Molecular Vs. Empirical Formulas

Molecular Formulas

boiling point

(may not be simplest ratio)

C₂H₄ ethene

$$C = C$$

-103.7°C

C₃H₆ propene

C₆H₁₂ 1-hexene

All 3 have same ratio but have different properties! Their **empirical formulas** are the same: CH₂ (simplest ratio)

Determining Empirical Formulas

A compound has 80% Carbon and 20 % H. Determine the Empirical Formula.

- 1. Convert % mass to mass: 80% C and 20 % H \$\frac{1}{4}\$ 80 g C and 20 g H.
- 2. Convert mass to moles:

$$\frac{80 \text{ g C}}{12 \text{ g C}} = 6.66 \text{ mol C}$$

$$\frac{20 \text{ g H} \quad 1 \text{ mole H}}{1 \text{ g H}} = 20 \text{ mol H}$$

3. Divide out all moles by the smallest value -give smallest ratio.

$$\frac{6.66}{6.66} = 1 \text{ C}$$
 $\frac{20.0}{6.66} = 3 \text{ H}$

CH₃ is the empirical formula

Determine the empirical formula of a substance with:

25.9 % N and 74.1 % O

$$\frac{74.1 \text{ g O}}{16 \text{ g O}} = 4.63 \text{ mol O}$$

find simplest ratio

$$\frac{1.85}{1.85} = 1 \text{ N}$$
 $\frac{4.63}{1.85} = 2.5 \text{ O}$

cannot have 1/2 of an atom

Multiply both by 2 to get whole number

$$1 N \times 2 = 2 N$$
 $2.5 O \times 2 = 5 O$

empirical formula: N_2O_5

Determining molecular formula from the empirical formula:

empirical formula:

CH₂ empirical weight; 14 g/mol potential molecular formulas:

mol. wt.

CH₂ 14g/mol

C₂H₄ 28 g/mol

C₃H₆ 42 g/mol

C₄H₈ 56 g/mol

C₅H₁₀ 70 g/mol

(Etc.)

Calculation: molecular wt. = multiple of subscript empirical wt.

Calculation: molecular wt. = multiple of subscript empirical wt.

85.7% C and 14.3% H with a molecular wt= 56 g/mol

$$\frac{85.7g \text{ C} | 1\text{mol C}}{12 \text{ g C}} = 7.14 \text{ mol C} \qquad \frac{7.14}{7.14} = 1 \text{ C}$$

$$\frac{14.3g \text{ H}}{1 \text{ g H}} = 14.3 \text{ mol H} \qquad \frac{14.3}{7.14} = 2 \text{ H}$$

empirical formula: CH₂

empirical weight: 14 g/mol

$$\frac{\text{molecular wt.}}{\text{empirical wt.}} = \frac{56\text{g/mol}}{14\text{g/mol}} = 4$$

$$\frac{14\text{g/mol}}{\text{(multiple of subscripts)}}$$

molecular formula = $4 \times (CH_2) = C_4H_8$

A compound has a molecular wt of 540g/mol.lt contains 60%C, 4.4%H and 35.6% O. What is its molecular formula?

A compound has a molecular wt of 540g/mol. It contains 60%C, 4.4%H and 35.6% O. What is its molecular formula?

empirical formula: C₉H₈O₄

Empirical weight:
$$(12x9) + (1x8) + (16x4) = 180g/mol$$

$$\frac{540g/\text{mol}}{180 \text{ g/mol}} = 3$$

molecular formula: C₂₇H₂₄O₁₂

Lactobionic Acid has a molecular wt of 358g/mol It contains 40.2%C, 6.2%H and 53.6% O. What is its molecular formula?

Lactobionic Acid has a molecular wt of 358.3g/mol It contains 40.2%C, 6.2%H and 53.6% O. What is its molecular formula?

$$\frac{40.23g \text{ C} | 1 \text{ mol C}}{12.01 \text{ g C}} = 3.349 \text{ mol C} \frac{3.349}{3.349} = 1.000 \quad \text{x6} = 6 \text{ C}$$

$$\frac{6.189g \text{ H} | 1 \text{ mol H}}{1.008 \text{ g H}} = 6.140 \text{ mol H} \quad \frac{6.140}{3.349} = 1.833 \quad \text{x6} = 11 \text{ H}$$

$$\frac{53.59g \text{ O} | 1 \text{ mol O}}{| 16.00 \text{ g} | 0} = 3.349 \text{ mol O} = \frac{3.349}{3.349} = 1.000 \text{ x6} = 6.0$$

empirical formula: C₆H₁₁O₆

Empirical weight: (12.01x6) + (1.008 x11) + (16.00x6) = 179.15g/mol

$$\frac{358.3g/mol}{179.15 g/mol} = 2$$

molecular formula: C₁₂H₂₂O₁₂