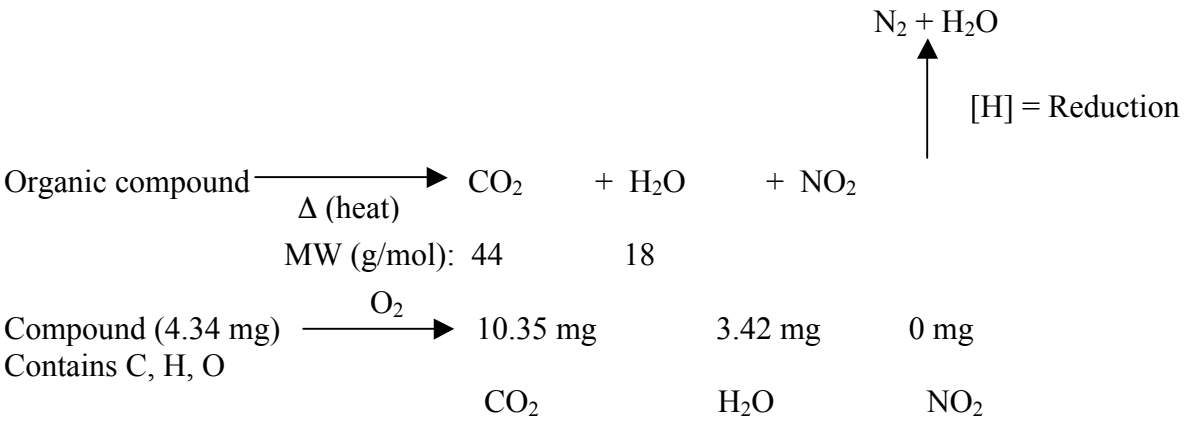
Quantitative Analysis

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



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

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

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

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

NB: H_2O contains two hydrogen. MW of H_2O = (2×1) + 16
H_2 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:

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

Mass of sample 4.34 mg

% H = 0.383 mg of H = 8.83%
4.34mg

% 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.