

Answer on Question #80594, Chemistry/ Organic Chemistry

Cumene is a compound containing only carbon and hydrogen that is used in the production of acetone and phenol in the chemical industry. Combustion of 47.6mg(47.6×10^{-3} g) produces some CO₂ and 42.8mg(42.8×10^{-3} g) water. The molar mass of cumene is between 115 and 125 g/mol. Determine the empirical and molecular formulas of the compound

Solution

Let cumene formula to be C_xH_y

1. In the process of combustion all hydrogen atoms of cumene reacted with oxygen to give H₂O. Find mass of hydrogen in H₂O:

$$n = m/M$$

$$n(\text{H}_2\text{O}) = m(\text{H}_2\text{O})/M(\text{H}_2\text{O}) = 42.8 \times 10^{-3} \text{ g} / 18 \text{ g/mol} = 2.38 \times 10^{-3} \text{ mol}$$

As one molecule of water contains 2 hydrogen atoms, then $n(\text{H}) = n(\text{H}_2\text{O}) \times 2 = 2.38 \times 10^{-3} \text{ mol} \times 2 = 4.76 \times 10^{-3} \text{ mol}$.

$$m = M \times n$$

$$m(\text{H}) = M(\text{H}) \times n(\text{H}) = 1 \text{ g/mol} \times 4.76 \times 10^{-3} \text{ mol} = 4.76 \times 10^{-3} \text{ g}.$$

2. Find mass of carbon in cumene:

$$m(\text{C}) = m(\text{C}_x\text{H}_y) - m(\text{H}) = 47.6 \times 10^{-3} \text{ g} - 4.76 \times 10^{-3} \text{ g} = 42.8 \times 10^{-3} \text{ g}$$

3. Find amount of substance of carbon and hydrogen in cumene:

$$n(\text{H}) = 4.76 \times 10^{-3} \text{ mol}.$$

$$n(\text{C}) = m(\text{C})/M(\text{C}) = 42.8 \times 10^{-3} \text{ g} / 12 \text{ g/mol} = 3.57 \times 10^{-3} \text{ mol}$$

4. Find ratio $n(\text{C}):n(\text{H})$ and determine empirical formula

$$\frac{n(\text{C})}{n(\text{H})} = \frac{3.57 \times 10^{-3} \text{ mol}}{4.76 \times 10^{-3} \text{ mol}} = \frac{3}{4}$$

Empirical formula is C₃H₄

5. To determine molecular formula we should find molar mass of empirical formula and multiply it on some integer number (let it be n). The result should be between numbers 115 and 125.

$$M(\text{C}_3\text{H}_4) = (12 \times 3 + 1 \times 4) \text{ g/mol} = 40 \text{ g/mol}$$

$$115 < 40 \times n < 125$$

$$2.875 < n < 3.125$$

So, the only integer number between 2.875 and 3.125 is 3.

Molecular formula is $(\text{C}_3\text{H}_4) \times 3 = \text{C}_9\text{H}_{12}$

Answer: empirical formula C₃H₄, molecular formula C₉H₁₂.