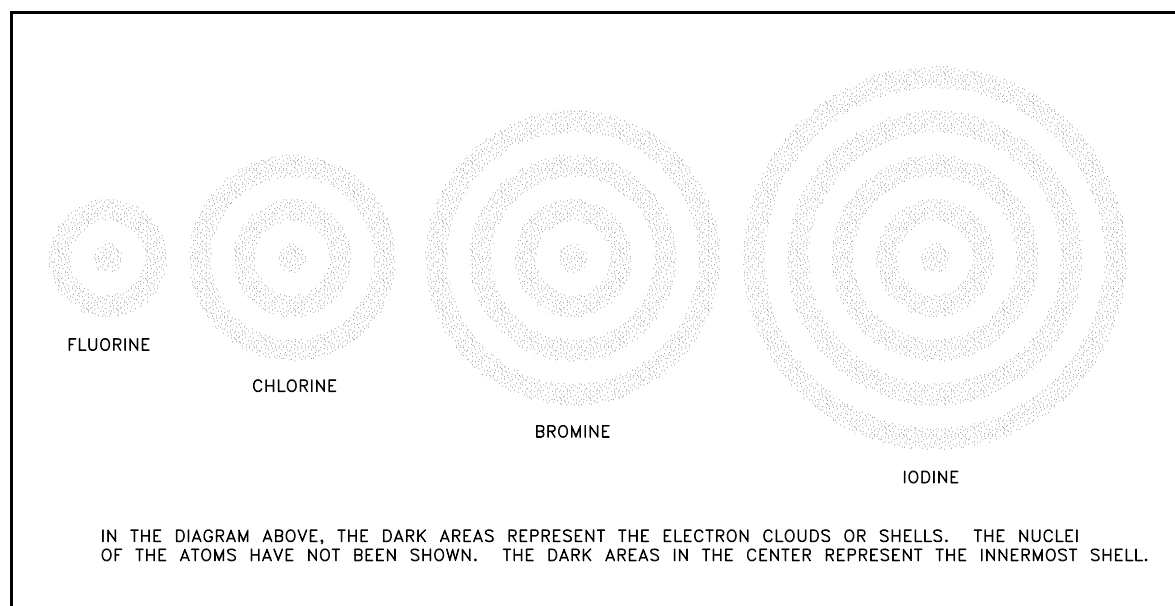
Figure 5   Electron Shells of Atoms

It is customary to speak of electron shells around the nucleus, and the shells are referred to by number. The first, or No. 1, shell is the one nearest the nucleus; the second, or No. 2, shell is next; then the third, or No. 3, shell; and so on in numerical order. In general, electrons closer to the nucleus have a lower energy state. Atomic electrons always seek the lowest energy state available.

The electron shells represent major energy states of electrons. Each shell contains one or more subshells called orbitals, each with a slightly different energy. In order of increasing energy, the orbitals are designated by the small letters s, p, d, f, g, h.

No two shells consist of the same number of orbitals. The first shell contains only one orbital, an s orbital. The second shell contains s and p orbitals. In general, each higher shell contains a new type of orbital:

> the first shell contains an s orbital,
> the second shell contains s and p orbitals,
> the third shell contains s, p, and d orbitals,
> the fourth shell contains s, p, d, and f orbitals,

and so on. Each orbital can hold a definite maximum number of electrons. There is also a limit to the number of electrons in each shell and the limit increases as one goes to higher shells. The numbers of electrons that can occupy the different orbitals and shells are shown in Table 4.

	TABLE 4		
	Electrons, Orbital, and Shell Relationships in Atomic Structure		
Shell Number	Type of Orbitals	Maximum Number of Electrons in Each Orbital	Maximum Total Electrons in shell
1	s	2	2
2	s	2	8
	p	6	
3	s	2	18
	p	6	
	d	10	
4	s	2	32
	p	6	
	d	10	
	f	14	
5	s	2	50
	p	6	
	d	10	
	f	14	
	g	18	

A more specific statement can now be made about which electrons are involved in chemical reactions. Chemical reactions involve primarily the electrons in the outermost shell of an atom. The term outermost shell refers to the shell farthest from the nucleus that has some or all of its allotted number of electrons. Some atoms have more than one partially-filled shell. All of the partially-filled shells have some effect on chemical behavior, but the outermost one has the greatest effect. The outermost shell is called the valence shell, and the electrons in that shell are called valence electrons. The term *valence* (of an atom) is defined as the number of electrons an element gains or loses, or the number of pairs of electrons it shares when it interacts with other elements.

The periodic chart is arranged so that the valence of an atom can be easily determined. For the elements in the A groups of the periodic chart, the number of valence electrons is the same as the group number; that is, carbon (C) is in Group IVA and has four valence electrons. The noble gases (Group 0) have eight in their valence shell with the exception of helium, which has two.

The arrangement in which the outermost shell is either completely filled (as with He and Ne) or contains eight electrons (as with Ne, Ar, Kr, Xe, Rn) is called the inert gas configuration. The inert gas configuration is exceptionally stable energetically because these inert gases are the least reactive of all the elements.

The first element in the periodic table, hydrogen, does not have properties that satisfactorily place it in any group. Hydrogen has two unique features: (a) the highest energy shell of a hydrogen atom can hold only two electrons, in contrast to all others (except helium) that can hold eight or more; and (b) when hydrogen loses its electron, the ion formed, H^+, is a bare nucleus. The hydrogen ion is very small in comparison with a positive ion of any other element, which must still have some electrons surrounding the nucleus. Hydrogen can either gain or lose an electron. It has some properties similar to Group IA elements, and some similar to Group VIIA elements.

The number of electrons in the outer, or valence, shell determines the relative activity of the element. The elements are arranged in the periodic table so that elements of the same group have the same number of electrons in the outer shell (except for the Transition Groups). The arrangement of electrons in the outer shell explains why some elements are chemically very active, some are not very active, and others are inert. In general, the fewer electrons an element must lose, gain, or share to reach a stable shell structure, the more chemically active the element is. The likelihood of elements forming compounds is strongly influenced by this valence shell and on the stability of the resulting molecule. The more stable the molecules are, the more likely these molecules are to form.

Summary

The important information from this chapter is summarized below.

Periodic Table Summary

- The subdivisions of the periodic table are periods, groups, and classes. The horizontal rows are called periods. The vertical columns are called groups. The entire table consists of three classes: metals, non-metals, and semi-metals.

- The subdivisions of the periodic chart have been explained such that the student should be able to identify them if given a periodic table.

- Elements of the same group share certain physical and chemical characteristics. Examples of the characteristics of several groups are listed below.

    Group 0 contains elements that are unreactive gases.
    Group IA contains elements that are chemically active soft metals.
    Group VIIA contains elements that are chemically active nonmetals.
    Groups IB through VIIB and VIII are called transition groups and elements found in them display properties of metals.

- The *valence* of an atom is defined as the number of electrons an element gains or loses, or the number of pairs of electrons it shares when it interacts with other elements.

CHEMICAL BONDING

The development of matter, no matter what the form, is the result of the practical application of the assumptions, hypotheses, theories, and laws that chemists have formulated from their research into the nature of matter, energy, and change. This chapter will address some of these theories and laws. Chemical bonds and how atoms bond to form molecules will be discussed. In addition, an introduction to organic chemistry is provided.

EO 2.1 DEFINE the following terms:

a.	Ionic bonds	c.	Covalent bonds
b.	Van der Waals forces	d.	Metallic bonds

EO 2.2 DESCRIBE the physical arrangement and bonding of a polar molecule.

EO 2.3 DESCRIBE the three basic laws of chemical reactions.

EO 2.4 STATE how elements combine to form chemical compounds.

EO 2.5 EXPLAIN the probability of any two elements combining to form a compound.

EO 2.6 DEFINE the following terms:

a.	Mixture	d.	Solute
b.	Solvent	e.	Solution
c.	Solubility	f.	Equilibrium

Chemical Bonding

As stated in the previous chapter, the number of electrons in the outer, or valence, shell determines the relative activity of the element. The arrangement of electrons in the outer shell explains why some elements are chemically very active, some are not very active, and others are inert. In general, the fewer electrons an element must lose, gain, or share to reach a stable shell structure, the more chemically active the element is. The likelihood of elements forming compounds is strongly influenced by the completion of the valence shell and by the stability of the resulting molecule. The more stable the resulting molecules are, the more likely these molecules are to form. For example, an atom that "needs" two electrons to completely fill the valence shell would rather react with another atom which must give up two electrons to satisfy its valence.

In the case of $H^+ + Br^-$, this is likely to take place because the exchange would satisfy the needs of both atoms. Although there is far more to consider than just the number of valence electrons, this is a good rule of thumb.

If the atom needed two electrons and only picked up one, it would still actively seek out an additional electron. The reaction of $H^+ + Te^2$ is far less likely to take place because the resulting molecule would still have an incomplete valence shell. Of course, the combining of two atoms, when both want to release or gain electrons, may take place (for example; H_2 or O_2) but is less probable when other atoms are available.

Atoms are joined or bonded together through this interaction of their electrons. There are several types of chemical bonds that hold atoms together; three will be discussed, ionic, covalent, and metallic.

Ionic Bonds

An *ionic bond* is formed when one or more electrons is wholly transferred from one element to another, and the elements are held together by the force of attraction due to the opposing charges. An example of ionic bonding is shown in Figure 6(A) for sodium chloride (table salt).

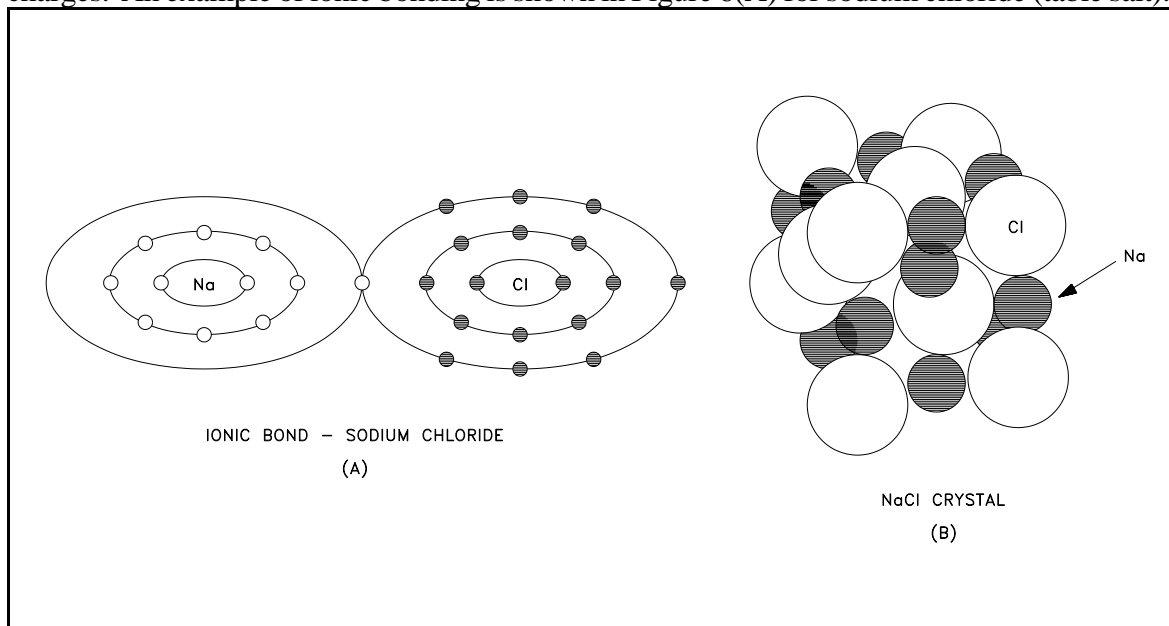IONIC BOND – SODIUM CHLORIDE
(A)

NaCl CRYSTAL
(B)

Figure 6   Ionic Bond, Sodium Chloride

The sodium atom loses the one electron in its outer shell to the chlorine atom, which uses the electron to fill its outer shell. When this occurs, the sodium atom is left with a +1 charge and the chlorine atom a -1 charge. The ionic bond is formed as a result of the attraction of the two oppositely-charged particles. No single negatively-charged ion has a greater tendency to bond to a particular positively-charged ion than to any other ion.

Because of this, the positive and negative ions arrange themselves in three dimensions, as shown in Figure 6(B), to balance the charges among several ions. In sodium chloride, for example, each chloride ion is surrounded by as many sodium ions as can easily crowd around it, namely six. Similarly, each sodium ion is surrounded by six chloride ions. Therefore, each chloride ion is bonded to the six nearest sodium ions and bonded to a lesser extent to the more distant sodium ions. Accordingly, the ionic bond is a force holding many atoms or ions together rather than a bond between two individual atoms or ions.

Covalent Bonds

A *covalent bond* is formed when one or more electrons from an atom pair off with one or more electrons from another atom and form overlapping electron shells in which both atoms share the paired electrons. Unlike an ionic bond, a covalent bond holds together specific atoms. Covalent bonding can be single covalent, double covalent, or triple covalent depending on the number of pairs of electrons shared. Figure 7 shows the bonding that occurs in the methane molecule, which consists of four single covalent bonds between one carbon atom and four hydrogen atoms.
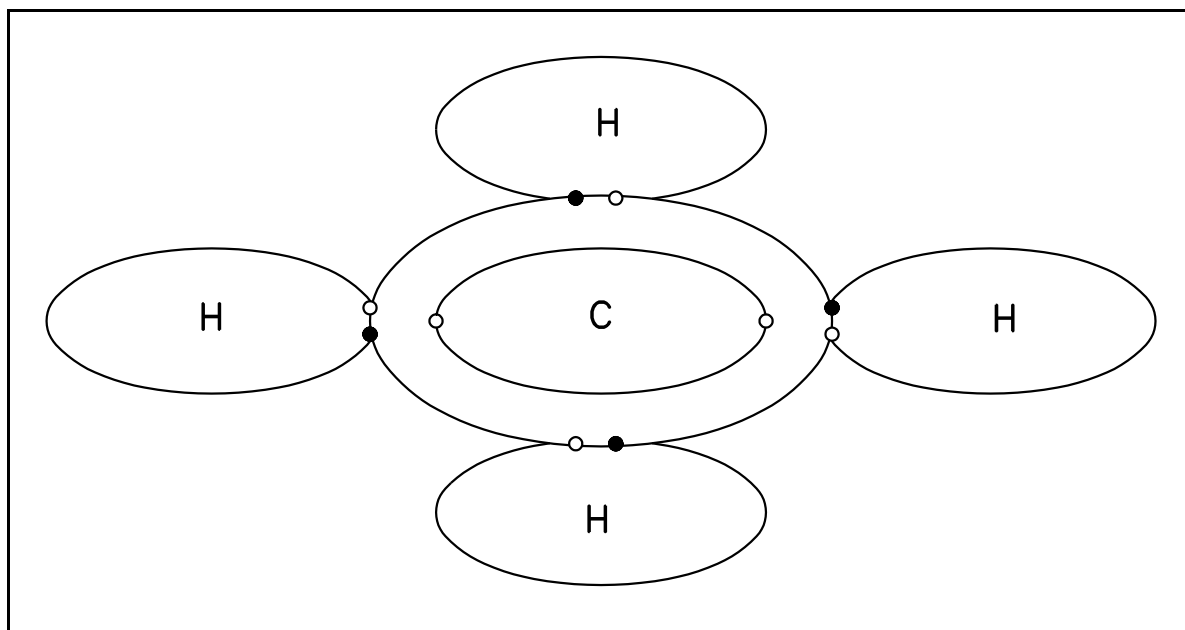

Figure 7 Covalent Bond, Methane CH_4

Two double covalent bonds result when carbon dioxide, which consists of one carbon atom and two oxygen atoms, is formed. Four pairs of electrons are shared by the carbon atom, two from each of the two oxygen atoms as shown in Figure 8. A combination of two electrons form a combination of lower energy than their energy when separated. This energy difference represents the force that binds specific atoms together.
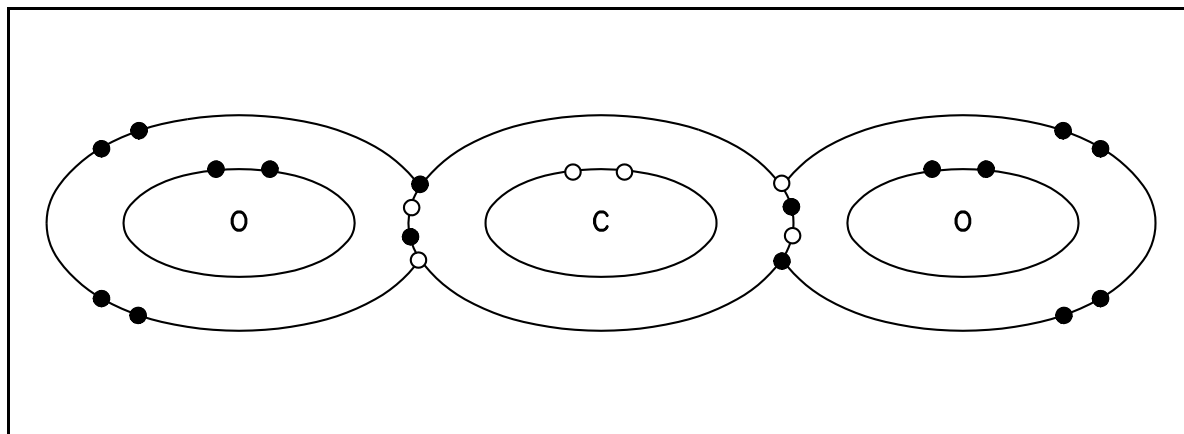
Figure 8 Formation of the Carbon Dioxide Molecule

When both shared electrons in a covalent bond come from the same atom, the bond is called a coordinate covalent bond. Although both shared electrons come from the same atom, a coordinate covalent bond is a single bond similar in properties to a covalent bond. Figure 9 illustrates the bonds of the negatively-charged chlorate ion. The ion consists of one chlorine atom and three oxygen atoms with a net charge of -1, and is formed with two coordinate covalent bonds and one covalent bond. The chlorine atom has effectively gained an electron through the covalent bond, which causes the overall negative charge.
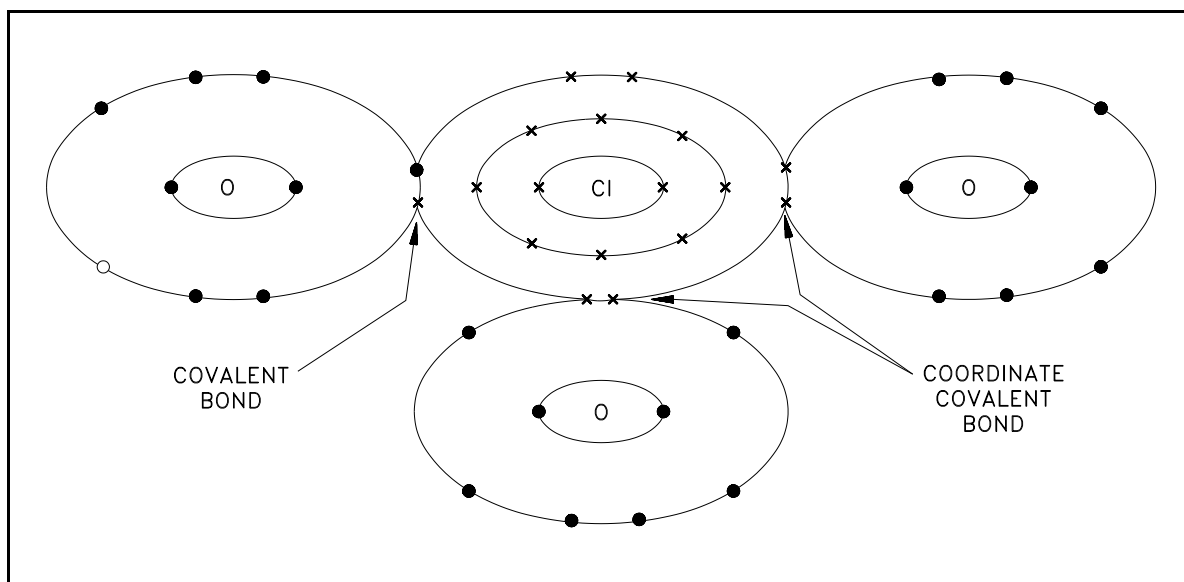
Figure 9 Coordinate Covalent Bond, Chlorate Ion ClO_3

Covalent bonds can be either polar or nonpolar. When the shared pair of electrons is not shared equally, one end of the bond is positive, and the other end is negative. This produces a bond with two poles called a polar covalent bond.

Molecules having polar covalent bonds are called dipolar or *polar molecules*. Water is an example of a polar molecule. When two atoms of the same element share one or more pairs of electrons (such as H or N), each atom exerts the same attraction for the shared electron pair or pairs. When the electron pairs are distributed or shared equally between the two like atoms, the bond is called a nonpolar covalent bond. If all the bonds in a molecule are of this kind, the molecule is called a nonpolar covalent molecule.

Metallic Bonds

Another chemical bonding mechanism is the *metallic bond*. In the metallic bond, an atom achieves a more stable configuration by sharing the electrons in its outer shell with many other atoms. Metallic bonds prevail in elements in which the valence electrons are not tightly bound with the nucleus, namely metals, thus the name metallic bonding. In this type of bond, each atom in a metal crystal contributes all the electrons in its valence shell to all other atoms in the crystal.

Another way of looking at this mechanism is to imagine that the valence electrons are not closely associated with individual atoms, but instead move around amongst the atoms within the crystal. Therefore, the individual atoms can "slip" over one another yet remain firmly held together by the electrostatic forces exerted by the electrons. This is why most metals can be hammered into thin sheets (malleable) or drawn into thin wires (ductile). When an electrical potential difference is applied, the electrons move freely between atoms, and a current flows.

Van der Waals Forces

In addition to chemical bonding between atoms, there is another type of attractive force that exists between atoms, ions, or molecules known as van der Waals forces.

These forces occur between the molecules of nonpolar covalent substances such as H_2, Cl_2, and He. These forces are generally believed to be caused by a temporary dipole, or unequal charge distribution, as electrons constantly move about in an atom, ion, or molecule. At a given instant, more electrons may be in one region than in another region, as illustrated in Figure 10.

The temporary dipole induces a similar temporary dipole on a nearby atom, ion, or molecule. Every instant, billions of these temporary dipoles form, break apart, and reform to act as a weak electrostatic force of attraction known as *van der Waals forces.*

It is important to note that van der Waals forces exist between all kinds of molecules. Some molecules may have these forces, as well as dipole or other intermolecular forces. Van der Waals forces, however, are the only intermolecular bonds between nonpolar covalent molecules such as H_2, Cl_2, and CH_4. The number of electrons in a substance increases as the gram molecular mass (mass in grams of one mole of compound) increases. Therefore, the strength of the van der Waals forces between substances increases with increasing gram molecular mass.
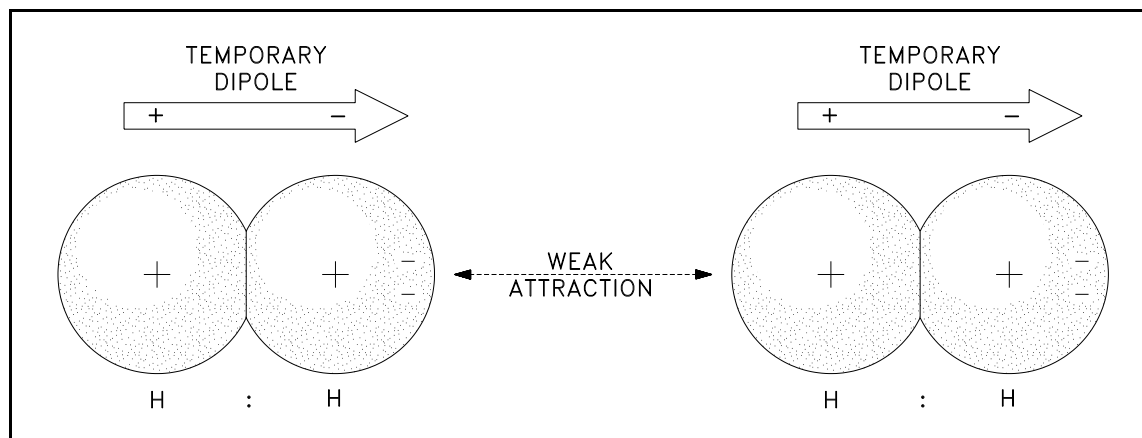
Figure 10   Van der Waals Forces

Van der Waals forces are small compared to the forces of chemical bonding and are significant only when the molecules are very close together.

Organic Chemistry

Organic chemistry is defined as the chemistry of carbon compounds. The compounds of carbon are in forms of living things and in synthetic fabrics and plastics. Organic chemistry is so broad a topic that it is usually subdivided into smaller areas. How the carbon is combined and what it is combined with determines the subdivision for a particular compound. These subdivisions are referred to as families or classes.

The carbon atoms can combine to form straight chains, rings, or branched chains. The bonds between carbon atoms can be single, double, triple or a combination of these. Other atoms (H, O, N, S, P) and the halogens can be attached to the carbon atoms to yield derivatives.

The large family of organic compounds containing only carbon and hydrogen are called hydrocarbons. These can be further divided into two broad classes, aliphatic (fatty) and aromatic (fragrant).

Aliphatic hydrocarbons are divided into two categories, saturated and unsaturated and into subdivisions alkanes, alkenes, and alkynes. These subdivisions reflect the type of bond between the carbon atoms.
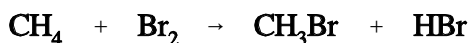
Alkanes

Alkanes are saturated compounds which have single bonds between carbon atoms and contain the maximum number of hydrogen atoms possible. Each carbon is flanked by four covalent bonds and each hydrogen atom shares one pair of electrons with a carbon atom, as illustrated in Figure 11.

The general formula for alkanes is C_nH_{2n+2}. The alkanes are colorless, practically odorless, insoluble in water, and readily soluble in nonpolar solvents such as benzene or ether.

Alkanes are low in reactivity. The reactions they do undergo are called halogenation, thermal decomposition (cracking), and combustion. These are summarized below.
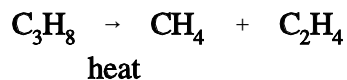

Figure 11 Alkane

Halogenation occurs when a hydrogen atom is replaced with a halogen atom. This is referred to as a substitution reaction. There is no limit to how many hydrogen atoms can be replaced in one molecule.

$$CH_4 \ + \ Br_2 \ \rightarrow \ CH_3Br \ + \ HBr$$

Thermal decomposition or cracking is the process of breaking large molecules into smaller ones. Using heat as a catalyst, propane can be broken into methane and ethylene:

$$CH_4(gas) \ + \ 2O_2(gas) \ \rightarrow \ CO_2(gas) \ + \ 2H_2O(liquid) \ + \ 213 \ kcal(heat)$$
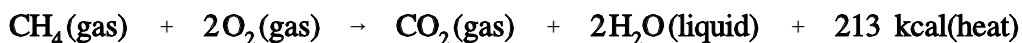
Combustion occurs when an alkane is burned, the products being carbon dioxide gas, water, and heat. These reactions are highly exothermic and as such the hydrocarbons are frequently used for fuel.

$$C_3H_8 \ \underset{heat}{\rightarrow} \ CH_4 \ + \ C_2H_4$$

Alkenes

Alkenes are hydrocarbons containing two fewer hydrogen atoms than the corresponding alkane. The general formula for alkenes is C_nH_{2n}. These molecules will have a double bond as illustrated in Figure 12.

Because there are fewer hydrogen atoms than the maximum possible, alkenes are unsaturated hydrocarbons. The chief source for alkenes is the cracking of alkanes.
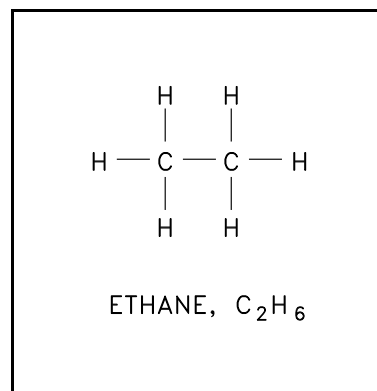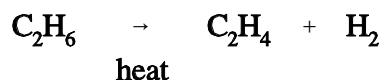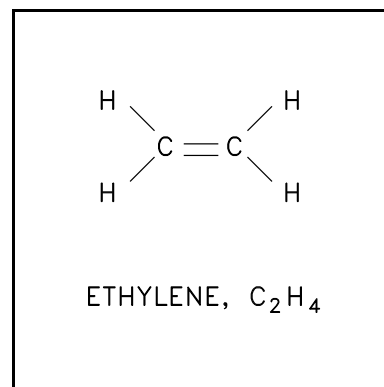

Figure 12 Alkene

$$C_2H_6 \ \underset{heat}{\rightarrow} \ C_2H_4 \ + \ H_2$$

Alkynes

The third of the aliphatic hydrocarbons are the *alkynes*. These compounds are unsaturated like the alkenes. They contain two fewer hydrogens than the corresponding alkane, C_nH_{2n-2}. The alkyne hydrocarbons contain a triple bond between at least one set of carbon atoms as illustrated in Figure 13.
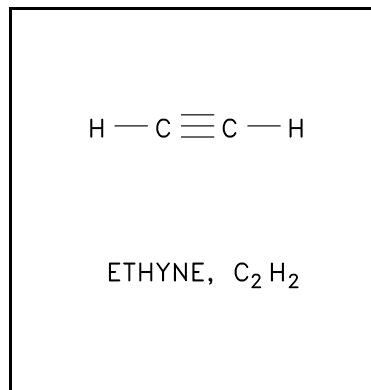
Figure 13 Alkyne

Aromatics

The other broad class of hydrocarbons is the aromatic hydrocarbon. Rather than being arranged in straight chains, as the aliphatics are, these are cyclic formations such as in benzene. The derivatives of cyclic hydrocarbons have pleasant (sometimes toxic) odors. The benzene in rubber cement is a familiar odor. The cyclic compounds have alternating single - double bonds as illustrated in Figure 14.

Aromatic hydrocarbons are very stable chemically, and act very much like alkanes. They will undergo substitution reactions rather than additions.
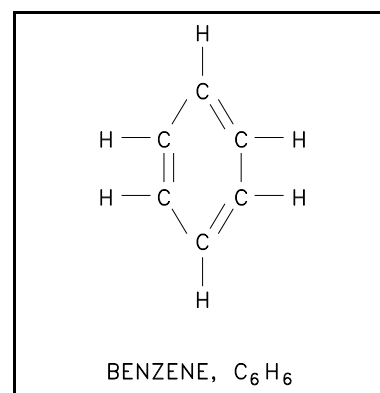
Figure 14 Aromatic

Alcohols

Alcohol is an aliphatic hydrocarbon with a hydroxyl (OH) group substituting for one or more hydrogens as illustrated in Figure 15.

The -OH functional group does not behave in an ionic manner in the case of alcohols. The alcohols are molecular, not ionic, in nature. Alcohols are versatile compounds which are often used to make nearly every other kind of aliphatic compound.
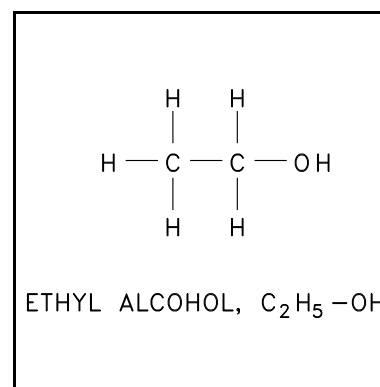
Figure 15 Alcohol

Aldehydes

Aldehydes are one of the oxidation products of the alcohols. Each of these compounds contain a carbonyl group (a carbon atom double bonded to an oxygen atom) as illustrated in Figure 16.

The term "aldehyde" is a contraction of the term "*al*cohol *dehyd*rogenation" indicating that two hydrogen atoms are removed from an end carbon when aldehydes are prepared from primary alcohols. The functional group (-C=O) is always at the end of the carbon chain.
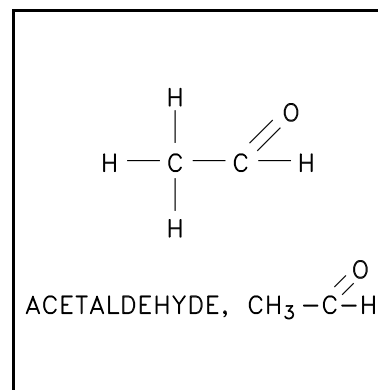
Figure 16 Aldehyde

Basic Chemical Laws

As previously stated, all matter is composed of atoms that which are capable of uniting to form chemical compounds. The various forms of matter can be summarized from a chemical point of view as follows.

1. Molecules are groups or clusters of atoms held together firmly by means of chemical bonding. There are two general types of molecules.

    a. Molecule of an element - Two single atoms of the same element, in certain cases, can become fastened to one another by a chemical bond to form a molecule. Examples of this are hydrogen (H_2), oxygen (O_2), and bromine (Br_2). Most gaseous elements exist as molecules of two atoms.

    b. Molecules of a compound - A compound contains at least two different kinds of atoms. Molecules are the ultimate particles of chemical compounds. Examples of compounds are hydrogen chloride (HCl), water (H_2O), methane (CH_4), and ammonia (NH_3).

2. Elements are substances that cannot be decomposed by ordinary types of chemical change nor made by chemical union.

3. Compounds are substances containing more than one constituent element and having properties different from those of the individual elements. The composition of a specific compound is always definite.

4. Mixtures consist of two or more substances intermingled with no constant percentage composition. Each component retains its original properties.

Forming Chemical Compounds

Chemistry and all other sciences are based on facts established through experimentation. A scientific law is a condensed statement of facts which has been discovered by experiment.

There are three basic laws that apply to chemical reactions. They are the Law of Conservation of Mass, the Law of Definite Proportions, and the Law of Multiple Proportions. These laws are described here to help the reader in understanding the reasons elements and compounds behave as they do.

1.   The Law of Conservation of Mass

        This law states that in a chemical reaction the total mass of the products equals the total mass of the reactants. Antoine Lavoisier, a French chemist, discovered that when tin reacts with air in a closed vessel, the weight of the vessel and its contents is the same after the reaction as it was before. Scientists later discovered that whenever energy (heat, light, radiation) is liberated during a reaction, a very small change in mass does occur, but this change is insignificant in ordinary chemical reactions.

2.   The Law of Definite Proportions

        This law states that no matter how a given chemical compound is prepared, it always contains the same elements in the same proportions by mass. John Dalton, an English physicist, discovered that when various metals are burned or oxidized in air, they always combine in definite proportions by weight.

        For example, one part by weight of oxygen always combines with 1.52 parts by weight of magnesium or 37.1 parts by weight of tin. This law results from the fact that a compound is formed by the combination of a definite number of atoms of one element with a definite number of atoms of another.

3.   The Law of Multiple Proportions

        This law states that if two elements combine to form more than one compound, the masses of one of the elements combining with a fixed mass of the other are in a simple ratio to one another. For example, carbon forms two common compounds with oxygen; carbon monoxide and carbon dioxide. With carbon monoxide (CO), 1.33 grams of oxygen are combined with 1 gram of carbon. With carbon dioxide (CO_2), 2.67 grams of oxygen are combined with 1 gram of carbon. Therefore, the masses of oxygen combining with a fixed mass of carbon are in the ratio 2:1.

Combining Elements

The Laws of Definite Proportions and Multiple Proportions and the related portions of atomic theory form the bases for most quantitative calculations involving chemical reactions. Applying the basic chemical laws to chemical bonding will help the reader to understand the probability and proportions involved in chemical reactions. Regardless of the type of bond (ionic, covalent, coordinate covalent, or metallic), specific amounts of one element will react with specific amounts of the element(s) with which it is combined.

If two substances are placed together in a container, in any ratio, the result is a *mixture*. When a teaspoon of sugar is added to a glass of water, it will slowly dissolve into the water and disappear from view. As a result, the molecules of sugar are evenly distributed throughout the water and become mixed with the water molecules. Because the sugar and water mixture is uniform throughout, it is said to be homogeneous. A homogeneous mixture of two or more substances is called a *solution*. The reason solutions are classified as mixtures rather than as compounds is because the composition is not of fixed proportion.

All solutions consist of a solvent and one or more solutes. The *solvent* is the material that dissolves the other substance(s). It is the dissolving medium. In the water-sugar solution, the water is the solvent. The substances that dissolve in the solution are called *solutes*. In the water-sugar solution, sugar is the solute. It is not always easy to identify which is the solvent and which is the solute (for example, a solution of half water and half alcohol).

Solutions can exist in any of the three states of matter, solid, liquid, or gas. The earth's atmosphere is a gaseous solution of nitrogen, oxygen, and lesser amounts of other gases. Wine (water and alcohol) and beer (water, alcohol, and CO_2) are examples of liquid solutions. Metal alloys are solid solutions (14-karat gold is gold combined with silver or copper).

One factor that determines the degree and/or rate at which a reaction takes place is solubility. *Solubility* is defined as the maximum amount of a substance that can dissolve in a given amount of solvent at a specific temperature. At this point, the solution is said to be saturated. A solution is saturated when equilibrium is established between the solute and the solvent at a particular temperature. *Equilibrium* is the point at which the rates of the forward and reverse reactions are exactly equal for a chemical reaction if the conditions of reaction are constant.

Kinetics is the study of the factors which affect the rates of chemical reactions. There are five principle factors to consider: concentration, temperature, pressure, the nature of the reactants, and the catalyst.

Summary

The important information in this chapter is summarized below.

Chemical Bonding Summary

• The following terms are defined in this chapter:

An ionic bond occurs where one or more electrons are wholly transferred from one element to another, and the elements are held together by the force of attraction due to the opposite polarity of the charge.

The van der Waals forces are attractions between the molecules of nonpolar covalent substances. These forces are generally believed to be caused by a temporary dipole, or unequal charge distribution, as electrons constantly move about in an atom, ion, or molecule.

A covalent bond is a bond in which one or more electrons from an atom pair off with one or more electrons from another atom and form overlapping electron shells in which both atoms share the paired electrons.

Metallic bonds are bonds where the atoms achieve a more stable configuration by sharing the electrons in their outer shell with many other atoms.

A mixture is defined as two substances placed together in a container, in any ratio and the composition is not of fixed proportion.

A solution is a homogeneous mixture of two or more substances.

A solute is defined as the substance that dissolves in a solution.

A solvent is defined as the material that dissolves the other substance(s) in a solution. It is the dissolving medium.

Solubility is defined as the maximum amount of a substance which will dissolve in a given amount of solvent at a specific temperature.

• When the shared pair of electrons which are forming the bond in a molecule are not shared equally, the resulting molecule will have a positive end and a negative end. This type of bond is a polar covalent bond. The molecules are called dipolar or polar molecules.

Chemical Bonding Summary (Cont.)

- In general, the fewer electrons an element must lose, gain, or share to reach a stable shell structure, the more chemically active the element is. The likelihood of elements forming compounds is strongly influenced by the valence shell and on the stability of the resulting molecule. The more stable the molecules are, the more likely these molecules are to form.

- Elements combine in specific ratios, regardless of the type of bond, to form molecules.

- The three basic laws of chemical reactions are discussed:

  (1) The Law of Conservation of Mass - "In a chemical reaction the total mass of the products equal the total mass of the reactants."

  (2) The Law of Definite Proportions - "No matter how a given chemical compound is prepared, it always contains the same elements in the same proportions by mass."

  (3) The Law of Multiple Proportions - "If two elements combine together to form more than one compound, then the masses of one of these elements combining with a fixed mass of the other are in a simple ratio to one another."

CHEMICAL EQUATIONS

This chapter will discuss the method of qualifying solutions. The balancing of the chemical equations will also be explained in this chapter.

EO 2.7   **STATE Le Chatelier's principle.**

EO 2.8   **DEFINE the following terms:**

a.	**ppm**	**c.**	**Density**
b.	**Molarity**	**d.**	**Normality**

EO 2.9   **BALANCE chemical equations that combine elements and/or compounds.**

Le Chatelier's Principle

The effect of temperature on solubility can be explained on the basis of *Le Chatelier's Principle* Le Chatelier's Principle states that if a stress (for example, heat, pressure, concentration of one reactant) is applied to an equilibrium, the system will adjust, if possible, to minimize the effect of the stress. This principle is of value in predicting how much a system will respond to a change in external conditions. Consider the case where the solubility process is endothermic (heat added).

$$\text{solid} + \text{heat} \rightleftharpoons \text{solution}$$

An increase in temperature puts a stress on the equilibrium condition and causes it to shift to the right. The stress is relieved because the dissolving process consumes some of the heat Therefore, the solubility (concentration) increases with an increase in temperature. If the process is exothermic (heat given off).

$$\text{solid} \rightleftharpoons \text{solution} + \text{heat}$$

A temperature rise will decrease the solubility by shifting the equilibrium to the left.

How much solute is dissolved in a solution is very important when the solution is being made for a specific use. To say there is a little, a lot, or a bit would not be very accurate if a specific concentration is required. There are a few common and accurate methods used to express concentration. These are density, molarity, normality, and parts per million.

Density

Density is the measure of the mass per unit volume of a material (density = mass/volume). Density is a characteristic of a substance; mass and volume are not. Mass and volume vary with size but density will remain constant. Temperature will affect the density of a substance and the temperature at which density for that substance was determined is usually reported along with the density value.

Molarity

A useful way to express exact concentrations of solutions is *molarity*. Molarity is defined as moles of solute per liter of solution. Molarity is symbolized by the capital letter M. It can be expressed mathematically as follows.

$$\text{molarity (M)} = \frac{\text{moles of solute (n)}}{\text{liters of solution (V)}}$$

Notice that the moles of solute are divided by the liters of solution not solvent. One liter of one molar solution will consist of one mole of solute plus enough solvent to make a final volume of one liter.

Example 1:

Prepare one molar solution of NaCl.

Solution:

a)   Calculate the molecular weight of the salt

1 atom of Na   = 22.989 amu
1 atom of Cl   = 35.453 amu
1 molecule of NaCl   = 58.442 amu

One mole is equal to the gram molecular weight, so one mole = 58.442 grams.

b)   58.442 grams of NaCl is weighed out and sufficient water is added to bring the solution to one liter.

Example 2:

     Prepare 3 liters of a 2M NaOH solution.

Solution:

     Calculate the amount of NaOH required to prepare the solution.

a) $\text{molarity (M)} = \dfrac{\text{moles of solute}}{\text{volume of solution } (\ell)}$

$$2M = \dfrac{X \text{ moles of solute}}{3 \text{ liters}}$$

b)   substituting: $(3 \text{ liters}) (2M) = 6 \text{ moles NaOH}$

$$\dfrac{40 \text{ grams NaOH}}{1 \text{ mole NaOH}} \times 6 \text{ moles NaOH} = 240 \text{ grams NaOH}$$
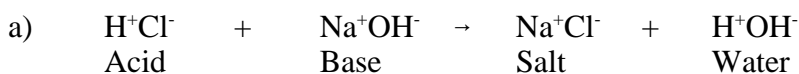
     Therefore, to prepare 3 liters of a 2M NaOH solution, 240 grams of NaOH must be weighed out and dissolved in water to make a volume of exactly 3 liters.

Normality

The normal concentration is another method for expressing the concentration of solutions. *Normality* (N) is defined as the number of equivalents of solute dissolved in one liter of solution.

$$\text{Normality (N)} = \dfrac{\text{equivalents of solute}}{\text{liter of solution}}$$

One equivalent of acid is the amount of acid necessary to give up one mole of hydrogen ions in a chemical reaction. One equivalent of base is the amount of base that reacts with one mole of hydrogen ions. When expressing the concentrations of bases, normality refers to the number of available hydroxyl ions. Because hydrogen and hydroxyl ions combine on a one-to-one basis, one OH^- is equivalent to one H^+ ion.

a) H^+Cl^- + Na^+OH^- → Na^+Cl^- + H^+OH^-
       Acid   Base   Salt   Water

b) H_2SO_4 + $2K^+OH^-$ → K_2SO_4 + $2H^+OH^-$
       Acid   Base   Salt   Water

Notice that in reaction a), one mole of HCl yields one equivalent per mole or one mole of H^+ ions. H_2SO_4 has two equivalents per mole or two H^+ ions because each mole of the compound can release two moles of hydrogen ions.

The number of equivalents of an acid or base can be determined from equivalent weight. The *equivalent weight* is defined as the molecular weight of the acid or base divided by the number of replaceable hydrogen or hydroxyl ions.

Example:

The equivalent weight of H_2SO_4 is:

$$\frac{98.0734 \text{ grams (molecular wt.)}}{2 \text{ } H^+ \text{ ions}} = 49 \text{ grams/equivalent}.$$

This means 49 grams of H_2SO_4 is equal to one equivalent of H_2SO_4. If there is a one liter solution that contains 78.32 grams H_2SO_4, the number of equivalents is:

$$\frac{78.32 \text{ grams } H_2SO_4}{1} \times \frac{1 \text{ equivalent}}{49 \text{ grams } H_2SO_4} = 1.6 \text{ equivalents}.$$

Since normality is equal to the number of equivalents per liter, the normality of this solution is 1.6 equivalents/liter, or 1.6 N.

Parts per Million

Another term used to describe the specific concentration of a solution is parts per million or ppm. The term *ppm* is defined as the concentration of a solution in units of one part of solute to one million parts solvent. One ppm equals one milligram of solute per liter of solution. Another term, parts per billion (ppb), is defined as one part solute per one billion parts solvent. One ppb is equal to one microgram solute per liter of solution. These two terms are usually used for very dilute solutions.
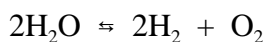
<u>Chemical Equations</u>

The chemical equation is simply a representation of a chemical reaction in the chemist's shorthand. In a chemical equation, the substances originally present are called the reactants and the new substances being formed are called the products. In the chemical reaction, the reactants are on the left of the arrow and the products are on the right of the arrow. For example, when looking at the combination of hydrogen and oxygen into water, the water molecule would be the product on the right.

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

If looking at the decomposition of water, the hydrogen and oxygen would be the products and the water is the reactant. The arrow means yields and is used to separate the reactants from the products. It also indicates the direction of the reaction as illustrated below.

$$2H_2O \rightarrow 2H_2 + O_2$$
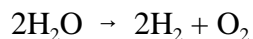
The single arrow in the above equation implies that the reaction will proceed in only one direction until it subsides or stops. If the reaction is reversible, that is, it can proceed left to right and right to left until it reaches an equilibrium, then a double arrow is used.

$$2H_2O \rightleftharpoons 2H_2 + O_2$$

When writing an equation, always place the reactant on the left and the products on the right even in the case of a reversible reaction.

A chemical equation represents not only the reaction, but also shows the number of atoms or molecules entering into and produced by the reaction. The formulas must be balanced correctly based on the valences of the constituent elements.

<u>Balancing Chemical Equations</u>

The number of atoms or molecules of each substance is shown by the coefficients in the equation. Because atoms cannot be created or destroyed in a chemical reaction, a chemical equation must be balanced so that there are exactly the same number of atoms of each element on each side of the equation.

Example:

   Explain the following chemical equation.

$$2Fe \;+\; 3H_2O \;\rightarrow\; Fe_2O_3 \;+\; 3H_2\uparrow$$
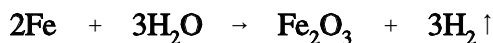
Solution:

   This chemical equation shows that iron reacts with water to form ferric oxide and hydrogen gas (the vertical arrow ↑ indicates a gas). This chemical equation also shows that for every two atoms of iron that react, three molecules of water are used to form one molecule of ferric oxide and three molecules of hydrogen gas. This is a balanced chemical equation. There are two iron atoms on each side of the equation; there are six hydrogen atoms on each side; and there are three oxygen atoms on each side.

There are no fixed rules for balancing chemical equations. Learning how is a matter of practice. The balancing of most equations can be accomplished by following the guidelines explained below.

Guidelines:

   a.   Once the correct chemical formula for a compound is written in an equation, do not modify it.

   b.   Select the compound with the greatest number of atoms. Then begin by balancing the element in that compound with the most atoms. There must be the same number of atoms of an element on each side of the equation. As a rule of thumb, this first element should not be hydrogen, oxygen, or a polyatomic ion.

   c.   Balance the atoms of each element in the compound by placing the appropriate coefficient in front of the chemical symbol or formula.

   d.   Next, balance the polyatomic ions. In some cases, the coefficient assigned in guideline 2 may have to be changed to balance the polyatomic ion.

   e.   Balance the hydrogen atoms next, then the oxygen atoms. If these elements appear in the polyatomic ion it should not be necessary to balance them again.

   f.   All coefficients will be whole numbers. The coefficients should be reduced to the lowest possible ratios.

   g.   As simple as it sounds, check off each element as it is accounted for since this will prevent double inclusion or a missed atom.

Example 1:
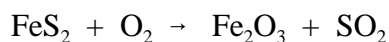
$$FeS_2 + O_2 \rightarrow Fe_2O_3 + SO_2$$

Solution 1:

Starting with Fe_2O_3 (see guideline b), write $2FeS_2 + O_2 \rightarrow Fe_2O_3 + SO_2$, which balances the Fe on each side of the equation.

Now there are 4 S atoms on the left side so balance the S atoms by writing $2FeS_2 + O_2 \rightarrow Fe_2O_3 + 4SO_2$.

Everything is balanced except the O. There are now 2 O atoms on the left and 11 O atoms on the right. To get 11 O atoms on the left write $2FeS_2 + 5.5O_2 \rightarrow Fe_2O_3 + 4SO_2$.

This makes both sides of the equation balanced except the coefficients must be whole numbers (guideline f). To meet guideline f, multiply both sides by two which will bring the left side to a whole number of O_2 molecules.

Thus, the solution is $4FeS_2 + 11O_2 \rightarrow 2Fe_2O_3 + 8SO_2$.

Example 2:
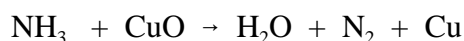
$$NH_3 + CuO \rightarrow H_2O + N_2 + Cu$$

Solution 2:

Start with NH_3 since there are two N atoms on the right of the equation. To balance the N atoms write $2NH_3 + CuO \rightarrow H_2O + N_2 + Cu$ (guideline b).

Since the H appears in only the NH_3 and H_2O and the NH_3 has been balanced, the H_2O will be balanced. Write $2NH_3 + CuO \rightarrow 3H_2O + N_2 + Cu$ (guideline e).

Oxygen appears only in CuO and in H_2O, and since the H_2O has been already been balanced write $2NH_3 + 3CuO \rightarrow 3H_2O + N_2 + Cu$ (guideline e).

That leaves the Cu to be balanced. Thus, the solution is $2NH_3 + 3CuO \rightarrow 3H_2O + N_2 + 3Cu$.

Example 3:

$$Na_2CO_3 + Ca(OH)_2 \rightarrow NaOH + CaCO_3$$
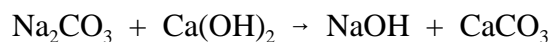
Solution 3:

There are two Na atoms on the left so start with the Na by writing
$Na_2CO_3 + Ca(OH)_2 \rightarrow 2NaOH + CaCO_3$ (guideline b).

By adding the 2, the equation is now completely balanced. This equation illustrates that not all equations are that hard to balance.

Most chemical equations do not indicate a number of important facts about the chemical reactions they represent. Chemical equations do not necessarily describe the path by which the substances reacting are converted to products.

$$2H_2 + O_2 \rightarrow 2H_2O$$
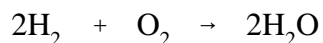
The equation would seem to imply that two molecules of hydrogen collide with one molecule of oxygen, and two molecules of water are produced. The actual mechanism by which this reaction takes place is much more complicated and involves a series of processes. Chemical equations do not indicate the rate at which the reaction proceeds, or even whether the reaction will occur in a finite time. In many cases, reactions will occur only under a particular set of circumstances and then only at a definite rate. Chemical equations do not show whether the reaction proceeds to completion or, if incomplete, the extent of reaction. In most cases, the substances that react never completely disappear; however, their concentration may be exceedingly small. Reactions that do not go to completion are usually represented in chemical equations by using double horizontal arrows ⇋. In general, a reaction will go to completion only if one or more of the products is removed from the field of the reaction. This is often accomplished if one of the products is a gas or is insoluble in the reaction mixture.

In the discussion of chemical equations, emphasis is normally placed on the number of atoms or molecules involved in the reaction. However, chemical equations are very effective in representing chemical reactions on a macroscopic scale. Practical chemical calculations involve very large numbers of atoms and molecules.

The equation weight in grams of a compound or element is defined as the gram molecular weight times the number of molecules of the compound, as shown by the coefficients of the chemical equation for the reaction. The sums of the equation weights on each side of a chemical equation must be equal. Chemical calculations are based on the fact that every fraction or multiple of the equation weights of substances that react gives a corresponding fraction or multiple of the equation weights of the products of the reaction. In other words, if 30 grams of a substance that has an equation weight of 15 grams reacts with some amount of another substance to form a product with an equation weight of 20 grams, then 40 grams of that product will be formed.

Example:

> How many grams of ferric oxide will be formed if 27.9 grams of iron reacts with water according to the following equation.

$$2Fe \quad + \quad 3H_2O \quad \rightarrow \quad Fe_2O_3 \quad + \quad 3H_2 \uparrow$$
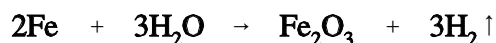
Solution:

> The equation weight of iron equals the gram atomic weight of iron times the number of atoms shown reacting in the equation, which is two. Using Table 2:

$$\text{Equation Weight Fe} \quad = \quad 2 \times 55.8 \text{ grams}$$
$$= \quad 111.6 \text{ grams}$$

Because 27.9 g of iron react, the fraction of the equation weight that reacts is:

$$\frac{27.9 \text{ grams}}{111.6 \text{ grams}} \quad = \quad \frac{1}{4}.$$

Thus, 1/4 of the equation weight of ferric oxide will be formed.

The equation weight of ferric oxide equals the gram molecular weight of ferric oxide times the number of molecules shown formed in the equation, which is one. Using Table 2:

$$\text{Equation Weight Fe}_2O_3 \quad = \quad 2(55.8 \text{ g}) \quad + \quad 3(16.0 \text{ g})$$
$$= \quad 111.6 \text{ g} \quad + \quad 48.0 \text{ g}$$
$$= \quad 159.6 \text{ g}$$

Thus, the amount of ferric oxide formed is:

$$\frac{1}{4} (159.6 \text{ g}) \quad = \quad 39.9 \text{ g}.$$

Summary

The important information from this chapter is summarized below.

Chemical Equations Summary

•   Le Chatelier's principle states that if a stress is applied to an equilibrium, the system will adjust to minimize the effect of the stress.

•   The following terms are defined:

> Density is the measure of the mass per unit volume of a material (density = mass/volume).

> Molarity is moles of solute per liter of solution. Molar solutions are symbolized by the capital letter M.

> Normality, (N), is defined as the number of equivalents of solute dissolved in one liter of solution.

> ppm expresses the concentration of a solution in units of one part of solute to one million parts solvent. One ppm equals one milligram of solute per liter of solution.

•   To balance chemical equations, the number of elemental constituents must be the same on each side of the equation.

ACIDS, BASES, SALTS, AND pH

Different substances respond differently in solution. How substances behave in water is of special interest to the power industry. The interactions of water and acids, bases, or salts are of special interest because water is used in many industries. This chapter will introduce the student to the general behavior of these substances.

EO 3.1	**DEFINE the following terms:**

        a.   **Acid**   e.   **Base**
        b.   **Salt**   f.   **pH**
        c.   **pOH**   g.   **Dissociation constant of water**
        d.   **Alkalies**

EO 3.2   **STATE the formula for pH.**

EO 3.3   **STATE the formula for pOH.**

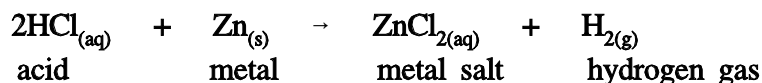**EO 3.4**   **CALCULATE the pH of a specified solution.**

Acids

Substances that form ions when they are dissolved in water are called electrolytes. The three types of electrolytes are acids, bases, and salts.

Acids are substances that dissociate in water to produce hydrogen (H^+). An example of a common acid is sulfuric acid, H_2SO_4. In solution, H_2SO_4 dissociates to form hydrogen and sulfate ions according to the following equation. The designation in parenthesis in the following formulas indicate the state of the reactants and the products, i.e., liquid (aq). solid (s), or gas (g).

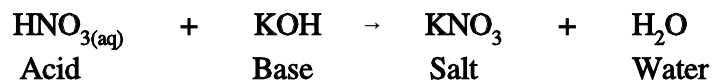$$H_2SO_{4(aq)} \rightarrow 2H^+ + SO_4^{--}$$
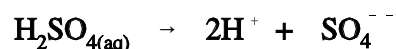
Additional examples of acids are vinegar, aspirin, and lemon juice. These substances share the following common properties.

1.   Acid solutions taste sour (acid means "sour" in Latin).

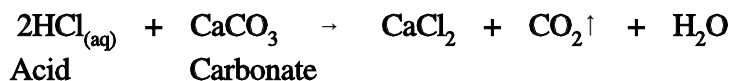2.   Acids react with many metals to form hydrogen gas.

$$2HCl_{(aq)} + Zn_{(s)} \rightarrow ZnCl_{2(aq)} + H_{2(g)}$$
$$\text{acid} \qquad \text{metal} \qquad \text{metal salt} \qquad \text{hydrogen gas}$$

3.   Acids turn litmus paper red.

4.   Acid solutions conduct electricity.

5.   Acids react with bases to form a salt and water.

Example:

$$HNO_{3(aq)} \quad + \quad KOH \quad \rightarrow \quad KNO_3 \quad + \quad H_2O$$
$$\text{Acid} \qquad\qquad \text{Base} \qquad \text{Salt} \qquad\qquad \text{Water}$$

6.   Acids react with carbonates to form CO_2 (carbon dioxide gas).

Example:

$$2HCl_{(aq)} \quad + \quad CaCO_3 \quad \rightarrow \quad CaCl_2 \quad + \quad CO_2\uparrow \quad + \quad H_2O$$
$$\text{Acid} \qquad\qquad \text{Carbonate}$$

Bases
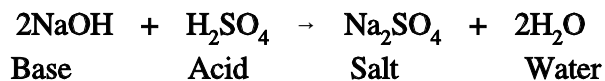
Bases are substances that produce hydroxide ions (OH^-) in water solutions. An example of a common base is sodium hydroxide, NaOH. In solution, it dissociates to form sodium ions and hydroxide ions according to the following equation:

$$NaOH_{(aq)} \quad \rightarrow \quad Na^+{}_{(aq)} \quad + \quad OH^-{}_{(aq)}.$$
$$\text{Base}$$
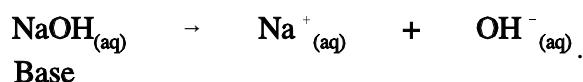
Common types of bases are lye, household ammonia, and most soaps. The following are four characteristic properties of bases.

1.   Basic solutions taste bitter and feel slippery to the touch.

2.   Bases turn litmus paper blue.

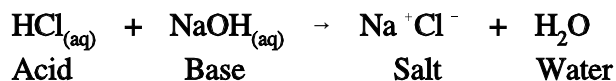3.   Basic solutions conduct electricity.

4.   Bases neutralize acids.

Example:

$$2NaOH \quad + \quad H_2SO_4 \quad \rightarrow \quad Na_2SO_4 \quad + \quad 2H_2O$$
$$\text{Base} \qquad\qquad \text{Acid} \qquad\qquad \text{Salt} \qquad\qquad \text{Water}$$

Salts

When an acid reacts with a base, two products are formed; water and a salt. A *salt* is an ionic compound composed of positive ions and negative ions. The ionic bond is what keeps salts in their molecular form. Some compounds look like salts, but are actually covalent compounds (have a covalent bond).

Example:

$$HCl_{(aq)} \quad + \quad NaOH_{(aq)} \quad \rightarrow \quad Na^+Cl^- \quad + \quad H_2O$$
$$\text{Acid} \qquad\qquad \text{Base} \qquad\qquad\quad \text{Salt} \qquad\quad \text{Water}$$

This type of acid-base reaction is called neutralization.

Certain soluble salts (principally sodium, potassium, magnesium, and calcium) that have the property of combining with acids to form neutral salts are called *alkalies*. Two of the common salts are sodium chloride (table salt) and calcium chloride (salt put on the road in winter). Unlike acids and bases, salts vary greatly in all their properties except their ionic characteristics. Salts may taste salty, sour, bitter, astringent, sweet, or tasteless. Solutions of salts may be acidic, basic, or neutral to acid-base indicators. Fused salts and aqueous solutions of salts conduct an electric current. The reactions of salts are numerous and varied.

pH

Many compounds dissolve in water and alter the hydrogen ion concentration. Compounds that produce hydrogen ions directly when dissolved in water are called acids, and those that produce hydroxyl ions directly when dissolved in water are called bases. To treat these aspects of chemistry more precisely, a quantitative system of expressing acidity or basicity (alkalinity) is needed. This need could be met by using the value of $[H^+]$, where $[H^+]$ is expressed in moles/liter, as a measure of acidity. But, in most cases $[H^+]$ is in the range of 10^1 to 10^{-14} moles/liter. Because numbers of this magnitude are inconvenient to work with, an alternate system for expressing the acidity of dilute solutions has been devised. This system is based on a quantity called *pH*. ph is defined as the negative logarithm of the hydrogen concentration, represented as $[H^+]$ in moles/liter.

$$pH \quad = \quad -\log [H^+] \tag{1-1}$$

$$[H^+] \quad = \quad 10^{-pH} \tag{1-2}$$

The negative logarithm is specified because the logarithm of any number less than 1 is negative; thus multiplication by -1 causes the values of pH to be positive over the range in which we are interested. (The term pH was first defined by a Danish chemist and is derived from p for the Danish word potenz (power) and H for hydrogen.)

Example 1:   The hydrogen concentration, $[H^+]$, of a solution is 4.8×10^{-8} moles/liter. What is the pH of the solution?

Solution 1:

$$pH = -\log\ [H^+]$$

$$= -\log\ (4.8 \times 10^{-8})$$

$$= 7.32$$

Example 2:   The pH of a solution is 3.83. What is the hydrogen concentration of the solution?

Solution 2:

$$[H^+] = 10^{-pH}$$

$$= 10^{-3.83}\ \text{moles/liter}$$

$$= 1.48 \times 10^{-4}\ \text{moles/liter}$$

pOH

It is also important to understand the relationship between the $[H^+]$ and the $[OH^-]$ concentrations. The *pOH* of a solution is defined as the negative logarithm of the hydroxyl concentration, represented as $[OH^-]$ in moles/liter.

$$pOH = -\log [OH^-] \tag{1-3}$$

$$[OH^-] = 10^{-pOH} \tag{1-4}$$

For water solutions, the product of the hydrogen ion concentration and the hydroxyl concentration is always 1×10^{-14} at 25°C. This means that the sum of pH and pOH is equal to 14 under these conditions.

$$[H^+] \times [OH^-] = 1 \times 10^{-14}$$

$$pH + pOH = 14$$

The following example illustrates this point.

Example: What is the hydrogen ion concentration [H⁺] and the hydroxyl concentration [OH⁻] in a solution with a pH of 5.5?

Solution:

$$[H^+] = 10^{-pH}$$

$$= 10^{-5.5}$$

$$= (10^{-6})(10^{.5})$$

$$= 3.16 \times 10^{-6} \text{ moles/liter}$$

since $pOH + pH = 14$

$$pOH = 14 - 5.5$$

$$pOH = 8.5$$

and $[OH^-] = 10^{-pOH}$

$$= 10^{-8.5}$$

$$= (10^{-9})(10^{.5})$$

$$= 3.16 \times 10^{-9} \text{ moles/liter}$$

Dissociation Constant

The product of ionic concentrations, $K_w = [H^+][OH^-]$, is called the Ion Product Constant for water, or more frequently, the Ionization Constant or *Dissociation Constant*. At 25°C, K_w equals 1 x 10⁻¹⁴. K_w varies with temperature and, at 37°C (body temperature), the value is about 3.4 x 10⁻¹⁴. Figure 17 illustrates the relationship of the Dissociation Constant with water temperature. As indicated earlier, a change in temperature causes a change in equilibrium in a chemical reaction. Because the ionization of water is an equilibrium process, it is also affected by temperature. The Dissociation (or Ionization) Constant, K_w, for water increases with increasing temperature up to about 500°F and then decreases. Experimental values of K_w at various temperatures are listed in Table 5 and graphed in Figure 16. Notice in Table 5 that the pH of pure water changes with temperature. For pure water at any temperature, however, $[H^+] = [OH^-]$. It should be noted that the equation pH + pOH = 14 is true only at or near 25°C (77°F).

Example: The hydroxyl concentration [OH⁻] of a water solution$^\circ$ at 25 C is 7.2×10^{-9} moles/liter. Calculate the pH of the solution.

Solution:

$$K_w = [H^+] \ [OH^-]$$

$$[H^+] = \frac{K_w}{[OH^-]}$$

$$pH = -\log \ [H^+]$$

$$= -\log \ (1.38 \times 10^{-6})$$

$$= \frac{1 \times 10^{-14}}{7.2 \times 10^{-9}}$$

$$= 5.86$$

$$= 1.38 \times 10^{-6}$$

TABLE 5			
Ion Product Constant and Neutral pH			
for Water at Various Temperatures			
Temperature		Ion Product Constant for Water	pH of Pure Water
F	C		
64.4	18	0.64×10^{-14}	7.10
77	25	1.0×10^{-14}	7.00
140	60	8.9×10^{-14}	6.54
212	100	6.1×10^{-13}	6.10
302	150	2.2×10^{-12}	5.83
392	200	5.0×10^{-12}	5.65
482	250	6.6×10^{-12}	5.59
572	300	6.4×10^{-12}	5.60
662	350	4.7×10^{-12}	5.66

At 25°C, an equilibrium exists between pure molecular water and its ions. The [H⁺] equals the [OH⁻] and both have values of 1×10^7 moles/liter. Using the pH definition, it follows that the pH of pure water at 25°C is 7. pH values less than 7 indicate an acidic solution and values greater than 7 indicate a basic or alkaline solution.
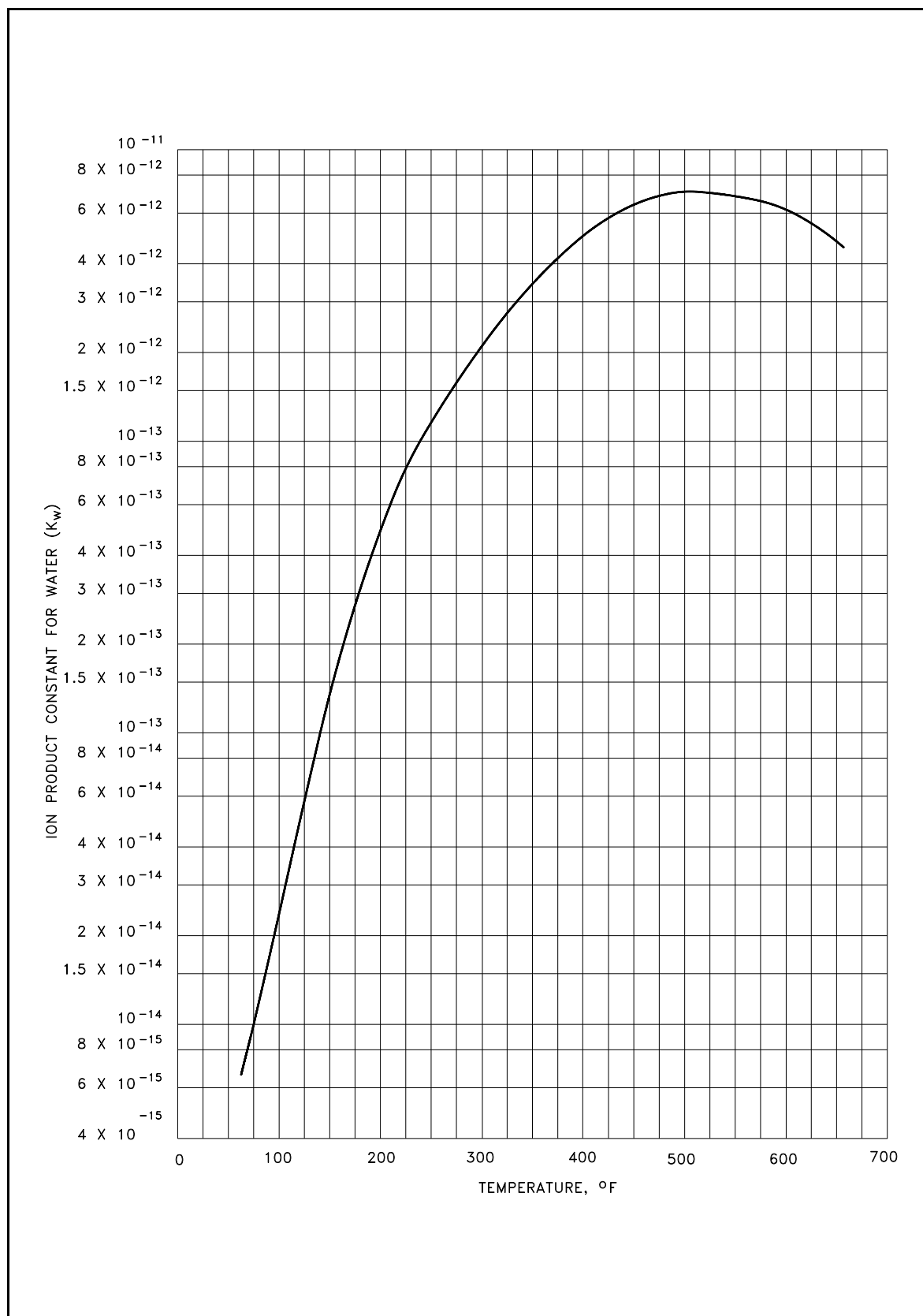
Figure 17   Ion Product Constant for Water

Summary

The important information in this chapter is summarized below.

Acids, Bases, Salts, and pH Summary

- The following terms are defined in this chapter:

    Acid - substances that produce hydrogen (H^+) in water solutions

    Base - substances that produce hydroxide ions (OH^-) in water solutions

    Salt - a compound composed of positive and negative ions held together with an ionic bond

    Alkalies - certain soluble salts, principally sodium, potassium, magnesium and calcium, that have the property of combining with acids to form neutral salts

    pH - the negative logarithm of the hydrogen concentration [H^+] in moles/liter

    pOH - the negative logarithm of the hydroxyl concentration [OH^-] in moles/liter

    Dissociation constant of water (K_w) - the product of ionic concentrations, ([H^+] [OH^-]); at 25°C $K_w = 1 \times 10^{-14}$

- The formula for pH is: $pH = -\log [H^+]$
  Therefore, $[H^+] = 10^{-pH}$

- The formula for pOH is: $pOH = -\log [OH^-]$
  Therefore, $[OH] = 10^{-pOH}$