Question

Complete combustion of 8.50 g of a hydrocarbon produced 26.2 g of CO_2 and 12.1 g of H_2O . What is the empirical formula for the hydrocarbon?

Solution

Number of moles of CO_2 and H_2O are

$$n_{CO_2} = \frac{m_{CO_2}}{M_{CO_2}} = \frac{26.2}{44} = 0.60 \text{ mol}$$
$$n_{H_{2O}} = \frac{m_{H_{2O}}}{M_{H_{2O}}} = \frac{12.1}{18} = 0.67 \text{ mol}$$

In general, formula for the hydrocarbon may be represented as C_xH_y . Then the combustion reaction may be given as

$$C_xH_y + (2x + y/2) O_2 \rightarrow x CO_2 + y/2 H_2O_2$$

From the equation of combustion we can see that

$$n_{C_xH_y} = \frac{n_{CO_2}}{x} = \frac{0.60}{x}$$

$$n_{C_xH_y} = \frac{2 \cdot n_{H_{2O}}}{y} = \frac{2 \cdot 0.67}{y} = \frac{1.34}{y}$$

$$M_{C_xH_y} = 12 \cdot x + 1 \cdot y$$

$$n_{C_xH_y} = \frac{m_{C_xH_y}}{M_{C_xH_y}} = \frac{8.50}{12x + y}$$

So, we have set of two equations with two unknown values

$$\begin{cases} \frac{8.50}{12x+y} = \frac{0.60}{x} \\ \frac{8.50}{12x+y} = \frac{1.34}{y} \\ \end{cases}$$

$$\begin{cases} 8.50x = 0.60(12x+y) \\ 8.50y = 1.34(12x+y) \\ 8.50y = 1.34(12x+y) \\ \end{cases}$$

$$\begin{cases} 7.20x + 0.60y - 8.50x = 0 \\ 16.08x + 1.34y - 8.50y = 0 \end{cases}$$

$\int 0.60y = 1.30x$

 $\int 7.16y = 16.08x$

Such set of equations has not one analytical solution.

Numerical solutions found in terms of minimum error (calculated until $x \approx 10$) are given in table.

Numerical solutions		Closest integer values		Difference between solution and closest integer	
х	У	х	У	Δx	Δy
1.996	4.480	2	4	0.004	0.480
2.993	6.721	3	7	0.007	0.279
3.991	8.961	4	9	0.009	0.039
4.989	11.201	5	11	0.011	0.201
5.987	13.441	6	13	0.013	0.441
6.984	15.682	7	16	0.016	0.318
7.982	17.922	8	18	0.018	0.078
8.980	20.162	9	20	0.020	0.162
9.978	22.402	10	22	0.022	0.402

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The solutions closest to integer values may be considered to be most feasible. Since hydrocarbon of empirical formula C_4H_9 does not exist, the empirical formula most likely is C_8H_{18} .

Answer: C₈H₁₈