Chem 261 September 4, 2018

Definitions

- Chemistry: Study of matter
- Organic Chemistry: Study of compounds containing carbon. Chemical symbol of carbon is C
- Chemical symbol: Code for chemical element
- Atom: Is the smallest possible particle that defines a complete chemical element
- They are composed of neutrons, protons (+), and electrons (-)
- Every atom is composed of a nucleus and one or more electrons bound to the nucleus
- Molecules: Discrete (bonded) arrangement of atoms
  - Changing the arrangement or connections changes the molecule and its physical properties
- Compound: Collection of molecules of the same type
  - Water (H_2O), Cholesterol (27 carbons, white crystalline powder, average male contains 80 g)
- Atomic Number: Number of protons in the nucleus of an atom (Z)
- Atomic Weight: Mass of protons (p^+) and neutron (N)
  - ^1H = Hydrogen = $1p^+ + 1e^-$
  - $^{12}C = 6p^+ + 6N$
  - $^{13}C = 6p^+ + 7N$ (Isotope of Carbon, Stable, 1.1% abundance)
  - $^{14}C = 6p^+ + 8N$ (Radioactive isotope with long half-life, $T_{1/2}$ = 5740 yrs)
    - 1N $\rightarrow$ $1p^+ + 1e^-$ to become ^{14}Nitrogen
- Molecular Weight (MW): Mass of atoms in a molecule
  - H_2O: MW = [(2 x 1 g/mol)H + (1 x 16 g/mol)O] = 18 g/mol

Basic Principles

1. Like charges repel, unlike charges attract.
2. Atoms want inert gas configuration of electrons
   - Same configuration as Helium, Neon, Argon, Xenon, and Krypton.

Mole Concept

- 1 mole = 6.02×10^{23} (Avogadro's number) (can be atoms, molecules etc.)
- 1 mole H = 1 g
- Mole concept relates to MW and Atomic weight
- 18 g of H_2O is 6.02×10^{23} molecules = 1 mole of H_2O or 6.02×10^{23} molecules of water
- Carbon has 12 grams per mol, Oxygen has 16 g per mol, so for CO_2 we can calculate that it has 44 g/mol
- D = ^2H, $1p^+ + 1N$ = 2 g/mol, it's an isotope
- D_2O = 20g/mol, known as heavy water.

Typical Molecule

- A few Angstroms (Å) in length: Bond length C-H is 1 Å, C-C is 1.5 Å
- 1 Å = 10^{-8} cm
- 1 Å = diameter of 1 hydrogen atom

Example: Cholesterol is 17 Å across. If you lined all of the cholesterol molecules in an 80 g bottle end to end it would wrap around the earth roughly 5,000,000 times.

Physical Properties

- Defined by chemical structure
- Melting point (mp) and boiling point (bp): Each compound has a characteristic mp and bp.
- Taste, appearance, odour, and biological properties (how it interacts with other molecules).
- Light Absorption
- Density (symbol is ρ, rho) (unit = g/cm^3)
- Density of water is 1g/cm^3, compounds that are less dense than water will float on top if they are not miscible (infinitely soluble)
- Absorption of radiation (light)
- Solubility

Purity of Compounds

- 1 mole of H_2O (6.02 x 10^{23} molecules) = 18 g, then add 1 x 10^6 other molecules (e.g. sugar) → the purity of the water would be 99.999 999 999 999 999%.
- Purity: A pure compound shows no change in physical properties upon attempts to further purify (purity is a relative term).
- Purity: A pure compound has a discrete and unique physical properties

Qualitative Test for Inorganic or Organic Compound

Qualitative: Determine if you have the compound of interest

Note that the structure of a molecule defines its physical properties

Organic	Inorganic
- Contains carbon - Low mp < 200 °C, low bp - Burns frequently in air - Soluble in non-polar solvents	- No carbon - High mp & bp - “Does not burn” - Soluble in H_2O

Non-Polar solvent: Hexane, Benzene, Diethyl ether etc

THERE ARE MANY EXCEPTIONS!!!

E.g. Common table sugar is an organic molecule, however it dissolves in water

Quantitative Analysis

Quantitative: How much of the compound of interest (quantity)
Amounts of atoms in a compound

$$N_2 + H_2O$$
$$\uparrow \; [H] = \text{Reduction}$$

$$\text{Organic compound} \xrightarrow[\Delta \text{ (heat)}]{} CO_2 + H_2O + NO_2$$

MW (g/mol): 44 18

$$\text{Compound (4.34 mg)} \xrightarrow{O_2} 10.35 \text{ mg} \quad 3.42 \text{ mg} \quad 0 \text{ mg}$$

Contains C, H, O

CO_2 H_2O NO_2

Note: Matter cannot be created or destroyed in a chemical reaction; therefore the amount of carbon in the CO_2 is equal to the amount of carbon in the starting sample.

Percent Composition

$$\text{Weight of carbon (in sample)} = \frac{12 \text{ g/mol of C}}{44 \text{ g/mol } CO_2} \times 10.35 \text{ mg of } CO_2 = 2.82 \text{ mg of C}$$

Molecular Weight (MW) of CO_2 = 12 (C) + 2×16 (O) = 44 g/mol

$$\text{Weight of hydrogen} = \frac{2(1 \text{ g/mol of H}) \times}{18 \text{ g/mol of } H_2O} \; 3.42 \text{ mg of } H_2O = 0.383 \text{ mg of H}$$

NB: H_2O contains two hydrogen. MW of $H_2O = \underbrace{(2\times1)}_{H_2} + \underbrace{16}_{O}$

Weight of oxygen = 4.34 mg – (2.82 mg of C + 0.383 mg of H) = 1.14 mg of O

Now one can calculate percentage composition:

% Composition:

$$\% \text{ C} = \frac{\text{Mass of carbon}}{\text{Mass of sample}} \times 100\% = \frac{2.82 \text{ mg of C}}{4.34 \text{ mg}} \times 100\% = 65.1\%$$

$$\% H = \frac{0.383 \text{ mg of H}}{4.34\text{mg}} = 8.83\%$$

$\% O = 100\% - 65.1\% - 8.83\% = 26.1\%$

The empirical (and with additional data, molecular formula) can be determined from % composition

Determining the empirical experimental formula:

Definition: Empirical formula is the ratio of atoms to each other in a molecular formula

There are three steps to calculate the empirical formula:

1) Divide each percentage (%) by the atomic weight of the element → crude ratio
2) Divide each crude ratio by the smallest crude ratio → refined ratio
3) Multiply the refined ratio by an integer value (x2, x3, x4…) → integral ratio

% Composition	Crude Ratio	Refined Ratio	Integral Ratio
65.1 % C	65.1 / 12.0 = 5.42 (% C / At Wt C)	5.42 / 1.63 = 3.34	3.34 x 3 = 10
8.83 % H	8.83 / 1.01 = 8.76	8.76 / 1.63 = 5.39	5.39 x 3 = 16
26.1 % O	26.1 / 16.0 = 1.63	1.63 / 1.63 = 1.00	1.00 x 3 = 3

From the integral ratio, the empirical formula is $C_{10}H_{16}O_3$. Using this formula an empirical weight can be calculated.

C: $10 \times 12 = 120$ g/mol
H: $16 \times 1 = 16$ g/mol
O: $3 \times 16 = 48$ g/mol

$C_{10}H_{16}O_3 = 184$ g/mol

Note: Suppose the molecular weight is given as 368 g/mol, then the molecular formula is obtained by multiplying the integral ratios by a factor of 2 and it would be $C_{20}H_{32}O_6$.

The molecular weight can be independently determined via mass spectrometry.