### **Definitions**

- Chemistry: Study of matter
- Organic Chemistry: Study of compounds containing carbon
- Atom: Is the smallest possible particle that defines a complete chemical element
- Molecules: Atoms connected in a particular arrangement
  - Changing the arrangement or connections changes the molecule and its physical properties.
- Compound: Collection of molecules of the same type
  - Water (H<sub>2</sub>O), Cholesterol (27 carbons, white crystalline powder, average male contains 80g)
- Atomic Number: number of protons in nucleus of atoms
- Atomic Weight: mass of protons and neutrons
- Molecular Weight (MW): mass of atoms in molecule
  - Hydrogen = H, Atomic number = 1, 1 proton =  $p^+ = (1H^+)$
  - Deuterium = D or d, Atomic number = 1, 1 proton and 1 neutron, Atomic Weight = 2 is an Isotope of Hydrogen
  - Tritium = T, Atomic number = 1, 1 proton and 2 neutrons, Atomic Weight = 3, radioactive isotope of hydrogen (half-life = 12.2 years)

### Mole Concept

- 1 mole =  $6.02 \times 10^{23}$  (Avogadro's number) (can be atoms, molecules etc)
- 1 mole H = 1 g
- $H_2O: MW = [(2 \times 1 \text{ g/mol})H + (1 \times 16 \text{ g/mol})O] = 18 \text{ g/mol}$
- 18g of H<sub>2</sub>O is  $6.02 \times 10^{23}$  molecules = 1 mole of H<sub>2</sub>O or  $6.02 \times 10^{23}$  molecules of water

# **Typical Molecule**

- A few Angstroms (Å) in length
- 1 Å =  $10^{-8}$  cm

Example: cholesterol is 18 Å across. If you lined all of the cholesterol molecules in a 80g bottle end to end it would wrap around the earth roughly 5,000,000 times.

# **Purity of Compounds**

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

# **Physical Properties**

- Defined by chemical structure.
- Melting point (mp) and Boiling point (bp): Each compounds has a characteristic mp and bp.
- Biological properties: Taste, appearance, odour
- Density  $(g/cm^3)$ .
- Absorption of radiation.

- Solubility

#### **Chemical Analysis**

- Qualitative Analysis
- Quantitative Analysis

### **Qualitative Test for Inorganic or Organic Compound**

- Qualitative: Determine if you have the compound of interest.

| Organic                           | Inorganic                     |  |
|-----------------------------------|-------------------------------|--|
| - Contains carbon                 | - No carbon                   |  |
| - Low mp $< 200 ^{\circ}\text{C}$ | - High mp                     |  |
| - Burn frequently                 | - "Does not burn"             |  |
| - Soluble in non-polar solvents   | - Soluble in H <sub>2</sub> O |  |

#### THERE ARE MANY EXCEPTIONS !!!

#### **Quantitative Analysis**

- Quantitative: How much of the compound of interest (quantity).

Organic compound 
$$\xrightarrow{O_2}$$
  $CO_2$  +  $H_2O$   $H_2O$  +  $H_2O$   
MW (g/mol) = 44 18  
Example:  
Compound contains  $\longrightarrow$  10.35 mg 3.42 mg 0 mg  
C, H, O (4.34 mg)

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.

Weight of carbon (in sample) =  $\frac{12 \text{ g/mol of C}}{44 \text{ g/mol CO}_2}$  x 10.35 mg of CO<sub>2</sub> = 2.82 mg of C

Weight of hydrogen =  $\frac{2(1 \text{ g/mol of H})}{18 \text{ g/mol of H}_2\text{O}}$  x 3.42 mg of H<sub>2</sub>O = 0.383 mg of H

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

Now one can calculate percentage composition

% Composition

% C = <u>Mass of carbon</u> = <u>2.82mg of C</u> = 65.1% Mass of sample 4.34mg % H = <u>0.383 mg of H</u> = 8.83% 4.34mg % O = 100% - 65% - 8.83% = 26.1%

The empirical can be determined from % composition.

Determining the empirical experimental formula:

- Definition: empirical formula is ratio of atoms to each other in a molecular formula
- Three steps to calculate the empirical formula:
  - i) divide each percentage (%) by the atomic weight of element  $\rightarrow$  crude ratio
  - ii) divide all crude ratio by the smallest crude ratio  $\rightarrow$  refined ratio
  - iii) Multiply the refined ratio by an integer value to get integral ratio

| % Composition | Crude ratio        | Refined ratio      | Integral ratio    |
|---------------|--------------------|--------------------|-------------------|
| 65.1 % C      | 65.1 / 12.0 = 5.42 | 5.42 / 1.63 = 3.34 | $3.34 \ge 3 = 10$ |
|               |                    |                    |                   |
| 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 | $1.00 \ge 3 = 3$  |

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

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

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  $C_{20}H_{32}O_6$ .