Laboratory 1: The Molecules of the Biodiesel Reaction

Topics Covered

- Organic molecules relevant to biodiesel and its production, including: hydrocarbons, fatty acids, alcohols, triglycerides, methyl esters, sodium/potassium hydroxides, sodium/potassium methoxides, and glycerol
- Categorization of chemicals, e.g., hydrocarbons, alcohols, esters
- 3-D configurations of fatty acids, methyl esters, and triglycerides

Equipment Needed

- Molecule model building kits or household items that can be used to build the models (such as toothpicks and gumdrops). Use different colors of gumdrops to designate different atomic species.

Background Information – Organic Chemistry

Organic chemistry is a science that deals with molecules and compounds that contain carbon. There are a vast number of gaseous, liquid, and solid substances that contain carbon. These are often energy sources like natural gas, propane, alcohol, gasoline, diesel fuel, biodiesel, coal, and biomass including wood.

When we talk about a "carbon footprint" we are referring to human activity that produces carbon dioxide (CO_2) and thus contributes to climate change: things like burning fossil fuels for heat, electricity, and transportation. We can reduce our carbon footprint by using biofuels such as biodiesel and ethanol. Because these fuels are made from plants that absorb carbon from the atmosphere as they grow, biofuels add less new carbon dioxide to the atmosphere than do fossil fuels.

Laboratory Procedure -- Constructing the Molecules of Biodiesel Production

Biodiesel is made when a triglyceride molecule (oil or fat) reacts with 3 molecules of an alcohol (usually methanol or ethanol) to produce 3 molecules of biodiesel (also called "methyl esters" or "ethyl esters") and one molecule of glycerol.

The structure of a molecule can be depicted using a chemical formula, a 2-dimensional structural chart, or a 3-dimensional model. In reality, all molecules are 3-dimensional, so we will be creating 3-dimensional models.

After you read the description and look at the models of each molecule, construct a model of that molecule using the molecule building kit, or other household items such as gumdrops and toothpicks.

Methanol is the most commonly used alcohol in biodiesel production. It is the simplest alcohol with the formula CH_3OH, and is sometimes abbreviated MeOH. It is colorless and highly volatile. It is used in the manufacture if many consumer and industrial products and as a high octane fuel in racing engines.

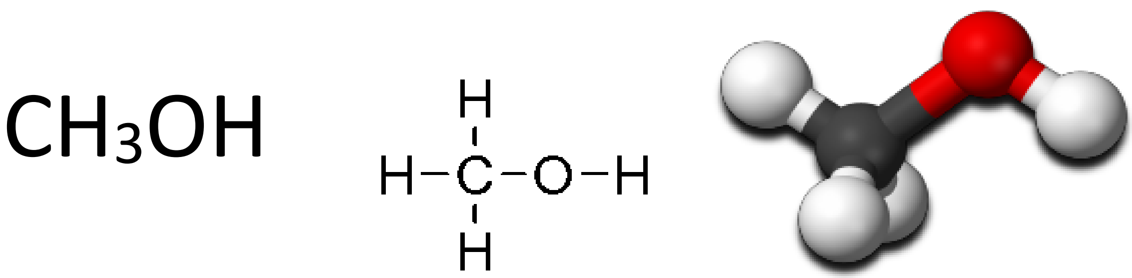

Figure 1 *Here are three different ways of depicting the methanol molecule: a molecular formula, a structural formula, and a 3-D ball-and-stick model. Molecule models become more complex as additional details are revealed about the molecular structure.*

Exercise 1: **Construct a model of a methanol molecule.**

Ethanol can also be used to make biodiesel. This type of alcohol is also called grain alcohol and is found in all alcoholic drinks. It can also be blended with gasoline as an octane booster and fuel extender for all gas-powered cars and trucks. Like methanol, it is also colorless and very volatile. It is a straight-chain hydrocarbon with a molecular formula C_2H_5OH, and is sometimes written EtOH.

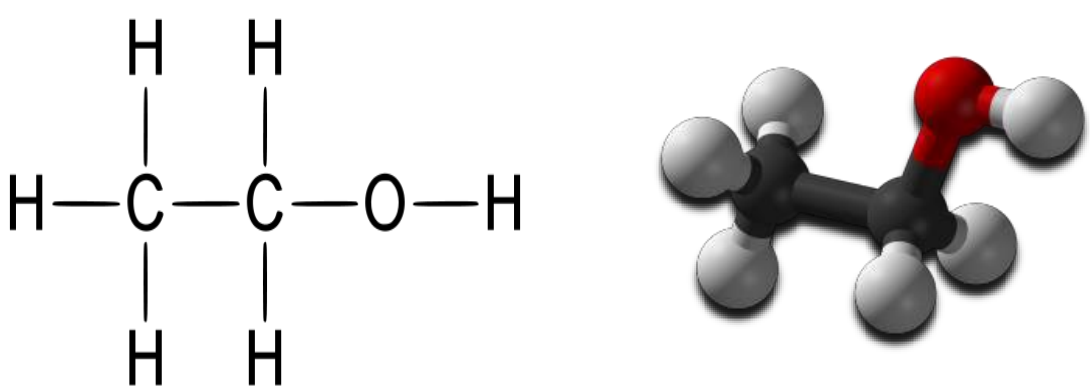

Figure 2 *Molecular structure and 3-D model of ethanol.*

Notice the relatively larger size and weight of the ethanol compared to methanol, putting it at a disadvantage as a reactant for biodiesel, since a larger quantity is needed.

<u>Exercise 2</u>: Construct a model of an ethanol molecule.

<u>Glycerol</u>, also called glycerin or glycerine, is a ubiquitous substance found in almost all cosmetics, in many pharmaceuticals, in personal care products like shampoos, lotions, and toothpaste, and in a lot of food items. Natural or vegetable-based glycerol has the molecular formula $C_3H_8O_3$ and forms the backbone of <u>triglycerides</u> (fats and oils). Glycerol is a byproduct of biodiesel production. It is also a byproduct of the soap-making process in which fats and oils are reacted with a strong base, forming sodium and/or potassium soaps, and releasing the glycerol.

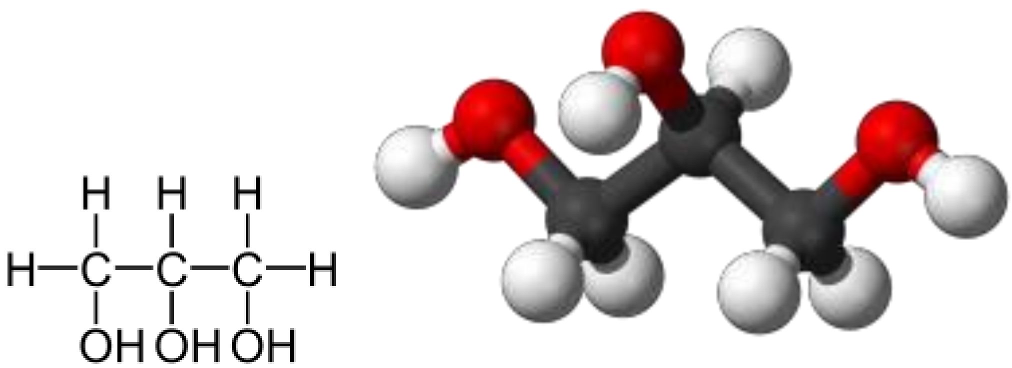

Figure 3 *Glycerol structure*

Glycerol can also be made synthetically based on petroleum refining. Before the biodiesel industry began to flourish, synthetic glycerol had a large share of the market with a price advantage. However, presently there is an abundance of natural glycerol coming from biodiesel production that has reduced the price of natural glycerol.

<u>Exercise 3</u>: Construct a model of a glycerol molecule.

<u>Fatty Acids</u> are part of triglycerides (fats and oils). In nature, they are made up of a chain consisting of an even number of carbons atoms from 4 to 28. Chains with an uneven number of carbons are much less common in nature.

Fatty acids are either saturated or unsaturated. Unsaturated fatty acids have double bonds between some of the carbons, whereas saturated fatty acids have no double bonds. Unsaturated fatty acids are generally classified as monounsaturated (they have one double bond), or polyunsaturated (they have two or more double bonds).

Fatty acids are often identified by name as well as by numbers in parentheses. The first number refers to the number of carbons, and the second number refers to the number of double bonds. Oleic acid (18:1) is a good example of a monounsaturated, with 18 carbons and one double bond.

Fatty acids have a carboxyl group (COOH) at one end. It is this end that combines with the hydroxyl group (HO-) on the glycerol molecule to form triglycerides.

Carbon atoms in a fatty acid are identified using the Greek alphabet, with the first carbon from the carboxyl group being labeled the alpha carbon, the next is the beta carbon, and so on. The last or terminal carbon is called the omega carbon. The most common form of linolenic acid (18:3) has three double bonds at 3, 6 and 9 carbons from the omega carbon. No doubt you have heard of Omega 3 and Omega 6 fatty acids as being essential in human nutrition. These names refer to the placement of the double bonds (counted from the last, or "omega," carbon.)

Double bonds can occur in a cis or trans configuration. In the cis arrangement, adjacent hydrogen atoms are on the same side of the double bond. This form is commonly found in nature, and causes the chains to be bent or hook-shaped (in the case of multiple double bonds). In trans fatty acids, adjacent hydrogen atoms are on opposite sides of the double bond, causing the chain to be straighter and to act more like a saturated fatty acid.

Notice in figures 4 – 6 we show three ways of illustrating fatty acids: the first is the space-filling model, where the atoms are shown touching each other; the second is the familiar stick-and-ball model; and the third is simply the structural formula. Another way to depict a molecule such as a fatty acid is with a line drawing that does not show the individual carbon and hydrogen atoms in the chain, as in figure 6.

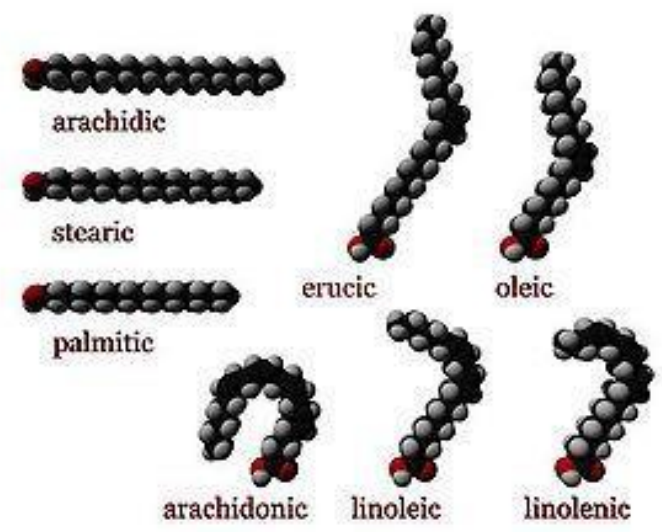

Figure 4 *Examples of different fatty acids*

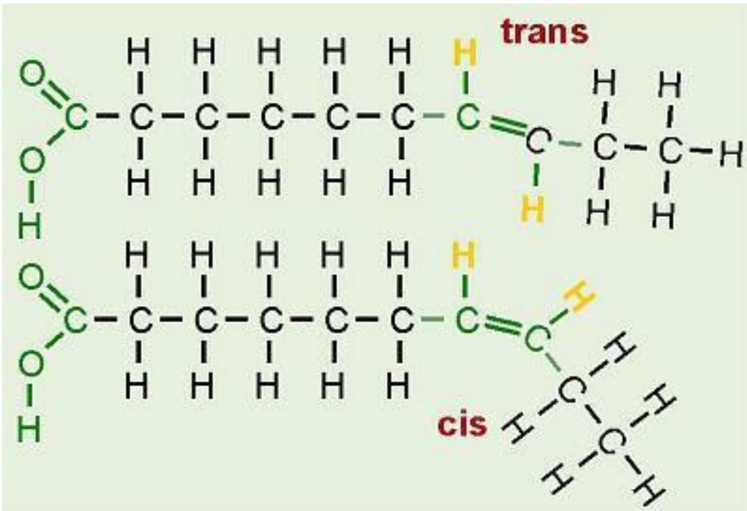

Figure 5 *cis vs. trans configuration*

Figure 6 *A polyunsaturated model*

Exercise 4: Construct models of a variety of fatty acids. Make saturated ones such as palmitic (14:0) and stearic (16:0), as well as some unsaturated fatty acids such as oleic (18:1) and linolenic (18:3).

Triglycerides are large and heavy molecules that are made up of three fatty acids connected to a glycerol backbone. They are commonly referred to as fats and oils, and are among a class of molecules called esters. Triglycerides are fatty acid esters of glycerol. The makeup of the fatty acids will vary based on the source. Animal fats tend to be more saturated (no double bonds) while plant oils are typically more unsaturated (having one or more double bonds).

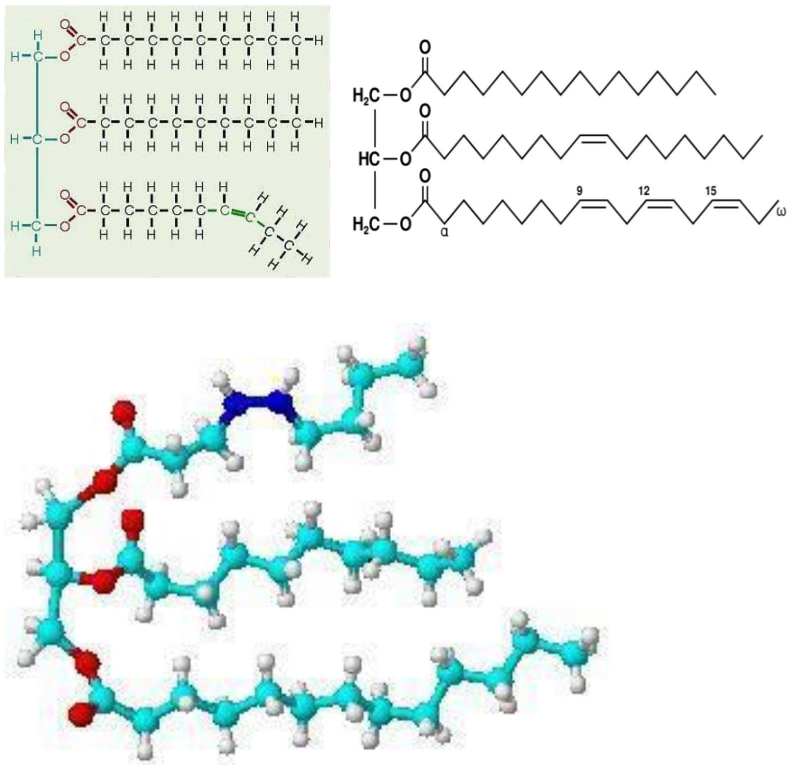

Figure 7 Molecular structure of triglycerides showing saturated and unsaturated fatty acids

<u>Exercise 5</u>: Using three fatty acids and a glycerol molecule, construct a triglyceride molecule.

Esters are a class of compounds derived from the reaction of an acid and an alcohol. For example, the reaction of fatty acids and methanol produce methyl esters, or biodiesel. The molecular formula for a methyl ester is RCO_2CH_3, where R represents a fatty acid. Triglycerides are also a type of ester. In fact the term "transesterification," which is the process of turning triglycerides into biodiesel, means the act of changing one type of ester into another.

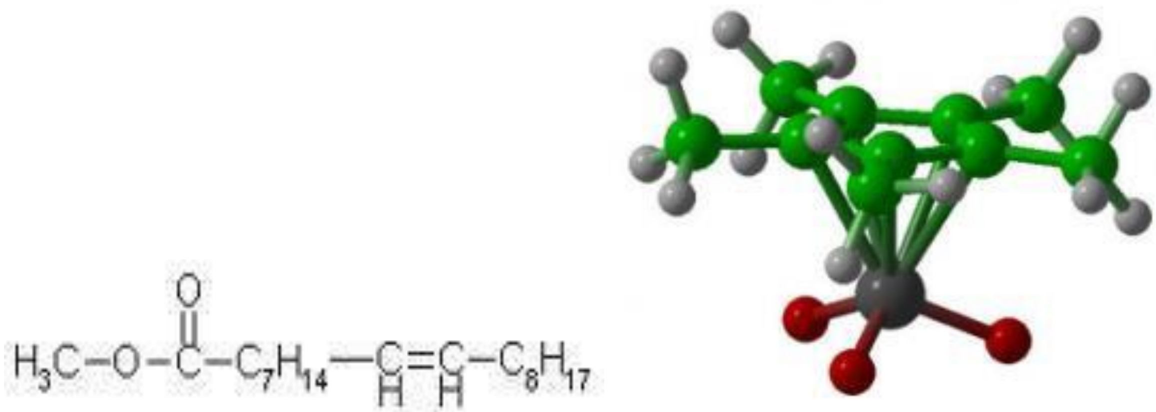

Figure 8 *Structure of a methyl oleate formula (18:1) and 3-D model of methyl caprylate (10:0).*

<u>Exercise 6</u>: Use 3 methanol molecules and 1 triglyceride molecule to construct 3 methyl ester molecules. Each methyl ester molecule may be different, depending on the fatty acid used to make it. You should have one glycerol molecule left over.

Additional Exercises

a. Write the molecular formula for oleic acid (18:1) and draw a diagram of the fatty acid chain.
b. On which carbon would you find the double bond in an Omega 3 fatty acid?