Empirical and Molecular Formulas

In which you will learn about (surprise, surprise):

- Empirical formulas
- Molecular formulas

Empirical Formulas

- The empirical formula for a compound is the formula with the smallest whole-number mole ratio of the elements.
  - The empirical formula might or might not be the same as the actual molecular formula!
  - The empirical formula = molecular formula for IONIC COMPOUNDS - ALWAYS!

Molecular Formulas

- If the empirical formula is different from the molecular formula, the molecular formula will always be a simple multiple of the empirical formula.
  - EX: The empirical formula for hydrogen peroxide is HO; the molecular formula is H_2O_2.
  - In both formulas, the ratio of oxygen to hydrogen is 1:1

Calculating Empirical Formulas

- Use the following poem to remember the steps:

Percent to mass

Mass to moles

Divide by small

Multiply ‘til whole

EXAMPLE PROBLEM

- Determine the empirical formula for methyl acetate, which has the following chemical analysis: 48.64% carbon, 8.16% hydrogen, and 43.20% oxygen.

Step One: Percent to Mass

- Let's assume we have a 100. g sample of methyl acetate. This means that each element's percent is also the number of grams of that element.
- 48.64% C = 48.64 g C
- 8.16% H = 8.16 g H
- 43.20% O = 43.20 g O

Step Two: Mass to Moles

- Convert each mass into moles using the molar mass of each element.
- $48.64 \text{ g C} \times \frac{1 \text{ mol C}}{12.0 \text{ g C}} = 4.053 \text{ mol C}$
- $8.16 \text{ g H} \times \frac{1 \text{ mol H}}{1.01 \text{ g H}} = 8.08 \text{ mol H}$
- $43.20 \text{ g O} \times \frac{1 \text{ mol O}}{16.0 \text{ g O}} = 2.700 \text{ mol O}$

Step Three: Divide by Small

- Oxygen accounts for the smallest number of moles in the formula, so divide each element by oxygen's number of moles: 2.700 mol
- Carbon: 4.053 mol / 2.700 mol = 1.501 = 1.5
- Hydrogen: 8.08 mol / 2.700 mol = 2.99 = 3
- Oxygen: 2.700 mol / 2.700 mol = 1.000 = 1

- Remember, we will want whole-number ratios

Step Four: Multiply 'Til Whole

- In the previous slide, the ratio of C:H:O is 1.5:3:1
- We need a whole-number ratio, so we can multiply everything by 2 to get rid of the 1.5

- C $\rightarrow$ 3, H $\rightarrow$ 6, O $\rightarrow$ 2

So, the final empirical formula is $C_3H_6O_2$

Calculating Molecular Formulas

- Sorry, no silly poem this time!
- Step 1 – Calculate the empirical formula (if needed)
- Step 2 – GIVEN molecular mass (experimental)/empirical formula molar mass = multiplier
- Step 3 – Multiply the empirical formula subscripts by the multiplier found in Step 2

EXAMPLE PROBLEM

- Chemical analysis indicates it is composed of 40.68% carbon, 5.08% hydrogen, and 52.24% oxygen and has a molar mass of 118.1 g/mol. Determine the empirical and molecular formulas for this compound.

Step One: Find Empirical Formula

- $40.68\ \%\ C = 40.68\ g\ C \times \frac{1 mol\ C}{12.0\ g\ C} = 3.390\ mol\ C$
- $5.08\ \%\ H = 5.08\ g\ H \times \frac{1\ mol\ H}{1.01\ g\ H} = 5.03\ mol\ H$
- $54.24\%\ O = 54.24\ g\ O \times \frac{1\ mol\ O}{16.0\ g\ O} = 3.390\ mol\ O$

C: H:O

$\frac{3.390\ mol}{3.390\ mol} = 1$ $\frac{5.03\ mol}{3.390\ mol} = 1.48$ OR 1.5 $\frac{3.390\ mol = 1}{3.390\ mol}$

multiply by 2 → $2(C_1H_{1.5}O_1) \rightarrow C_2H_3O_2$

Step Two: Divide Molar Masses

- Molar mass empirical formula → $C_2H_3O_2$

C 2(12.01)= 24.02

H 3(1.008)=   3.024

O 2(16.00)= 32.00

59.044 g/mol

- Given molar mass = 118.1 g/mol
- Multiplier = $\frac{118.1 \text{ g/mol}}{59.0 \text{ g/mol}} = 2$

Step Three: Use Multiplier

- Empirical Formula = $C_2H_3O_2$
- x 2 from step two $2(C_2H_3O_2)$
- Molecular formula = $C_4H_6O_4$

HOMEWORK QUESTIONS

- 1) What information must a chemist obtain in order to determine the empirical formula of an unknown compound?
- 2) What information must a chemist have to determine the molecular formula of a compound?
- 3) A compound containing barium, carbon, and oxygen has the following percent composition: 69.58% Ba, 6.09% C, 24.32% O. What is the empirical formula for this compound?

HOMEWORK CONTINUED

- 4) What is the empirical and molecular formula of Vitamin D_3 if it contains 84.31% C, 11.53% H, and 4.16% O, with a molar mass of 384 g/mol?