Determining Chemical Formula

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Empirical Formula Determination

Empirical Formula

* The empirical formula is the simplest formula of a compound.
* It tells us the relative number of atoms in a compound.
* It does not tell us how many atoms of each type are in the molecule of the compound.

- Step 1: List Given Values
- Step 2: Calculate Mass(m) of Each Element in a 100g sample
- Step 3: Convert mass (m) into Amount (n)
  - $n = m / M$
- Step 4: State Amount Ratio
- Step 5: Calculate the Lowest Whole-Number

Example

* A certain compound contains 5.9 % hydrogen and 94.1 % oxygen. Determine the empirical formula of the compound.

Example

Element	Mass in 100 g sample	Amount (n) $n = m / M$	Ratio
Hydrogen	5.9 g	$n = \frac{5.9\ g}{1\ g/mol}$ $n = 5.9\ mol$	5.9/5.9 =1
Oxygen	94.1 g	$n = \frac{94.1\ g}{16\ g/mol}$ $n = 5.9$	5.9/5.9 =1

- Therefore the empirical formula of this compound is HO
- **If the ratio ends up with .5, then multiply all be 2 to get whole numbers

Example

* Determine the empirical formula for a compound that contains 69.88% iron and 30.12% oxygen.

Example

Element	Mass in 100 g sample	Amount (n) n= m / M	Ratio
Iron	69.88 g	n= $\frac{69.88\ g}{55.85\ g/mol}$ n= 1.2512 mol	1.2512/1.2512 =1
Oxygen	30.12 g	n= $\frac{30.12\ g}{16.00\ g/mol}$ n= 1.882 mol	1.882/1.2312 =0.5

Example

* Therefore the empirical formula would be $FeO_{0.5}$
  * However you cannot have decimals, so you must find the closest whole number ratio
  * Fe_2O

Finding Whole Number Ratios

* If you have a whole number ratio of:
  * $HO_{0.5}$
  * $AlCl_{0.33}$
  * $BI_{0.667}$

Finding Whole Number Ratios

* If you have a whole number ratio of:
  * $HO_{0.5}$ x2 H_2O
  * $Al_{0.33}Cl$ x3 $AlCl_3$
  * $B_{0.667}O$ x3 B_2O_3

Molecular Formula Determination

Molecular Formula

* The molecular formula shows the actual number of atoms of each element in a molecule or compound.
* There is a direct relationship between the empirical and molecular formula.
    * Eg. The empirical formula for glucose is CH_2O and the molecular formula is $C_6H_{12}O_6$

Steps to Determine Molecular Formula

- Step 1: Use the Steps to Determine the Empirical Formula If Not Given
- Step 2: List Given Values
- Step 3: Determine Molar Mass of Empirical Formula
- Step 4: Determine Ratio of Molar Mass of Compound to Molar Mass of Empirical Formula.
- Step 5: Calculate Molecular Formula

Example

* The empirical formula of a compound is HCO_2. If the compound has a molecular mass of 90 g/mol, determine it's molecular formula.

- Step 1: Empirical formula is HCO_2.
- Step 2:
  - Given: Empirical Formula HCO_2
  - Given: M = 90.0 g/mol

- Step 3: Determine the Molar Mass of the empirical formula
- HCO_2:
  - H = 1 x 1.0 g = 1 g
  - C= 1 x 12.0 g = 12 g
  - O = 2 x 16 g = 32 g
- =45.0g/mol

* Step 4: Determine Ratio of Molar Mass of Compound to Molar Mass of Empirical Formula

$$\frac{M_{compound}}{M_{HCO_2}} = \frac{90\ g/mol}{45\ g/mol}$$

$$=2$$

* Step 5: Calculate the Molecular Formula

Molecular Formula = 2(empirical formula)

$= 2 \times HCO_2$

$= C_2H_2O_4$

Hydrates

Hydrates

* A hydrate is a compound with a specific number of water molecules bound to each formula unit.

    * Example: $CaSO_4 \cdot 2H_2O_{(s)}$

Hydrates

* Compounds in an ionic state can be hydrates(with water) or anhydrous(without water).
* While the water doesn't interfere with chemical activity, they do change the mass.