General chemistry

Chapter 1

Introduction

References for general chemistry course

- Chang, R. (1986). General chemistry. Fifth edition.
- Mortimer, Ch. Chemistry. Sixth edition.

Definition of chemistry

- It is the study of composition, structure, properties of the matter and the changes it undergoes.
  - *Composition:* What is it made of?
  - *Structure:* How is it put together?
  - *Properties:* What characteristics does it have? (physical and chemical properties).
  - *Reactions:* How does it behave with other substances?

Matter

- **Definition:**

Matter is anything that occupies space and has a mass.

- **States of matter:**

Matter can exist in three states: solid, liquid, and gas. The three states of matter can be interconverted without changing the composition of the substance.

States of matter

Classification of matter

Substances

- **A substance:** is matter that has a definite or constant composition and distinct properties.
  - Examples are oxygen, water, table salt (sodium chloride) and carbon dioxide.
  - Substances differ from one another in composition and can be identified by their appearance, smell, taste, and other properties.
  - ***A substance can be either an element or a compound.***

Elements

- **An element:** is a substance that cannot be separated into simpler substances by chemical means (one type of atoms).
  - Examples: oxygen, hydrogen, nitrogen and chlorine.

Compounds

- **A compound:** is a substance composed of two or more elements chemically united in fixed proportions. Compounds can be separated only by chemical means into their pure components.
- Examples: Hydrogen gas burns in oxygen gas to form water, a compound whose properties are distinctly different from those of the starting materials. Water is made up of two parts of hydrogen and one part of oxygen. This composition does not change, regardless of the source of water.

Mixtures

- **A mixture:** is a combination of two or more substances in which the substances retain their distinct identities. Mixtures do not have constant composition. They can be separated by physical means into their components.
- They are either ***homogeneous or heterogeneous***.

Homogeneous mixtures

- In homogeneous mixtures: all portions of a material are in the same state, have no visible boundaries, and are uniform throughout.
- Homogeneous mixtures are also called solutions. Although most solutions we encounter are liquid, solutions can also be solid or gas.

- **Examples:**
  - A solution of salt and water.
  - Air is a solution of nitrogen, oxygen, water vapor, carbon dioxide, and several other gases.
  - Tap water is a solution of small amounts of several substances in water.
  - Alloys are solid solutions of two or more metals such as he gray substance still used by some dentists to fill tooth.

Heterogeneous mixtures

- If the composition of a material is not completely uniform, then it is heterogeneous.
- The components of heterogeneous mixtures can usually be separated by simple means.
- **Examples**:
  - A mixture of water with sand.
  - A mixture of oil and water.
  - Mixtures that appear to be homogeneous are often found to be heterogeneous after microscopic examination. Milk, for example, appears to be homogeneous, but when examined under a microscope, it clearly consists of tiny globules of fat and protein dispersed in water.

Mixtures

Classification of matter (summary)

(a) Atoms of an element (b) Molecules of an element (c) Molecules of a compound (d) Mixture of elements and a compound

Physical and chemical properties

- A **physical property** can be measured and observed without changing the composition or identity of a substance.
- Ex.: melting point, freezing points, mass……etc.
- **A chemical property** a chemical change in which the original substances will have vanished and a chemically different substance will have taken their place.
- Possible indicators of chemical change include a change in color, odor, temperature, and the formation of a gas or solid from a liquid.
- Ex.: Hydrogen gas burns in oxygen gas to form water.

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Chapter 2
Atoms, Molecules, Ions and chemical formulas

Atoms

Definition

It is the basic unit of an element that can enter into chemical combination.

Structure

- An atom consists of a very dense central nucleus made up of **protons and neutrons.** Around the nucleus **electrons** move and shown as clouds.
- Protons are positively charged, neutrons have no charge, and electrons are negatively charged.

Atomic symbol

- **X** denotes the symbol of the element.
- **Z** denotes the number of protons in the nucleus is called the **atomic number**.
- In a neutral atom: The number of protons = the number of electrons.
- **(A) denotes** the **mass number** which is:

$$\underset{(A)}{\text{mass number}} = \underset{(Z)}{\text{number of protons}} + \text{number of neutrons}$$
$$= \text{atomic number} + \text{number of neutrons}$$

Molecules

- A **molecule** is an aggregate of at least two atoms held together by chemical forces or bonds.
- **Examples**:
  - ***Molecules of the same element:*** nitrogen (N_2), oxygen (O_2), iodine (I_2) and ozone (O_3).
  - ***Molecules contain atoms of different elements (compounds):*** hydrogen chloride (HCl), carbon monoxide (CO), water (H_2O) and ammonia (NH_3).

Ions

- An **ion** is an atom or a group of atoms that has a net positive or negative charge as electrons may be lost or gained.
- The loss of electrons results in a ***cation,*** *an ion with a net positive charge.*

  Examples: Na^+, Mg^{2+}, Fe^{3+}, NH_4^+ (ammonium ion).
- Gain of electrons results in an ***anion***, *an ion whose net charge is negative*

  Examples: Cl^-, S^{2-}, N^{3-}, OH^- (hydroxide ion), CN^- (cyanide ion).

The charge of an ion

- Charge of ion = number of protons - number of electrons
- So, number of electrons = number of protons - charge of ion
- **Problems:**

1- How many electrons are there in $_{13}Al^{+3}$?

$_{13}Al^{+3}$ have 13 proton .

number of electrons = number of protons - charge of ion

$= 13 - (+3) = 10$

2- How many electrons are there in $_{16}S^{-2}$?

$_{16}S^{-2}$ have 16 proton .

number of electrons = number of protons - charge of ion

$= 16 - (-2) = 18$

3- What is the atomic symbol of F that contain 9 protons and 10 neutrons and 10 electrons?

Z = 9, A= 9+10= 19

Charge of ion = number of protons - number of electrons

= 9 – 10= -1

So, atomic symbol is ($^{19}_{9}\mathbf{F}^{-}$), so it is anion.

4- What is the atomic symbol of Fe that contain 26 protons and 30 neutrons and 24 electrons?

Z = 26, A= 26+30= 56

Charge of ion = number of protons - number of electrons

= 26 – 24= +2

So, atomic symbol is ($^{56}_{26}\mathbf{Fe}^{+2}$), so it is cation.

Isotopes

- **Isotopes** are atoms of the same element that have the same number of protons but different numbers of neutrons.

- **Give the number of protons, neutrons, and electrons in each of the following species:**

(a) $^{199}_{80}Hg$ (b) $^{200}_{80}Hg$.

- **Solution**

(a) There are 80 protons. The number of neutrons is 199 - 80 = 119. The number of electrons is 80.

(b) The number of protons is 80. The number of neutrons is 200 – 80 = 120. The number of electrons is 80.

The species in (a) and (b) are chemically similar isotopes of mercury.

Chemical Formulas

- **Chemical formula:** formula that represent the composition of molecules in terms of chemical symbols and ratio.
- **Three types of chemical formulas:** molecular, empirical and structural formulas.

  1- Molecular Formula: shows the exact number of atoms in each element in a molecule.

  2- Empirical formula: shows the simplest whole-number ratio of atoms, but not necessarily the actual number of atoms.

  3- Structural formula: shows how atoms are bonded to one another in a molecule.

Chemical Formulas

- For many molecules, the molecular formula and empirical formula are one and the same.

	Hydrogen	Water	Ammonia	Methane
Molecular formula = empirical formula	H_2	H_2O	NH_3	CH_4
Structural formula	H–H	H–O–H	H–N–H | H	H | H–C–H | H

Chemical Formulas

For other molecules, the molecular formula and empirical formula are not the same.

	Hydrogen peroxide	Hydrazine	Acetylene	Glucose
Molecular formula	H_2O_2	N_2H_4	C_2H_2	$C_6H_{12}O_6$
Empirical formula	HO	NH_2	CH	CH_2O
Structural formula				

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Chapter 3

Stoichiometry

Definition of Stoichiometry

- Studying the quantitative relationships of atoms and molecules. These relationships in turn will help us to explain the composition of compounds and the ways in which composition changes.

Atomic weight

- The atomic weight or atomic mass is the weight of one atom of the element, and is expressed in the unit u= amu = atomic mass unit = Dalton (Da)
- Atomic weights of the elements is written in the periodic table in the subscript.
- ***Numerically,*** Atomic weight ≈ Mass number.

Molecular weight

- The **molecular weight** (called molecular mass) is the sum of the atomic weights (in amu) in the molecule.
- It is calculated weight.
- For example,

Molecular mass of H_2O = 2*(atomic mass of H) + atomic mass of O

= 2*(1.008 amu) + 16.00 amu = 18.02 amu

Molecular mass of H_2 = 2*(atomic mass of H)

= 2*(1.008 amu)

= 2 amu

Mole

- In any real situation, we deal with macroscopic samples containing enormous numbers of atoms. Therefore, it is convenient to have a special unit to describe a very large number of atoms. This special unit is the mole.
- The **mole (mol)** is the amount of a substance that contains **Avogadro's number (N_A)** of particles.

$$N_A = 6.0221415 \times 10^{23}$$

Mole

- 1 mole of hydrogen atoms contains 6.022×10^{23} H atoms.
- 1 mole of hydrogen molecules contains 6.022×10^{23} H molecules.
- 1 mole of water molecules contains 6.022×10^{23} water molecules.
- As the mole of substances have the same number of particles, they differ in their molar mass.

Molar mass

- It is the mass (in grams or kilograms) of 1 mole of units (such as atoms or molecules) of a substance.
- ***<u>Notes:</u>***

  A- For an element (found as atoms): the molar mass (in grams) is ***numerically*** equal to its atomic weight in amu.
- **Examples:**

1. The atomic mass of sodium (Na) is 22.99 amu and its molar mass is 22.99 g
2. The atomic mass of phosphorus is 30.97 amu and its molar mass is 30.97 g; and so on.

Molar mass

- ***Notes:***

  B- For an element (found as a molecule) or for a compound: The molar mass (in grams) is ***numerically*** equal to its molecular weight in amu.

- **Examples:**

Molecular mass of H_2O = 2*(atomic mass of H) + atomic mass of O

= 2*(1.008 amu) + 16.00 amu = 18.02 amu

Similarly,

Molar mass of H_2O =2*(molar mass of H atoms)+ molar mass of O atoms

= 2*(1.008 g) + 16.00 g = 18.02 g

Relationship between mass and no. of moles of a substance

- A knowledge of the molar mass enables us to calculate the numbers of moles or the mass of a given quantity of a substance.
- Mass of substance (m) =No. of moles (n) X Molar mass (M)
- No. of moles= mass of substance/ Molar mass

m= mass

n= # of moles

M= molar mass

Examples

- **Zinc (Zn) is a silvery metal. How many moles of Zn are there in 23.3 g of Zn?**

From periodic table, Molar mass (M)= 65.39 g

No. of moles (n) = mass of substance (m)/Molar mass (M)

$$(n) = 23.3 / 65.39 = 0.356 \text{ mol}$$

- **Calculate the number of grams of lead (Pb) in 12.4 moles of lead?**

Mass of substance (m) =No. of moles (n) X Molar mass (M)

$$(m) = 12.4 \times 207 = 2567 \text{ g}$$

Examples

- **How many moles of CH_4 are present in 6.07 g of CH_4?**

Molar Mass of CH_4= 1*12 + 4*1= 16 g

No. of moles (n) = mass of substance (m)/Molar mass (M)

n= 6.07/16= 0.378 mol

- **Calculate the mass of chloroform ($CHCl_3$) in 1.66 moles of Chloroform?**

Molar Mass of $CHCl_3$ = 1*12 +1*1+ 3*35 = 118 g

Mass of substance (m) =No. of moles (n) X Molar mass (M)

= 1.66 * 118 = 196 g

Elemental analysis
and
Percent composition of compounds

A- Determination of Percent composition from molecular formula

- In case that the molecular formula of the compound is known, the percent composition is used to verify the purity of a compound for use in a laboratory experiment.
- This is done by comparing the result of the percent composition obtained experimentally for a sample (elemental analysis), with the percent composition calculated from the formula of the sample.

Percent composition

- The **percent composition** is the percent by mass of each element in a compound.
- If the molecular formula is known, percent composition can be calculated from the following equation:

$$\text{percent composition of an element} = \frac{\text{Mass of element in one mole of the compound}}{\text{molar mass of compound}} \times 100\%$$

- As m=n * M, and n represent the no. of moles of the element in one mole of the compound so:

$$\text{percent composition of an element} = \frac{n \times \text{molar mass of element}}{\text{molar mass of compound}} \times 100\%$$

Problem

Phosphoric acid (H_3PO_4).Calculate the percent composition by mass of H, P, and O in this compound?

molar mass of H_3PO_4 is 97.99 g (calculated).

1 mole of H_3PO_4 contains 3 mole of H, 1 mole of P, 4 mole of O

$$\text{percent composition of an element} = \frac{n \times \text{molar mass of element}}{\text{molar mass of compound}} \times 100\%$$

The percent by mass of each of the elements in H_3PO_4 is calculated as follows:

$$\%H = \frac{3(1.008\ g)\ H}{97.99\ g\ H_3PO_4} \times 100\% = 3.086\%$$

$$\%P = \frac{30.97\ g\ P}{97.99\ g\ H_3PO_4} \times 100\% = 31.61\%$$

$$\%O = \frac{4(16.00\ g)\ O}{97.99\ g\ H_3PO_4} \times 100\% = 65.31\%$$

Note: The sum of the percentages is 100.01%.

B- Determination of Percent composition from elemental analysis (experimentally)

- Elemental analysis of a compound analyze a certain mass of a sample and give the masses of individual elements in that sample mass (experimentally). So the percentage composition can be calculated as follows:
- **Percent composition of an element=**

  mass of an element/mass of the sample X 100%

Problem

- Elemental analysis of 2.5 g sample of nicotine shows that it contains 1.85 g of C, 0.218 g of H and 0.432 g of N. Calculate the percentage composition of nicotine?

- **Percent composition of an element=**

mass of an element/mass of the sample X 100%

%C = 1.85/2.5 * 100%= 74%

% H= 0.218/2.5*100%= 8.72%

% N= 0.432/2.5*100%= 17.3%

How elemental analysis is done Experimentally?

- Elemental analysis, determines the amounts of Carbon (C), Hydrogen (H), Nitrogen (N), Sulfur (S) and Oxygen (O) present in a sample.
- The most common technique of CHNSO elemental analysis is based on the combustion of the sample.
- The combustion products CO_2, H_2O, N_2, SO_2 are measured and thus the ratio of the elements in the original sample is determined.
- The final amounts of each element are typically given as a percentage of the original sample weight.

How elemental analysis is done Experimentally?

- When ethanol is burned, carbon dioxide (CO2) and water (H2O) are given off.
- Molecular oxygen was added in the combustion process, but some of the oxygen may also have come from the original ethanol sample.
- The masses of CO2 and of H2O produced can be determined by measuring the increase in mass of the CO2 and H2O absorbers,

- **Suppose that in one experiment the combustion of 11.5 g of a compound (contain C, H and O) produced 22.0 g of CO_2 and 13.5 g of H_2O. Calculate the mass percentage of C,H and O in the sample?**

1 mole of CO_2 ≏ 1 mole of C

22/44 mol ≏ ??

- n_C = 0.5 mol So, m_C= 0.5 x 12 = 6 g

1 mole of H_2O ≏ 2 mole of H

13.5/18 mol ≏ ??

- n_H = 1.5 mol So, m_H= 1.5 x 1 = 1.5 g

- Then,

$$\begin{aligned}\text{mass of O} &= \text{mass of sample} - (\text{mass of C} + \text{mass of H})\\ &= 11.5\text{ g} - (6.00\text{ g} + 1.51\text{ g})\\ &= 4.0\text{ g}\end{aligned}$$

- To calculate % by mass

%C = 6/11.5 * 100%= 52.17%

% H= 1.5/11.5*100%= 13.04%

% O= 4/11.5*100%= 34.78%

Derivation the empirical formula of the compounds from elemental analysis

Steps

Given the percent composition by mass of a compound, we can determine its empirical formula.

Problem 1

- **Ascorbic acid (vitamin C) cures scurvy. It is composed of 40.92 %(C), 4.58% (H), and 54.50% (O) by mass. Determine its empirical formula?**

1. If we have 100 g of ascorbic acid, then each percentage can be converted directly to grams. In this sample, there will be 40.92 g of C, 4.58 g of H, and 54.50 g of O.
2. we need to convert the grams of each element to moles:

$n = m/M$

$n_C = 40.92/12.01 = 3.407$ mol C

$n_H = 4.58/1.008 = 4.54$ mol H

$n_O = 54.50/16.00 = 3.406$ mol O

3. we arrive at the formula $C_{3.407}H_{4.54}O_{3.406}$, divide all the subscripts by the smallest subscript ٣.٤٠٦

4. This gives $CH_{1.33}O$ as the formula for ascorbic acid. Next, we need to convert 1.33, the subscript for H, into an integer. This can be done by multiply all the subscripts by 3 and obtain the empirical formula for ascorbic acid as:

$$C_3H_4O_3$$

Problem 2

- **A 1.261 g sample of Caffeine was analyzed to see that it have 0.624 g C, 0.065 g H, 0.364 g N and 0.208 g O. what is the empirical formula of caffeine?**

1. we need to convert the grams of each element to moles:

   $n = m/M$

   $n_C = 0.624/12.01 = 0.052$ mol C

   $n_H = 0.065/1.008 = 0.065$ mol H

   $n_N = 0.364/14.0 = 0.026$ mol N

   $n_O = 0.208/16.00 = 0.0130$ mol O

2. we arrive at the formula $C_{0.052}H_{0.065}N_{0.026}O_{0.0130}$, divide all the subscripts by the smallest subscript 0.0130.
3. This gives $C_4H_5N_2O$ as the formula for caffeine.

Problem 3

- **Suppose that in one experiment the combustion of 11.5 g of a compound (contain C, H and O) produced 22.0 g of CO_2 and 13.5 g of H_2O. Calculate the empirical formula of the compound?**

1 mole of CO_2 ≏ 1 mole of C

22/44 mol ≏ ??

- n_C = 0.5 mol So, m_C= 0.5 x 12 = 6 g

1 mole of H_2O ≏ 2 mole of H

13.5/18 mol ≏ ??

- n_H = 1.5 mol So, m_H= 1.5 x 1 = 1.5 g
- Then,

$$\begin{aligned}\text{mass of O} &= \text{mass of sample} - (\text{mass of C} + \text{mass of H})\\ &= 11.5\text{ g} - (6.00\text{ g} + 1.51\text{ g})\\ &= 4.0\text{ g}\end{aligned}$$

- n_O= 4/16 = 0.25 mol
- So,

$C_{0.50}H_{1.5}O_{0.25}$ divide the subscripts by 0.25, C_2H_6O

Determination of Molecular Formulas from empirical formula

Steps

- The formula calculated from elemental analysis is always the empirical formula.
- To calculate the actual, molecular formula we must know the *approximate* molar mass of the compound experimentally.
- The integral relationship between the empirical and molecular formulas could be obtained from the following ratio:

$$\text{No. of folds} = \frac{\text{molar mass}}{\text{empirical molar mass}}$$

- Molecular formula = No. of folds *(empirical formula)

Problem 3

- From problem 2, calculate the molecular formula of caffeine if you know that its molar mass ≈ 194.19 g/mol?

1. Empirical molar mass of $C_4H_5N_2O$ = 97 g/mol

2. No. of folds = $\frac{\text{molar mass}}{\text{empirical molar mass}}$

$= 194.19/97 \approx 2$

3. Molecular formula = 2 (empirical formula)
4. Molecular formula is $C_8H_{10}N_4O_2$

Chemical Reactions and Chemical Equations

Definitions

- A **chemical reaction,** a process in which a substance (or substances) is changed into one or more new substances.

- A **chemical equation** uses chemical symbols to show what happens during a chemical reaction.

Writing Chemical Equations

- For the following reaction:

$$2H_2 + O_2 \longrightarrow 2H_2O$$

1. The "plus" sign means "reacts with" and the arrow means "to yield."
2. We refer to H2 and O2 in the Equation as reactants, and Water is the product.
3. **Reactants,** are the starting materials in a chemical reaction and written on the left of the arrow.
4. **Products,** are the substances formed as a result of a chemical reaction and written on the right of the arrow.

5. Chemists often indicate the physical states of the reactants and products by using the letters *g*, *l*, and *s* to denote gas, liquid, and solid, respectively. *aq* denotes the aqueous (that is, water) environment.

$$2CO(g) + O_2(g) \longrightarrow 2CO_2(g)$$
$$2HgO(s) \longrightarrow 2Hg(l) + O_2(g)$$

$$NaCl(s) \xrightarrow{H_2O} NaCl(aq)$$

TABLE 3.1 Interpretation of a Chemical Equation

$2H_2$	$+ O_2$	$\longrightarrow$	$2H_2O$
Two molecules	+ one molecule	$\longrightarrow$	two molecules
2 moles	+ 1 mole	$\longrightarrow$	2 moles
$\underbrace{2(2.02\text{ g}) = 4.04\text{ g} + 32.00\text{ g}}_{36.04\text{ g reactants}}$		$\longrightarrow$	$\underbrace{2(18.02\text{ g}) = 36.04\text{ g}}_{36.04\text{ g product}}$

Balancing Chemical Equations

1. Identify all reactants and products and write their correct formulas on the left side and right side of the equation, respectively.
2. Begin balancing the equation to conform with the law of conservation of mass, there must be the same number of each type of atom on both sides of the arrow.
3. We can change the coefficients (the numbers preceding the formulas) but not the subscripts (the numbers within formulas).
4. First, look for elements that appear only once on each side of the equation with the same number of atoms on each side: The formulas containing these elements must have the same coefficient. Therefore, there is no need to adjust the coefficients of these elements at this point.
5. Next, look for elements that appear only once on each side of the equation but in unequal numbers of atoms. Balance these elements.
6. Finally, balance elements that appear in two or more formulas on the same side of the equation.
7. Check your balanced equation to be sure that you have the same total number of each type of atoms on both sides of the equation arrow.

Example 1

- Small amounts of oxygen gas can be prepared by heating potassium chlorate ($KClO_3$). The products are oxygen gas (O_2) and potassium chloride (KCl). From this information, we write

$$KClO_3 \longrightarrow KCl + O_2$$

- All three elements (K, Cl, and O) appear only once on each side of the equation, but only for K and Cl do we have equal numbers of atoms on both sides. Thus, $KClO_3$ and KCl must have the same coefficient.
- The next step is to make the number of O atoms the same on both sides of the equation:

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

Example 1

- Finally, we balance the K and Cl atoms :

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

- As a final check the number of atoms on each side for the reactants and products.

Example 2

- The combustion (that is, burning) of the natural gas component ethane (C2H6) in oxygen or air, yields carbon dioxide (CO2) and water. The unbalanced equation is:

$$C_2H_6 + O_2 \longrightarrow CO_2 + H_2O$$

- We see that the number of atoms is not the same on both sides of the equation for any of the elements (C, H, and O). In addition, C and H appear only once on each side of the equation; O appears in two compounds on the right side (CO2 and H2O).
- First, balance the C atoms:

$$C_2H_6 + O_2 \longrightarrow 2CO_2 + H_2O$$

- Then, balance the H atoms:

$$C_2H_6 + O_2 \longrightarrow 2CO_2 + 3H_2O$$

Example 2

- At this stage, the C and H atoms are balanced, but the O atoms are not, so balance them:

$$C_2H_6 + \frac{7}{2}O_2 \longrightarrow 2CO_2 + 3H_2O$$

- However, we normally prefer to express the coefficients as whole numbers rather than as fractions. Therefore, we multiply the entire equation by 2 to get:

$$2C_2H_6 + 7O_2 \longrightarrow 4CO_2 + 6H_2O$$

- As a final check the number of atoms on each side for the reactants and products.

Amounts of Reactants and Products

The mole method

- A basic question raised in the chemical laboratory is "How much product will be formed from specific amounts of reactants?".
- Or in some cases, we might ask the reverse question: "How much reactants must be used to obtain a specific amount of product?"
- For example, the combustion of carbon monoxide in air produces carbon dioxide:

$$2CO(g) + O_2(g) \longrightarrow 2CO_2(g)$$

- This equation can be read as "2 moles of carbon monoxide gas combine with 1 mole of oxygen gas to form 2 moles of carbon dioxide gas." In stoichiometric calculations, we say that two moles of CO are equivalent to two moles of CO_2, that is,

$$2 \text{ mol } CO \simeq 2 \text{ mol } CO_2$$

- where the symbol $\simeq$ means "stoichiometrically equivalent to" or simply "equivalent to."
- Similarly, we have 1 mol O_2 $\simeq$ 2 mol CO_2 and 2 mol CO $\simeq$ 1 mol O_2.

The mole method

- The mole method used to calculate the amount of reactants or products in a chemical reaction by their molar ratios.
- First convert the quantity of reactant A (in grams or other units) to number of moles.
- Next, use the mole ratio in the balanced equation to calculate the number of moles of product B formed.
- Finally, convert moles of product to grams of product.
- If the grams of the products are given to calculate the grams of the reactants, do the same procedure above.

Summary for the mole method

Example

- **A general overall equation for the degradation of glucose ($C_6H_{12}O_6$) to carbon dioxide (CO_2) and water (H_2O):**

$$C_6H_{12}O_6 + 6O_2 \longrightarrow 6CO_2 + 6H_2O$$

If 856 g of $C_6H_{12}O_6$ is consumed by a person over a certain period, what is the mass of CO_2 produced?

1. From the equation:

   1 mole of $C_6H_{12}O_6$ ≙ 6 moles of CO_2

2. no. of moles of $C_6H_{12}O_6$ (n)= mass (m)/ molar mass(M)

   = 856/ 180= 4.750 mol $C_6H_{12}O_6$

3. no. of moles of C= 4.750 X 6 = 28.50 mol CO_2
4. Mass of CO_2 (m) = n*M= 28.5 X 44 = 1.25 X 10^3 g CO_2

Limiting Reagents

Definitions

- When a chemist carries out a reaction, the reactants are usually not present in exact stoichiometric amounts indicated by the balanced equation.
- Because the goal of a reaction is to produce the maximum quantity of a useful compound from the reactants, frequently a large excess of one reactant is supplied to ensure that the more expensive reactant is completely converted to the desired product. Consequently, some reactant will be left over at the end of the reaction.
- The reactant used up (finished) first in a reaction is called the **limiting reagent**.
- **Excess reagents** are the reactants present in quantities greater than necessary to react with the quantity of the limiting reagent.
- In practice, chemists usually choose the more expensive chemical as the limiting reagent so that all or most of it will be consumed in the reaction.

Calculations

- In stoichiometric calculations involving limiting reagents, the first step is to decide which reactant is the limiting reagent.
- **How to determine the limiting reagent?**

1. Calculate the no. of moles for each reactant from the data given.
2. For each reactant, divide the no. of moles calculated from step 1 by the no. of moles indicated in the balanced equation.
3. Compare the two ratios obtained from step 2, the smallest ratio is for the limiting reagent.

- After the limiting reagent has been identified, the rest of the problem can be solved as outlined in the mole method.

Problem

- **Urea [(NH2)2CO] is prepared by reacting ammonia with carbon dioxide:**

$$2NH_3(g) + CO_2(g) \longrightarrow (NH_2)_2CO(aq) + H_2O(l)$$

- **In one process, 637.2 g of NH3 are treated with 1142 g of CO2.**

  (a) Which of the two reactants is the limiting reagent?

  (b) Calculate the mass of (NH2)2CO formed.

  (c) How much excess reagent (in grams) is left at the end of the reaction?

  Solution for a:

1. No. of moles of NH3 = m/M= 637.2/17.03= 37.42 mol

   No. of moles of CO2 = m/M= 1142/44= 25.95 mol

2. For NH3, 37.42/2= 18.71

   For CO2, 25.95/1= 25.95

3. As 18.71 is smaller than 25.95, so NH3 is the limiting reagent.

- **Solution for b:**
- Use the mole method and regarding that NH_3 is the limiting reagent

1. From the equation:

   2 mole of NH_3 ≏ 1 mole of $(NH_2)_2CO$

2. no. of moles of NH_3 reacted in equation = 37.42 mol
3. no. of moles of $(NH_2)_2CO$= 37.42/2= 18.71 mol
4. Mass of $(NH_2)_2CO$ = n*M= 18.71 X 60.06 = 1124 g

- **Solution for c:**

1. From the equation:

   2 mole of NH_3 ≃ 1 mole of reacted CO_2

2. no. of moles of NH_3 reacted in equation = 37.42 mol
3. no. of moles of reacted CO_2= 37.42/2= 18.71 mol
4. Mass of reacted CO_2 = n*M= 18.71 X 44 = 823.24 g
5. Mass of excess CO_2= 1142-823.24= 318.76 g

Reaction Yield

Definitions

- The amount of limiting reagent present at the start of a reaction determines the theoretical yield of the reaction.
- **Theoretical yield** is the maximum amount of product that would result if all the limiting reagent reacted.
- In practice, the actual yield is almost always less than the theoretical yield.
- **Actual yield** is the amount of product actually obtained from a reaction.
- To determine how efficient a given reaction is, chemists often figure the percent yield.
- **Percent yield** describes the proportion of the actual yield to the theoretical yield. It is calculated as follows:

$$\% \text{ yield} = \frac{\text{actual yield}}{\text{theoritical yield}} \times 100\%$$

Problem

- From the previous problem, if you know that actual yield of urea is 1000 g, calculate the reaction yield?

$$\% \text{ yield} = \frac{\text{actual yield}}{\text{theoritical yield}} \times 100\%$$

= 1000/1124 X 100% = 89%

General chemistry

Chapter 4
The Electronic Structure of Atoms

Introduction

- An electron possesses both particle (has a mass) and wave properties (an electron move around the nucleus as standing waves).
- **Atomic orbitals** defines the distribution of electron density in three-dimensional space around the nucleus.
- An atomic orbital has a characteristic energy, as well as a characteristic distribution of electron density.

the electron density in an electron wave

90% of the electron density is inside the two lobes drawn on the electron wave

these balloons represent the region of space which contains 90% of the electron density for this particular electron wave

Quantum numbers

- Quantum numbers describe the distribution of electrons in atomic orbitals and label electrons that reside in them in terms of its wave characters.
- In quantum mechanics, three quantum numbers are required to describe the distribution of electrons in atoms. They are called the ***principal quantum number***, the ***angular momentum quantum number***, and the ***magnetic quantum number***. A fourth quantum number— the ***spin quantum number***—describes the behavior of a specific electron and completes the description of electrons in atoms.

The Principal Quantum Number (n)

- The principal quantum number (n) can have integral values 1, 2, 3, and so forth.
- It describes the shell or the level to which the electron belongs.
- The principal quantum number relates to the average distance of the electron from the nucleus in a particular orbital.
- The larger n is, the greater the average distance of an electron in the orbital from the nucleus and therefore the larger the orbital.

The Angular Momentum Quantum Number (*l*) or subsidiary Quantum Number

- Each shell is divided into subshell or sublevels assigned *l* number.
- Each shell or principal level of quantum number *n* contains *n* subshells. For example, if *n* = 2, then there are two subshells (two values of *l*)
- The values of *l* depend on the value of n. For a given value of n, *l* has possible integral values from 0 to (n -1).
- It tells us the "shape" of the orbitals.
- Thus, if *l*=0, we have an s orbital; if *l* =1, we have a p orbital; and so on.

ℓ	0	1	2	3	4	5
Name of orbital	*s*	*p*	*d*	*f*	*g*	*h*

The Magnetic Quantum Number (m_l)

- The magnetic quantum number $\boldsymbol{m_l}$ describes the orientation of the orbital in space
- The values of $\boldsymbol{m_l}$ can vary from - l to l.
- The number of $\boldsymbol{m_l}$ values indicates the number of orbitals in a subshell with a particular l value.
- There are (2 l +1) integral values of $\boldsymbol{m_l}$ as follows: if l =0, then there are (2 l + 1)= 1 orbital and the value of $\boldsymbol{m_l}$ = 0. If l = 1, then there are (2 l + 1)= 3 orbitals have three values of $\boldsymbol{m_l}$, namely, -1, 0, 1 and so on.

The Electron Spin Quantum Number (m_s)

- Electrons spin on their own axes, so can generate a magnetic field, and it is this motion that causes an electron to behave like a magnet.
- There are two possible spinning motions of an electron, one clockwise and the other counterclockwise.
- The electron spin quantum number (m_s), describe electron spinning and has a value of $+\frac{1}{2}$ or $-\frac{1}{2}$.

Summary

n (shell)	*l* (sub-shell) (0 to n-1)	symbol of *l* subshell	m_l (-*l* to +*l*)	no. of orbitals in the subshell (2*l* +1)	Total no. of orbitals in the shell (n^2)	Total no. of electrons in the shell ($2 n^2$)
1	0	s	0	1	1	2
2	0 1	s p	0 -1,0,+1	1 3	4	8
3	0 1 2	s p d	0 -1,0,+1 -2,-1,0,+1,+2	1 3 5	9	18
4	0 1 2 3	s p d f	0 -1,0,+1 -2,-1,0,+1,+2 -3,-2,-1,0,+1,+2,+3	1 3 5 7	16	32

Atomic Orbitals

- **s Orbitals**

All s orbitals are spherical.

They increase in size as n increases, so 1s< 2s <3s

- **p Orbitals**

These three p orbitals are identical in size, shape, and energy; they differ from one another only in orientation.

Each p orbital can be thought of as two lobes on opposite sides of the nucleus.

They increase in size as n increases, so 2p< 3p< 4p.

Atomic Orbitals

d Orbitals

All the five d orbitals in an atom are identical in energy. They differ from one another in orientation. They increase in size as n increases.

Notes

- When we write the subshell, we write first the n number followed by the symbol of the l number.
- **For example:**

In 2s and 2p subshells, 2 denotes the value of n, and s and p denote the symbol of l number.

- The four quantum numbers n, l , m_l , and m_s enable us to label completely an electron in any orbital in any atom.
- In a sense, we can regard the set of four quantum numbers as the "address" of an electron in an atom.
- We use the simplified notation (n, l , m_l, m_s).

The Energies of Orbitals

- The energy of an electron in many-electron atoms in such an atom depends on ***n*** and ***l*** values.
- For the same subshell (l), the energy increases as n increase. (1s<2s<3s).
- In the same shell (n), the energy increase as l increase (3s<3p<3d).
- Between subshells in different shells, there are overlap. For example, the 3d energy level is very close to the 4s energy level.
- It turns out that the total energy of an atom is lower when the 4s subshell is filled before a 3d subshell (the energy of repulsion between the electrons in d orbitals make increase in the atom energy).

Ground state and excited state

- A **ground state** of an atom is the lowest possible energy (stable state) of an atom in which all the electrons in the atom are as close to the nucleus as possible.
- An **excited state** of an atom in which the electronic configurations gives the atom a higher energy than the ground state.

Ground state Electron Configuration

- The **Ground state electron configuration** of the atom determines how the electrons are distributed among the various atomic orbitals. It is important to understand electronic behavior.
- The next figure shows the order in which atomic subshells are filled in a many-electron atom.
- Start with the 1s orbital and move downward, following the direction of the arrows.

Electron Configuration

- To write the electron configuration we write the symbol of the subshell (n+ symbol of *l*) and provide the number of its electrons in the superscript as follows:

- The electron configuration can also be represented by an *orbital diagram* that shows the spin of the electron:

- The upward arrow denotes one of the two possible spinning motions of the electron. (Alternatively, we could have represented the electron with a downward arrow.) The box represents an atomic orbital.

The Building-Up Principle

- It is used in writing electron configurations for the elements. This process is based on the Aufbau principle.
- The **Aufbau principle** dictates that as protons are added one by one to the nucleus (as Z increase) to build up the elements, electrons are similarly added to the atomic orbitals.
- The electron configurations of elements (except hydrogen and helium) could be represented by a **noble gas core,** which shows in brackets the noble gas element that most nearly precedes the element being considered, followed by the symbol for the highest filled subshells in the outermost shells.

1	H	$1s^1$
2	He	$1s^2$
3	Li	$[He]2s^1$
4	Be	$[He]2s^2$
5	B	$[He]2s^22p^1$
6	C	$[He]2s^22p^2$
7	N	$[He]2s^22p^3$
8	O	$[He]2s^22p^4$
9	F	$[He]2s^22p^5$
10	Ne	$[He]2s^22p^6$
11	Na	$[Ne]3s^1$
12	Mg	$[Ne]3s^2$
13	Al	$[Ne]3s^23p^1$
14	Si	$[Ne]3s^23p^2$
15	P	$[Ne]3s^23p^3$
16	S	$[Ne]3s^23p^4$
17	Cl	$[Ne]3s^23p^5$
18	Ar	$[Ne]3s^23p^6$

The Pauli Exclusion Principle

- This principle states that no two electrons in an atom can have the same four quantum numbers.
- If two electrons in an atom should have the same n, l , and m_l values (that is, these two electrons are in the *same* atomic orbital), then they must have different values of m_s.
- In other words, only two electrons may occupy the same atomic orbital, and these electrons must have opposite spins.
- Consider the helium atom, which has two electrons. The right way of placing two electrons in the

1s orbital are as follows:

He $\boxed{\uparrow\downarrow}$

$1s^2$

Hund's rule

- This rule states that the most stable arrangement of electrons in subshells is the one with the greatest number of parallel spins.

Paramagnetism & diamagnetism

- Atoms in which one or more electrons are unpaired and are attracted by a magnet are paramagnetic.

- Atoms in which all the electron spins are paired (cancel each other) and are slightly repelled by a magnet are diamagnetic.

Irregularities

- The electron configuration of chromium (Z=24) is $[Ar]4s^1 3d^5$ and not $[Ar]4s^2 3d^4$, as we might expect. A similar break in the pattern is observed for copper (Z=29), whose electron configuration is $[Ar]4s^1 3d^{10}$ rather than $[Ar]4s^2 3d^9$.
- The reason for these irregularities is that a slightly greater stability is associated with the half-filled ($3d^5$) and completely filled ($3d^{10}$) subshells.
- The electron configuration of gadolinium (Z=64) is $[Xe]6s^2 4f^7 5d^1$ rather than $[Xe]6s^2 4f^8$. Like chromium, gadolinium gains extra stability by having a half-filled subshell ($4f^7$).

	1 1A	2 2A	3 3B	4 4B	5 5B	6 6B	7 7B	8	9 8B	10	11 1B	12 2B	13 3A	14 4A	15 5A	16 6A	17 7A	18 8A
1	1 **H** $1s^1$																	2 **He** $1s^2$
2	3 **Li** $2s^1$	4 **Be** $2s^2$											5 **B** $2s^22p^1$	6 **C** $2s^22p^2$	7 **N** $2s^22p^3$	8 **O** $2s^22p^4$	9 **F** $2s^22p^5$	10 **Ne** $2s^22p^6$
3	11 **Na** $3s^1$	12 **Mg** $3s^2$											13 **Al** $3s^23p^1$	14 **Si** $3s^23p^2$	15 **P** $3s^23p^3$	16 **S** $3s^23p^4$	17 **Cl** $3s^23p^5$	18 **Ar** $3s^23p^6$
4	19 **K** $4s^1$	20 **Ca** $4s^2$	21 **Sc** $4s^23d^1$	22 **Ti** $4s^23d^2$	23 **V** $4s^23d^3$	24 **Cr** $4s^13d^5$	25 **Mn** $4s^23d^5$	26 **Fe** $4s^23d^6$	27 **Co** $4s^23d^7$	28 **Ni** $4s^23d^8$	29 **Cu** $4s^13d^{10}$	30 **Zn** $4s^23d^{10}$	31 **Ga** $4s^24p^1$	32 **Ge** $4s^24p^2$	33 **As** $4s^24p^3$	34 **Se** $4s^24p^4$	35 **Br** $4s^24p^5$	36 **Kr** $4s^24p^6$
5	37 **Rb** $5s^1$	38 **Sr** $5s^2$	39 **Y** $5s^24d^1$	40 **Zr** $5s^24d^2$	41 **Nb** $5s^14d^4$	42 **Mo** $5s^14d^5$	43 **Tc** $5s^24d^5$	44 **Ru** $5s^14d^7$	45 **Rh** $5s^14d^8$	46 **Pd** $4d^{10}$	47 **Ag** $5s^14d^{10}$	48 **Cd** $5s^24d^{10}$	49 **In** $5s^25p^1$	50 **Sn** $5s^25p^2$	51 **Sb** $5s^25p^3$	52 **Te** $5s^25p^4$	53 **I** $5s^25p^5$	54 **Xe** $5s^25p^6$
6	55 **Cs** $6s^1$	56 **Ba** $6s^2$	57 **La** $6s^25d^1$	72 **Hf** $6s^25d^2$	73 **Ta** $6s^25d^3$	74 **W** $6s^25d^4$	75 **Re** $6s^25d^5$	76 **Os** $6s^25d^6$	77 **Ir** $6s^25d^7$	78 **Pt** $6s^15d^9$	79 **Au** $6s^15d^{10}$	80 **Hg** $6s^25d^{10}$	81 **Tl** $6s^26p^1$	82 **Pb** $6s^26p^2$	83 **Bi** $6s^26p^3$	84 **Po** $6s^26p^4$	85 **At** $6s^26p^5$	86 **Rn** $6s^26p^6$
7	87 **Fr** $7s^1$	88 **Ra** $7s^2$	89 **Ac** $7s^26d^1$	104 **Rf** $7s^26d^2$	105 **Db** $7s^26d^3$	106 **Sg** $7s^26d^4$	107 **Bh** $7s^26d^5$	108 **Hs** $7s^26d^6$	109 **Mt** $7s^26d^7$	110 **Ds** $7s^26d^8$	111 **Rg** $7s^26d^9$	112 $7s^26d^{10}$	(113)	114 $7s^27p^2$	(115)	116 $7s^27p^4$	(117)	(118)

58 **Ce** $6s^24f^15d^1$	59 **Pr** $6s^24f^3$	60 **Nd** $6s^24f^4$	61 **Pm** $6s^24f^5$	62 **Sm** $6s^24f^6$	63 **Eu** $6s^24f^7$	64 **Gd** $6s^24f^75d^1$	65 **Tb** $6s^24f^9$	66 **Dy** $6s^24f^{10}$	67 **Ho** $6s^24f^{11}$	68 **Er** $6s^24f^{12}$	69 **Tm** $6s^24f^{13}$	70 **Yb** $6s^24f^{14}$	71 **Lu** $6s^24f^{14}5d^1$
90 **Th** $7s^26d^2$	91 **Pa** $7s^25f^26d^1$	92 **U** $7s^25f^36d^1$	93 **Np** $7s^25f^46d^1$	94 **Pu** $7s^25f^6$	95 **Am** $7s^25f^7$	96 **Cm** $7s^25f^76d^1$	97 **Bk** $7s^25f^9$	98 **Cf** $7s^25f^{10}$	99 **Es** $7s^25f^{11}$	100 **Fm** $7s^25f^{12}$	101 **Md** $7s^25f^{13}$	102 **No** $7s^25f^{14}$	103 **Lr** $7s^25f^{14}6d^1$

Summary
General Rules for Assigning Electrons to Atomic Orbitals

- Each shell or principal level of quantum number n contains n subshells. For example, if $n = 2$, then there are two subshells (two values of l) of angular momentum quantum numbers 0 and 1.
- Each subshell of quantum number l contains $(2l + 1)$ orbitals. For example, if $l = 1$, then there are three p orbitals.
- No more than two electrons can be placed in each orbital. They must have opposite spins, or different electron spin quantum numbers. Therefore, the maximum number of electrons is simply twice the number of orbitals that are employed.
- A quick way to determine the maximum number of electrons that an atom can have in a principal level n is to use the formula $2n^2$.
- No two electrons in the same atom can have the same four quantum numbers. (This is the Pauli exclusion principle).
- The most stable arrangement of electrons in a subshell is the one that has the greatest number of parallel spins. This is Hund's rule.
- Atoms in which one or more electrons are unpaired are paramagnetic. Atoms in which all the electron spins are paired are diamagnetic.
- In a hydrogen atom, the energy of the electron depends only on its principal quantum number n. In a many-electron atom, the energy of an electron depends on both n and its angular momentum quantum number l.

General chemistry

Chapter 5
Periodic table

Periodic table

- **Periodic table**—a chart in which elements are arranged by atomic number (shown above the element symbol) in horizontal rows called ***periods*** and in vertical columns known as ***groups or families***.
- The periodic table is a handy tool that correlates the properties of the elements in a systematic way and helps us to make predictions about chemical behavior.

Notes

- A **block** of the periodic table is a set of chemical elements having their differentiating electrons predominately in the same type of atomic orbital.
- **A differentiating electron** is the electron that differentiates an element from the previous one.

Periodic Classification of the Elements

- Elements are grouped according to their outer-shell electron configurations, which account for their similar chemical behavior.
- According to the type of subshell being filled by the differentiating electron, the elements can be divided into categories:

1. **The Representative elements** (also called main group elements) the elements in Groups 1A through 7A, in which the differentiating electron is filled in the s subshells (s-block) or in the p subshell (p-block) of the highest principal quantum number.

2- **The noble gases**, with the exception of helium, the noble gases (the Group 8A elements) all have a completely filled s and p subshells of the highest principal quantum number. The electron configurations are $1s^2$ for helium and ns^2np^6 for the other noble gases, in which n is the principal quantum number for the outermost shell.

3- **The transition elements (or transition metals)**, are the elements in Groups 1B and 3B through 8B, in which the differentiating electron is filled in the d subshells (d-block).

4- **The Group 2B elements are Zn, Cd, and Hg**, which are neither representative elements nor transition metals.

5- **The inner transition elements (the lanthanides, and the actinides)**, in which the differentiating electron is filled in the f subshells (f-block).

Main-group elements
s-block
1A
2A
1s
2s
3s
4s
5s
6s
7s
Transition elements
d-block
3B 4B 5B 6B 7B 8B 1B 2B
3d
4d
5d
6d
p-block
3A 4A 5A 6A 7A
8A
1s
2p
3p
4p
5p
6p
Inner-transition elements
f-block
4f
5f

Representative elements

Noble gases

Transition metals

Zinc
Cadmium
Mercury

Lanthanides

Actinides

1 1A	2 2A	3 3B	4 4B	5 5B	6 6B	7 7B	8	9 8B	10	11 1B	12 2B	13 3A	14 4A	15 5A	16 6A	17 7A	18 8A
1 H																	2 He
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
55 Cs	56 Ba	57 La	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
87 Fr	88 Ra	89 Ac	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112	(113)	114	(115)	116	(117)	(118)

58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

	1 1A	2 2A	3 3B	4 4B	5 5B	6 6B	7 7B	8	9 8B	10	11 1B	12 2B	13 3A	14 4A	15 5A	16 6A	17 7A	18 8A
1	1 **H** $1s^1$																	2 **He** $1s^2$
2	3 **Li** $2s^1$	4 **Be** $2s^2$											5 **B** $2s^22p^1$	6 **C** $2s^22p^2$	7 **N** $2s^22p^3$	8 **O** $2s^22p^4$	9 **F** $2s^22p^5$	10 **Ne** $2s^22p^6$
3	11 **Na** $3s^1$	12 **Mg** $3s^2$											13 **Al** $3s^23p^1$	14 **Si** $3s^23p^2$	15 **P** $3s^23p^3$	16 **S** $3s^23p^4$	17 **Cl** $3s^23p^5$	18 **Ar** $3s^23p^6$
4	19 **K** $4s^1$	20 **Ca** $4s^2$	21 **Sc** $4s^23d^1$	22 **Ti** $4s^23d^2$	23 **V** $4s^23d^3$	24 **Cr** $4s^13d^5$	25 **Mn** $4s^23d^5$	26 **Fe** $4s^23d^6$	27 **Co** $4s^23d^7$	28 **Ni** $4s^23d^8$	29 **Cu** $4s^13d^{10}$	30 **Zn** $4s^23d^{10}$	31 **Ga** $4s^24p^1$	32 **Ge** $4s^24p^2$	33 **As** $4s^24p^3$	34 **Se** $4s^24p^4$	35 **Br** $4s^24p^5$	36 **Kr** $4s^24p^6$
5	37 **Rb** $5s^1$	38 **Sr** $5s^2$	39 **Y** $5s^24d^1$	40 **Zr** $5s^24d^2$	41 **Nb** $5s^14d^4$	42 **Mo** $5s^14d^5$	43 **Tc** $5s^24d^5$	44 **Ru** $5s^14d^7$	45 **Rh** $5s^14d^8$	46 **Pd** $4d^{10}$	47 **Ag** $5s^14d^{10}$	48 **Cd** $5s^24d^{10}$	49 **In** $5s^25p^1$	50 **Sn** $5s^25p^2$	51 **Sb** $5s^25p^3$	52 **Te** $5s^25p^4$	53 **I** $5s^25p^5$	54 **Xe** $5s^25p^6$
6	55 **Cs** $6s^1$	56 **Ba** $6s^2$	57 **La** $6s^25d^1$	72 **Hf** $6s^25d^2$	73 **Ta** $6s^25d^3$	74 **W** $6s^25d^4$	75 **Re** $6s^25d^5$	76 **Os** $6s^25d^6$	77 **Ir** $6s^25d^7$	78 **Pt** $6s^15d^9$	79 **Au** $6s^15d^{10}$	80 **Hg** $6s^25d^{10}$	81 **Tl** $6s^26p^1$	82 **Pb** $6s^26p^2$	83 **Bi** $6s^26p^3$	84 **Po** $6s^26p^4$	85 **At** $6s^26p^5$	86 **Rn** $6s^26p^6$
7	87 **Fr** $7s^1$	88 **Ra** $7s^2$	89 **Ac** $7s^26d^1$	104 **Rf** $7s^26d^2$	105 **Db** $7s^26d^3$	106 **Sg** $7s^26d^4$	107 **Bh** $7s^26d^5$	108 **Hs** $7s^26d^6$	109 **Mt** $7s^26d^7$	110 **Ds** $7s^26d^8$	111 **Rg** $7s^26d^9$	112 $7s^26d^{10}$	(113)	114 $7s^27p^2$	(115)	116 $7s^27p^4$	(117)	(118)

58 **Ce** $6s^24f^15d^1$	59 **Pr** $6s^24f^3$	60 **Nd** $6s^24f^4$	61 **Pm** $6s^24f^5$	62 **Sm** $6s^24f^6$	63 **Eu** $6s^24f^7$	64 **Gd** $6s^24f^75d^1$	65 **Tb** $6s^24f^9$	66 **Dy** $6s^24f^{10}$	67 **Ho** $6s^24f^{11}$	68 **Er** $6s^24f^{12}$	69 **Tm** $6s^24f^{13}$	70 **Yb** $6s^24f^{14}$	71 **Lu** $6s^24f^{14}5d^1$
90 **Th** $7s^26d^2$	91 **Pa** $7s^25f^26d^1$	92 **U** $7s^25f^36d^1$	93 **Np** $7s^25f^46d^1$	94 **Pu** $7s^25f^6$	95 **Am** $7s^25f^7$	96 **Cm** $7s^25f^76d^1$	97 **Bk** $7s^25f^9$	98 **Cf** $7s^25f^{10}$	99 **Es** $7s^25f^{11}$	100 **Fm** $7s^25f^{12}$	101 **Md** $7s^25f^{13}$	102 **No** $7s^25f^{14}$	103 **Lr** $7s^25f^{14}6d^1$

Figure 8.1

The ground-state electron configurations of the elements. For simplicity, only the configurations of the outer electrons are shown.

Special names

- For convenience, some element groups have special names.
- The Group 1A elements are called ***alkali metals.***
- The Group 2A elements are called ***alkaline earth metals.***
- The Group 7Aare known as ***halogens.***
- The Group 8A are called ***noble gases*** (or ***inert*** or ***rare gases***).
- **Lanthanides,** are the ***rare earth series or metals.***

Determination of the period number and group number from electron configuration

A- For representative elements (groups A)

- ***Period number:*** it equals to the number of the highest energy level.
- ***Group number:*** it equals the sum of electrons in the highest energy level (valance electrons).

B- For transition metals

- ***Period number:*** it equals to the number of the highest energy level.
- ***Group number:***
  - If number of electrons of d<6, Group number = number of electrons +2
  - If number of electrons of d=6,7,8 , Group number = 8
  - If number of electrons of d=9,10, Group number = 1,2 respectively.

Electron Configurations of Cations and Anion

- Because many ionic compounds are made up of monatomic anions and/or cations, it is helpful to know how to write the electron configurations of these ionic species.

1. **Ions Derived from Representative Elements**

In the formation of a cation from the neutral atom of a representative element, one or more electrons are removed from the highest occupied n shell. Here are the electron configurations of some neutral atoms and their corresponding cations:

Na: $[Ne]3s^1$	Na^+: [Ne]
Mg: [Ne] $3s^2$	Mg^{2+}: [Ne]
Al: $[Ne]3s^2 3p^1$	Al^{3+}: [Ne]

Note that each ion has a stable noble gas configuration.

- In the formation of an anion, one or more electrons are added to the highest partially filled n shell. Consider these examples:

H: $1s^1$	H^-: $1s^2$ or [He]
F: $1s^2 2s^2 2p^5$	F^-: $1s^2 2s^2 2p^6$ or [Ne]
O: $1s^2 2s^2 2p^4$	O^{2-}: $1s^2 2s^2 2p^6$ or [Ne]
N: $1s^2 2s^2 2p^3$	N^{3-}: $1s^2 2s^2 2p^6$ or [Ne]

- Again, all the anions have stable noble gas configurations. Thus, a characteristic of most representative elements is that ions derived from their neutral atoms have the noble gas outer electron configuration ns^2np^6.

Isoelectronicity

- Ions, or atoms and ions, that have the same number of electrons, and hence the same ground-state electron configuration, are said to be **isoelectronic.**
- Thus, H^- and He are isoelectronic.
- Al^{+3}, Mg^{+2}, Na^+ , N^{-3}, O^{-2} ,F^{-1} and Ne are isoelectronic; and so on.

Cations Derived from Transition Metals

- When a cation is formed from an atom of a transition metal, electrons are always removed first from the *ns* orbital and then from the (*n*-1)*d* orbitals (although the 4*s* orbital is always filled before the 3*d* orbital).
- This is because the 3d orbital is more stable than the 4s orbital in transition metal ***ions. (not as the atoms)***
- Keep in mind that most transition metals can form more than one cation and that frequently the cations are not isoelectronic with the preceding noble gases.

Periodic Variation in Physical Properties

- As we have seen, the electron configurations of the elements show a periodic variation with increasing atomic number. Consequently, there are also periodic variations in physical and chemical behavior.
- With a group, there is similarities in physical and chemical characters as there outer electron configuration is similar.
- Physical characters include: atomic sizes, ionization energy, electron affinity and metallic characters.

Atomic size

- A number of physical properties, including density, melting point, and boiling point, are related to the sizes of atoms.
- The size of an atom can be defined in terms of its ***atomic radius***, which is *one-half the distance between the two nuclei in two adjacent metal atoms (for mono atoms) or as one-half the distance between the centers of the atoms in the molecule (di atoms).*

Increasing atomic radius
1A
2A
3A
4A
5A
6A
7A
8A
H
37
He
31
B
C
N
O
F
Ne
Li
Be
152
112
85
77
75
73
72
70
Na
Mg
Al
Si
P
S
Cl
Ar
186
160
143
118
110
103
99
98
K
Ca
Ga
Ge
As
Se
Br
Kr
227
197
135
123
120
117
114
112
Rb
Sr
In
Sn
Sb
Te
I
Xe
248
215
166
140
141
143
133
131
Cs
Ba
Tl
Pb
Bi
Po
At
Rn
265
222
171
175
155
164
142
140
Increasing atomic radius

Atomic size

- Periodic **trends** are clearly evident. The atomic radius is determined to a large extent by the strength of the attraction between the nucleus and the ***outer-shell electrons.***
- In the **same period, as nuclear charge increases**, the stronger the hold of the nucleus on outer-shell electrons, and the smaller the atomic radius. Hence, the atomic radius decreases steadily from left to right.
- Within a **group** of elements we find that atomic radius increases with increasing atomic number. This is because that orbital size increases with the increasing the **number of principal levels**, so does the average distance of a outer shells from the nucleus.

Ionic Radius

- Ionic radius is the radius of a cation or an anion. Ionic radius affects the physical and chemical properties of an ionic compound. When a neutral atom is converted to an ion, we expect a change in size.
- If the atom forms an ***anion, its size (or radius) increases***, because the nuclear charge remains the same but the **repulsion** resulting from the additional electron(s) enlarges the domain of the electron cloud.
- On the other hand, removing one or more electrons from an atom reduces electron-electron repulsion but the nuclear charge remains the same, so the electron cloud shrinks, and the ***cation is smaller* than the atom.**

Ionic Radius

- **Compare the ionic radius with atomic radius for each element.**

Ionic Radius

- From top to bottom, both the atomic radius and the ionic radius increase within a group.
- In the same period, the size of anions is larger than the size of cations.

Ionic Radius

- Focusing on isoelectronic cations, we see that the radii of tripositive ions are smaller than those of dipositive which in turn are smaller than unipositive ions.

- The radius of isoelectronic anions increases as we go from ions with uninegative charge to those with dinegative charge and so on.

Ionic Radius

- Comparing isoelectronic ions, cations are smaller than anions.

Ionization Energy

- Ionization energy is the minimum energy (in kJ/mol) required to remove an electron from a gaseous atom in its ground state.
- The magnitude of ionization energy is a measure of how "tightly" the electron is held in the atom.
- The higher the ionization energy, the more difficult it is to remove the electron.
- For a many-electron atom, the amount of energy required to remove the first electron from the atom in its ground state, is called the first ionization energy (I_1) described by the following equation:

$$\text{energy} + X(g) \longrightarrow X^+(g) + e^-$$

X represents an atom of any element and e^- is an electron.

Ionization Energy

- The second ionization energy (I2) and the third ionization energy (I3) are shown in the following equations:

$$\text{energy} + X^{+}(g) \longrightarrow X^{2+}(g) + e^{-} \quad \text{second ionization}$$
$$\text{energy} + X^{2+}(g) \longrightarrow X^{3+}(g) + e^{-} \quad \text{third ionization}$$

- When an electron is removed from an atom, the repulsion among the remaining electrons decreases and the effective nuclear charge increases, so more energy is needed to remove another electron from the positively charged ion.
- Thus, ionization energies always increase in the following order:

$$I_1 < I_2 < I_3 < \cdot$$

Ionization Energy

- Ionization is always an endothermic process, that means the energy absorbed by atoms (or ions) in the ionization process has a positive value.
- Note that, apart from small irregularities, the first ionization energies of elements in a period increase with increasing atomic number.
- This trend is due to the increase in effective nuclear charge from left to right (as in the case of atomic radii variation). A larger effective nuclear charge means a more tightly held outer electron, and hence a higher first ionization energy.

Ionization Energy

- For a given group, ionization energy decreases with increasing atomic number (that is, as we move down the group).
- Elements in the same group have similar outer electron configurations. However, as the principal quantum number n increases, so does the average distance of a valence electron from the nucleus. A greater separation between the valance electrons and the nucleus means a weaker attraction (+ shielding effect of the inner sub-shells), so that it becomes increasingly easier to remove the first electron as we go from element to element down a group.

The increase in first ionization energy from left to right across a period and from bottom to top in a group for representative elements.

Electron Affinity

- It is a measure to the ability of atoms to accept one or more electrons.
- There is an increase in the tendency to accept electrons (electron affinity values increase) from left to right across a period.
- The values vary within a given group.
- Halogens (Group 7A) have the highest electron affinity values. This is not surprising when we realize that by accepting an electron, each halogen atom assumes the stable electron configuration of the noble gas immediately to its right.
- Group 1A and 2A have low electron affinity.

Metallic character

- Elements are further classified into metals, non-metals, and metalloids based on their properties, which are correlated with their placement in the periodic table.
- Metallic character of the elements decreases from left to right across a period and increases from top to bottom within a group.
- Group 7A are the most reactive non-metals and group 1A are the most reactive metals.
- Metalloids have properties intermediate between the metals and nonmetals. Metalloids are useful in the semiconductor industry. The physical properties of metalloids tend to be metallic, but their chemical properties tend to be non-metallic.

1 1A	2 2A	3 3B	4 4B	5 5B	6 6B	7 7B	8	9 8B	10	11 1B	12 2B	13 3A	14 4A	15 5A	16 6A	17 7A	18 8A
1 H																	2 He
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
55 Cs	56 Ba	57 La	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
87 Fr	88 Ra	89 Ac	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112	(113)	114	(115)	116	(117)	(118)

58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

Metals

Metalloids

Nonmetals

Metallic characters

Characteristic physical properties of metallic and non-metallic elements	
Metallic Elements	**Nonmetallic elements**
Distinguishing luster (shine)	Non-lustrous, various colors
Metals are solids at room temperature except mercury	Gases (oxygen) and solids (carbon) except bromine
Malleable and ductile (flexible), hard as solids	Brittle, hard or soft
Conduct heat and electricity	Poor conductors
Metals have high melting and boiling points	The melting points of non-metals are generally lower than metals

Metallic characters

Characteristic chemical properties of metallic and non-metallic elements	
Metals typically have 1 to 3 electrons in the outermost shell of their atoms	Non-Metals typically have more than 3 electrons in the outermost shell of their atoms
Metals tend to have low ionization energies and low electron affinity and *typically lose electrons (i.e. are **oxidized**).* when reacting with non-metals (tend to become ***cation) and form ionic bonds***	Non-metals tend to have high ionization energies and high electron affinity and *typically* gain or share electrons with other atoms. They are electronegative in character. Nonmetals, when reacting with metals, tend to gain electrons and become ***anions and form ionic bonds*** Nonmetals, when reacting with other non-metals, share electrons and form covalent bonds.
Most metal oxides are basic and ionic. They dissolve in water to form ***metal hydroxides***: $Na_2O(s)+H_2O(l)\rightarrow 2NaOH(aq)$ $CaO(s)+H_2O(l)\rightarrow Ca(OH)_2(aq)$	They generally form covalent, acidic or neutral oxides with oxygen that that dissolve in water to form acids: $P_4O_{10}(s) + 6H_2O(l) \longrightarrow 4H_3PO_4(aq)$ $SO_3(g) + H_2O(l) \longrightarrow H_2SO_4(aq)$
Metal oxides exhibit their ***basic*** chemical nature by reacting with ***acids*** to form metal ***salts*** and water: $MgO(s)+HCl(aq)\rightarrow MgCl_2(aq)+H_2O(l)$ $NiO(s)+H_2SO_4(aq)\rightarrow NiSO_4(aq)+H_2O(l)$	Nonmetallic oxides are acidic can combine with bases to form salts. $CO_2(g)+2NaOH(aq)\rightarrow Na_2CO_3(aq)+H_2O(l)$
Form cations in aqueous solution	Form anions in aqueous solution

Summary

Ionization energy
Electron affinity
Atomic radius
Nonmetallic character
Metallic character
Ionization energy
Atomic radius

General chemistry

Chapter 6

Chemical bonding

I- Ionic Bond

Introduction

- Atoms combine to achieve a more stable electron configuration. Maximum stability results when an atom is isoelectronic with a noble gas.
- **OCTET RULE**
- A stable arrangement is attended when the atom is surrounded by eight electrons. This octet can be made up by own electrons and some electrons which are shared. Thus, an atom continues to form bonds until an octet of electrons is made. This is known as octet rule by Lewis.

Lewis dot symbol

- When discussing the octet rule, we do not consider *d* or *f* electrons. Only the s and p electrons are involved in the octet rule **(valance electrons),** making it a useful rule for the *main group elements*, an octet in these atoms corresponds to an electron configurations ending with s^2p^6.
- **Lewis dot symbol** consists of the symbol of an element and one dot for each valence electron in an atom of the element.
- Note that, except for helium, the number of valence electrons each atom has is the same as the group number of the element (for the main groups).

1 1A	2 2A	13 3A	14 4A	15 5A	16 6A	17 7A	18 8A
H							He
Li	Be	B	C	N	O	F	Ne
Na	Mg	Al	Si	P	S	Cl	Ar
K	Ca	Ga	Ge	As	Se	Br	Kr
Rb	Sr	In	Sn	Sb	Te	I	Xe
Cs	Ba	Tl	Pb	Bi	Po	At	Rn
Fr	Ra						

Lewis dot symbols for the representative elements and the noble gases. The number of unpaired dots corresponds to the number of bonds an atom of the element can form in a compound.

The Ionic Bond

- An ***ionic bond*** is *the electrostatic force that holds ions together in an ionic compound.*
- Atoms of elements with low ionization energies tend to form cations, while those with high electron affinities tend to form anions.
- **Monatomic ions** contain only one atom as Na^+ and Cl^-. **Polyatomic ions** are ions containing more than one atom, such as OH^- and CN^- .
- As a rough rule, the elements most likely to form cations in ionic compounds are the alkali metals (Group 1A) and alkaline earth metals (Group 2A), and the elements most likely to form anions are the halogens and oxygen.

1A	2 2A	3 3B	4 4B	5 5B	6 6B	7 7B	8	9 8B	10	11 1B	12 2B	13 3A	14 4A	15 5A	16 6A	17 7A	8A
Li^+													C^{4-}	N^{3-}	O^{2-}	F^-	
Na^+	Mg^{2+}											Al^{3+}		P^{3-}	S^{2-}	Cl^-	
K^+	Ca^{2+}				Cr^{2+} Cr^{3+}	Mn^{2+} Mn^{3+}	Fe^{2+} Fe^{3+}	Co^{2+} Co^{3+}	Ni^{2+} Ni^{3+}	Cu^+ Cu^{2+}	Zn^{2+}				Se^{2-}	Br^-	
Rb^+	Sr^{2+}									Ag^+	Cd^{2+}		Sn^{2+} Sn^{4+}		Te^{2-}	I^-	
Cs^+	Ba^{2+}									Au^+ Au^{3+}	Hg_2^{2+} Hg^{2+}		Pb^{2+} Pb^{4+}				

Figure 2.10

Common monatomic ions arranged according to their positions in the periodic table. Note that the Hg_2^{2+} ion contains two atoms.

Formula of Ionic Compounds

- The formulas of ionic compounds are usually the same as their empirical formulas.
- In order for ionic compounds to be electrically neutral, the sum of the charges on the cation and anion in each formula unit must be zero.
- Knowing the symbols and charges of the cations and anions is essential for formula of ionic compounds. For the monoatomic ions, you can figure out the charges from the position of the element in the periodic chart.
- If the charges are numerically equal, then no subscripts are necessary.
- If the charges on the cation and anion are numerically different, we apply the following rule to make the formula electrically neutral:

The subscript of the cation is numerically equal to the charge on the anion, and the subscript of the anion is numerically equal to the charge on the cation.

Crossover rule for ionic compounds

#12 Write formulas for compounds formed from these pairs of ions.

a. NH_4^{+1} and SO_3^{-2} $(NH_4)_2SO_3$

Always use parenthesis when you have more than one polyatomic ion (positive or negative) to avoid interpreting it as 42.

b. calcium ion and phosphate ion

Ca^{+2} and PO_4^{-3}

$Ca_3(PO4)_2$

Formula of Ionic Compounds and Lewis dot symbols

- In the formation of LiF, the following reaction occur:

$$2Li + F_2 \longrightarrow 2LiF$$

- Using Lewis dot symbols, we represent the formation of ionic bond between lithium and fluorine like this:

- We normally write the empirical formulas of ionic compounds without showing the charges. The + and - are shown here to emphasize the transfer of electrons. The compound itself is electrically neutral.

- Calcium burns in oxygen to form calcium oxide:

$$2Ca(s) + O_2(g) \longrightarrow 2CaO(s)$$

$$\cdot Ca \cdot + \cdot \ddot{\underset{\cdot\cdot}{O}} \cdot \longrightarrow Ca^{2+} \; : \ddot{\underset{\cdot\cdot}{O}} :^{2-}$$

$$[Ar]4s^2 \quad 1s^2 2s^2 2p^4 \quad [Ar] \quad [Ne]$$

- Lithium burns in air to form lithium oxide (Li2O):

$$4Li(s) + O_2(g) \longrightarrow 2Li_2O(s)$$

$$2 \cdot Li + \cdot \ddot{\underset{\cdot\cdot}{O}} \cdot \longrightarrow 2Li^+ \; : \ddot{\underset{\cdot\cdot}{O}} :^{2-} \text{ (or } Li_2O)$$

$$1s^2 2s^1 \quad 1s^2 2s^2 2p^4 \quad [He] \quad [Ne]$$

- When magnesium reacts with nitrogen at elevated temperatures, magnesium nitride (Mg3N2), forms:

$$3Mg(s) + N_2(g) \longrightarrow Mg_3N_2(s)$$

$$3 \cdot Mg \cdot + 2 \cdot \ddot{\underset{\cdot\cdot}{N}} \cdot \longrightarrow 3Mg^{2+} \; 2 : \ddot{\underset{\cdot\cdot}{N}} :^{3-} \text{ (or } Mg_3N_2)$$

$$[Ne]3s^2 \quad 1s^2 2s^2 2p^3 \quad [Ne] \quad [Ne]$$

Notes

- Although beryllium and magnesium related to group 2A and are metals, most beryllium compounds and some magnesium compounds (MgH_2, for example) are molecular rather than ionic in nature.
- Boron is a metalloid from group 3A, does not form binary ionic compounds. Other metallic elements in Group 3A form ionic and many molecular compounds.
- Take care that the following elements normally exist as diatomic molecules: hydrogen (H_2), nitrogen (N_2) and oxygen (O_2), as well as the Group 7A elements—fluorine (F_2), chlorine (Cl_2), bromine (Br_2), and iodine (I_2).

Naming ionic Compounds

- Metal cations take their names from the elements.

Na^+	sodium ion (or sodium cation)
K^+	potassium ion (or potassium cation)
Mg^{2+}	magnesium ion (or magnesium cation)
Al^{3+}	aluminum ion (or aluminum cation)

- The anion is named by taking the first part of the element name and adding "-ide.

Group 5A	Group 6A	Group 7A
N Nitride (N^{3-})	O Oxide (O^{2-})	F Fluoride (F^-)
P Phosphide (P^{3-})	S Sulfide (S^{2-})	Cl Chloride (Cl^-)
	Se Selenide (Se^{2-})	Br Bromide (Br^-)
	Te Telluride (Te^{2-})	I Iodide (I^-)

Naming ionic Compounds

- Many ionic compounds are **binary compounds,** or compounds formed from just two elements. For binary ionic compounds the first element named is the metal cation, followed by the nonmetallic anion.
- Thus, NaCl is sodium chloride. Potassium bromide (KBr), zinc iodide (ZnI_2), and aluminum oxide (Al_2O_3).

Naming ionic Compounds

- Other ionic substances are called **ternary compounds,** meaning compounds consisting of three elements.
- The “-ide” ending is also used for certain anion groups containing different elements, such as hydroxide (OH) and cyanide (CN).
- Thus, the compounds LiOH and KCN are named lithium hydroxide and potassium cyanide.

Some of the names and charges of common polyatomic cations and anions are listed in Table IV.

Table IV

Cations		Anions		
+1	**+2**	**–1**	**–2**	**–3**
NH_4^+ ammonium	VO^{2+} vanadyl	OH^- hydroxide		
H_3O^+ hydronium		CN^- cyanide	CrO_4^{2-} chromate	
NO^+ nitrosyl		MnO_4^- permanganate	$Cr_2O_7^{2-}$ dichromate	
		NO_2^- nitrite	SO_3^{2-} sulfite	AsO_3^{3-} arsenite
		NO_3^- nitrate	SO_4^{2-} sulfate	AsO_4^{3-} arsenate
		ClO^- hypochlorite		
		ClO_2^- chlorite		
		ClO_3^- chlorate		
		ClO_4^- perchlorate		
		HCO_3^- bicarbonate or hydrogen carbonate	CO_3^{2-} carbonate	
		$H_2PO_4^-$ dihydrogen phosphate	HPO_4^{2-} hydrogen phosphate	PO_4^{3-} phosphate
		CH_3COO^- acetate	$C_2O_4^{2-}$ oxalate	

Naming ionic Compounds

- Certain metals, especially the *transition metals,* can form more than one type of cation.
- Example: Iron can form two cations: Fe^{+2} and Fe^{+3}. For designating different cations of the *same* element use Roman numerals. The Roman numeral I is used for one positive charge, II for two positive charges, and so on. This is called the *Stock system*.
- In this system, the Fe^{+2} and Fe^{+3} ions are called iron (II) and iron (III), and the compounds $FeCl_2$ and $FeCl_3$ are called iron (II) chloride and iron (III) chloride, respectively.
- The old style system has different suffixes in their names. For example, Fe^{2+} is called the ferrous ion, and Fe^{3+} is called the ferric ion; Cu^{+} is the cuprous ion, and Cu^{2+} is the cupric ion. Notice that the ion with the lesser charge ends with –ous and the one with greater charges ends with –ic. In

Examples

KI	potassium ion + iodide ion = potassium iodide
$CoCl_2$	cobalt(II) ion + two chloride ions = cobalt(II) chloride
$CoCl_3$	cobalt(III) ion + three chloride ions = cobalt(III) chloride
Hg_2Cl_2	mercury(I) ion + two chloride ions = mercury(I) chloride or mercurous chloride
$AgNO_3$	silver ion + nitrate ion = silver nitrate It is not called silver(I) nitrate because Ag^+ is the only stable ion of silver.
$(NH_4)_2S$	two ammonium ions + sulfide ion = ammonium sulfide
$Al(HCO_3)_3$	aluminum ion + bicarbonate ion = aluminum bicarbonate or aluminum hydrogen carbonate

Cations of metals from groups 1A, 2A, and 3A have constant charges and do NOT get Roman Numerals in their names

a.	Barium nitride	Ba^{+2}	N^{-3}	Ba_3N_2
b.	Indium Fluoride	In^{+3}	F^{-1}	InF_3
c.	Calcium oxide	Ca^{+2}	O^{-2}	CaO
d.	Sodium nitride	Na^{+1}	N^{-3}	Na_3N
e.	Magnesium chloride	Mg^{+2}	Cl^{-1}	$MgCl_2$
f.	Potassium oxide	K^{+1}	O^{-2}	K_2O
g.	Magnesium oxide	Mg^{+2}	O^{-2}	MgO
h.	Potassium sulfide	K^{+1}	S^{-2}	K_2S
i.	Lithium nitride	Li^{+}	N^{-3}	Li_3N
j.	Strontium fluoride	Sr^{+2}	F^{-1}	SrF_2
k.	Aluminum sulfide	Al^{+3}	S^{-2}	Al_2S_3

Cations of Transition metals and metals from group 4A (Pb and Sn) and metals from group 5A (Bi) get Roman Numerals in their names

a.	SnO_2	oxide = O^{-2}	Tin (IV) oxide
b.	Mn_2O_7	oxide = O^{-2}	Manganese (VII) oxide
c.	FeN	nitride = N^{-3}	Iron (III) nitride
d.	Cu_3N_2	nitride = N^{-3}	Copper (II) nitride
e.	TiF_3	fluoride = F^{-1}	Titanium (III) fluoride
f.	Cu_2S	sulfide = S^{-2}	Copper (I) sulfide
g.	Fe_2S_3	sulfide = S^{-2}	Iron (III) sulfide
h.	CuBr	bromide = Br^{-1}	Copper (I) bromide
i.	Co_3N_2	nitride = N^{-3}	Cobalt (II) nitride
j.	CoF_2	fluoride = F^{-1}	Cobalt (II) fluoride

Nomenclature of multivalent cations

Systematic (new) common (old)

Symbol	Stock name	Classical name
Cu^{+}	Copper(I) ion	Cuprous ion
Cu^{2+}	Copper(II) ion	Cupric ion
Fe^{2+}	Iron(II) ion	Ferrous ion
Fe^{3+}	Iron(III) ion	Ferric ion
$^{*}Hg_2^{2+}$	Mercury(I) ion	Mercurous ion
Hg^{2+}	Mercury(II) ion	Mercuric ion
Pb^{2+}	Lead(II) ion	Plumbous ion
Pb^{4+}	Lead(IV) ion	Plumbic ion
Sn^{2+}	Tin(II) ion	Stannous ion
Sn^{4+}	Tin(IV) ion	Stannic ion
Cr^{2+}	Chromium(II) ion	Chromous ion
Cr^{3+}	Chromium(III) ion	Chromic ion
Mn^{2+}	Manganese(II) ion	Manganous ion
Mn^{3+}	Manganese(III) ion	Manganic ion
Co^{2+}	Cobalt(II) ion	Cobaltous ion
Co^{3+}	Cobalt(III) ion	Cobaltic ion

Ionic Compounds with Polyatomic Ions (ternary compounds)

a. $Co(NO_3)_2$ Cobalt (II) nitrate

b. $NaNO_2$ Sodium nitrite

c. $Cu_3(PO_3)_2$ Copper (II) phosphite

d. $Ba(CN)_2$ Barium cyanide

e. $Al_2(SO_4)_3$ Aluminum sulfate

f. $KClO_3$ Potassium chlorate

$Zn_3(PO_4)_2$ ____zinc phosphate____

NH_4NO_3 ____ammonium nitrate_

$Al(OH)_3$ ____aluminum hydroxid

$CuC_2H_3O_2$ ___copper (I) acetate__

$PbSO_3$ _____lead (II) sulfite___

$NaClO_3$ _____sodium chlorate__

$(NH_4)_3PO_4$ ___ammonium phosphate__

$NaHSO_4$ _____sodium hydrogen sulfate_

potassium permanganate _____$KMnO_4$__

sodium hydrogen carbonate _____$NaHCO_3$_

zinc nitrate _____$Zn(NO_3)_2$_

aluminum sulfite _____$Al_2(SO_3)_3$_

magnesium hydroxide _____$Mg(OH)_2$_

aluminum sulfate _____$Al_2(SO_4)_3$_

copper (II) sulfate _____$CuSO_4$___

. lead (IV) chromate _____$Pb(CrO_4)_2$_

Lattice Energy of Ionic Compounds

- **Ionic bonding** is the attraction between positively- and negatively-charged ions. These oppositely charged ions attract each other to form ionic networks (or **lattices**).
- When many ions attract each other, they form large, ordered, crystal lattices in which each ion is surrounded by ions of the opposite charge.

Lattice Energy of Ionic Compounds

- Thus, the overall stability of a solid ionic compound depends on the interactions of all these ions and not merely on the interaction of a single cation with a single anion.
- A quantitative measure of the stability of any ionic solid is its **lattice energy**, defined as the energy required to completely separate one mole of a solid ionic compound into gaseous ions.
- The larger the lattice energy, the more stable the solid and the more tightly held the ions, and so the solid has a higher melting point.

Lattice Energy of Ionic Compounds

- The lattice energy between two doubly charged species > that between a doubly charged ion and a singly charged ion > that between singly charged anions and cations.

Lattice Energies and Melting Points of Some Ionic Compounds

	Lattice Energy (kJ/mol)	Melting Point (°C)
LiF	1017	845
LiCl	828	610
NaCl	788	801
NaBr	736	750
$MgCl_2$	2527	714
MgO	3890	2800
CaO	3414	2580

Chapter 6

II- The Covalent Bond

Introduction

- **Covalent bond is** a bond in which two electrons are shared by two atoms.
- In a covalent bond, each electron in a shared pair is attracted to the nuclei of both atoms. This attraction holds the two atoms together.
- Covalent bonding between many-electron atoms involves only the valence electrons.
- The formation of these molecules illustrates the octet rule to achieve the stable noble gas configuration by sharing electrons.

Lewis structure

- The structures we use to represent covalent compounds, such as H2 and F2, are called Lewis structures.
- A Lewis structure is a representation of covalent bonding in which shared electron pairs are shown either as lines or as pairs of dots between two atoms, and lone pairs are shown as pairs of dots on individual atoms. Only valence electrons are shown in a Lewis structure.
- The formation of the F2 molecule can be represented as follows:

- For the sake of simplicity, the shared pair of electrons is often represented by a single line.

Lone pairs

- Note that only two valence electrons participate in the formation of F2. The other, nonbonding electrons, are called lone pairs. (these are pairs of valence electrons that are not involved in covalent bond formation). Thus, each F in F2 has three lone pairs of electrons.

Bond order

- Atoms can form different types of covalent bonds.
- In a single bond, two atoms are held together by one electron pair as F2 molecule.
- If two atoms share two pairs of electrons, the covalent bond is called a double bond, such as: carbon dioxide (CO2) and ethylene (C2H4):

Bond order

- A triple bond arises when two atoms share three pairs of electrons, as in the nitrogen molecule (N2) and acetylene molecule (C2H2):

Bond length

- Bond length is defined as the distance between the nuclei of two covalently bonded atoms in a molecule.
- Triple bonds are shorter than double bonds, which, in turn, are shorter than single bonds.
- The shorter multiple bonds are also

more stable than single bonds.

Bond Type	Bond Length (pm)
C—H	107
C—O	143
C=O	121
C—C	154
C=C	133
C≡C	120
C—N	143
C=N	138
C≡N	116
N—O	136
N=O	122
O—H	96

Electronegativity

- Electronegativity is the ability of an atom to attract the electrons toward itself in a chemical bond.
- Elements with high electronegativity have a greater tendency to attract electrons than do elements with low electronegativity.
- As we might expect, electronegativity is related to electron affinity and ionization energy.
- In general, electronegativity increases from left to right across a period in the periodic table, as the metallic character of the elements decreases.
- Within each group, electronegativity decreases with increasing atomic number, and increasing metallic character.

Increasing electronegativity

Increasing electronegativity

H 2.1	2A	3A	4A	5A	6A	7A	8A
Li 1.0	Be 1.5	B 2.0	C 2.5	N 3.0	O 3.5	F 4.0	
Na 0.9	Mg 1.2	Al 1.5	Si 1.8	P 2.1	S 2.5	Cl 3.0	
K 0.8	Ca 1.0	Ga 1.6	Ge 1.8	As 2.0	Se 2.4	Br 2.8	Kr 3.0
Rb 0.8	Sr 1.0	In 1.7	Sn 1.8	Sb 1.9	Te 2.1	I 2.5	Xe 2.6
Cs 0.7	Ba 0.9	Tl 1.8	Pb 1.9	Bi 1.9	Po 2.0	At 2.2	
Fr 0.7	Ra 0.9						

Writing Lewis Structures

1. **Write the skeletal structure of the compound**, using chemical symbols and placing bonded atoms next to one another. In general, the least electronegative atom occupies the central position. Hydrogen and fluorine usually occupy the terminal (end) positions in the Lewis structure.
2. **Count the total number of valence electrons present**. For polyatomic anions, add the number of negative charges to that total. For polyatomic cations, we subtract the number of positive charges from this total.
3. **Draw a single covalent bond between the central atom and each of the surrounding atoms**. **Complete the octets of the atoms** bonded to the central atom except a hydrogen atom is complete with only two electrons. Electrons belonging to the central or surrounding atoms must be shown as lone pairs if they are not involved in bonding. The total number of electrons to be used is that determined in step 2.
4. After completing steps 1–3, if the central atom has fewer than eight electrons, **try adding double or triple bonds between the surrounding atoms and the central atom**, using lone pairs from the surrounding atoms to complete the octet of the central atom.

Examples

- **Write the Lewis structure for nitrogen trifluoride (NF_3)?**

Step 1: The N atom is less electronegative than F, so the skeletal structure of NF_3 is

F N F

F

Step 2: There are 5+ (3 X 7)= 26, valence electrons to account for in NF_3.

Step 3: We draw a single covalent bond between N and each F, and complete the octets for the F atoms. We place the remaining two electrons on N.

Examples

- **Write the Lewis structure for nitric acid (HNO_3)?**

Step 1: The skeletal structure of HNO_3 is

O N O H

O

Step 2: There are 5 +(3 *6) + 1 = 24, valence electrons to account for in HNO_3.

Step 3: We draw a single covalent bond between N and each of the three O atoms and between one O atom and the H atom. Then we fill in electrons to comply with the octet rule for the O atoms:

Step 4: We see that this structure satisfies the octet rule for all the O atoms but not for the N atom. The N atom has only six electrons. Therefore, we move a lone pair from one of the end O atoms to form another bond with N.

Now the octet rule is also satisfied for the N atom.

Examples

- **Write the Lewis structure for the carbonate ion (CO_3) $^{-2}$**

Step 1: C is less electronegative than O. Therefore, it is most likely to occupy a central position as follows:

O

O C O

Step 2: Thus, the total number of electrons is 4 + (3* 6)+2 = 24.

Step 3: We draw a single covalent bond between C and each O and comply with the octet rule for the O atoms. This structure shows all 24 electrons.

Step 4: Although the octet rule is satisfied for the O atoms, it is not for the C atom. Therefore, we move a lone pair from one of the O atoms to form another bond with C.

Now the octet rule is also satisfied for the C atom.

Resonance

- A resonance structure is one of two or more Lewis structures for a particular molecule that cannot be represented accurately by only one Lewis structure. For example:

1- Ozone:

2- Carbonate ion:

3- Benzene:

- The double-headed arrow indicates that the structures shown are resonance structures.

Resonance

- ***Remember this important rule for drawing resonance structures:*** The positions of electrons (that is, bonds), but not those of atoms, can be rearranged in different resonance structures. In other words, the same atoms must be bonded to one another in all the resonance structures for a given species.
- Draw resonance structures (including formal charges) for the nitrate ion, NO_3^-

Formal Charges

- Sometimes there is more than one acceptable Lewis structure for a given species. In such cases, we can often select the most plausible Lewis structure by using formal charges.
- An atom's formal charge is the electrical charge difference between the valence electrons in an isolated atom and the number of electrons assigned to that atom in a Lewis structure.
- To assign the number of electrons on an atom in a Lewis structure, we proceed as follows:
  1. All the atom's nonbonding electrons (lone pairs) are assigned to the atom.
  2. We break the bond(s) between the atom and other atom(s) and assign half of the bonding electrons to the atom.

Rules of Formal Charges

- When you write formal charges, these rules are helpful:

1. For molecules, the sum of the formal charges must add up to zero because molecules are electrically neutral species.
2. For cations, the sum of the formal charges must equal the positive charge.
3. For anions, the sum of the formal charges must equal the negative charge.
4. A Lewis structure in which there are no formal charges is preferable to one in which formal charges are present.
5. Lewis structures with large formal charges (-2, -3, and/or +2, +3, and so on) are less plausible than those with small formal charges.
6. Among Lewis structures having similar distributions of formal charges, the most plausible structure is the one in which negative formal charges are placed on the more electronegative atoms.

Examples

- The ozone molecule (O_3).

Valence e^-	6	6	6
e^- assigned to atom	6	5	7
Difference (formal charge)	0	+1	−1

- The carbonate ion $(CO_3)^{-2}$

Examples

- Formaldehyde (CH_2O). The two possible skeletal structures

- Although both structures satisfy the octet rule, (b) is the more likely structure because it carries no formal charges, and because in (a) the more electronegative ion (O) carry a positive charge while the less electronegative ion carry a negative charge (less plausible).

Problems

- **Write the Lewis structure and formal charges for the following compounds:**

A- Formic acid (HCOOH).

B- The nitrite ion $(NO_2)^-$.

C- Carbon disulfide (CS2).

D- Ammonium ion $(NH_4)^+$.

Exceptions to the Octet Rule
1- The Incomplete Octet

- In some compounds, the number of electrons surrounding the central atom in a stable molecule is fewer than eight.
- The Lewis structure of BeH2 is

- Elements in Group 3A, particularly boron and aluminum, also tend to form compounds in which they are surrounded by fewer than eight electrons.
- The Lewis structure of boron trifluoride is

Exceptions to the Octet Rule

2. Odd-Electron Molecules

- Some molecules contain an odd number of electrons. Among them are nitric oxide (NO) and nitrogen dioxide (NO2): the octet rule clearly cannot be satisfied for all the atoms in any of these molecules.

- Odd-electron molecules are sometimes called radicals. Many radicals are highly reactive. The reason is that there is a tendency for the unpaired electron to form a covalent bond with an unpaired electron on another molecule. For example, when two nitrogen dioxide molecules collide, they form dinitrogen tetroxide in which the octet rule is satisfied for both the N and O atoms:

Exceptions to the Octet Rule
3- The Expanded Octet

- Atoms of the second-period elements cannot have more than eight valence electrons around the central atom, but atoms of elements in and beyond the third period of the periodic table form some compounds in which more than eight electrons surround the central atom.
- One compound in which there is an expanded octet is sulfur hexafluoride, a very stable compound.

Examples

- Draw the Lewis structure for phosphorus pentafluoride (PF_5).

- Draw the Lewis structure for aluminum triiodide (AlI_3).

- Draw the Lewis structure for$POCl_3$.

Nomenclature

- Naming binary molecular compounds is similar to naming binary ionic compounds.
- We place the name of the first element in the formula first, and the second element is named by adding "-ide" to the root of the element name. Some examples are:
  - HCl: Hydrogen chloride.
  - SiC: Silicon carbide
  - HBr: Hydrogen bromide

Greek Prefixes Used in Naming Molecular Compounds

Prefix	Meaning
mono-	1
di-	2
tri-	3
tetra-	4
penta-	5
hexa-	6
hepta-	7
octa-	8
nona-	9
deca-	10

Nomenclature

- It is quite common for one pair of elements to form several different compounds.
- In these cases, confusion in naming the compounds is avoided by the use of Greek prefixes to denote the number of atoms of each element present.
- Consider these examples:
  - CO Carbon monoxide
  - CO_2 Carbon dioxide
  - SO_2 Sulfur dioxide
  - SO_3 Sulfur trioxide
  - NO_2 Nitrogen dioxide
  - N_2O_4 Dinitrogen tetroxide

Notes

- The prefix “mono-” may be omitted for the first element. For example, PCl_3 is named phosphorus trichloride, not monophosphorus trichloride. Thus, the absence of a prefix for the first element usually means that only one atom of that element is present in the molecule.
- For oxides, the ending “a” in the prefix is sometimes omitted. For example, N_2O_4 may be called dinitrogen tetroxide rather than dinitrogen tetraoxide.

Nomenclature

- Exceptions to the use of Greek prefixes are molecular compounds containing hydrogen.
- Traditionally, many of these compounds are called either by their common, nonsystematic names or by names that do not specifically indicate the number of H atoms present:

B_2H_6 Diborane	PH_3 Phosphine
CH_4 Methane	H_2O Water
SiH_4 Silane	H_2S Hydrogen sulfide
NH_3 Ammonia	

- Note that even the order of writing the elements in the formulas is irregular. These examples show that H is written first in water and hydrogen sulfide, whereas H is written last in the other compounds.

Bond enthalpy

- The stability and strength of a covalent bond is measured in terms of its bond enthalpy, which is the enthalpy change required to break a particular bond in 1 mole of gaseous molecules.
- As stated earlier, triple bonds are stronger than double bonds, which, in turn, are stronger than single bonds.

Bond	Bond Enthalpy
H—F	568.2
H—Cl	431.9
H—Br	366.1
H—I	298.3
C—H	414
C—C	347
C=C	620
C≡C	812
C—N	276
C=N	615
C≡N	891

Problems

- **Name the following molecular compounds:**

(a) $SiCl_4$ (b) P_4O_{10} (c) NF_3 and (d) Cl_2O_7.

- **Write chemical formulas for the following molecular compounds:**

(a) carbon disulfide (b) disilicon hexabromide

(c) sulfur tetrafluoride (d) dinitrogen pentoxide.

- **Draw Lewis structures for the following compounds:**

HBr, H_2S, CH_4, ICl, PH_3, N_2H_4, $COBr_2$

- **Write Lewis structures for these species and Show formal charges and resonance forms if found :**

NO^+, NH_4^+ , CN^- , ClO_3^- , $HClO_3$, SO_4^- , H_2SO_4, PO_4^{-3} , H_3PO_4, OCN^-, CNO^-, N_2O, N_3^- , HN_3

سؤال مهم جدا

الحل موجود ضمن مراجعة الشابتر وتتم مناقشته في المحاضرة

General chemistry

Chapter 7

Molecular Geometry and Hybridization of Atomic Orbitals

Molecular Geometry

- Molecular geometry is the three-dimensional arrangement of atoms in a molecule. Recall that the geometry of a molecule is determined only by the arrangement of atoms.
- A molecule's geometry affects its physical and chemical properties, such as solubility, melting point, boiling point, density, and the types of reactions it undergoes.
- This approach to the study of molecular geometry is called the **valence-shell electron-pair repulsion (VSEPR) model, because it accounts for the geometric arrangements of electron pairs around a central atom in terms of the electrostatic repulsion between electron pairs.**
- **Electron pairs include bonding and non-bonding (lone) pairs.**

VSEPR model

- **Two general rules govern the use of the VSEPR model:**

1. As far as electron-pair repulsion is concerned, double bonds and triple bonds can be treated like single bonds. This approximation is good for qualitative purposes.

    - However, you should realize that in reality multiple bonds are "larger" than single bonds; that is, because there are two or three bonds between two atoms, the electron density occupies more space.

2. If a molecule has two or more resonance structures, we can apply the VSEPR model to any one of them. Formal charges are usually not shown.

A- Molecules in which the central atom has no lone pairs

- Here, we will consider molecules that contain atoms of only two elements, A and B, of which A is the central atom. These molecules have the general formula AB*x*, where *x* is an integer (*x* *often* is between 2 and 6).
- As a result of mutual repulsion, the electron pairs stay as far from one another as possible.
- Molecules in which the central atom has no lone pairs have one of five arrangements of bonding pairs.
- Here, arrangements of electron pairs is the same as geometry of molecules.

A- Molecules in which the central atom has no lone pairs					
Molecular formula	**No. of Electron pair groups** (bonding)	**Molecular geometry**		**Description of the shape**	**Examples**
AB_2	2	**B—A—B linear**		Because the bonding pairs repel each other, they must be at opposite ends of a straight line in order for them to be as far apart as possible. Thus, the BAB angle is predicted to be 180.	**Beryllium Chloride ($BeCl_2$)**
AB_3	3			In the most stable arrangement, the three BF bonds point to the corners of a planar equilateral triangle with B in the center of the triangle.	**Boron Trifluoride (BF_3)**
AB_4	4			A tetrahedron has four sides or faces, all of which are equilateral triangles	**Methane (CH_4)**
AB_5	5			The central atom (P in this case) is at the center of the common triangle with the surrounding atoms positioned at the five corners of the trigonal bipyramid.	**Phosphorus Pentachloride (PCl_5)**
AB_6	6			An octahedron has eight sides. It can be generated by joining two square pyramids on a common base.	**Sulfur Hexafluoride (SF_6)**

B- Molecules in which the central atom has one or more lone pairs

- Determining the geometry of a molecule is more complicated if the central atom has both lone pairs and bonding pairs.
- Here, we will we designate molecules with lone pairs as AB_xE_y, where A is the central atom, B is a surrounding atom, and E is a lone pair on A. Both x and y are integers; (x = 2, 3, . . . ,) and (y = 1, 2, ...).
- Here, arrangements of electron pairs is not the same as geometry of molecules.

B- Molecules in which the central atom has one or more lone pairs						
Molecular formula	No. of bonding pairs	No. of lone pairs	Molecular geometry		Description of the shape	Examples
AB_2E	2	1	Bent (angular)	SO_2	VSEPR treats double bonds as though they were single that the overall arrangement of three electron pairs is trigonal planar. But because one of the electron pairs is a lone pair, the SO2 **Molecular geometry** has a "bent" shape.	**Sulfur Dioxide (SO_2)**
AB_2E_2	2	2	Bent (angular)		Water has two lone pairs on the central O atom. These lone pairs tend to be as far from each other as possible. Consequently, the two OH bonding pairs are pushed toward each other,	**Water (H2O)**
AB_3E	3	1	Trigonal pyramidal		The overall arrangement of four electron pairs is tetrahedral. But in NH3 one of the electron pairs is a lone pair, so the geometry of NH3 is trigonal pyramidal (so called because it looks like a pyramid, with the N atom at the apex).	**Ammonia (NH3)**

- Electrons in a bond are held by the attractive forces exerted by the nuclei of the two bonded atoms. So bonding electrons take up less space than lone-pair electrons, which are associated with only one particular atom.
- Because lone-pair electrons in a molecule occupy more space, they experience greater repulsion from neighboring lone pairs and bonding pairs.
- In such molecules there are three types of repulsive forces:
  - Those between two bonding pairs.
  - Those between two lone pairs.
  - Those between a bonding pair and a lone pair.
- In general, according to the VSEPR model, the repulsive forces decrease in the following order:
  - lone-pair vs. lone-pair > lone-pair vs. bonding pair repulsion > bonding-pair vs. bonding pair repulsion

(a)

(b)

Geometry of molecules with more than one central atom

- The overall geometry of molecules with more than one central atom is difficult to define in most cases. Often we can describe only the shape around each of the central atoms.
- **Example: methanol, CH_3OH**.

Tetrahedral about the C atom.

Bent about the O atom.

Guidelines for Applying the VSEPR Model

1. Write the Lewis structure of the molecule, considering only the electron pairs around the central atom.

2. Count the number of electron pairs around the central atom (bonding pairs and lone pairs) using the VSEPR model. Treat double and triple bonds as though they were single bonds.

3. Refer to the previous tables to predict the geometry of the molecule.

Examples

Carbonate ion

Lewis structure

Molecular geometry
(trigonal planar)

hydronium ion

trigonal pyramidal

Problems

Use the VSEPR model to predict the geometry of the following molecules and ions:

(a) AsH_3, (b) OF_2, (c) $AlCl_4^-$, (d) C_2H_4.

Lewis structure				
Molecular geometry	trigonal pyramidal	bent	tetrahedral	The arrangement around each C atom has a trigonal planar shape

Valence Bond Theory

- It give a more complete explanation of chemical bond formation in terms of quantum mechanics.
- It assumes that the electrons in a molecule occupy atomic orbitals of the individual atoms taking in consideration energy changes in chemical bond formation.
- The **Lewis theory** describes the H—H bond in terms of the pairing of the two electrons on the H atoms. In the framework of **valence bond theory**, the covalent H—H bond is formed by the overlap of the two 1s orbitals in the H atoms. Each orbital has a single electron.

Top to bottom: As two H atoms approach each other, their 1s orbitals begin to interact and each electron begins to feel the attraction of the other proton.

Gradually, the electron density builds up in the region between the two nuclei (red color).

Eventually, a stable H_2 molecule is formed when the internuclear distance is 74 pm.

Valence Bond Theory

- F2 molecule forms when the 2p orbital (containing the unpaired electrons) in the two F atoms overlap to form a covalent bond.

- Similarly, the formation of the HF molecule can be explained by the overlap of the 1s orbital in H with the 2p orbital in F.

Valence Bond Theory

- In each case, VB theory accounts for the changes in energy between the reacting atoms.
- Because the orbitals involved are not the same kind in all cases, we can see why the bond enthalpies and bond lengths in H_2, F_2, and HF might be different.
- Lewis theory treats all covalent bonds the same way and offers no explanation for the differences among covalent bonds.

Hybridization

- The concept of atomic orbital overlap should apply also to polyatomic molecules.
- The overlap of bonding orbitals is substantially increased through a process called *hybridization*, which results in the formation of stronger bonds.
- **Hybridization** is the term applied to the mixing of atomic orbitals in an atom (usually a central atom) to generate a set of hybrid orbitals.
- **Hybrid orbitals**, which are atomic orbitals obtained when two or more nonequivalent orbitals of the same atom combine in preparation for covalent bond formation.
- The number of hybrid orbitals generated is equal to the number of pure atomic orbitals that participate in the hybridization process

Hybridization

- ***It is important to understand the relationship between hybridization and the VSEPR model. We use hybridization to describe the bonding scheme only when the arrangement of electron pairs (both bonding and lone pairs) has been predicted using VSEPR.***

sp^3 Hybridization

- **CH_4 molecule.**
- Focusing only on the valence electrons, we can represent the orbital diagram of C as

- By promoting a 2s electron to the 2p orbital, we get the excited state:

- The 2*s* and 2*p* orbitals then mix to form 4 hybrid orbitals:

- The 4 C—H bonds are formed by the overlap of the C sp^3 orbitals with the 1s orbitals of the H atoms. Thus, CH_4 is a tetrahedral molecule.

z
y
x
2s
2p_x
2p_y
2p_z
Hybridization
sp³

H
C
H
H
H

sp^3 Hybridization

- **Ammonia (NH_3)**
- The orbital diagram of N

- As the orbital diagram for the sp^3 hybridized N atom

- Three of the four hybrid orbitals form covalent N—H bonds, and the fourth hybrid orbital accommodates the lone pair on nitrogen

sp Hybridization

- The beryllium chloride ($BeCl_2$) molecule is predicted to be linear by VSEPR.
- The orbital diagram for the valence electrons in Be is

- First, we promote a 2s electron to a 2p orbital, resulting in exited state

- The 2s and 2p orbitals mixed, or hybridized, to form two equivalent sp hybrid orbitals

- Each of the BeCl bonds is then formed by the overlap of a Be sp hybrid orbital and a Cl 3p orbital, and the resulting $BeCl_2$ molecule has a linear geometry

z
y
x
2s
z
y
x
$2p_x$
Hybridization
z
y
x
sp
z
y
x
sp

Cl
Be
Cl

sp^2 Hybridization

- BF_3 (boron trifluoride) molecule, known to have trigonal planar geometry based on VSEPR.
- The orbital diagram of B is

- We promote a 2s electron to an empty 2p orbital:

- Mixing the 2s orbital with the two 2p orbitals generates three sp^2 hybrid orbitals

- Each of the BF bonds is formed by the overlap of a boron sp^2 hybrid orbital and a fluorine 2p orbital

orbitals of fluorine. The BF_3 molecule is planar, and all FBF angles are 120°.

sp^3d Hybridization

- PBr_5, five pairs of electrons around P.
- The orbital diagram of the ground-state P atom is

- Promoting a 3s electron into a 3d orbital results in the following excited state:

- Mixing the one 3s, three 3p, and one 3d orbitals generates five sp^3d hybrid orbitals:

- These hybrid orbitals overlap with the 4p orbitals of Br to form five covalent P—Br bonds.

sp^3d^2 Hybridization

- SF_6 molecule has six electron pairs around P.
- The orbital diagram of S is

- Because the 3d level is quite close in energy to the 3s and 3p levels, we can promote 3s and 3p electrons to two of the 3d orbitals

- Mixing the 3s, three 3p, and two 3d orbitals generates six sp3d2 hybrid orbitals

- The six S—F bonds are formed by the overlap of the hybrid orbitals of the S atom with the 2p orbitals of the F atoms

Important note

- Second period elements, unlike third-period elements, do not have 2d energy levels, so they can never expand their valence shells. Hence, atoms of second-period elements can never be surrounded by more than eight electrons in any of their compounds (no expanded octet).

Hybridization in Molecules Containing Double and Triple Bonds

- Ethylene molecule, C_2H_4, The Lewis structure of C_2H_4 is

- There are **three electron pairs** around each C atom, the arrangement around each C atom has a trigonal planar. So each C atom has sp^2 hybrid orbitals

The sp^2 hybridization of a carbon atom. The 2s orbital is mixed with only two 2p orbitals to form three equivalent sp^2 hybrid orbitals. This process leaves an electron in the unhybridized orbital, the $2p_z$ orbital.

Each carbon atom in the C2H4 molecule has three sp^2 hybrid orbitals and one unhybridized $2p_z$ orbital, which is perpendicular to the plane of the hybrid orbitals.

Bonding in ethylene, C_2H_4.

(a) Top view of the sigma bonds between carbon atoms and between carbon and hydrogen atoms using the three sp2 hybridized orbitals. All the atoms lie in the same plane, making C_2H_4 a planar molecule. **(b)** Side view showing how the two $2p_z$ orbitals on the two carbon atoms overlap, leading to the formation of a pi bond.

(c) The interactions in (a) and (b) lead to the formation of the sigma bonds and the pi bond in ethylene. Note that the pi bond lies above and below the plane of the molecule.

- The acetylene molecule (C_2H_2) contains a carbon-carbon triple bond. Because the molecule is linear, we can explain its geometry and bonding by assuming that each C atom is sp-hybridized by mixing the 2s with the $2p_x$ orbital.
- The two sp hybrid orbitals of each C atom form one sigma bond with a hydrogen 1s orbital and another sigma bond with the other C atom. In addition, two pi bonds are formed by the sideways overlap of the unhybridized 2py and 2pz orbitals. Thus, the $C{\equiv}C$ bond is made up of one sigma bond and two pi bonds.

Ground state
2s
2p
Promotion of electron
2s
2p
sp-Hybridized state
sp orbitals
2p_y 2p_z

H 1s
H 1s
C
C

2p_z
2p_z
C
C
2p_y
2p_y

H
σ
C
π
π
π
C
π
σ
H

Sigma and pi bonds

- Although we normally represent the carbon-carbon double bond as C=C (as in a Lewis structure), it is important to keep in mind that the two bonds are different types: One is a sigma bond and the other is a pi bond. The trible bond is made up of one sigma bond and two pi bonds.
- Sigma bonds (σ bonds), covalent bonds formed by orbitals overlapping end-to-end, with the electron density concentrated between the nuclei of the bonding atoms.
- The second type is called a pi bond (π bond), which is defined as a covalent bond formed by sideways overlapping orbitals with electron density concentrated above and below the plane of the nuclei of the bonding atoms.
- In fact, the bond enthalpies of the carbon-carbon pi and sigma bonds are about 270 kJ/mol and 350 kJ/mol, respectively. So the sigma bond is stronger than pi bonds.