Combustion Analysis Notes

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You may encounter a moderately difficult combustion analysis problem like the one below:

> $1.80\ g$ of an unknown substance was combusted in excess oxygen to produce $2.64\ g$ of CO_2 gas and $1.08\ g$ of H_2O vapor. A separate analysis gave the molar mass of the substance as $180\ {}^{g}/_{mol}$. Using these data find both the empirical and molecular formulas for the unknown substance.

For this sort of problem, we should recognize that the substance (we can call it X) contains at least C and H atoms, and may contain O as well. The general form of the reaction is:

$$X + O_2(g) \longrightarrow CO_2(g) + H_2O(g)$$

Without the chemical formula for X, we cannot balance the equation, but it is still useful because we note three things:

- The C atoms which make up the CO_2 can only come from X
- The H atoms which make up the H_2O can only come from X
- Since O is in potentially *every* chemical species in this equation, we cannot directly measure the amount which came from X

The first step is to find the number of C and H atoms, which we know must have come from X:

$$\frac{2.64\ g\ \text{CO}_2}{1}\left|\frac{1\ mol\ \text{CO}_2}{44.0098\ g\ \text{CO}_2}\right|\frac{1\ mol\ \text{C atoms}}{1\ mol\ \text{CO}_2} = 0.0600\ mol\ \text{C atoms}$$

$$\frac{1.08\ g\ \text{H}_2\text{O}}{1}\left|\frac{1\ mol\ \text{H}_2\text{O}}{18.0153\ g\ \text{H}_{2\text{O}}}\right|\frac{2\ mol\ \text{H atoms}}{1\ mol\ \text{H}_2\text{O}} = 0.120\ mol\ \text{H atoms}$$

Now that we know exactly how many C and H atoms X contains, we can see how much they weigh together.

$$\frac{0.0600\ mol\ \text{C atoms}}{1}\left|\frac{12.011\ g}{1\ mol\ \text{C atoms}}\right. = 0.721\ g$$

$$\frac{0.120\ mol\ \text{H atoms}}{1}\left|\frac{1.00794\ g}{1\ mol\ \text{H atoms}}\right. = 0.121\ g$$

$$0.721\ g + 0.121\ g = 0.842\ g$$

This falls far short of the original mass of X, which means that there must be some O present in X. In order to count how many O atoms there are, we must find the mass that they make up.

$$m_{(\text{O atoms})} = m_{(total)} - m_{(\text{C and H atoms})}$$

$$1.80\ g - 0.842\ g = 0.96\ g$$

$$\frac{0.96\ g}{1}\left|\frac{1\ mol\ \text{O atoms}}{15.9994\ g}\right. = 0.0600\ \text{O atoms}$$

Now we have:

Element	C	H	O
Moles	0.0600	$.120$	0.0600

To get a reduced molar ratio, divide all moles by the smallest number (that is, by 0.0600) to get:

Element	C	H	O
Moles	1	2	1

So the empirical formula is: CH_2O, and the mass for the empirical formula is $30.03{}^{g}/_{mol}$. Molecules with this empirical formula are called "hydrocarbons" because they are carbon with a water.

To find the *molecular formula*, we need to recognize that it will be some multiple of the empirical formula (i.e. CH_2O, $C_2H_4O_2$, $C_3H_6O_3$, $C_4H_8O_4$, etc.).

$$M_{\text{Molecular}} = n \times M_{\text{Empirical}}, \text{ so } n = \frac{M_{\text{Molecular}}}{M_{\text{Empirical}}} = \frac{180{}^{g}/_{mol}}{30.03{}^{g}/_{mol}} = 5.994 \approx 6$$

This gives us the actual molecular formula: $C_6H_{12}O_6$