Introduction to Biodiesel Chemistry
Terms and Background Information

Basic Organic Chemistry

Organic chemistry is the branch of chemistry that deals with *organic compounds.*

Organic compounds are compounds that (with a few exceptions such as carbon dioxide gas) contain the element carbon.

The properties of *organic compounds* are dependent primarily on the physical structure of the molecules and by the presence of *functional groups*, which categorize *organic compounds* in different groupings, such as *alcohols, acids, esters, aldehydes, or ketones,* just to name a few.

If a component of an organic compound is not important to the reaction being defined, it is often represented on paper as *R*, which indicates "organic rest."

What is Biodiesel?

Biodiesel is composed of *mono alkyl esters* of *long chain fatty acids* derived from renewable *lipid* sources, such as vegetable oil or animal fats.

Esters are *organic compounds* composed of an *alcohol* and an *organic acid.*

Alcohols are *organic compounds* that contain a functional group OH (hydroxide).

Carboxylic acids are *organic compounds* that contain a functional group COOH (carboxyl).

Long chain fatty acids are *carboxylic acids* that are composed of single chains of 12 to 24 carbons with a carboxyl group.

What is Vegetable Oil?

Vegetable oil is composed of *triglycerides* of *long chain fatty acids* attached to *glycerol,* which is a type of *alcohol.* Each *triglyceride* contains one *glycerol* and three *long chain fatty acids.*

The process used to make *biodiesel* is called *transesterification* because it is a process of transforming one type of *ester* into another.

prepared by John Bush for Biodiesel Collective Conference 2008
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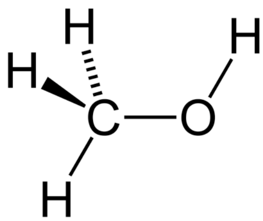
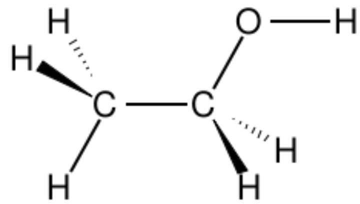
<u>Examples of Organic Compounds</u>

Alcohols – containing a hydroxyl group OH

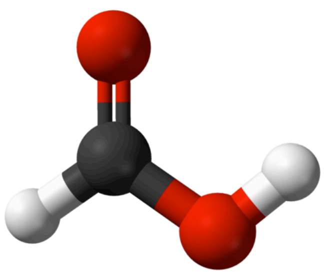


Methanol
CH_3OH

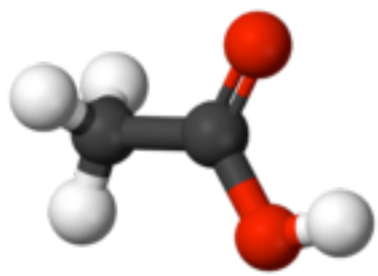


Ethanol
CH_3CH_2OH

Carboxylic Acids – containing a carboxyl group COOH

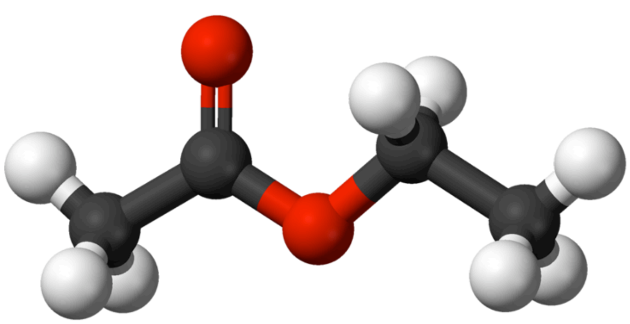


Formic (Methanoic) Acid
CH_2O_2



Acetic (Ethanoic) Acid
CH_3COOH

Esters – alcohols bonded to acids



Ethyl Acetate
$C_4H_8O_2$

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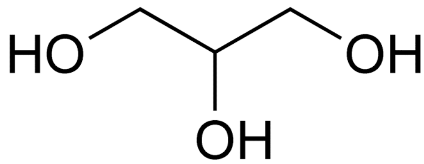
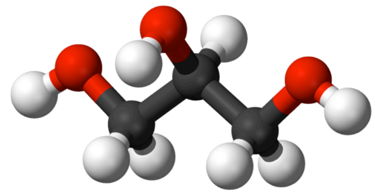
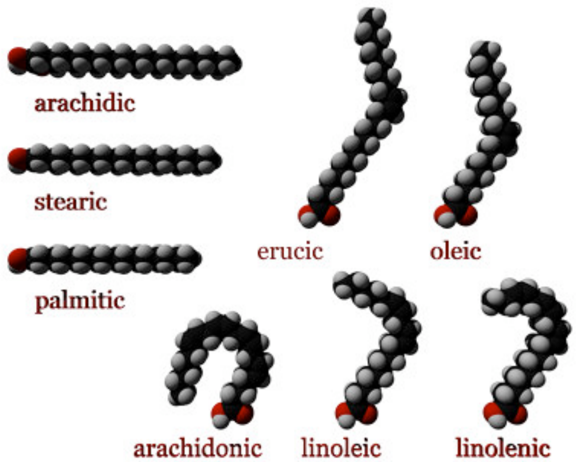
Glycerol, Fatty Acids, Triglycerides, and Biodiesel

Glycerol (Glycerine)

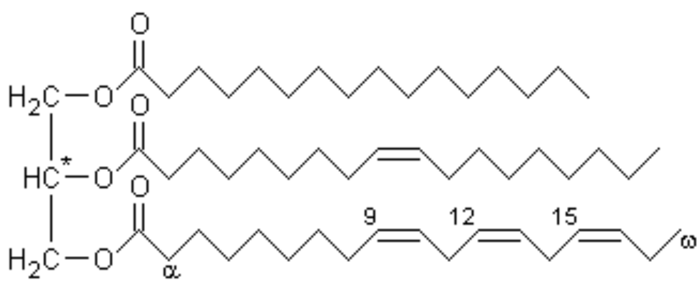




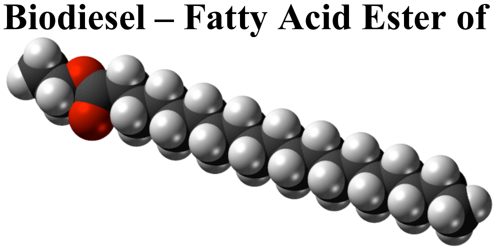
Fatty Acids



Triglyceride – Fatty Acid Ester of Glycerol



Biodiesel – Fatty Acid Ester of a Simple Alcohol



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Biodiesel Chemistry
Reactions Contributing to Methyl Ester Production

1. Transesterification of Fats (Triglycerides) to form Fatty Acid Methyl Esters and Glycerol

   1 Triglyceride + 3 Methanol $\leftrightarrow$ 3 Methyl Ester + 1 Glycerol

   - The fatty acid *R* groups remain unchanged
   - This reaction is facilitated with a strong base catalyst

2. Reaction of Catalyst (NaOH) with Methanol

   $CH_3OH + NaOH \rightarrow CH_3O\text{-}Na + H_2O$

   - $CH_3O\text{-}Na$ exists as the anion CH_3O^- and the cation Na^+

3. The reaction of Methoxide with Triglyceride

```
          O                                  O
          ||                                 ||
CH2-O-C-R                         CH2-O-C-R
|                                 |
|        O                        |                        O
|        ||                       |                        ||
CH-O-C-R  +  CH3O-    →          CH-O-        +       CH3O-C-R
|                                 |
|          O                      |          O
|          ||                     |          ||
CH2-O-C-R                         CH2-O-C-R
```

Triglyceride + Methoxide → Triglyceride Anion + Methyl Ester

   - The triglyceride anion then needs a proton to form a diglyceride. If the proton comes from another methanol, a new methoxide ion is formed, regenerating the catalyst.

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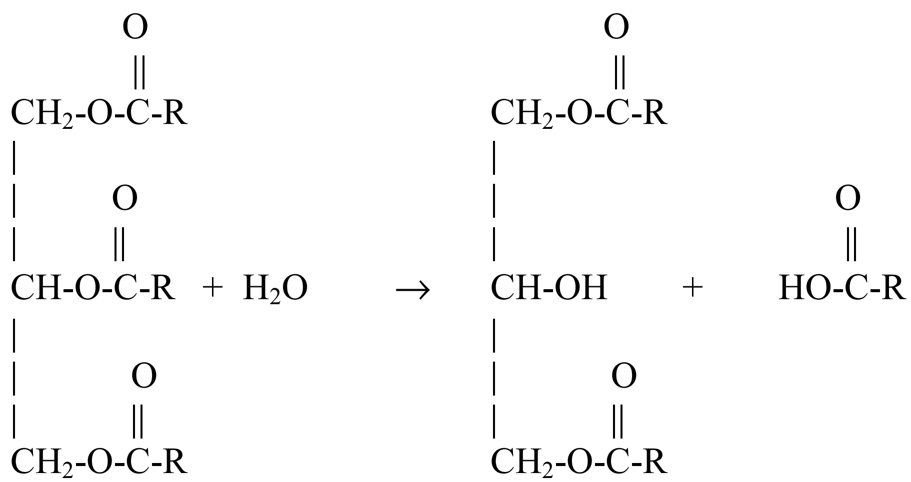
Biodiesel Chemistry
Reactions Inhibiting Methyl Ester Production

1. Hydrolysis of Triglyceride to form Diglyceride and Free Fatty Acid



- This reaction is particularly prevalent in deep fryers, and is the primary reason used cooking oil contains free fatty acids
- It can also happen during biodiesel processing. The presence of a base catalyst facilitates this reaction in a similar way as it facilitates transesterification, except the end result is soap.

2. Reaction of Alkali Catalyst with Free Fatty Acid to form Soap

$$NaOH + HOC(O)R \rightarrow H_2O + Na\text{-}OC(O)R$$

- Note that water is also a product

Summary:

Water can react in a similar way as methanol with triglycerides, except it results in free fatty acid production. Free fatty acids form soaps with alkali catalysts. Therefore, either the presence of water or free fatty acids will limit the effectiveness of the catalyst and inhibit the completion of the transesterification reaction that produces methyl ester.

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