

Determining Chemical Formula

J KROPAC

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	$n = \frac{5.9 \text{ g}}{1 \text{ g/mol}}$ $n = 5.9 \text{ mol}$	$\frac{5.9}{5.9}$ $= 1$
Oxygen	94.1 g	$n = \frac{94.1 \text{ g}}{16 \text{ g/mol}}$ $n = 5.9$	$\frac{5.9}{5.9}$ $= 1$

- * Therefore the empirical formula of this compound is H_2O
- * **If the ratio ends up with .5, then multiply all by 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	$n = \frac{69.88 \text{ g}}{55.85 \text{ g/mol}}$ $n = 1.2512 \text{ mol}$	$1.2512 / 1.2512 = 1$
Oxygen	30.12 g	$n = \frac{30.12 \text{ g}}{16.00 \text{ g/mol}}$ $n = 1.882 \text{ mol}$	$1.882 / 1.2312 = 0.5$

Example

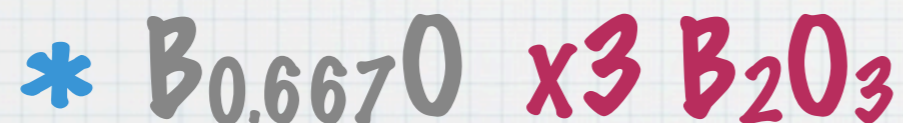
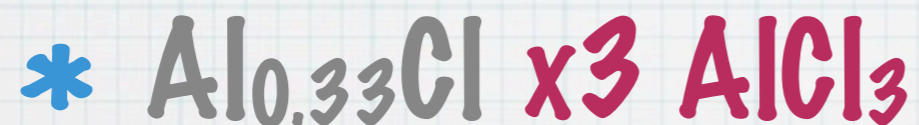
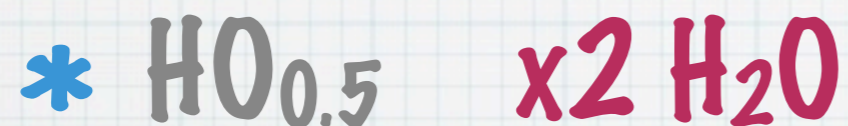
- * Therefore the empirical formula would be $\text{FeO}_{0.5}$
- * However you cannot have decimals, so you must find the closest whole number ratio
- * Fe_2O

Finding Whole Number Ratios

- * If you have a whole number ratio of:
 - * $\text{H}_2\text{O}_{0.5}$
 - * $\text{AlCl}_3_{0.33}$
 - * $\text{B}_2\text{O}_3_{0.667}$

Finding Whole Number Ratios

* If you have a whole number ratio of:



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 $\text{C}_6\text{H}_{12}\text{O}_6$

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 its molecular formula.

* Step 1: Empirical formula is HCO_2 .

* Step 2:

* Given: Empirical Formula HCO_2

* Given: $M = 90.0 \text{ g/mol}$

* Step 3: Determine the Molar Mass of the empirical formula

* HCO_2 :

* $\text{H} = 1 \times 1.0 \text{ g} = 1 \text{ g}$

* $\text{C} = 1 \times 12.0 \text{ g} = 12 \text{ g}$

* $\text{O} = 2 \times 16 \text{ g} = 32 \text{ g}$

* $= 45.0 \text{ g/mol}$

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

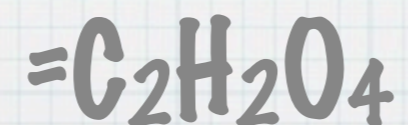
$$\underline{M_{\text{compound}}} = \underline{90 \text{ g/mol}}$$

$$M_{\text{HCO}_2} \quad 45 \text{ g/mol}$$

$$= 2$$

*** Step 5: Calculate the Molecular Formula**

Molecular Formula = 2(empirical formula)



Hydrates

Hydrates

- * A hydrate is a compound with a specific number of water molecules bound to each formula unit.
- * Example: $\text{CaSO}_4 \cdot 2\text{H}_2\text{O}_{(s)}$



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.