Determining Chemical Formula

Empirical Formula

* The empirical formula is the simplest formula of a compound.
* Tells us the relative number of atoms, does not tell us how many atoms of each type.
    * eg. The empirical formula of glucose is CH_2O (The real formula is $C_6H_{12}O_6$)

Steps Used to Determine Empirical Formula

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

Example

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

Example

* Consider 100g of the compound

Element	Mass in Sample		
Hydrogen	5.9		
Oxygen	94.1		

Example

* Consider 100g of the compound

Element	Mass in Sample	Moles $n=m/M$	
Hydrogen	5.9	$n=5.9/1$ $n=5.9$	
Oxygen	94.1	$n=94.1/16$ $n=5.9$	

Example

* Consider 100g of the compound

Element	Mass in Sample	Moles n=m/M	Ratio
Hydrogen	5.9	n=5.9/1 n=5.9	5.9/5.9=1
Oxygen	94.1	n=94.1/16 n= 5.9	5.9/5.9 =1

Example

* 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

* A certain compound contains 11.2 % hydrogen and 88.8% oxygen. Determine the empirical formula of the compound.

Example

* Consider 100g of the compound

Element	Mass in Sample		
Hydrogen	11.2		
Oxygen	88.8		

Example

* Consider 100g of the compound

Element	Mass in Sample	Moles $n=m/M$	
Hydrogen	11.2	$n=11.2/1$ $n=11.2$	
Oxygen	88.8	$n=88.8/16$ $n=5.55$	

Example

* Consider 100g of the compound

Element	Mass in Sample	Moles $n=m/M$	Ratio
Hydrogen	11.2	$n=11.2/1$ $n=11.2$	$11.2/5.55$ $=2$
Oxygen	88.8	$n=88.8/16$ $n=5.55$	$5.55/5.55$ $=1$

Example

* Therefore the empirical formula of this compound is H_2O

Molecular Formula Determination

Molecular Formula

* The molecular formula show the actual number of atoms of each element in a molecule or compound.

Steps to Determine Molecular Formula

* Step 1: Use the Steps to Determine the Empirical Formula If Not Given
* Step 2: Determine Molar Mass of Empirical Formula
* Step 3: Determine Ratio of Molar Mass of Compound to Molar Mass of Empirical Formula.
* Step 4: 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.

Example

* Step 1:
  * Given: Empirical Formula HCO_2
  * Given: M = 90.0 g/mol

Example

* Step 2: 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

Example

* Step 3: Determine Ratio of Molar Mass of Compound to Molar Mass of Empirical Formula
  * $M_{compound}$ / M_{HCO2}
  * = 90 / 451
  * =2

Example

* Step 4: Calculate the Molecular Formula
  * Molecular Formula = 2(empirical formula)
    * 2 x HCO_2
    * $C_2H_2O_4$

Example

* The analysis of a compound shows that it is made up of 21.9 % Na, 45.7 % C, 1.9% H and 30.5% O

* What is the molecular formula of a compound if its molecular mass is 210.0g/mol?

Example

Element	Mass in Sample		
Sodium	21.9		
Carbon	45.7		
Hydrogen	1.9		
Oxygen	30.5		

Example

Element	Mass in Sample	Moles	
Sodium	21.9	21.9/23 =0.952	
Carbon	45.7	45.7/12 =3.81	
Hydrogen	1.9	1.9/1 =1.9	
Oxygen	30.5	30.5/16.0 =1.91	

Example

Element	Mass in Sample	Moles	Ratio
Sodium	21.9	21.9/23 =0.952	0.952/0.952 =1
Carbon	45.7	45.7/12 =3.81	3.81/0.952 =4
Hydrogen	1.9	1.9/1 =1.9	1.9/0.952 =2
Oxygen	30.5	30.5/16.0 =1.91	1.91/0.952 =2

Example

Element	Mass in Sample	Moles	Ratio
Sodium	21.9	21.9/23 =0.952	0.952/0.952 =1
Carbon	45.7	45.7/12 =3.81	3.81/0.952 =4
Hydrogen	1.9	1.9/1 =1.9	1.9/0.952 =2
Oxygen	30.5	30.5/16.0 =1.91	1.91/0.952 =2

Empirical Formula = $NaC_4H_2O_2$

Example

* Determine Molar Mass of Empirical Formula
  * $NaC_4H_2O_2$
    * Na= 1 x 23.0g = 23 g
    * C = 4 x 12.0 g = 48 g
    * H = 2 x 1.0 g = 2 g
    * O = 2 x 16 g = 32 g
    * 105.0 g/mol

Example

* Determine Ratio of Molar Mass of Compound to Molar Mass of Empirical Formula
    * $M_{Compound}$/ $M_{NaC4H2O2}$
    * =210.0 g/mol / 105.0 g/mol
    * =2

Example

* Calculate Molecular Formula
  * Molecular Formula = 2 (empirical formula)
  * $=2(NaC_4H_2O_2)$
  * $= Na_2C_8H_4O_4$