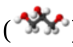
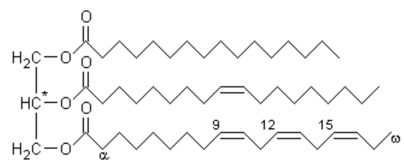
3.5.1: Foods- Burning or Metabolizing Fats and Sugars

The caloric value for fats is about 9 Cal/g, while for carbohydrates (sugars or starches) and proteins, it's about 4 Cal/g [1], so a teaspoon of sugar is only about 20 Calories, but a teaspoon of oil is about 45 calories. Our body stores fats as a long term, high energy per gram energy source, while sugars can be metabolized quickly, but don't give as much energy per gram. The energy is released when each is metabolized, giving the same amount of energy as combustion in air.

Fats and Oils

Vegetable fats and oils are all triglycerides, which contain a glycerol () three carbon "backbone" with 3 long chain *"fatty acids"* attached through ester linkages, as in the figure below. The actual shape is shown in the Jmol model, which can be rotated with the mouse. Triglycerides are called "fats" when they're solids or semisolids, and "oils" when they're liquids.

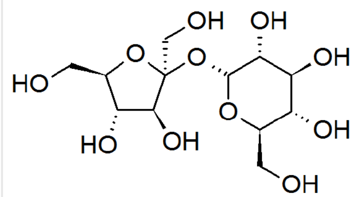


A triglyceride, overall unsaturated, with the glycerol "backbone" on the left, and saturated palmitic acid, monounsaturated oleic acid, and polyunsaturated alpha-linolenic acid. Carbon atoms are at each bend in the structure, and hydrogen atoms are omitted.

The long chain fatty acids may be *saturated* with hydrogen atoms, in which case they have all single bonds like the top fatty acid in the Figure (which is palmitic acid). If they have fewer hydrogen atoms, they are *unsaturated* and have double bonds like the middle fatty acid in the Figure (which is oleic acid). The bottom fatty acid is *polyunsaturated*, with multiple double bonds (it is linolenic acid). Various cooking oils have |known concentrations of saturated and unsaturated fatty acids.

Carbohydrates

Carbohydrates are made up of simple sugar units. The sucrose (ordinary table sugar) molecule shown below is made of a glucose and fructose "monosaccharides".



Sucrose,$C_{12}H_{22}O_{11}$ (C atoms are at each bend, H atoms are not shown)

A key to why fats have more than twice the caloric value of sugars comes from the combustion reactions:

A typical sugar combustion reaction is

$C_{12}H_{22}O_{11} + 6\ O_2 \rightarrow 6\ CO_2 + 6\ H_2O$

It requires 6 mol O_2 for every 6 mol of C, a 1:1 ratio. Since the molar mass of sucrose is 180 g/mol, about 0.033 mol O_2 is required per gram.

While a typical fat combustion might be

$C_{56}H_{108}O_6 + 80\ O_2 \rightarrow 56\ CO_2 + 54\ H_2O$

It requires 80 mol O_2 for every 56 mol of C, a 1.42:1 ratio. Or, since the molar mass of the fat shown is 878 g/mol, about 0.091 mol O_2 is required per gram. *The fat requires much more oxygen to burn, and consequently produces more energy.* We see why by looking at the C:O mole ratios in fats and sugars:

In the fat above,

$\text{S}\left(\frac{\text{C}}{\text{O}}\right) = \frac{56\text{ mol C}}{6\text{ mol O}}$ (a 9.3:1 ratio). Or for the sugar,
$\text{S}\left(\frac{\text{C}}{\text{O}}\right) = \frac{6\text{ mol C}}{6\text{ mol O}}$ (a 1:1 ratio).

Since the sugar is already more oxygenated, it produces less energy when it is burned.

Looking at it another way, the carbon, which reacts with oxygen and releases energy in combustion, is a bigger part of the fat:

In fat: $S\left(\frac{\text{C}}{\text{C}_{56}\text{H}_{108}\text{O}_6}\right) = \frac{56\text{ mol C}}{1\text{ mol C}_{56}\text{H}_{108}\text{O}_6}$ or 56 mol C/877.5 g $C_{56}H_{108}O_6$ = 0.064 mol C/g fat.

In Sugar: $S\left(\frac{\text{C}}{\text{C}_6\text{H}_{12}\text{O}_6}\right) = \frac{6\text{ mol C}}{1\text{ mol C}_6\text{H}_{12}\text{O}_6}$ or 6 mol C/180 g $C_6H_{12}O_6$ = 0.033 mol C/g fat.

We'll see below that these ratios actually allow us to determine the chemical formula for a fat, sugar, or any other compound.

Stoichiometric ratios derived from formulas instead of equations are involved in the most common procedure for determining the empirical formulas of compounds which contain only C, H, and O. A weighed quantity of the substance to be analyzed is placed in a combustion train and heated in a stream of dry O_2. All the H in the compound is converted to $H_2O(g)$ which is trapped selectively in a previously weighed absorption tube. All the C is converted to $CO_2(g)$ and this is absorbed selectively in a second tube. The increase of mass of each tube tells, respectively, how much H_2O and CO_2 were produced by combustion of the sample

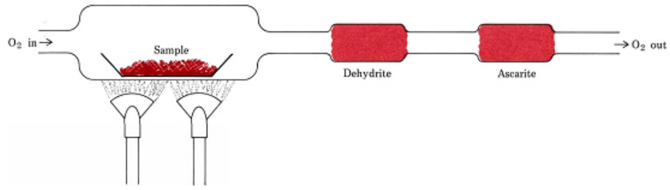


Illustration of a combustion train shows O 2 entering a heated chamber in which the sample is placed. This chamber leads straight to a the first tube which has dehydrite. This leads to the second tube containing ascarite. At the exit, O 2 passes out.

EXAMPLE 1 A 1.000 g sample of a fat was burned in a combustion train, producing 2.784 g of CO_2 and 1.140 g of H_2O. Determine the empirical formula of the fat.

Solution

We need to know the amount of C, the amount of H, and the amount of O in the sample. The ratio of these gives the subscripts in the formula. The first two may be obtained from the masses of CO_2 and H_2O using the molar masses and the stoichiometric ratios

$S\left(\frac{\text{C}}{\text{CO}_2}\right) = \frac{1 \text{ mol C}}{1 \text{ mol CO}_2}$ $S\left(\frac{\text{H}}{\text{H}_2\text{O}}\right) = \frac{2 \text{ mol H}}{1 \text{ mol H}_2\text{O}}$ Thus

$n_{\text{C}} = 2.784 \text{ g CO}_2 \times \frac{1 \text{ mol CO}_2}{44.01 \text{ g CO}_2} \times \frac{1 \text{ mol C}}{1 \text{ mol CO}_2} = 0.06326 \text{ mol C}$

$n_{\text{H}} = 1.140 \text{ g H}_2\text{O} \times \frac{1 \text{ mol H}_2\text{O}}{18.02 \text{ g H}_2\text{O}} \times \frac{2 \text{ mol H}}{1 \text{ mol H}_2\text{O}} = 0.1265 \text{ mol H}$ The compound may also have contained oxygen. To see if it does, calculate the masses of C and H and subtract from the total mass of sample

$$m_{\text{C}} = 0.06326 \text{ mol C} \times \frac{12.01 \text{ g C}}{1 \text{ mol C}} = 0.7598 \text{ g C} \tag{3.5.1.1}$$

$$\tag{3.5.1.2}$$

$$m_{\text{H}} = 0.1265 \text{ mol H} \times \frac{1.008 \text{ g H}}{1 \text{ mol H}} = 0.1275\text{g H} \tag{3.5.1.3}$$

Thus we have 1.000 g sample – 0.7598 g C – 0.1275 g H = 0.1128 g O and $n_{\text{O}} = 0.1128 \text{ g O} \times \frac{1 \text{ mol O}}{16.00 \text{ g O}} = 0.007050 \text{ mol O}$ The ratios of the amounts of the elements in ascorbic acid are therefore $\frac{n_{\text{H}}}{n_{\text{O}}} = \frac{0.1265 \text{ mol H}}{0.00705 \text{ mol C}} = \frac{17.94 \text{ mol H}}{1 \text{ mol O}}$

$\frac{n_{\text{C}}}{n_{\text{O}}} = \frac{20.06326 \text{ mol O}}{0.00705 \text{ mol O}} = \frac{8.97 \text{ mol C}}{1 \text{ mol C}}$

Since n_C:n_H:n_O is 9 mol C : 18 mol H : 1 mol O, the empirical formula is $C_9H_{18}O_1$.

Because most fats have 3 fatty acids bonded to glycerol with 2 oxygen atoms in each "ester" bond, the molecular formula is probably $C_{54}H_{108}O_6$. This molecule would contain the 3 carbon glycerol backbone, the 3 fatty acid chains would share the remaining 51 carbon atoms, and would be of average length 51/3 = 17 carbon atoms.

EXAMPLE 2 A 6.49-mg sample of ascorbic acid (vitamin C) was burned in a combustion train. 9.74 mg CO_2 and 2.64 mg H_2O were formed. Determine the empirical formula of ascorbic acid.

Solution

We need to know the amount of C, the amount of H, and the amount of O in the sample. The ratio of these gives the subscripts in the formula. The first two may be obtained from the masses of CO_2 and H_2O using the molar masses and the stoichiometric ratios

$S\left(\frac{\text{C}}{\text{CO}_2}\right) = \frac{1 \text{ mol C}}{1 \text{ mol CO}_2}$ $S\left(\frac{\text{H}}{\text{H}_2\text{O}}\right) = \frac{2 \text{ mol H}}{1 \text{ mol H}_2\text{O}}$ Thus

$n_{\text{C}} = 9.74 \times 10^{-3}\text{g CO}_2 \times \frac{1 \text{ mol CO}_2}{44.01 \text{ g CO}_2} \times \frac{1 \text{ mol C}}{1 \text{ mol CO}_2} = 2.21 \times 10^{-4} \text{ mol C}$

$n_{\text{H}} = 2.64 \times 10^{-3}\text{g H}_2\text{O} \times \frac{1 \text{ mol H}_2\text{O}}{18.02 \text{ g H}_2\text{O}} \times \frac{2 \text{ mol H}}{1 \text{ mol H}_2\text{O}} = 2.93 \times 10^{-4} \text{ mol H}$ The compound may also have contained oxygen. To see if it does, calculate the masses of C and H and subtract from the total mass of sample

$$m_{\text{C}} = 2.21 \times 10^{-4} \text{ mol C} \times \frac{12.01 \text{ g C}}{1 \text{ mol C}} = 2.65 \times 10^{-3}\text{g C} = 2.65 \text{ mg C} \tag{3.5.1.4}$$

$$\tag{3.5.1.5}$$

$$m_{\text{C}} = 2.93 \times 10^{-4} \text{ mol H} \times \frac{1.008 \text{ g H}}{1 \text{ mol H}} = 2.95 \times 10^{-4}\text{g H} = 0.295 \text{ mg H} \tag{3.5.1.6}$$

Thus we have 6.49 mg sample – 2.65 mg C – 0.295 mg H = 3.54 mg O and $n_{\text{O}} = 3.54 \times 10^{-3}\ \text{g O} \times \frac{1\ \text{mol O}}{16.00\ \text{g O}} = 2.21 \times 10^{-4}\ \text{mol O}$ The ratios of the amounts of the elements in ascorbic acid are therefore

$$\frac{n_{\text{H}}}{n_{\text{C}}} = \frac{2.93 \times 10^{-4}\ \text{mol H}}{2.21 \times 10^{-4}\ \text{mol C}} = \frac{1.33\ \text{mol H}}{1\ \text{mol C}} = \frac{1\frac{1}{3}\ \text{mol H}}{1\ \text{mol C}} = \frac{4\ \text{mol H}}{3\ \text{mol C}}$$

$$\frac{n_{\text{O}}}{n_{\text{C}}} = \frac{2.21 \times 10^{-4}\ \text{mol O}}{2.21 \times 10^{-4}\ \text{mol C}} = \frac{1\ \text{mol O}}{1\ \text{mol C}} = \frac{3\ \text{mol O}}{3\ \text{mol C}}$$

Since n_C:n_H:n_O is 3 mol C:4 mol H:3 mol O, the empirical formula is $C_3H_4O_3$.

A drawing of a molecule of ascorbic acid is shown here. You can determine by counting the atoms that the molecular formula is $C_6H_8O_6$—exactly double the empirical formula. It is also evident that there is more to know about a molecule than just how many atoms of each kind are present. In ascorbic acid, as in other molecules, the way the atoms are connected together and their arrangement in three-dimensional space are quite important. A picture showing which atoms are connected to which is called a **structural formula**. Empirical formulas may be obtained from percent composition or combustion-train experiments, and, if the molecular weight is known, molecular formulas may be determined from the same data. More complicated experiments are required to find structural formulas. In Example 2 we obtained the mass of O by subtracting the masses of C and H from the total mass of sample. This assumed that only C, H, and O were present. Sometimes such an assumption may be incorrect. When penicillin was first isolated and analyzed, the fact that it contained sulfur was missed. This mistake was not discovered for some time because the atomic weight of sulfur is almost exactly twice that of oxygen. Two atoms of oxygen were substituted in place of one sulfur atom in the formula.

A 3D representation of L-Ascorbic Acid <chemeddl-jmol2>ascorbic|size=300</chemeddl-jmol2>

References

1. ↑ Wolke,R.L. "What Einstein Told His Cook", W.W. Norton & Co., NY, 2002, p.65