Combustion Analysis - Alternative Approaches

Combustion Analysis is a method of determining the empirical formula by completing combusting a compound and determining the amounts of elements in sample of the original compound by using the products and relating the elements in the products to those in the original compound. If a compound with C, H and one other element is completely combusted all the C needs to wind up in the CO_2 and all the H needs to wind up in the H_2O. If there's O in the original compound it winds up in both the CO_2 and H_2O but that doesn't matter since it's mass is determined using the law of conservation of mass. If the third element isn't oxygen this can still be done as long as the C winds up only in the CO_2 and the H winds up only in the H_2O. The third element winds up in products containing that element and oxygen only.

Below I'll show two ways of approaching the problem.

We'll do this using problem 3.55(b) from the 13th edition of the book.

Menthol is composed of C, H and O. A 0.1005-g sample is combusted, producing 0.2829 g of CO_2 and 0.1159 g of H_2O. What is the empirical formula and the molecular formula if the molar mass is 156 g/mol?

1) **<u>As done in lecture</u>**:

Using mass fractions to determine the mass of C and H first and then using those, the mass of the sample and the law of conservation of mass to determine the mass of the third element (oxygen in this case). Then use the masses to determine the moles of each element. Then you proceed as usual to get mole ratios and the empirical formula.

a) **<u>Determine mass of C and H using mass fractions and mass of O</u>**:

A mass fraction is the ratio you get for an element when doing a % composition problem.

$$? \text{ g C} = 0.2829 \text{ g } CO_2 \times \frac{12.01 \text{ g C}}{44.01 \text{ g } CO_2} = 0.0772\underline{\mathbf{0}}12 \text{ g C}$$

Mass fraction of C in CO_2

$$? \text{ g H} = 0.1159 \text{ g } H_2O \times \frac{2(1.008) \text{ g H}}{18.02 \text{ g } H_2O} = 0.0129\underline{\mathbf{6}}63 \text{ g H}$$

Mass fraction of H in H_2O

$$\text{mass O} = 0.1005 \text{ g} - 0.0772\underline{\mathbf{0}}12 \text{ g} - 0.0129\underline{\mathbf{6}}63 \text{ g} = 0.010\underline{\mathbf{3}}323 \text{ g O}$$

b) **Determine moles**:

$$? \text{ mol C} = 0.0772\underline{\mathbf{0}}12 \text{ g C} \times \frac{1 \text{ mol C}}{12.01 \text{ g C}} = 0.00642\underline{\mathbf{8}}08 \text{ mol C}$$

$$? \text{ mol H} = 0.0129\underline{\mathbf{6}}63 \text{ g H} \times \frac{1 \text{ mol H}}{1.008 \text{ g H}} = 0.0128\underline{\mathbf{6}}34 \text{ mol H}$$

$$? \text{ mol O} = 0.010\underline{\mathbf{3}}323 \text{ g O} \times \frac{1 \text{ mol O}}{16.00 \text{ g O}} = 0.00064\underline{\mathbf{5}}769 \text{ mol O}$$

c) **Determine the mole ratio**:

Divide each by the smallest moles.

$$\text{C: } \frac{0.00642\underline{\mathbf{8}}08 \text{ mol C}}{0.00064\underline{\mathbf{5}}769 \text{ mol O}} = 9.954 = 10$$

$$\text{H: } \frac{0.0128\underline{\mathbf{6}}34 \text{ mol H}}{0.00064\underline{\mathbf{5}}769 \text{ mol O}} = 19.91 = 20$$

$$\text{O: } \frac{0.00064\underline{\mathbf{5}}769 \text{ mol O}}{0.00064\underline{\mathbf{5}}769 \text{ mol O}} = 1.00$$

d) **Empirical Formula**:

$C_{10}H_{20}O$

e) **Molecular Formula**:

Need FW of $C_{10}H_{20}O$: EFW = 10(12.01) + 20 (1.008) + 16.00 = 156.2$\underline{\mathbf{6}}$ amu or g/mol

Get multiplying factor:

$$n = \frac{\text{MW}}{\text{EFW}} = \frac{156 \text{ g/mol}}{156.2\underline{\mathbf{6}} \text{ g/mol}} = 1$$

So the molecular formula is the same as the empirical formula, $C_{10}H_{20}O$

2) **Alternative way**:

Use the masses of CO_2 and H_2O to first determine moles of C and H in the original compound, since they're needed anyway, and then their masses. Then you use these to get the masses of C and H and then the mass of O as above and then the moles of O as above.

a) **Determine moles of C and H using molar masses**:

$$? \text{ mol C} = 0.2829 \text{ g } CO_2 \times \frac{1 \text{ mol } CO_2}{44.01 \text{ g } CO_2} \times \frac{1 \text{ mol C}}{1 \text{ mol } CO_2} = 0.00642\underline{\mathbf{8}}08 \text{ mol C}$$

$$? \text{ mol H} = 0.1159 \text{ g } H_2O \times \frac{1 \text{ mol } H_2O}{18.02 \text{ g } H_2O} \times \frac{2 \text{ mol H}}{1 \text{ mol } H_2O} = 0.0128\underline{\mathbf{6}}34 \text{ mol H}$$

b) **Determine the masses of C and H from their moles and then mass of O**:

$$? \text{ g C} = 0.00642\underline{\mathbf{8}}08 \text{ mol C} \times \frac{12.01 \text{ g C}}{1 \text{ mol C}} = 0.0772\underline{\mathbf{0}}12 \text{ g C}$$

$$? \text{ g H} = 0.0128\underline{\mathbf{6}}34 \text{ mol H} \times \frac{1.008 \text{ g H}}{1 \text{ mol H}} = 0.0129\underline{\mathbf{6}}63 \text{ g H}$$

Then proceed to get the mass of O in the compound as above in method 1. Then proceed as in parts (b) - (e) to finish the problem. This essentially amounts to the same amount of work and calculations but in slightly different order in the first couple of steps.