Determination Molecular Formula by Combustion Analysis and Gas Laws

Complete combustion of 1.110 g of a gaseous hydrocarbon yields 3.613g CO_2, and 1.109g H_2O. A 0.288-g sample of the hydrocarbon occupies a volume of 131 mL at 24.8°C and 753mmHg. What is the molecular formula of the hydrocarbon??

Solution:
The goal of the problem is to first determine the simplest formula for C_xH_y from the combustion analysis. Then, using the ideal gas law, determine the molar mass of the compound. The ratio of the molecular molar mass and empirical molar mass will give the appropriate factor to convert the empirical formula into the molecular formula.

$$n_{\mathrm{C}} = \left(3.613 \text{ g } CO_2 \Big/ 44.01 \tfrac{\text{g}}{\text{mol}} \right) \times \frac{1 \text{ mol C}}{1 \text{ mol } CO_2} = 0.08209 \text{ mol C}$$

$$n_{\mathrm{H}} = \left(1.109 \text{ g } H_2O \Big/ 18.015 \tfrac{\text{g}}{\text{mol}} \right) \times \frac{2 \text{ mol H}}{1 \text{ mol } H_2O} = 0.1231 \text{ mol H}$$

It is somewhat important to be sure that the hydrocarbon is only carbon and hydrogen. This can be easily accomplished by converting these molar quantities of C and H into mass and adding them together. If the sum of the masses adds to 1.110 g, then there is no other atom in the hydrocarbon. Without further proof, suffice it to say that the hydrocarbon is only C and H.

Now, normalize to the least common multiple (*i.e.*, divide by the smallest *n*)....

$x = 1 \quad y = 1.5$

so the empirical formula is C_2H_3

Determine the molar mass of the compound:

$$\frac{PV}{nT} = R \quad \text{and} \quad n = \frac{m}{M} \quad \text{so} \quad \frac{PVM}{mT} = R \quad \text{and} \quad M = \frac{mTR}{PV}$$

$V = 0.131 \text{ L}$

$$P = \left(753 \text{ mmHg} \Big/ 760 \tfrac{\text{mmHg}}{\text{atm}} \right) = 0.9908 \text{ atm}$$

$T = 24.8° + 273.2 \text{ K} = 298.0 \text{ K}$

$$M = \frac{mTR}{PV} = \frac{(0.288 \text{ g})(298.0 \text{ K})\left(0.082059 \tfrac{\text{L}\cdot\text{atm}}{\text{mol}\cdot\text{K}}\right)}{(0.9908 \text{ atm})(0.131 \text{ L})} = 54.26 \tfrac{\text{g}}{\text{mol}}$$

Finally, determine the factor and molecular formula:

$$f = \frac{54.26 \frac{\text{g}}{\text{mol}}}{27.044 \frac{\text{g}}{\text{mol}}} = 2$$

Molecular formula is C_4H_6