Calculating molecular formulas for compounds

ethylene glycol : $C_2H_6O_2$ molecular formula

CH_3O empirical formula

isopropanol : C_3H_8O molecular = empirical formula

glucose : $C_6H_{12}O_6$ molecular formula

CH_2O empirical formula

How do I get from an empirical to a molecular formula ?

1. Given : empirical formula C_2H_3O

molar mass = 86.09 g/mol

2. Molecular F. = empirical F · n

$$n = \frac{\text{molecular formula}}{\text{empirical formula}}$$

$$n = \frac{\text{molar mass (molecular)}}{\text{molar mass (empirical)}}$$

3. molar mass (empirical) =

$2 \cdot 12.01\ g/mol + 3 \cdot 1.008\ g/mol +$

$1 \cdot 16.00\ g/mol =$

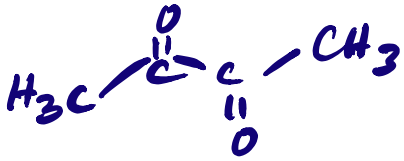
$43.04\ g/mol$

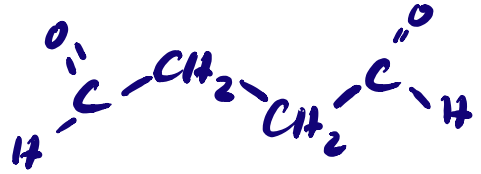
$$n = \frac{86.09\ g/mol}{43.04\ g/mol} \approx 2$$

4. Molecular formula:

$$C_2H_3O \times 2 \rightarrow C_4H_6O_2$$

Structural Formula:

butanedione 

succindialdehyde 

Combustion Reactions

Combustion of propane C_3H_8

1. $C_3H_8(g) + O_2(g) \rightarrow CO_2(g) + H_2O(g)$

2. Balance "C"

$C_3H_8(g) + O_2(g) \rightarrow 3CO_2(g) + H_2O(g)$

Balance "H"

$C_3H_8(g) + O_2(g) \rightarrow 3CO_2(g) + 4H_2O(g)$

3. Balance "elements"

$C_3H_8(g) + 5O_2(g) \rightarrow 3CO_2(g) + 4H_2O(g)$

4. Resolve fractions n/a

5. check

Vanillin is a compound containing carbon, hydrogen and oxygen. the combustion of 30.4 mg vanillin produces 70.4 mg of CO_2 and 14.4 mg H_2O. The mass spectrum of vanillin shows molecular ion line at 152 amu. Use this information to determine the molecular formula!

Given:

30.4 mg Vanillin

70.4 mg CO_2

14.4 mg H_2O

Mw: 152 amu

1. Calculate # moles of C and H produced

$$\text{mass } (CO_2) = 70.4 \text{ mg} \cdot \frac{1 \text{ g}}{1000 \text{ mg}} = 0.0704 \text{ g}$$

$$\text{mass } (H_2O) = 14.4 \text{ mg} \cdot \frac{1 \text{ g}}{1000 \text{ mg}} = 0.0144 \text{ g}$$

$$M_w\ (CO_2) = 44.01 \text{ g/mol}$$

$$M_w\ (H_2O) = 18.02 \text{ g/mol}$$

$$\#\text{moles C} = 0.0704 \text{g}(CO_2) \cdot \frac{1 \text{mol}(CO_2)}{44.01 \text{g}(CO_2)} \cdot \frac{1 \text{mol C}}{1 \text{mol}(CO_2)}$$

$= 1.60 \cdot 10^{-3}$ mol

$$\#\text{ moles } (H) = 0.0144\,g\,(H_2O) \cdot \frac{1\,\text{mol}\,(H_2O)}{18.02\,g\,(H_2O)} \cdot \frac{2\,\text{mol}\,(H)}{1\,\text{mol}\,(H_2O)}$$

$$= 1.60 \cdot 10^{-3}\ \text{mol}$$

2. Calculate # moles (O)

$$\text{mass}\,(C) = 1.60 \cdot 10^{-3}\,\text{mol}\,(C) \cdot \frac{12.01\,g\,(C)}{1\,\text{mol}\,(C)}$$

$$= 1.92 \cdot 10^{-2}\,g$$

$$\text{mass}\,(H) = 1.60 \cdot 10^{-3}\,\text{mol}\,(H) \cdot \frac{1.008\,g\,(H)}{1\,\text{mol}\,(H)}$$

$$= 1.61 \cdot 10^{-3}\,g$$

$$\text{mass}\,(O) = \text{total mass} - \text{mass}\,(C) - \text{mass}\,(H)$$

$$= 0.0304\,g - 0.0192\,g - 0.00161\,g$$

$$= 9.59 \cdot 10^{-3}\,g$$

$$\text{moles}\,(O) = 9.59 \cdot 10^{-3}\,g \cdot \frac{1\,\text{mol}\,(O)}{16.00\,g\,(O)}$$

$$= 5.99 \cdot 10^{-4}\ \text{mol}$$

3. Calculate empirical formula

$$C: \frac{1.60 \cdot 10^{-3}\,mol}{5.99 \cdot 10^{-4}\,mol} = 2.67$$

$$H: \frac{1.60 \cdot 10^{-3}\,mol}{5.99 \cdot 10^{-4}\,mol} = 2.67$$

$$O: \frac{5.99 \cdot 10^{-4}\,mol}{5.99 \cdot 10^{-4}\,mol} = 1$$

$$C_{2.67}H_{2.67}O_1 \times 3 = C_8H_8O_3$$

4. Calculate molecular formula

$$M_w\,(C_8H_8O_3) = 152.14\ g/mol$$

$$n = \frac{M_w(\text{vanillin})}{M_w\,(C_8H_8O_3)} = \frac{152\ g/mol}{152.14\ g/mol} \simeq 1$$

Molecular Formula $C_8H_8O_3$