CHAPTER 3

CHEMICAL COMPOUNDS

KEY CONCEPTS:

1. MOLECULAR VS. IONIC COMPOUNDS

2. MOLECULAR VS. EMPIRICAL FORMULAS

3. MOLECULAR MASS VS. MOLAR MASS

4. COMBUSTION ANALYSIS

5. OXIDATION STATES

6. NAMING INORGANIC COMPOUNDS

Molecular Compounds

- **molecule:** an assembly of at least two atoms, held together in a discrete conformation by chemical forces
- **ion:** a molecule that has gained or lost an electron
  - cation: positively charged
  - anion: negatively charged
- **ionic compound:** a stable ionic lattice formed of cations and anions

Chemical Formulas

Molecular formula:

- indicates the exact number of atoms of each element contained in the smallest chemical unit of a substance

Empirical formula:

- indicates the simplest whole number RATIO in which elements are present in a substance

Hydrogen peroxide is a molecule that contains 2 atoms of H and two atoms of O

The molecular formula is H_2O_2

The empirical formula is HO

Molecular Mass/Molecular Weight

Molecular Mass

molecular mass = sum of atomic mass of each atom in the molecule (in amu)

Molar Mass of Molecules

mass in grams of 1 mole of the molecule

H_20

Molecular Mass: mass of one molecule 18.015 amu

Molar Mass: mass of one mole of molecules 18.015 g/mol

GLUCOSE ($C_6H_{12}O_6$)

Molecular Mass: Use the naturally occurring mixture of isotopes,

$$6 \times 12.01 + 12 \times 1.01 + 6 \times 16.00 = \mathbf{180.18\ amu}$$

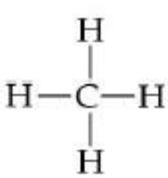
Exact Mass: Use the most abundant isotopes,

$$6 \times 12.000000 + 12 \times 1.007825 + 6 \times 15.994915$$

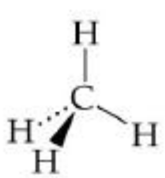
$$= \mathbf{180.06339\ amu}$$

Picturing Molecules

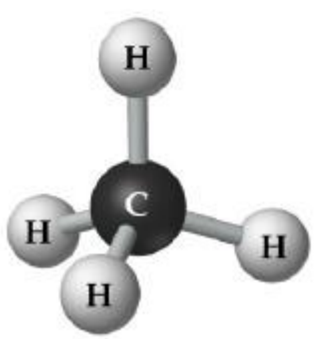
Molecules occupy three dimensional space:



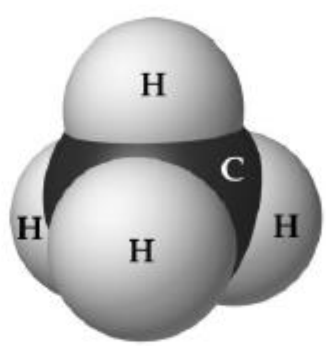
Structural formula



Perspective drawing



Ball-and-stick model

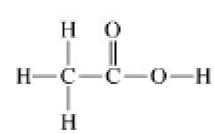


Space-filling model

Empirical formula: CH_2O

Molecular formula: $C_2H_4O_2$

Structural formula:



Determination of Empirical Formula Combustion Analysis

Example 1: Using Combustion Data

Complete combustion of a 1.505 g sample of an unknown compound consisting of C, H and S yields 3.149 g CO_2, 0.645 g H_2O and 1.146 g of SO_2. What is the empirical formula for the unknown?

Solution

Step 1: Convert the mass of each product into moles.

$$? \text{ mol C} = 3.149 \text{ g } CO_2 \bullet \frac{\text{mol } CO_2}{44.010 \text{ g } CO_2} \bullet \frac{1 \text{ mol C}}{1 \text{ mol } CO_2} = 0.07155 \text{ mol C}$$

$$? \text{ mol H} = 0.645 \text{ g } H_2O \bullet \frac{\text{mol } H_2O}{18.02 \text{ g } H_2O} \bullet \frac{2 \text{ mol H}}{1 \text{ mol } H_2O} = 0.07160 \text{ mol H}$$

$$? \text{ mol S} = 1.146 \text{ g } SO_2 \bullet \frac{\text{mol } SO_2}{64.06 \text{ g } SO_2} \bullet \frac{1 \text{ mol S}}{1 \text{ mol } SO_2} = 0.01789 \text{ mol S}$$

Solution

Step 2: Write a tentative formula. $C_{0.07155}H_{0.07160}S_{0.01789}$

Step 3: Divide by the smallest value.

$$C_{\frac{0.07155}{0.01789}}H_{\frac{0.07160}{0.01789}}S_{\frac{0.01789}{0.01789}} = C_4H_4S$$

empirical formula

N.B. To determine the ***molecular formula***, we need to know the ***molecular mass***!

Example 2: Using Combustion Data

When an unknown compound is decomposed into its constituent elements, it is found to contain 71.65% Cl, 24.27% C, and 4.07% H by mass. What is the empirical formula for the unknown?

Solution

Step 1: Determine the number of moles of each element in a 100 g sample.

$$? \text{ mol Cl} = 100 \text{ g sample} \bullet \frac{71.65 \text{ g Cl}}{100 \text{ g sample}} \bullet \frac{\text{mol Cl}}{35.45 \text{ g Cl}} = 2.021 \text{ mol Cl}$$

$$? \text{ mol C} = 100 \text{ g sample} \bullet \frac{24.27 \text{ g C}}{100 \text{ g sample}} \bullet \frac{\text{mol C}}{12.01 \text{ g C}} = 2.021 \text{ mol C}$$

$$? \text{ mol H} = 100 \text{ g sample} \bullet \frac{4.07 \text{ g H}}{100 \text{ g sample}} \bullet \frac{\text{mol H}}{1.008 \text{ g H}} = 4.04 \text{ mol H}$$

Step 2: Write a tentative formula. $Cl_{2.021}\ C_{2.021}\ H_{4.04}$

Step 3: Divide by the smallest value.

$$Cl_{\frac{2.021}{2.021}}C_{\frac{2.021}{2.021}}H_{\frac{4.04}{2.021}} = Cl_1C_1H_2$$

empirical formula

N.B. To determine the ***molecular formula***, we need to know the ***molecular mass***!

Step 1: Determine the mass of the *empirical formula*.

$$\text{EF mass} = 1 \text{ Cl} \bullet \frac{35.45 \text{ amu}}{\text{Cl}} + 1 \text{ C} \bullet \frac{12.01 \text{ amu}}{\text{C}} + 2 \text{ H} \bullet \frac{1.008 \text{ amu}}{\text{H}} = 49.48 \text{ amu}$$

Step 2: Divide the MF mass by the EF mass.

$$\text{Stoichiometric factor} = \frac{\text{MF mass}}{\text{EF mass}} = \frac{98.96 \text{ amu}}{49.48 \text{ amu}} = 2$$

Step 3. Multiply the empirical formula by the stoichiometric factor to obtain the *molecular formula*.

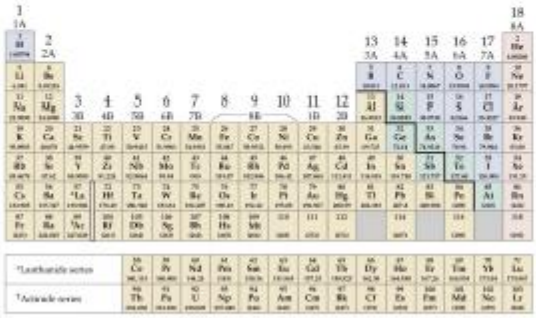
$$Cl_1C_1H_2 \bullet 2 = Cl_2C_2H_4$$

Therefore, the correct molecular formula is $Cl_2C_2H_4$.

Oxidation States

Metals tend to lose electrons.

$Na \rightarrow Na^+ + e^-$



Non-metals tend to gain electrons.

$Cl + e^- \rightarrow Cl^-$

Reducing agents

Oxidizing agents

We use the ***Oxidation State*** to keep track of the number of electrons that have been gained or lost by an element.

Oxidation Numbers – A useful means of electron "accounting"

- Oxidation number for an ion: the charge on the ion.
- Oxidation number for an atom: the hypothetical charge that atom would have if it was an ion.

Oxidation State Rules, p. 82-83

Oxidation numbers are assigned by a series of rules:

1. If the atom is in its elemental form, the oxidation number is zero. e.g., Cl_2, H_2, P_4.
2. For a monoatomic ion, the charge on the ion is the oxidation state.
3. Nonmetal *usually* have negative oxidation numbers:
   a) Oxidation number of O is usually –2. (peroxide ion, O_2^{2-}, has oxygen with an oxidation number of –1.
   b) Oxidation number of H is +1 when bonded to nonmetals and –1 when bonded to metals.
   c) The oxidation number of F is –1.
4. The sum of the oxidation numbers for the atom is the charge on the molecule (zero for a neutral molecule).
5. In their compounds, the alkali metals and the alkaline earths have OS of +1 and +2 respectively.

- if two rules contradict each other, follow the rule that appears *higher* in the list.
- the sum of the oxidation states of all the atoms *must be equal to* the charge of the ion or molecule
- for a multi-atom species, label the easy oxidation states, and solve for the unknown atoms

Naming binary compounds

- prefixes are used to indicate the numbers of each element in the compound (Table 3.2)

Number	Prefix	Example
1	*mono-*	NO: nitrogen monoxide
2	*di-*	NO_2: nitrogen dioxide
3	*tri-*	N_2O_3: dinitrogen trioxide
4	*tetra-*	N_2O_4: dinitrogen tetroxide
5	*penta-*	N_2O_5: dinitrogen pentoxide
6	*hexa-*	SF_6: sulfur hexafluoride

Naming inorganic compounds

- Some examples:

KNO_3	**potassium nitrate**
NH_4Cl	**ammonium chloride**
$KMnO_4$	**potassium permanganate**
$Ca(SCN)_2$	**calcium thiocyanate**

- Hydrates:
  - an ionic compound containing a fixed number of molecules of water

$CaCl_2 \cdot 6H_2O$ = calcium chloride hexahydrate

$MgSO_4 \cdot 2H_2O$ = magnesium sulfate dihydrate

Ions

When # protons ≠ # electrons, the species has a net charge and is called an **ION**.

- When an atom or molecule loses electrons, it becomes positively charged. Positively charged ions are called *cations*.

$$Na \rightarrow Na^{+} + e^{-}$$

- When an atom or molecule gains electrons, it becomes negatively charged. Negatively charged ions are called *anions*.

$$Cl + e^{-} \rightarrow Cl^{-}$$

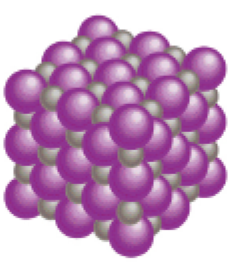
Ionic compounds

- Atoms of almost all elements can gain *or* lose electrons to form charged species called *ions*.
- Compounds composed of ions are known as *ionic compounds*.

Metals tend to lose electrons to form positively charged ions called ***cations***.

Non-metals tend to gain electrons to form negatively charged ions called ***anions***.

Ionic compounds



- there are no distinct molecules, so the empirical formula is used
- as shown in the figure, each Na^{+} is associated with 6 Cl^{-}, and each Cl^{-} is associated with 6 Na^{+}
- NaCl = an ionic compound formed of two ions with charges of +1 and -1
- however, other ionic compounds can have different lattice structures with different charges, but:

the overall crystal must be electrically neutral!

Naming Ionic Compounds

- for ionic compounds, the cation is named first, then the anion
- prefixes are avoided when possible
- if necessary, the oxidation state of the cation is added as Roman numeral in brackets

KBr	potassium bromide
$CaCl_2$	calcium chloride
Al_2O_3	aluminum oxide
FeI_2	iron (II) iodide

- Sometimes, the anion or cation is *polyatomic*:
  - NH_4^+ : ammonium
  - CO_3^{2-}: carbonate
  - OH^- : hydroxide
- the suffixes *–ite* and *-ate* and the prefixes *hypo-* and *per-* are used to indicate the oxidation state of the nonmetal atom in an oxoanion

Increasing number of oxygen atoms

ClO^-	hypochlorite
ClO_2^-	chlorite
ClO_3^-	chlorate
ClO_4^-	perchlorate

TABLE 3.3 Some Common Polyatomic Ions

Name	Formula	Typical Compound	Name	Formula	Typical Compound
Cation			**Anions**		
Ammonium ion	NH_4^+	NH_4Cl	Nitrite ion	NO_2^-	$NaNO_2$
Anions			Nitrate ion	NO_3^-	$NaNO_3$
Acetate ion	$C_2H_3O_2^-$	$NaC_2H_3O_2$	Oxalate ion	$C_2O_4^{2-}$	$Na_2C_2O_4$
Carbonate ion	CO_3^{2-}	Na_2CO_3	Permanganate ion	MnO_4^-	$NaMnO_4$
Hydrogen carbonate ion[a] (or bicarbonate ion)	HCO_3^-	$NaHCO_3$	Phosphate ion	PO_4^{3-}	Na_3PO_4
			Hydrogen phosphate ion[a]	HPO_4^{2-}	Na_2HPO_4
Hypochlorite ion	ClO^-	$NaClO$	Dihydrogen phosphate ion[a]	$H_2PO_4^-$	NaH_2PO_4
Chlorite ion	ClO_2^-	$NaClO_2$	Sulfite ion	SO_3^{2-}	Na_2SO_3
Chlorate ion	ClO_3^-	$NaClO_3$	Hydrogen sulfite ion[a] (or bisulfite ion)	HSO_3^-	$NaHSO_3$
Perchlorate ion	ClO_4^-	$NaClO_4$			
Chromate ion	CrO_4^{2-}	Na_2CrO_4	Sulfate ion	SO_4^{2-}	Na_2SO_4
Dichromate ion	$Cr_2O_7^{2-}$	$Na_2Cr_2O_7$	Hydrogen sulfate ion[a] (or bisulfate ion)	HSO_4^-	$NaHSO_4$
Cyanide ion	CN^-	$NaCN$			
Hydroxide ion	OH^-	$NaOH$	Thiosulfate ion	$S_2O_3^{2-}$	$Na_2S_2O_3$

Naming acids and bases

Brønsted-Lowry definitions:

- acids are proton donors
- bases are proton acceptors

Binary acids (or hydroacids)

- A hydroacid is a compound with the general formula « XH_n » that loses H^+ in water
- they are named used the prefix *hydro-* and the suffix *–ic*:
  - HF : hydrofluoric acid
  - HI : hydroiodic acid
  - H_2S: hydrosulfuric acid

Naming oxoacids

- an oxoacid is a compound with the general formula « H_mXO_n » that loses H^+ in water

oxoacid = oxoanion + H^+ ions

- their names are based on the oxoanion from which they are formed

-ite becomes *–ous*

-ate becomes *-ic*

ClO^-	hypochlorite
ClO_2^-	chlorite
ClO_3^-	chlorate
ClO_4^-	perchlorate

HClO	hypochlorous acid
$HClO_2$	chlorous acid
$HClO_3$	chloric acid
$HClO_4$	perchloric acid