Chapter 7 Notes – Chemistry; Chemical Formulas and Chemical Compounds

Molecules and Molecular Compounds

- A **molecule** consists of two or more atoms bounded together.

Molecules and Chemical Formulas

- Each molecule has a **chemical formula.**
- The chemical formula indicates:

1. Which atoms are found in the molecule, and
2. In what proportion they are found.

- A molecule made up of two atoms is called a **diatomic molecule.**
- Different forms of an element which have different chemical formulas are know as allotropes.
  - Allotropes differ in their chemical and physical properties.
- Compounds composed of molecules are **molecular compounds.**
  - These contain at least two types of atoms.
  - Most molecular substances contain only nonmetals.

Molecular and Empirical Formulas

- **Molecular formulas**
  - Give the actual numbers and types of atoms in a molecule.
  - Examples: H_2O, CO_2, CO, CH_4, H_2O_2, O_2, O_3, and C_2H_4.
- **Empirical formulas**
  - give the relative numbers and types of atoms in a molecule (they give the lowest whole-number ratio of atoms in a molecule).
  - Examples: H_2O, CO_2, CO, CH_4,HO, CH_2.

Picturing Molecules

- Molecules occupy three-dimensional space.
- However, we often represent them in two dimensions.
- The **structural formula** gives the connectivity between individual atoms in a molecule.
- The structural formula may or may not be used to show the three-dimensional shape of the molecule.
- If the structural formula does show the shape of the molecule then either a perspective drawing, ball-and -stick model or space filling model is used.
  - *Perspective drawings* use dashed lines and wedges to represent bonds receding and emerging from the plane of the paper.
  - *Ball-and-stick models* show atoms as contracted spheres and the bonds as sticks.
    - The angles in the ball-and-stick model are accurate.
    - *Space-filling models* give an accurate representation of the relative sizes of the atoms and the 3D shape of the molecule.

Ions and Ionic Compounds

- If electrons are added to or removed from a neutral atom, an **ion** is formed.
- When an atom or molecule loses electrons it becomes positively charged.
  - Positively charged ions are called **cations.**
- When an atom or molecule gains electrons it becomes negatively charged.
  - Negatively charged ions are called **anions**.
- In general, metal atoms tend to lose enough electrons to have the same number of electrons as the nearest noble gas (group 8A).
- The number of electrons an atom loses is related to its position on the periodic table.

Ionic Compounds

- A great deal of chemistry involves the transfer of electrons between species.
- Example:
  - To form NaCl, the neutral sodium atom, Na must lose an electron to become a cation: Na+
  - The electron cannot be lost entirely, so it is transferred to a chlorine atom, Cl, which then becomes an anion: Cl-.
  - The Na+ and Cl- ions are attracted to form an ionic NaCl lattice which crystallizes.
- NaCl is an example of an **ionic compound –** consisting of positively charged cations and negatively charged anions.
  - Important: Note that there are no easily identified NaCl molecules in the ionic lattice. Therefore, we cannot use molecular formulas to describe ionic substances.
- In general, ionic compounds are combinations of metals and nonmetals, whereas molecular compounds are composed of nonmetals only.
- Writing empirical formulas for ionic compounds.
  - You need to know the ions of which it is composed.
  - The formula must reflect the electrical neutrality of the compound.
  - You must combine cations and anions in a ratio so that the total positive charge is equal to the total negative charge.
  - Example: Consider the formation of Mg_3N_2
    - Mg loses two electrons to become Mg^{2+}
    - Nitrogen gains three electrons to become N^{3-}
    - For a neutral species, the number of electrons lost and gained must be equal.
    - However, Mg can only lose electrons in twos and N can only accept electrons in threes.
    - Therefore, Mg needs to to lose sin electrons (2x3) and N gains those six electrons (3x2).
    - That is , 3Mg atoms need to form $3Mg^{2+}$ ions (total 3x2 positive charges) and 2N atoms need to form $2N^{3-}$ ions (total 2x3 negative charges).
    - Therefore, the formula is Mg_3N_2.

Chemistry and Life: Elements Required by Living Organisms

- Of the 115 elements known, only 26 are required for life.
- Water accounts for more than 70% of the mass of the cell.
- Carbon is the most common solid constituent of cells.
- The most important elements for life are H,C,N,O,P, and S.
- The next most important ions are Na+, Mg2+,K+, Ca2+, and Cl-.
- The other 15 elements are only needed in trace amounts.

Naming Inorganic Compounds

- Chemical nomenclature: the naming of substances.
- Common names: traditional names for substances (e.g., water, ammonia)
- Systemic names: naming based on a systemic set of rules.
  - Divided into organic compounds (those containing C, usually in combination with H,O,N, or S) and inorganic compounds (all other compounds).

Names and Formulas of Ionic Compounds

1. Positive Ions (Cations)

- Cations formed from a metal have the same name as the metal.
  - Example: Na+ = sodium ion
  - Ions formed from a single atom are called *monatomic ions.*
- Many transition metals exhibit variable charge.

- If the metal can form more than one cation, then the charge is indicated in parentheses in the name.
  - Examples: Cu+ = copper (I) ion; Cu+2 = copper (II) ion.
- An alternative nomenclature method uses the endings *-ous* and *-ic* to represent the lower and higher charged ions respectively.
  - Examples: Cu+ = cuprous ion; Cu+2 = cupric ion.
- Cations formed from non-metals end in **-ium**.
  - Examples: NH_4+ = ammonium ion; H_3O+ = hydronium ion

2. Negative Ions (Anions)

- Monoatomic anions (with only one atom) use the ending **-ide.**
  - Example: Cl- is the chloride ion.
- Some polyatomic anions also use the -ide ending.
  - Examples: hydroxide, cyanide, and peroxide ions.
- Polyatomic anions (with many atoms) containing oxygen are called **oxyanions.**
  - Their names end in **-ate** or **-ite.** (The one with more oxygen are called **-ate.**)
  - Examples: NO_3- is nitr**ate**, NO_2- is nitr**ite**.
- Polyatomic anions containing oxygen with more than two members in the series are named as follows (in order of **decreasing oxygen**):
- **per-...-ate** example: ClO_4- **per**chlor**ate**
- **-ate** ClO_3- chlor**ate**
- **-ite** ClO_2- chlor**ite**
- **hypo-...-ite** ClO- **hypo**chlor**ite**
- Polyatomic anions containing oxygen with additional hydrogens are named by adding hydrogen or bi- (one H), dihydrogen (two H) etc. to the name as follows:
- CO_3- is the carbon**ate** anion
- HCO_3- is the hydrogen carbonate (or **bi**carbonate) anion.
- H_2PO_4- is the **dihydrogen** phosphate anion.

3. Ionic Compounds

- These are named cation then anion
- Example: $BaBr_2$ = barium bromide

Names and Formulas of Acids

- Acids: Substances that yield hydrogen ions when dissolved in water (Arrhenius definition).
  - The names of acids are related to the names of anions:
  - -ide becomes **hydro...-ic** acid; example: HCl **hydro**chlor**ic** acid
  - -ate becomes -**ic** acid; $HClO_4$ perchlor**ic** acid
  - -ite becomes -**ous** acid HClO hypochlor**ous** acid

Names and Formulas for Binary Molecular Compounds

- Binary molecular compounds have two elements.
- The most metallic element (i.e. the one to the farthest left on the periodic table) is usually written first. Exception NH_3
- If both elements are in the same group, the lower one is written first.
- Greek prefixes are used to indicate the number of atoms (e.g., mono, di, tri).
  - The prefix mono is never used with the first element (i.e. carbon monoxide, CO).
- Examples;
  - Cl_2O is **di**chlorine *mon*oxide
  - N_2O_4 is **di**nitrogen *tetr*oxide

- NF_3 nitrogen *trif*luoride
- P_4S_{10} is **tetra**phosphorus *deca*sulfide

Oxidation Numbers

- Electrons are not explicitly shown in chemical equations.
- **Oxidation numbers** (or *oxidation states*) help keep track of electrons during chemical reactions.
- Oxidation numbers are assigned to atoms using specific rules.
  - For an atom in its *elemental form*, the oxidation number is always zero.
  - For any *monatomic ion*, the oxidation number equals the charge on the ion.
  - *Nonmetals* usually have negative oxidation numbers.
    - The oxidation number of *oxygen* is usually -2.
      - The major exception is in peroxides (containing the O_2 -2 ion).
  - The oxidation number of *hydrogen* is +1 when bonded to nonmetals and -1 when bonded to metals.
  - The oxidation number of *fluorine* is -1 in all compounds. The other *halogens* have an oxidation number of -1 in most binary compounds.
  - The *sum of the oxidation numbers* of all atoms in a neutral compound is zero.
  - The sum of the oxidation numbers in a polyatomic ion equals the charge on the ion.
- The oxidation of an element is evidenced by its increase in oxidation number; reduction is accompanied by its decrease in oxidation number.

Empirical Formulas from Analysis

- Recall that the empirical formula gives the *relative* number of atoms in a molecule.
- Finding empirical formula from mass percent data:
  - We start with the mass percent of elements (i.e. empirical data) and calculate a formula.
  - Assume we start with 100 g of sample.
  - The mass percent then translates as the number of grams of each element in 100 g of sample.
  - From these masses, the number of moles can be calculated (using the atomic weights from the periodic table).
  - The lowest whole-number ratio of moles is the empirical formula.
- Finding the empirical mass percent of elements from the empirical formula.
  - If we have the empirical formula, we know how many moles of each element is present in one mole of the same.
  - Then we use molar masses (or atomic weights) to convert to grams of each element.
  - We divide the number of grams of element by grams of 1 mole of sample to get the fraction of each element in 1 mole of sample.
  - Multiply each fraction by 100 to convert to a percent.

Molecular Formula from Empirical Formula

- The empirical formula (relative ratio of elements in the molecule) may not be the molecular formula (actual ratio of elements in the molecule).
- Example: ascorbic acid (vitamin C) has an empirical formula $C_3H_4O_3$.
  - The molecular formula is $C_6H_8O_6$.
  - To get the molecular formula from the empirical formula, we need to know the molecular weight, (MW).
  - The ratio of the MW to the formula weight (FW) of the empirical formula must be a whole number.