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 - Low mp < 200 °C - Burn frequently - Soluble in non-polar solvents	- No carbon - High mp - "Does not burn" - Soluble in H_2O

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).

$$NO_2 \xrightarrow{[H] = \text{reduction}} N_2 + H_2O$$

$$\text{Organic compound} \xrightarrow[\Delta \text{ (heat)}]{O_2} CO_2 + H_2O + NO_2$$

MW (g/mol) = 44 (for CO_2), 18 (for H_2O)

Compound contains C, H, O (4.34 mg) $\longrightarrow$ 10.35 mg (CO_2), 3.42 mg (H_2O), 0 mg (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.

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

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

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:-

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

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

% O = 100% - 65% - 8.83% = 26.1%

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

Quantitative analysis of organic compound (from last class)

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 → crude ratio
  ii) Divide all crude ratio by the smallest crude ratio → 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 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.

Gas Law: (different kinds of units for pressure and volume can be used provided the value of the gas constant is adjusted to those units)

PV = nRT P=Pressure in mmHg
V=Volume in L
n=moles
T=temperature in °K; °K and °C are same size but 0 °K = minus 273 °C

$$R \text{ is a constant } \frac{0.082 \text{ L} \cdot \text{atm.}}{\text{mol} \cdot {}^\circ\text{K}}$$

Sample Question- What volume will 3 mL of N_2 gas occupy at standard pressure and temperature (STP)?

Standard Pressure is 1 atmosphere or 760 mm Hg; Standard temperature is 273 °K

$$\frac{P_1V_1}{P_2V_2} = \frac{nRT_1}{nRT_2} \quad \text{divide equations to give} \quad \frac{P_1V_1}{P_2V_2} = \frac{T_1}{T_2}$$

$P_1 = 760$ mmHg $\quad T_1 = 273$ °K
$P_2 = 750$ mmHg $\quad T_2 = 298$ °K $\quad V_2 = 3$ mL

Solve for V_1

$$V_1 = \frac{T_1P_2V_2}{T_2P_1} = \frac{(273\ {}^\circ\text{K})(750 \text{ mmHg})(3 \text{ mL})}{(298\ {}^\circ\text{K})(760 \text{ mmHg})}$$

= 2.71 mL is the answer

Question: How many moles of N_2 is 2.71 mL at STP and what is its mass?

NOTE: 1 mole of an ideal gas occupies 22.4 L at STP.

$$2.71 \times 10^{-3} \text{ L} \times \frac{1 \text{ mole}}{22.4 \text{ L}} = 1.21 \times 10^{-4} \text{ moles of } N_2$$

1.21×10^{-4} mol × 28 g/mol = 3.4 mg of N_2
