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Find empirical formula of hydrocarbon

When a compound containing carbon and hydrogen is the subject of combustion with oxygen in a special combustion device, all carbon is converted into CO2 and hydrogen into H2O (Figure \(\PageIndex{2}\)). The amount of carbon produced can be determined by measuring the amount of carbon produced. This is captured by sodium hydroxide, and thus we can monitor the mass of CO2 produced by determining the increase in the mass of the CO2 trap. Likewise, we can determine the amount of H produced by the amount of H2O trapped by magnesium perchlorate. One of the most common ways to determine the elemental composition of an unknown hydrocarbon is an analytical procedure called combustion analysis. A small, carefully balanced sample of an unknown compound that may contain carbon, hydrogen, nitrogen, and/or sulfur is burned in an oxygen atmosphere. Other elements, such as metals, can be determined by other methods, and the quantities of the resulting gaseous products (CO2, H2O, N2 and SO2) are determined by one of several possible methods. A procedure used in combustion analysis is thematically outlined in Figure \(\PageIndex{3}\) and a typical combustion analysis is illustrated in Examples \(\PageIndex{3}\) and \(\PageIndex{4}\)). Example \(\PageIndex{3}\)): Combustion of isopropyl alcohol What is the empirical form of isopropyl alcohol (which contains only C, H and O) if the combustion of a 0.255 gram of isopropyl alcohol sample produces 0.561 grams of CO2 and 0.306 grams of H2O? Solution Based on this amount of C and H in the sample, \(\frac{0.561\text{ g CO}_2}{44.0\text{ g CO}_2}\times\frac{1\text{ mol CO}_2}{12.01\text{ g C}}=0.0128\text{ mol C}\) Since a mole CO2 consists of a mole of C and two moles of O, if we have 0.0128 mole CO2 in our sample, then we know that we have 0.0128 moles of C in the sample. How many grams of C is that? \(\frac{0.0128\text{ mol C}}{1\text{ mol C}}\times 12.01\text{ g C/mol}=0.154\text{ g C}\) What about hydrogen? \(\frac{0.306\text{ g H}_2\text{O}}{18.0\text{ g H}_2\text{O}}\times\frac{1\text{ mol H}_2\text{O}}{2\text{ mol H}}=0.0084\text{ mol H}\) Since a mole H2O consists of a mole of oxygen and two moles of hydrogen, if we have 0.017 moles of H2O, then we have 2* (0.017) = 0.034 moles of hydrogen. Since hydrogen is about 1 gram/mole, we need 0.034 grams of hydrogen in our original sample. When we add our carbon and hydrogen together we get: 0.154 grams (C) + 0.034 grams (H) = 0.188 grams But we know we burned 0.255 grams of isopropyl alcohol. The 'missing' mass must be from oxygen atoms in isopropyl alcohol: 0.255 grams - 0.188 grams = 0.067 grams of oxygen So much oxygen is how many moles? \(\frac{0.067\text{ g O}}{16.0\text{ g O/mol}}=0.0042\text{ mol O}\) Overall why we have: 0.0128 Moles Carbon moles Hydrogen 0.0042 Moles Oxygen Divide by the smallest molar amount to normalize: C = 3.05 atoms H = 8.1 atoms O = 1 atom Within experimental error, the most likely empirical formula for propanol would be C3H8O Example \(\PageIndex{4}\)): Combustion of Naphthalene Naphthalene, the active ingredient in a number of mothballs, is an organic compound containing carbon and hydrogen only. Complete combustion of a 20.10 mg sample of naphthalen in oxygen yielded 69.00 mg CO2 and 11.30 mg H2O. Determine the empirical formula of naphthalene. Given: mass of sample and mass of combustion products Requested: empirical formula strategy: Use the masses and molar masses in the combustion products, CO2 and H2O, to calculate the amounts of carbon and hydrogen found in the original sample of naphthalen. Use these masses and molar masses of the elements to calculate the empirical formula of naphthalene. Solution: A When incinerated, 1 mole \(\frac{1\text{ mol CO}_2}{44.01\text{ g CO}_2}\times\frac{1\text{ mol C}}{12.01\text{ g C}}=0.0227\text{ mol C}\) is produced for every 1 mole of CO2. Similarly, 1 mol H2O is produced for every 2 mol hydrogen atoms found in the sample. The masses of carbon and hydrogen in the original sample can be calculated from these conditions, the masses of CO2 and H2O and their molar masses. Since the units of molar mass are grams per mole, we must first convert the masses from milligram to gram: \(\frac{69.00\text{ mg CO}_2}{1000\text{ mg}}\times\frac{1\text{ mol CO}_2}{44.01\text{ g CO}_2}\times\frac{1\text{ mol C}}{12.01\text{ g C}}=0.00125\text{ mol C}\) \(\frac{11.30\text{ mg H}_2\text{O}}{1000\text{ mg}}\times\frac{1\text{ mol H}_2\text{O}}{18.02\text{ g H}_2\text{O}}\times\frac{2\text{ mol H}}{2\text{ mol H}}=0.00125\text{ mol H}\) B To get the relative number of atoms of both elements present, we need to calculate the number of moles of each and divide by the number of moles of the element in the day in the smallest amount: \(\frac{0.00125\text{ mol C}}{0.00125\text{ mol C}}=1\text{ C}\) \(\frac{0.00125\text{ mol H}}{0.00125\text{ mol H}}=1\text{ H}\) Divide each number by the number of moles of the item in the smaller giving amount \(\frac{1\text{ C}}{1\text{ C}}=1\text{ C}\) \(\frac{1\text{ H}}{1\text{ H}}=1\text{ H}\) C \(\frac{1\text{ C}}{1\text{ C}}=1\text{ C}\) \(\frac{1\text{ H}}{1\text{ H}}=1\text{ H}\) The empirical formula of naphthalene is C10H8, which is consistent with our results. \$begin{array}{l} \text{What is the molecular formula for a connection, that contains only carbon and hydrogen if the combustion of } 1.05\text{ g of the compound produces } 3.30\text{ g of CO}_2 \text{ and } 1.35\text{ g of H}_2\text{O?} \\ \text{Solution: } 1.05\text{ g of compound} \times \frac{1\text{ mol CO}_2}{44.01\text{ g CO}_2} \times \frac{1\text{ mol C}}{12.01\text{ g C}} = 0.0047\text{ mol C} \\ 1.35\text{ g of H}_2\text{O} \times \frac{1\text{ mol H}_2\text{O}}{18.02\text{ g H}_2\text{O}} \times \frac{2\text{ mol H}}{2\text{ mol H}} = 0.0150\text{ mol H} \\ \text{Divide by the smallest number of moles: } \frac{0.0047\text{ mol C}}{0.0047\text{ mol C}} = 1\text{ C} \quad \frac{0.0150\text{ mol H}}{0.0047\text{ mol C}} = 3.19\text{ H} \\ \text{The empirical formula is } \text{C}_1\text{H}_{3.19} \\ \text{Round to the nearest whole number: } \text{C}_1\text{H}_3 \\ \text{The empirical formula is } \text{CH}_3 \end{array}\$ Obtaining Empirical and Molecular Formulas from Combustion Data Empirical and molecular formulas for compounds that contain only carbon and hydrogen (CaHb) or carbon , hydrogen and oxygen (CaHbOc) can be determined with a process called combustion analysis. The steps for this procedure are Way a sample of the compound to be analyzed and put it in the apparatus shown in the image below. Burn the connection completely. The only products for burning a compound containing only carbon and hydrogen (CaHb) or carbon, hydrogen and oxygen (CaHbOc) are carbon dioxide and water. H2O and CO2 are pulled through two tubes. One tube contains a substance that absorbs water and the other contains a substance that absorbs carbon dioxide. Each of these pipes is weighed before and after combustion. The increase in mass in the first tube is the mass of H2O that is formed in combustion, and the increase in mass of the second tube is the mass of CO2 formed. Suppose that all the carbon in the compound has been converted into CO2 and trapped in the second tube. The carbon mass in the compound is calculated from the carbon mass of the measured carbon mass. Suppose that all the hydrogen in the compound has been converted into H2O and trapped in the first tube. The hydrogen mass is calculated in the connection from the measured body of water. If the compound contains oxygen as well as carbon and hydrogen, the oxygen mass is calculated by subtracting the mass of carbon and hydrogen from the total mass of the original sample of the compound. Use this data to determine the empirical and molecular formulas in the usual way. Combustion analysis apparatus A compound containing carbon and hydrogen (CaHb) or carbon, hydrogen and oxygen (CaHbOc) is completely burned to form H2O and CO2. The products are drawn two tubes. The first tube absorbs water, and the second tube absorbs carbon dioxide. To illustrate how empirical and molecular formulas can be determined from data from combustion analysis, let's consider a substance called trioxane. Formaldehyde, CH2O, is unstable as a pure gas that easily forms a mixture of a substance called trioxane and a polymer called paraformaldehyde. Therefore, formaldehyde is dissolved in a solvent, such as water, before it is sold and used. The molecular formula trioxan, which contains carbon, hydrogen and oxygen, can be determined using data from two different experiments. In the first trial, 17,471 g of trioxan is cut into the apparatus shown above, forming 10,477 g of H2O and 25,612 g of CO2. In the second experiment, the molecular mass of trioxane is found to be 90,079. We can get the molecular formula of a compound from its empirical formula and its molecular mass. (See the text for a reminder of how to do this.) To get the empirical formula, we need to determine the mass in grams of carbon, hydrogen and oxygen in 17,471 g of trioxane. That is why we need to take these general steps. First convert from the data given to grams of carbon, hydrogen and oxygen. Second, determine the empirical formula from grams of carbon, hydrogen and oxygen. Thirdly, the molecular formula is determined by the empirical formula and the given molecular mass. Because we assume that all carbon in trioxan has reacted to form in CO2, we can find the mass of carbon in 17,471 g trioxan by calculating the mass of carbon in 25,612 g of CO2. Because we assume that all hydrogen in the trioxane has reacted to form H2O, we can find the mass of hydrogen in 17,471 g of trioxane by calculating the mass of hydrogen in 10,477 g H2O. Because trioxan contains only carbon, hydrogen and oxygen, we can calculate the oxygen mass by subtracting the masses of carbon and hydrogen from the total mass of trioxane. ? g O = 17,471 g trioxan - 6.9899 g C - 1.1724 g H = 9.309 g O We now calculate the empirical formula, the empirical formula mass and the molecular formula. Sample Study Sheet: Calculating molecular formulas from Combustion Data Tip-off – You want to calculate the molecular formula for a compound that contains only carbon and hydrogen (CaHb) or carbon, hydrogen and oxygen (CaHbOc), and you get its molecular mass and the masses of CO2 and H2O formed in the combustion of a given mass of the compound. General procedure Calculate the number of grams of carbon in the compound by calculating the number of grams of carbon in the given amount of CO2. The number of grams of hydrogen in the compound is calculated by calculating the number of grams of hydrogen in the given amount of H2O. If the compound contains oxygen, calculate the number of grams of oxygen in it by subtracting the masses of carbon hydrogen from the given total mass of the compound. ? g O = (given) g total - (calculated) g C - (calculated) g H Calculate the empirical formula for the compound based on grams of carbon, hydrogen and oxygen. The formula mass of the empirical formula is calculated, and the given molecular mass is divided by the empirical formula mass to obtain n. Multiply each of the subscripts in the empirical formula by n to get the molecular formula. EXAMPLE - Obtaining a molecular formula from combustion data: Dianabol is one of the anabolic steroids that have been used by some athletes to increase the size and strength of their muscles. It is similar to the male hormone testosterone. Some studies suggest that the desired effects of the drug are minimal, and the side effects, which include sterility and increased risk of liver cancer and heart disease, keep most people from using it. The molecular formula of Dianabol, which consists of carbon, hydrogen and oxygen, can be determined using data from two different experiments. In the first experiment, 14,765 g dianabol is burned and 43,257 g co2 and 12,395 g of H2O are formed. In the second experiment, the molecular mass of Dianabol is found to be 300.44. What is the molecular formula for Dianabol? Solution: Solution: