MATERIALS AND METHODS

Material and method are described in this section. A high efficiency computer is used to determine a geometrical parameter of triolein structure, the energy of reaction step in transesterification mechanism, and the total energy of the transesterification mechanism. All of this calculations can compute by GAUSSAIN 03W and GaussViewW software.

Materials

The materials which are used in this work are shown in the following list.

1. Personal computer:

    - Intel® Xeon™ CPU3.0 GHz processor, 2.0 GB of RAM
    - Intel® Pentium® 4 CPU 3.00 GHz processor, 2.0 GB of RAM
    - AMD Athlon™ 64 bit CPU 2.0 GHz processor, 1 GB of RAM
    - AMD Athlon™ 64 bit CPU 2.0 GHz processor, 1 GB of RAM
    - AMD Athlon™ 64 bit CPU 2.0 GHz processor, 1 GB of RAM
    - AMD Athlon™ 64 bit CPU 2.0 GHz processor, 256 GB of RAM
    - AMD Athlon™ XP 2400+ CPU 2.0 GHz processor, 1.5 GB of RAM
    - AMD Athlon™ XP 2200+ CPU 2.0 GHz processor, 256 GB of RAM

2. GAUSSIAN 03W and GaussViewW for windows software.

Methods

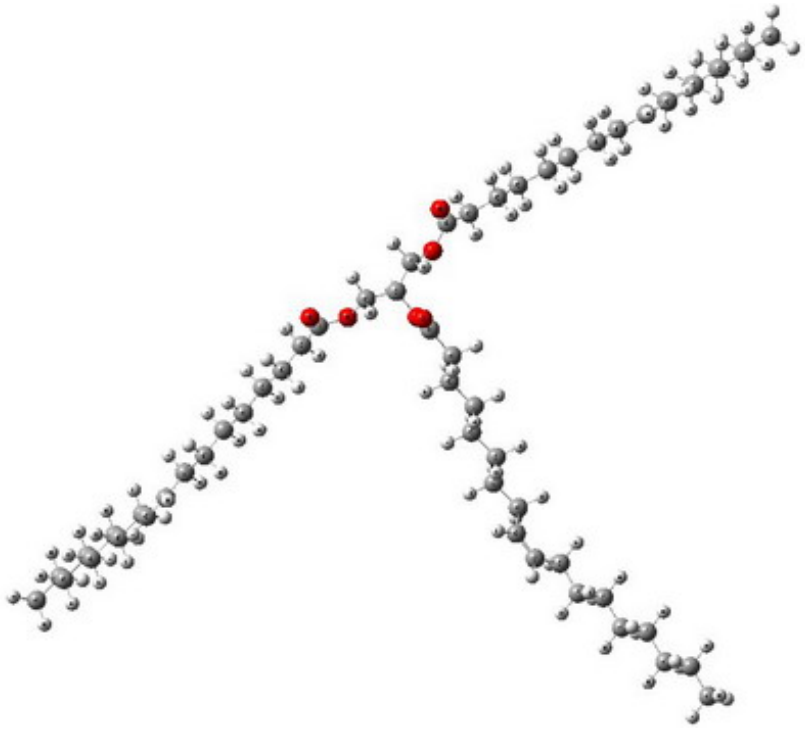
Molecular Modeling is the specific method to determine any molecular structures and also transport mechanism during the operation. This technique has many advantages, for example, to eliminate the need of use real chemicals; to save not only resources but also to reduce researcher exposure to toxic chemicals; called greener science.

Geometrical Parameters

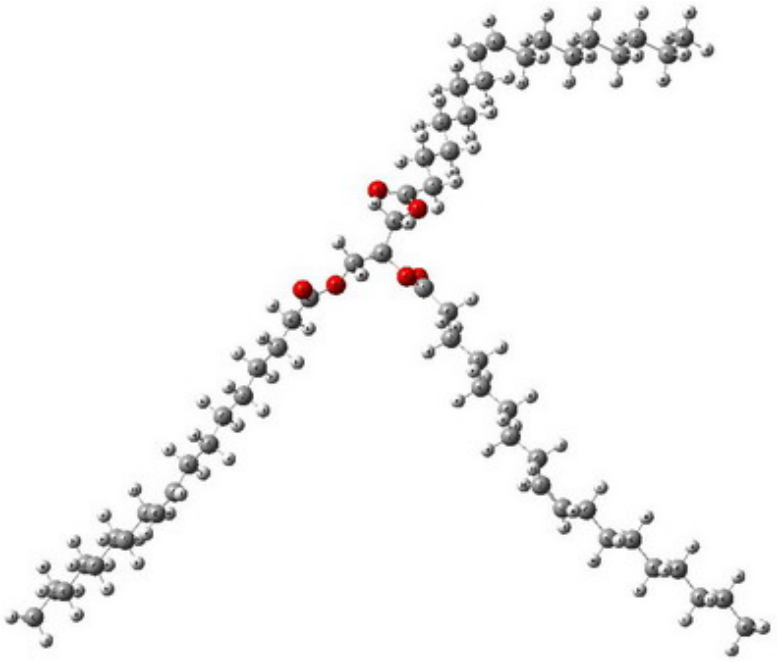
The geometries of all molecules were constructed by GaussViewW and the GAUSSIAN 03W is used to predict many properties of molecules and reactions. A stable molecular structure is shown with a minimum molecular energy. In this thesis, geometrical parameters of molecules are determined in the gas phase calculation that input a “NONE” model of a solvation function into GAUSSIAN 03W. The calculation in the liquid phase can be determined either by input a “DEFAULT” model of a solvation function then choose the solvent that system need. The exact structures or possible structures with a lowest molecular energy will be parted of the molecular study to complete the transesterification mechanism.

At first, the geometries of the triolein were constructed but it is difficult to predict because of its large molecule and unavailable. Other substances such as alcohol (methanol or ethanol etc.), catalyst (sodium methoxide, potassium methoxide etc.) can be modeled directly.

There are two possible geometrical molecular structures of triolein as shown in Fig. 6(a) and Fig 6(b). The optimum bond lengths and angles of triolein molecule calculated with the semiempirical AM1, PM3 and *ab initio* Hartree-Fock.



(a)

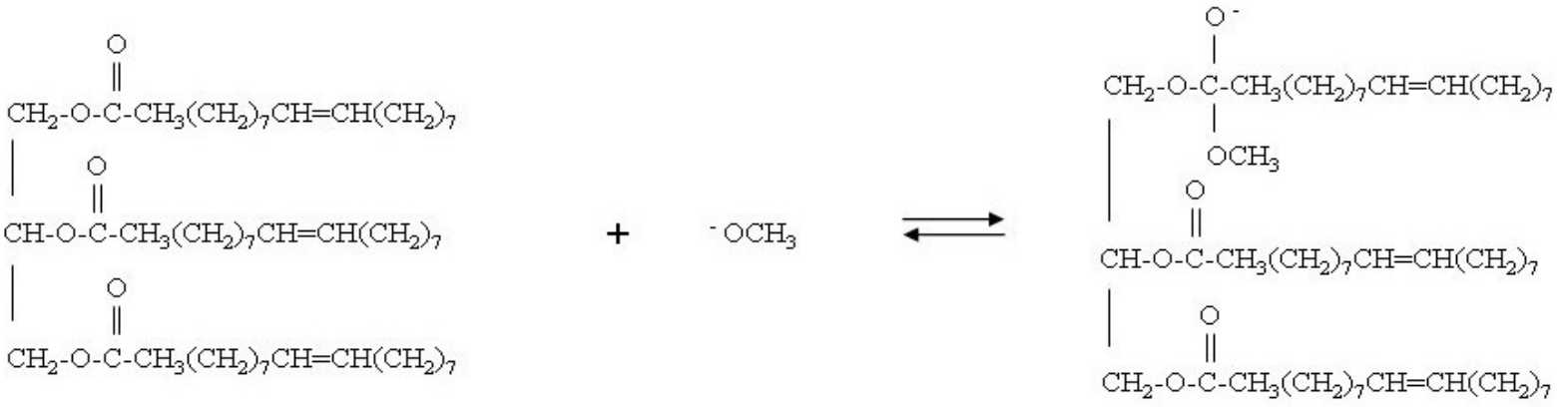


(b)

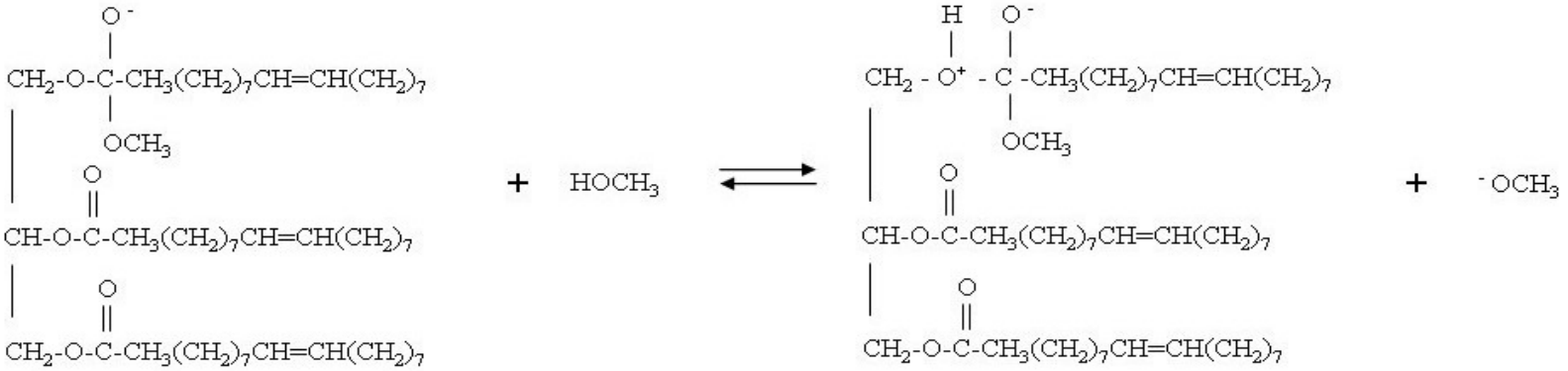
Figure 6 Molecular structure of triolein: (a) 1st triolein (b) 2nd triolein.

Transesterification mechanism

The transesterification can be divided into 3 steps for each of glycerides (mono-, di-, and triglyceride) as shown in Fig. 2 and 3. These step referred to an experimental results [ref]. In this thesis, in each step, the reaction will be constructed and optimized by GaussViewW and GUASSIAN 03W respectively. In the first step, the reactants are composed of glyceride and catalyst as methoxide to form intermediate1. The second step, the reactant are composed of intermediate1 and methanol as an alcohol to form intermediate2. The last step, intermediate2 is reformed to fatty acid alkyl ester or methyl ester and glycerol. All three steps of all molecules that are triolein, diolein, and monoolein were shown in Fig. 7-13

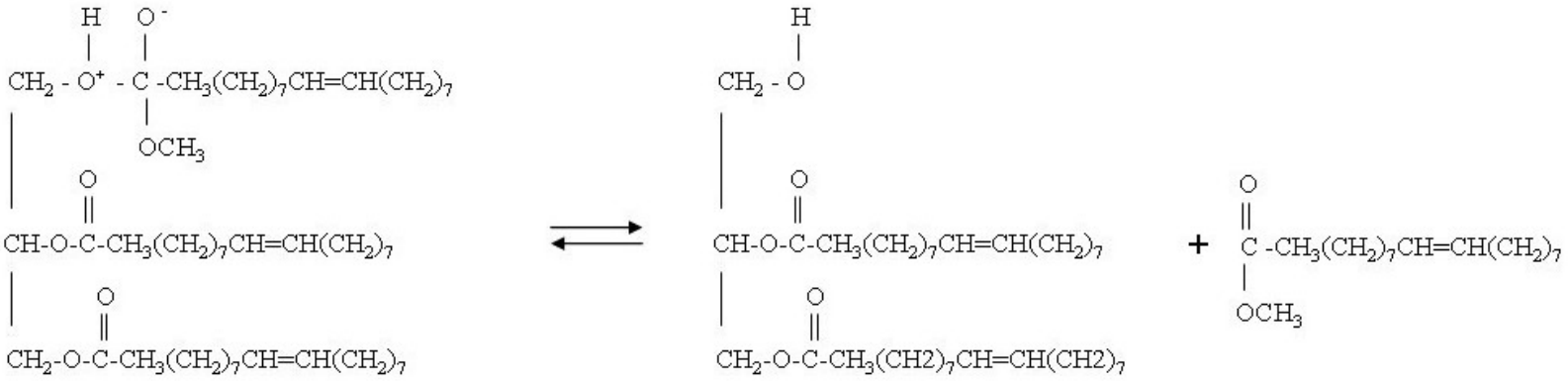


(a.1)



(a.2)1

Figure 7 Transesterification mechanism type1.



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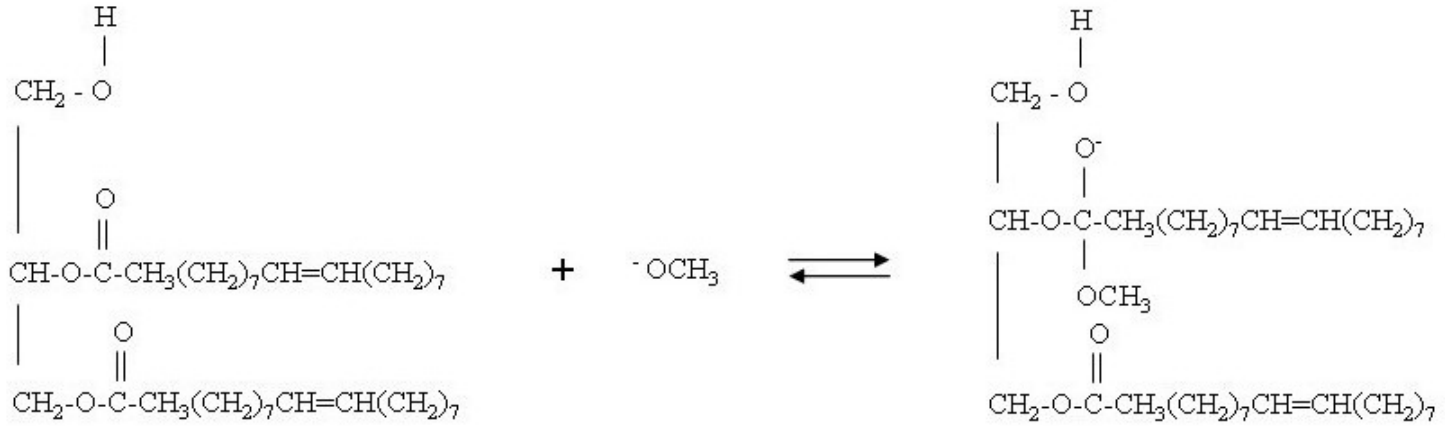
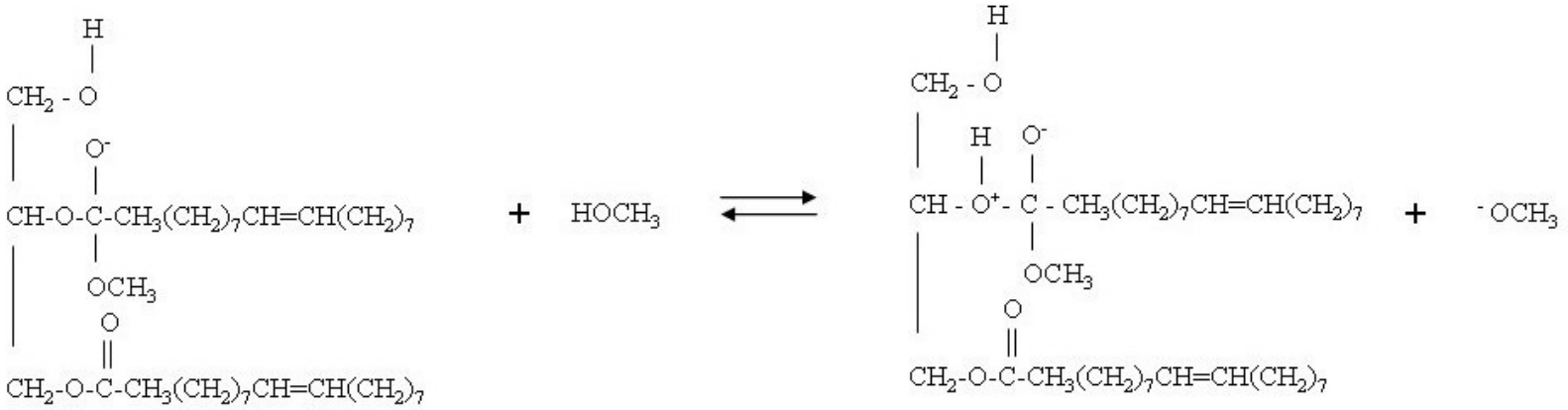


(b.1)

Figure 7 Transesterification mechanism type1. (Cont'd)



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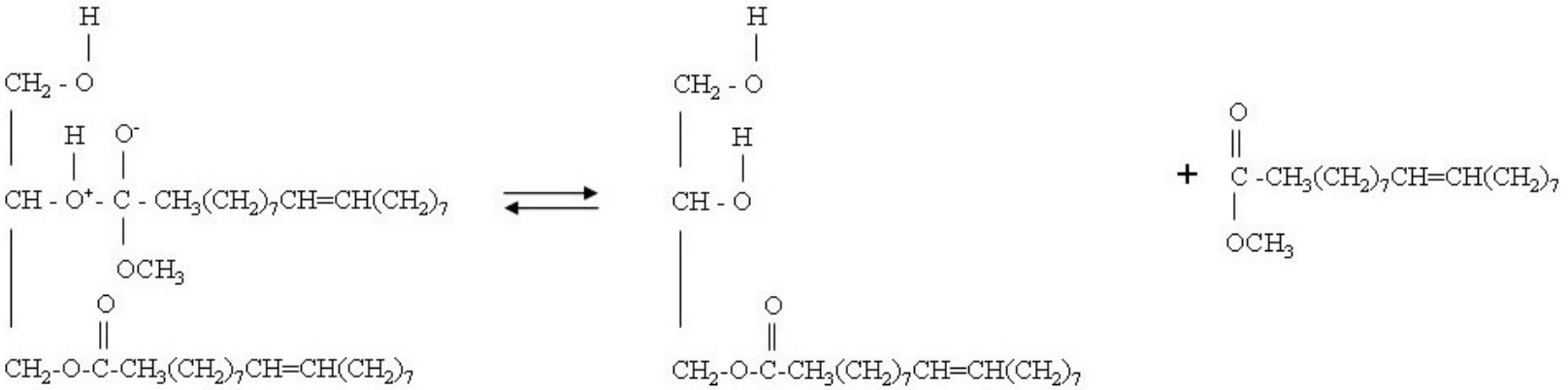

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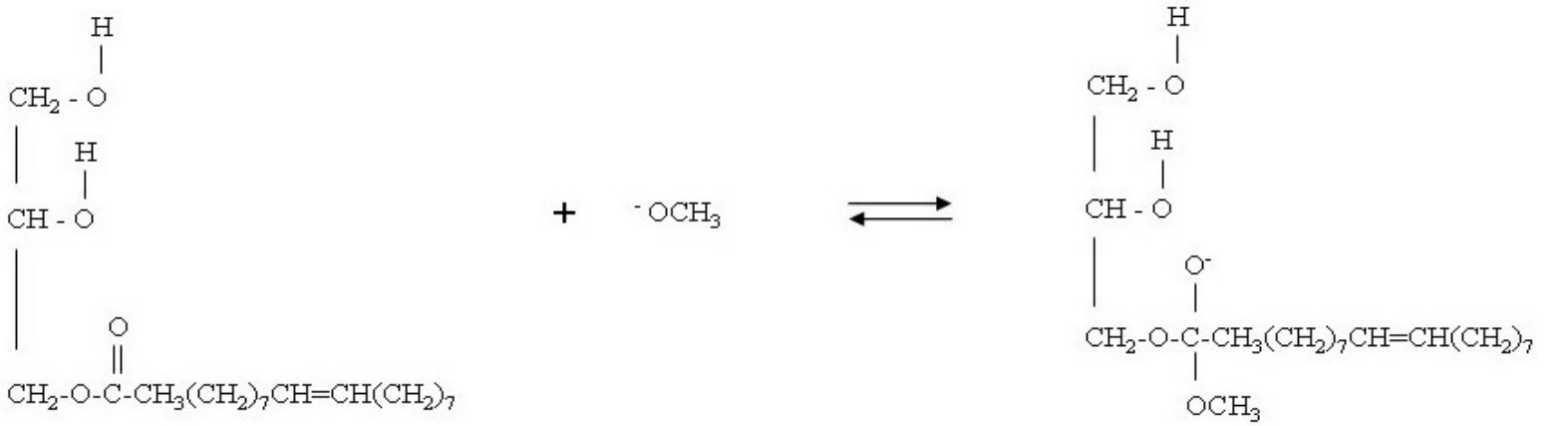
Figure 7 Transesterification mechanism type1. (Cont'd)



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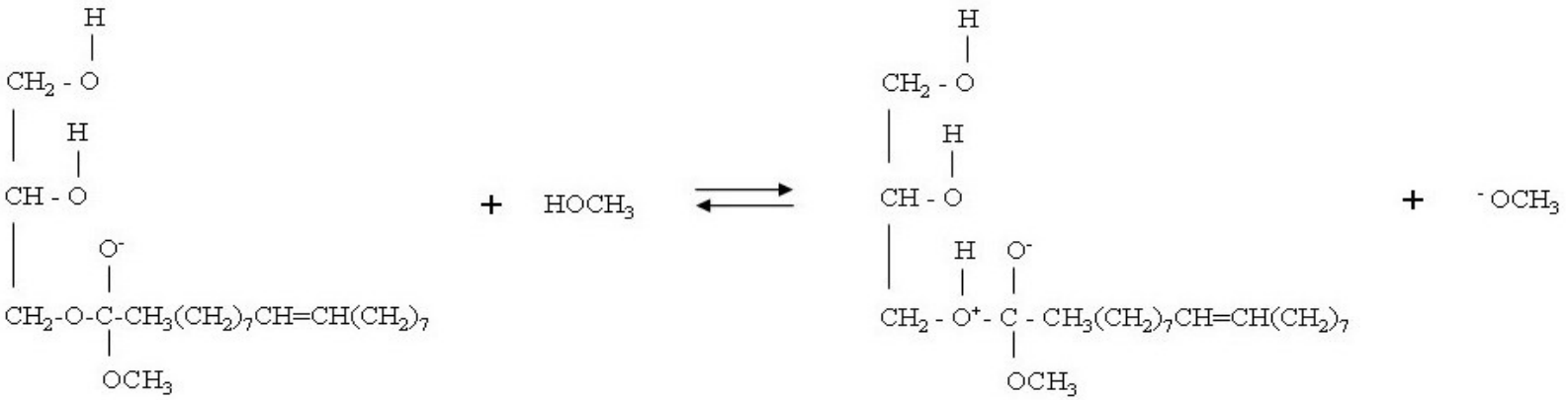

(c.2)

Figure 7 Transesterification mechanism type1. (Cont'd)

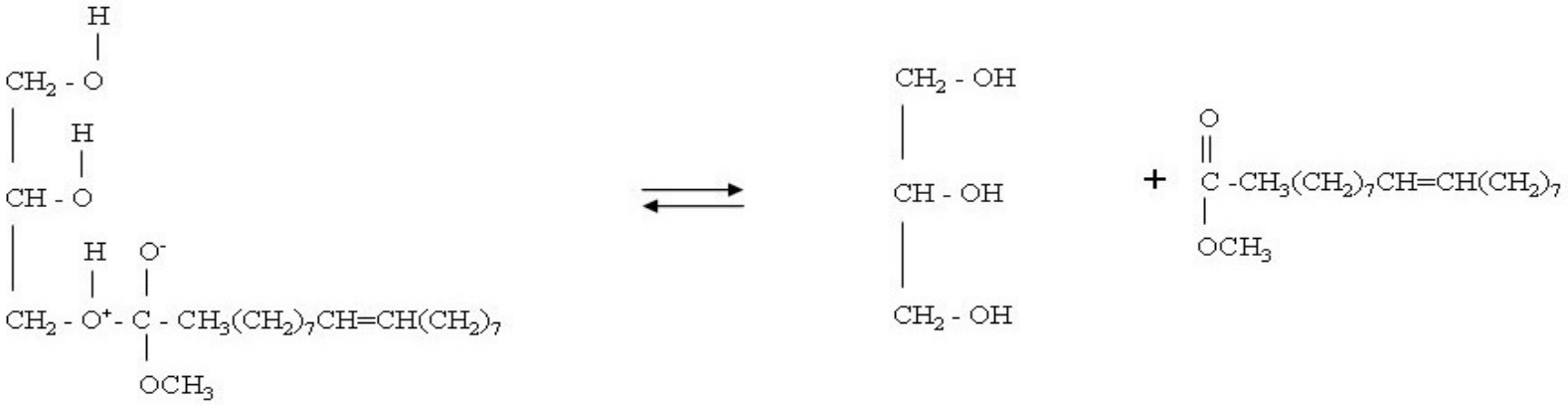

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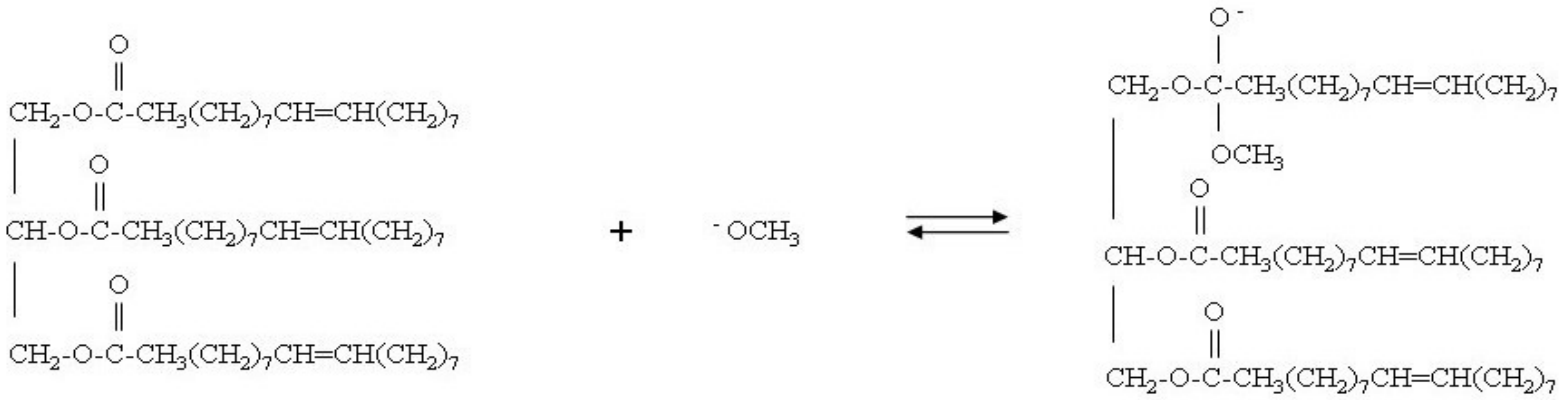
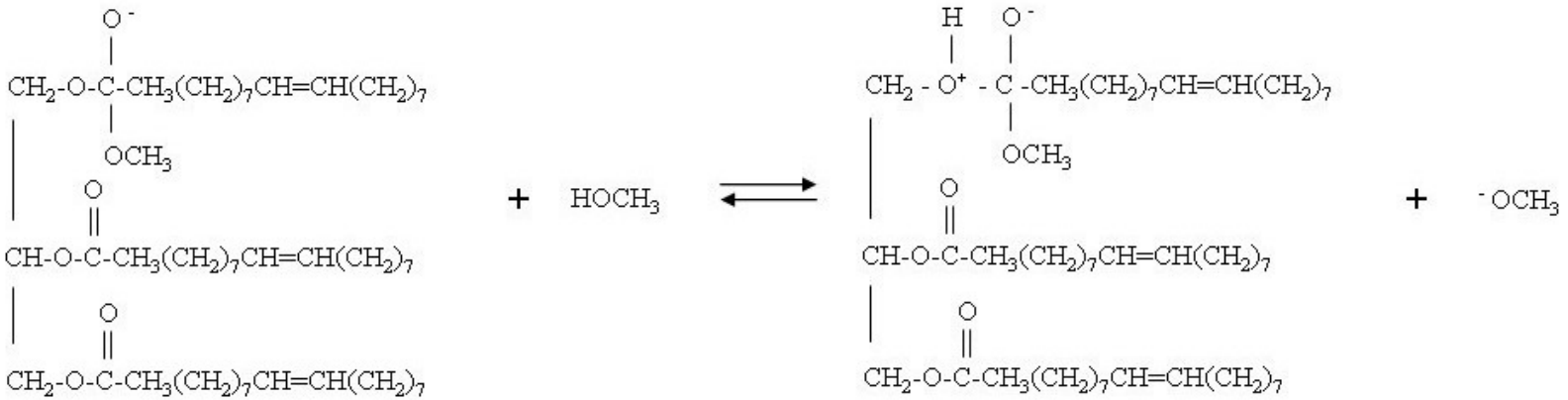
Figure 7 Transesterification mechanism type1. (Cont'd)

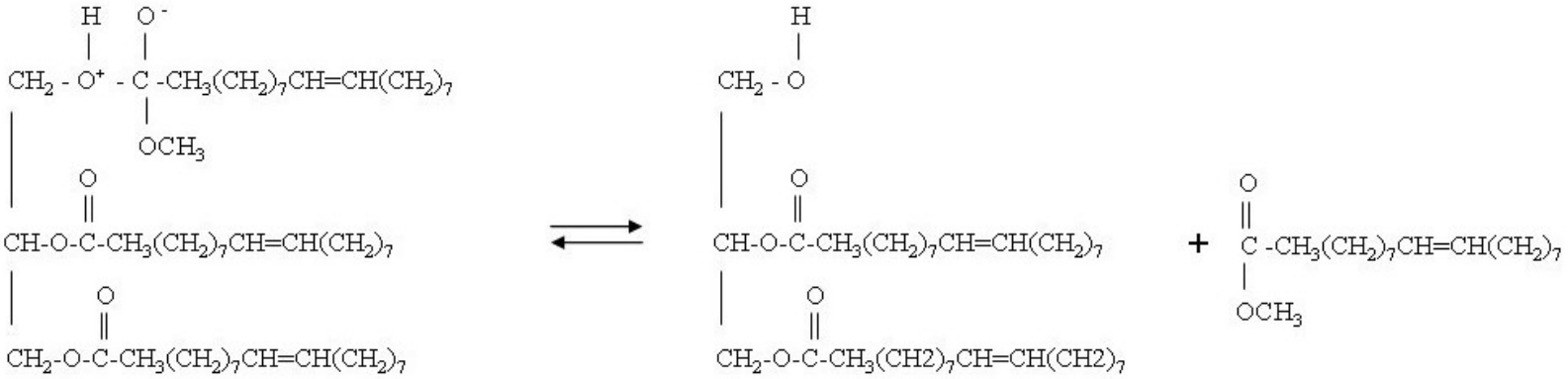


(a.1)

Figure 8 Transesterification mechanism type2.



(a.2)



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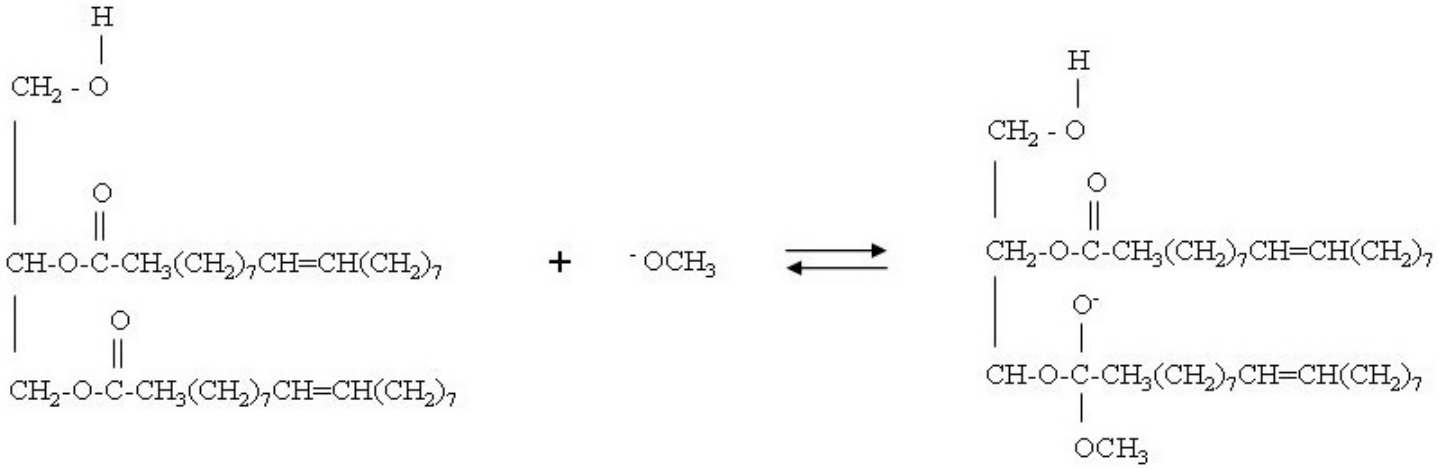

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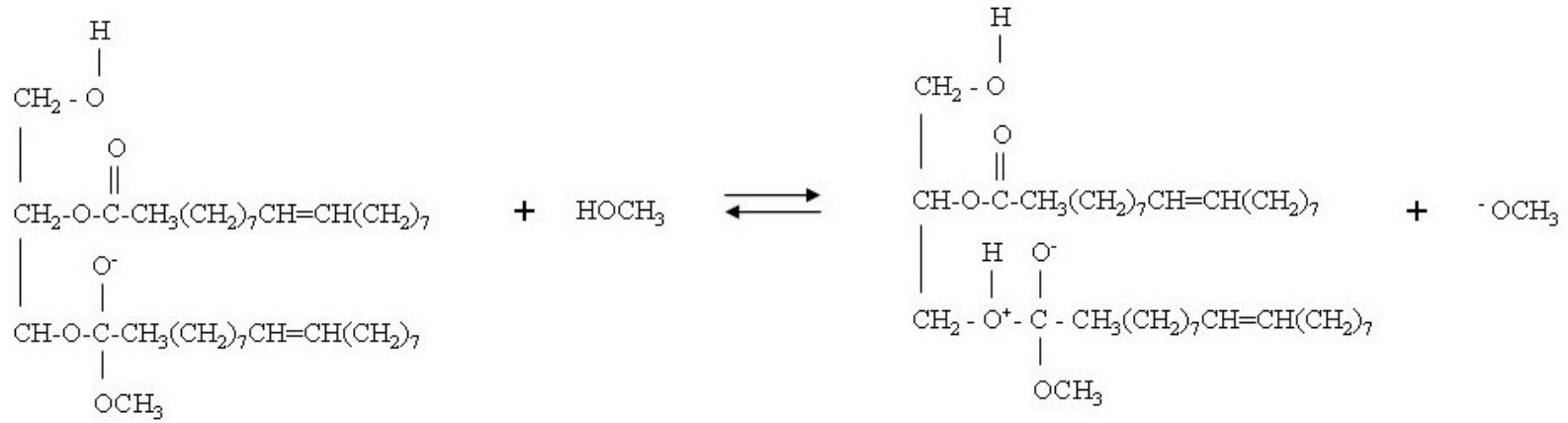

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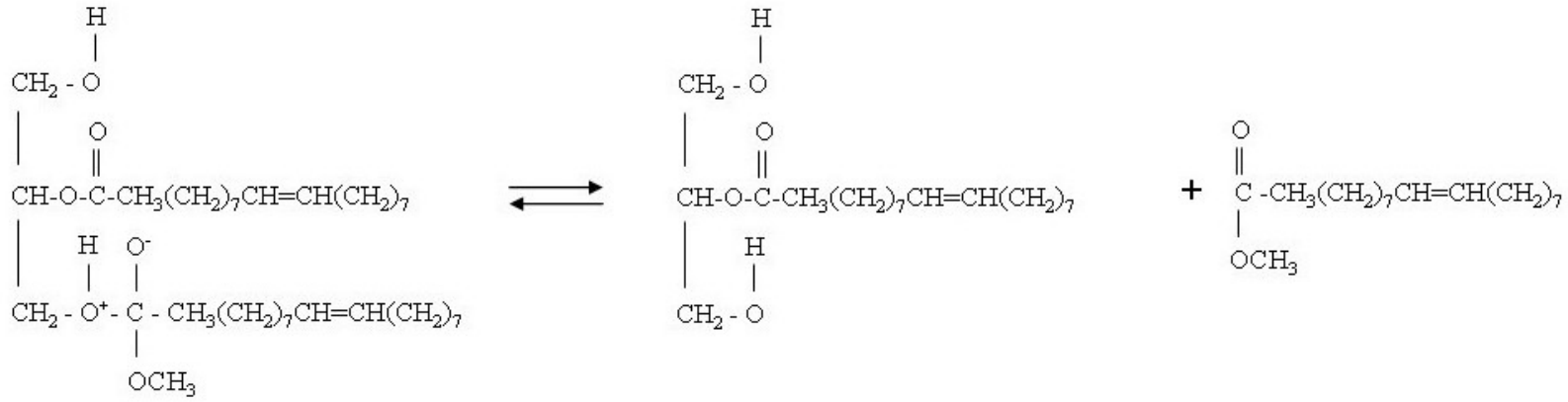

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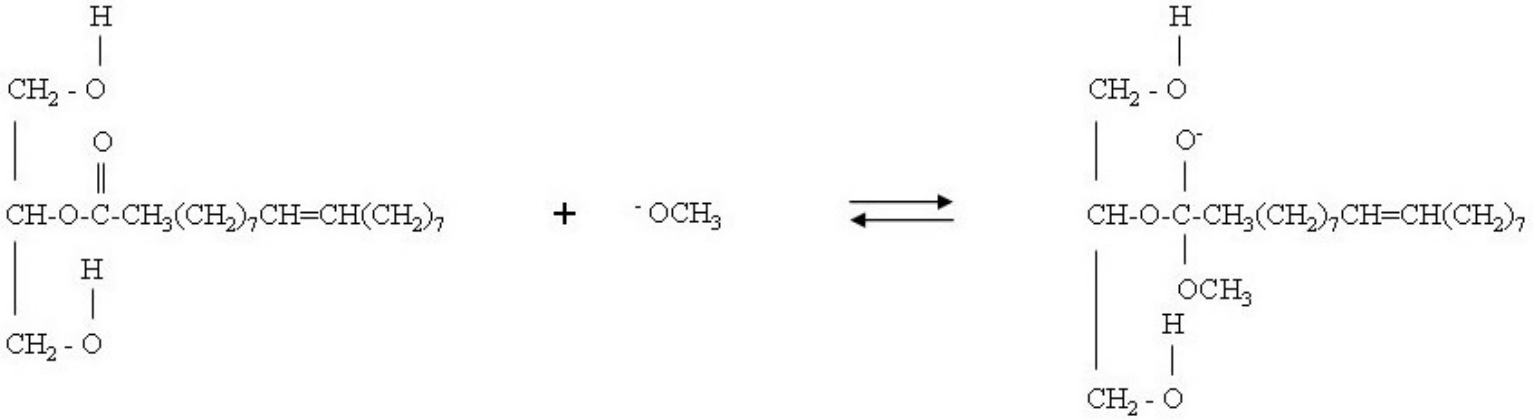

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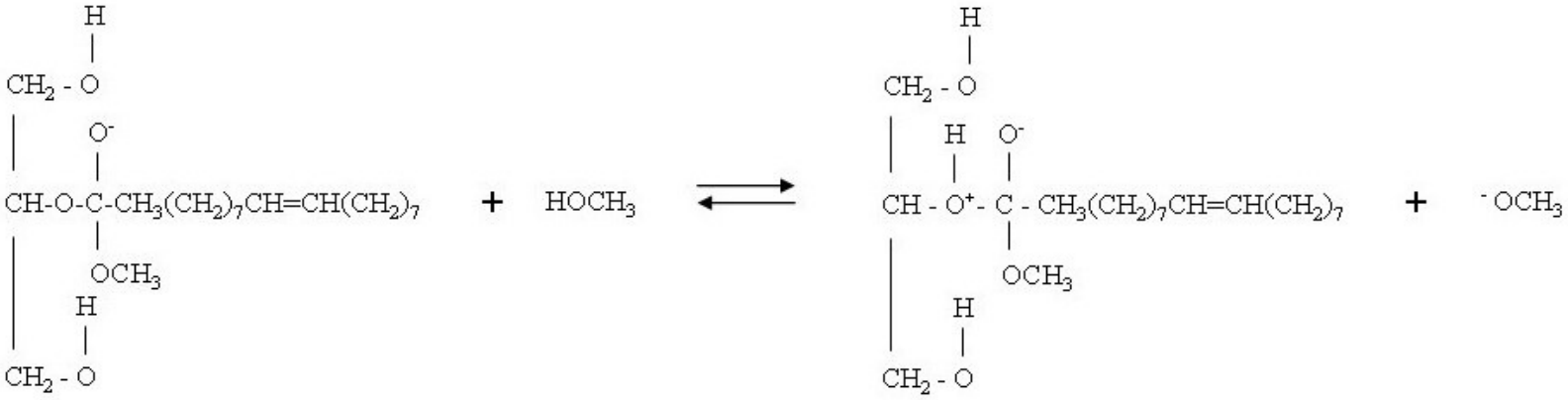

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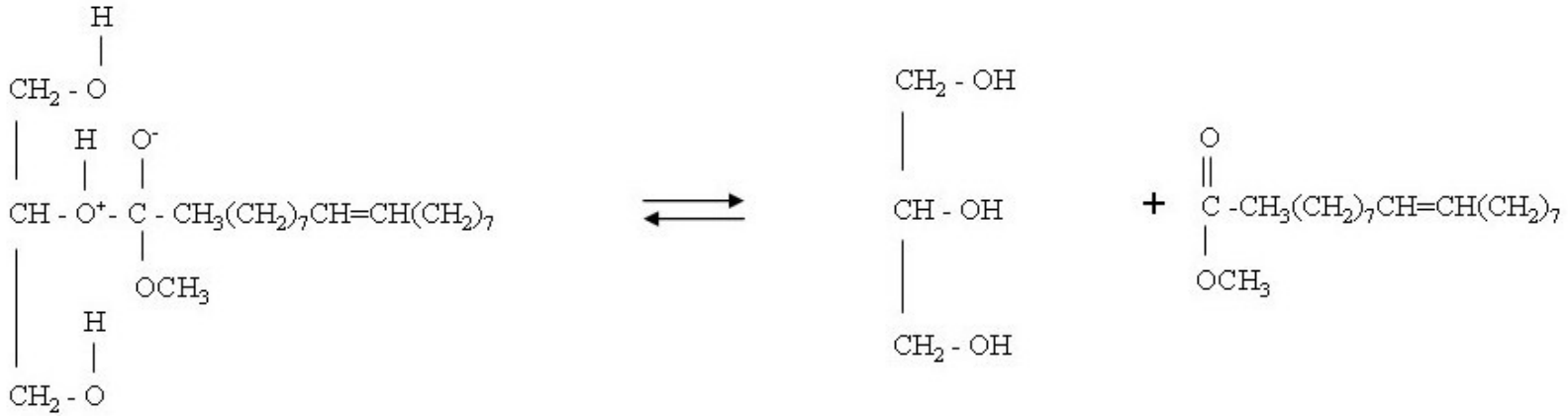

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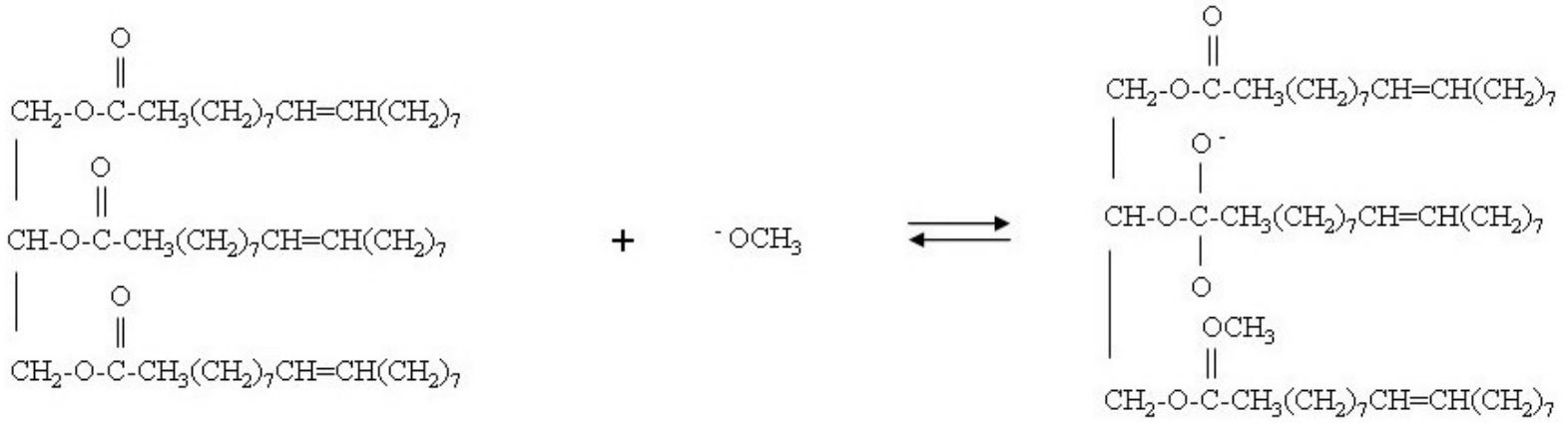

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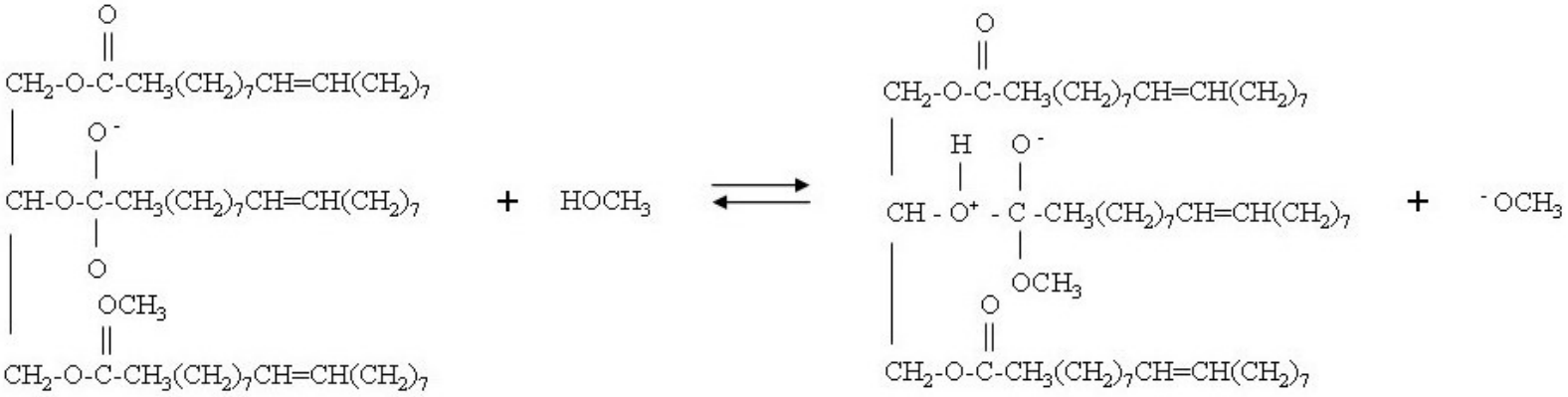
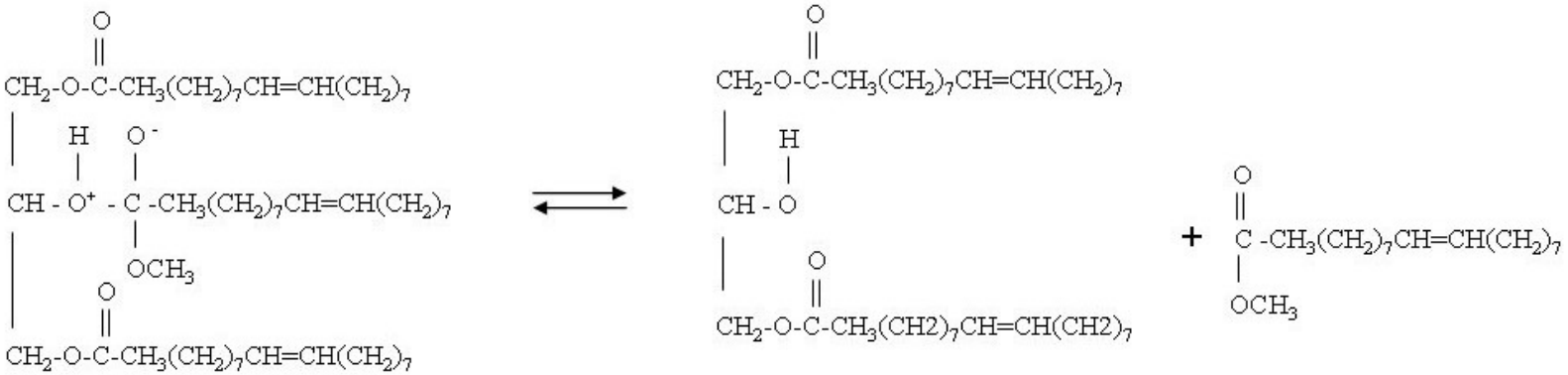


(a.2)

Figure 9 Transesterification mechanism of triolein type3.



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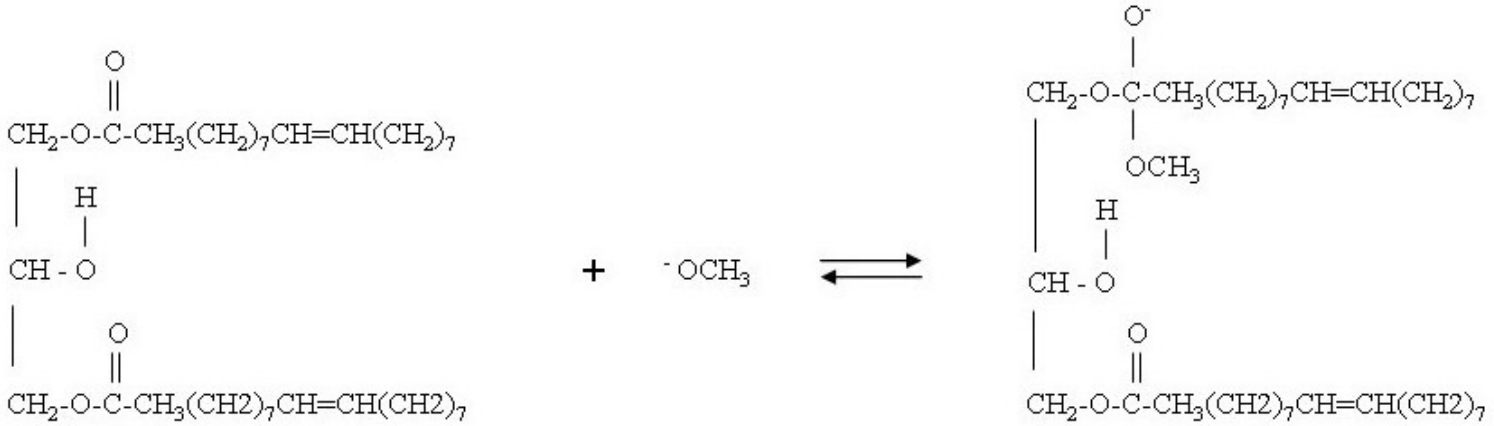

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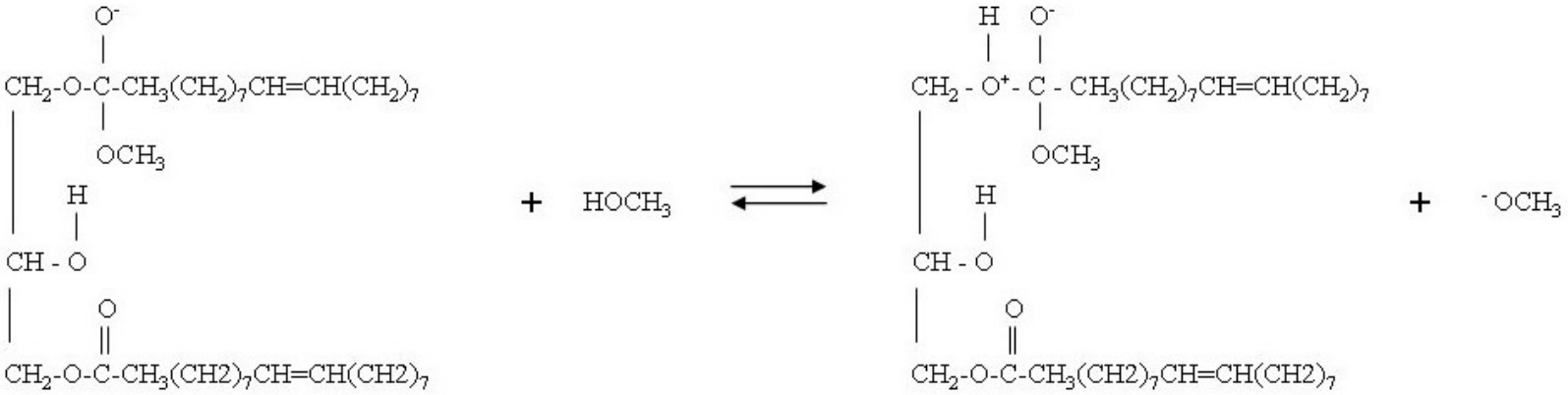
Figure 9 Transesterification mechanism of triolein type3. (Cont'd)



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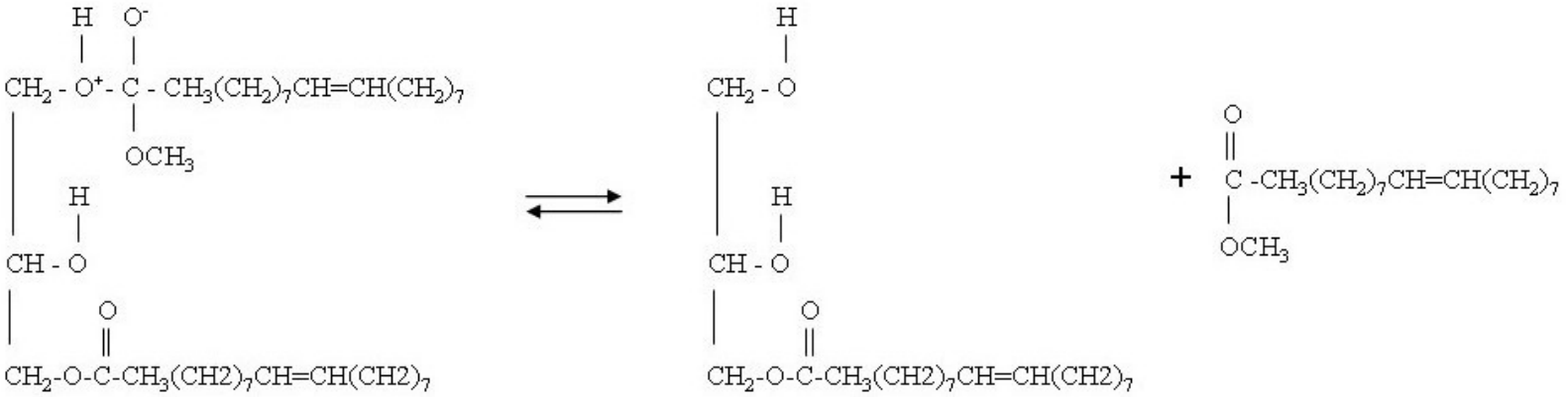

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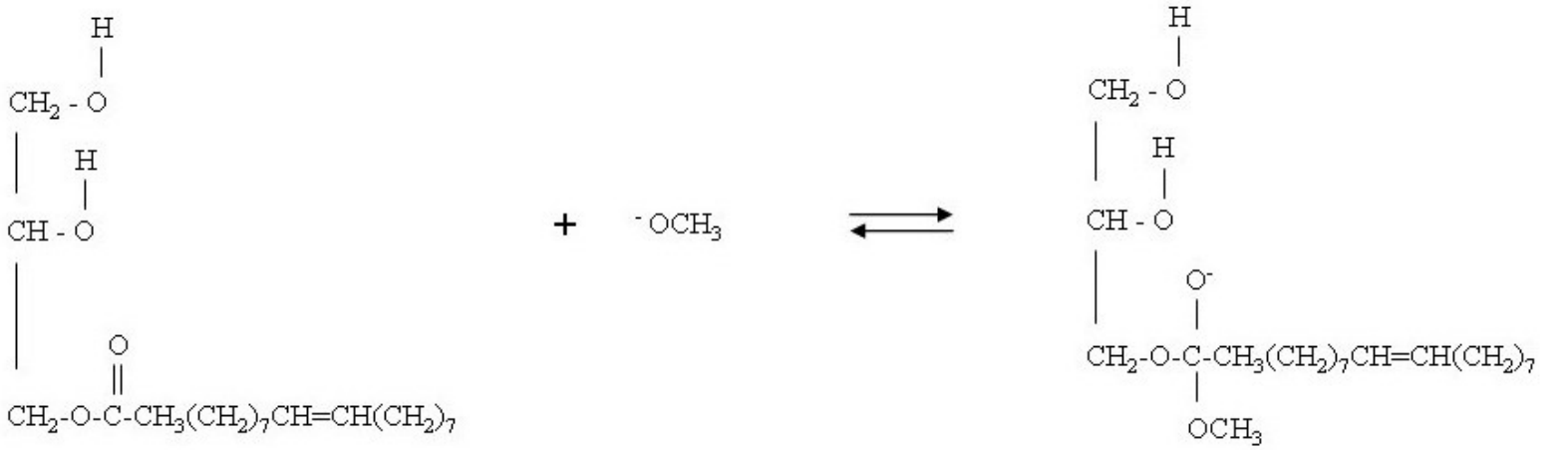
Figure 9 Transesterification mechanism of triolein type3. (Cont'd)



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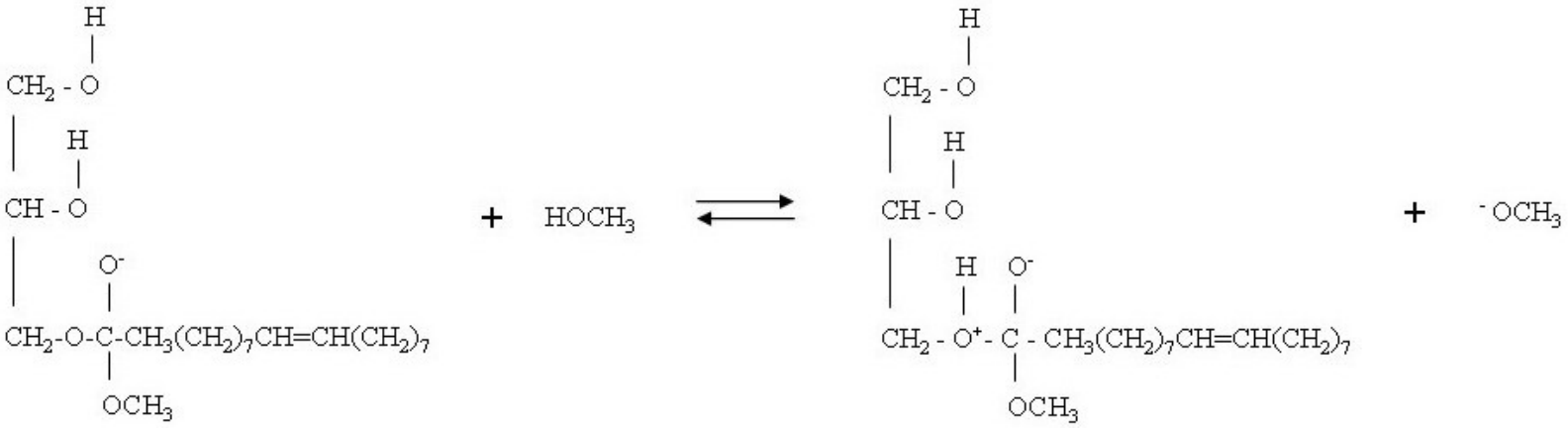

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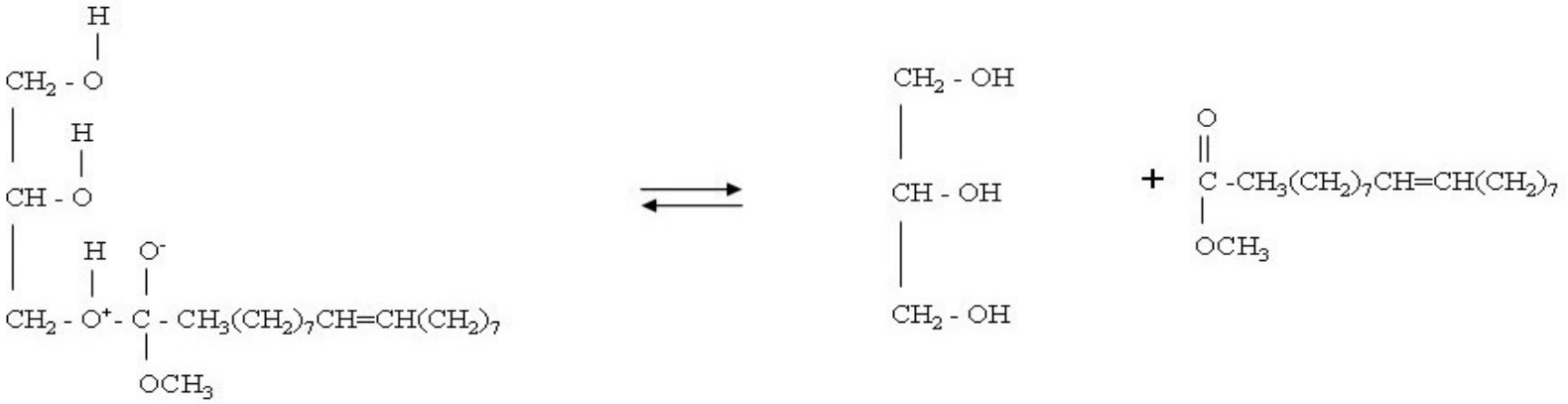

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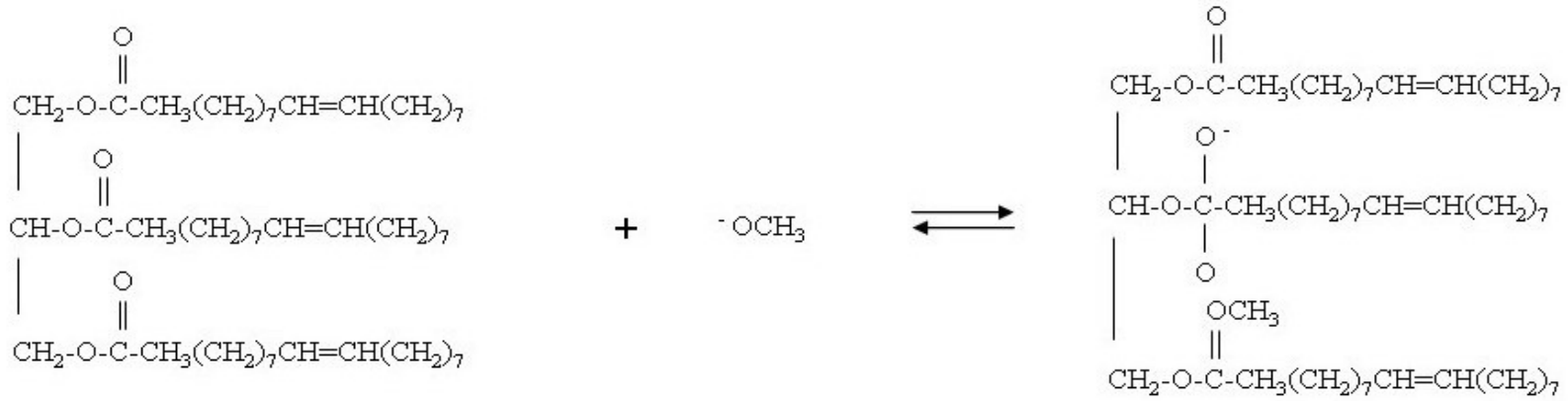
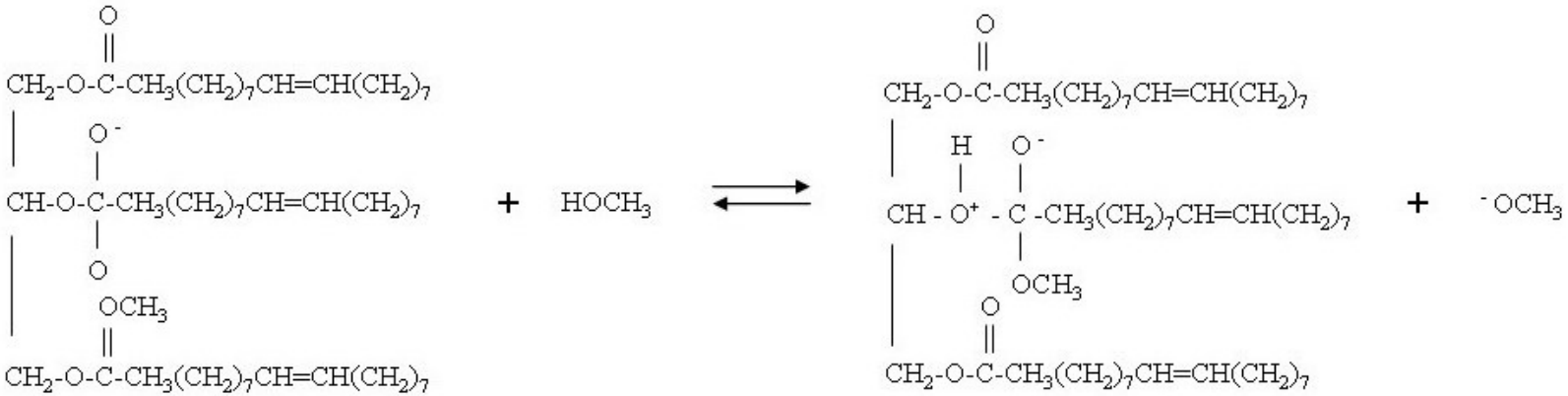
Figure 9 Transesterification mechanism of triolein type3. (Cont'd)



(a.1)

Figure 10 Transesterification mechanism type4.



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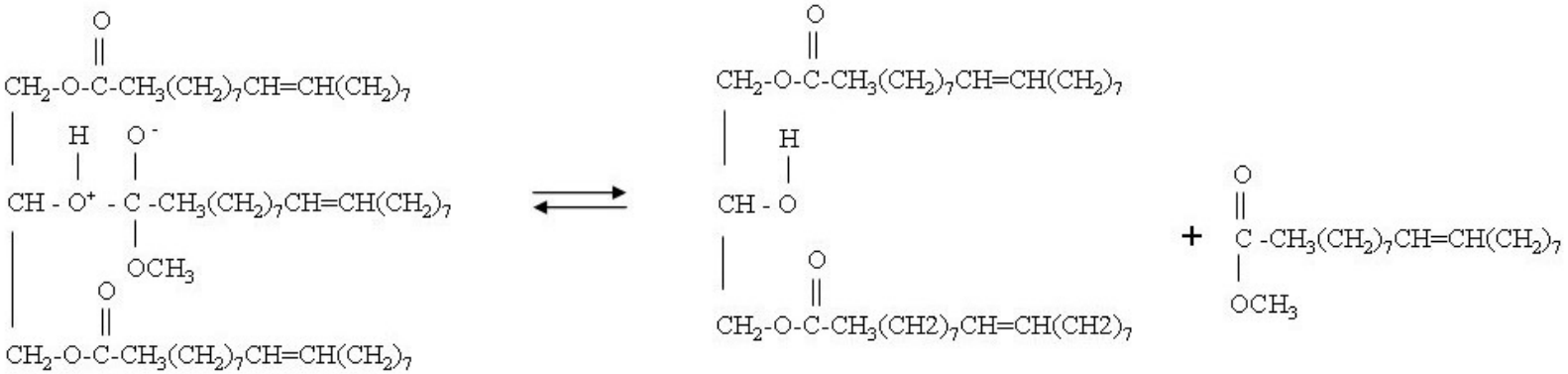

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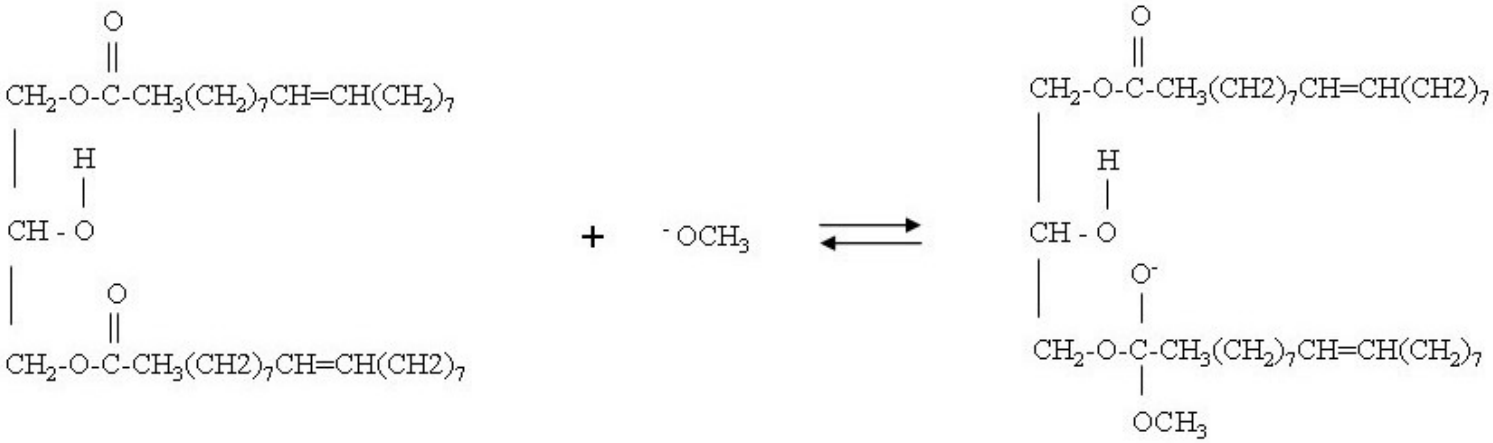
Figure 10 Transesterification mechanism type4. (Cont'd)



(b.1)

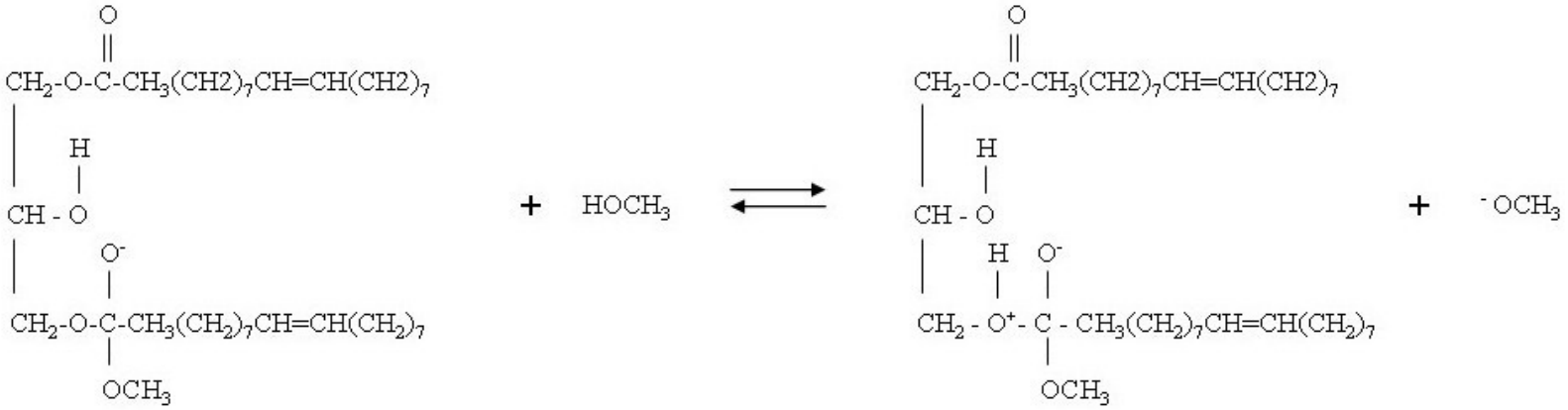


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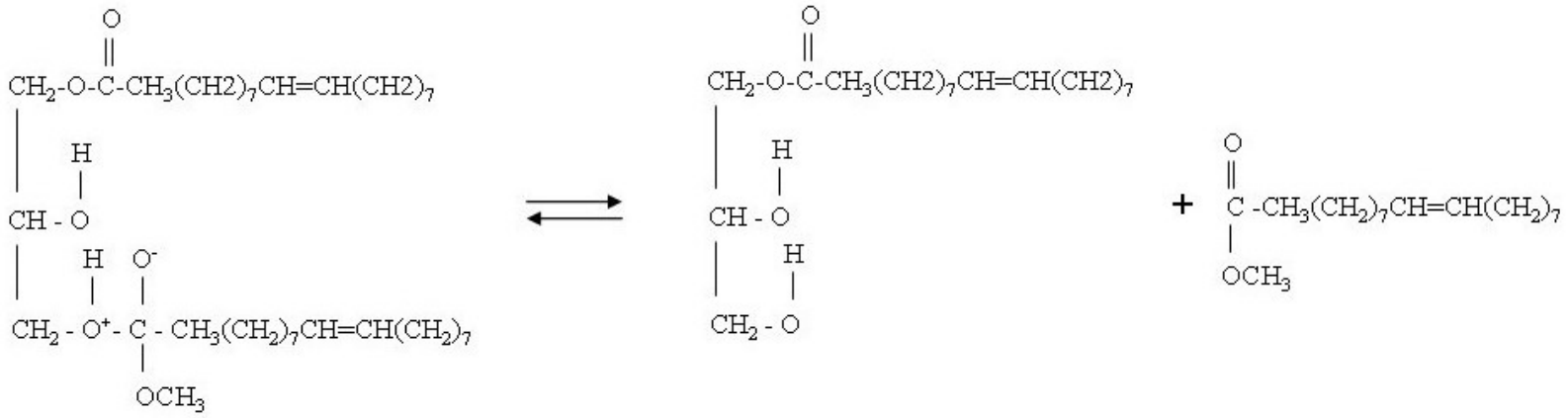
Figure 10 Transesterification mechanism type4. (Cont'd)



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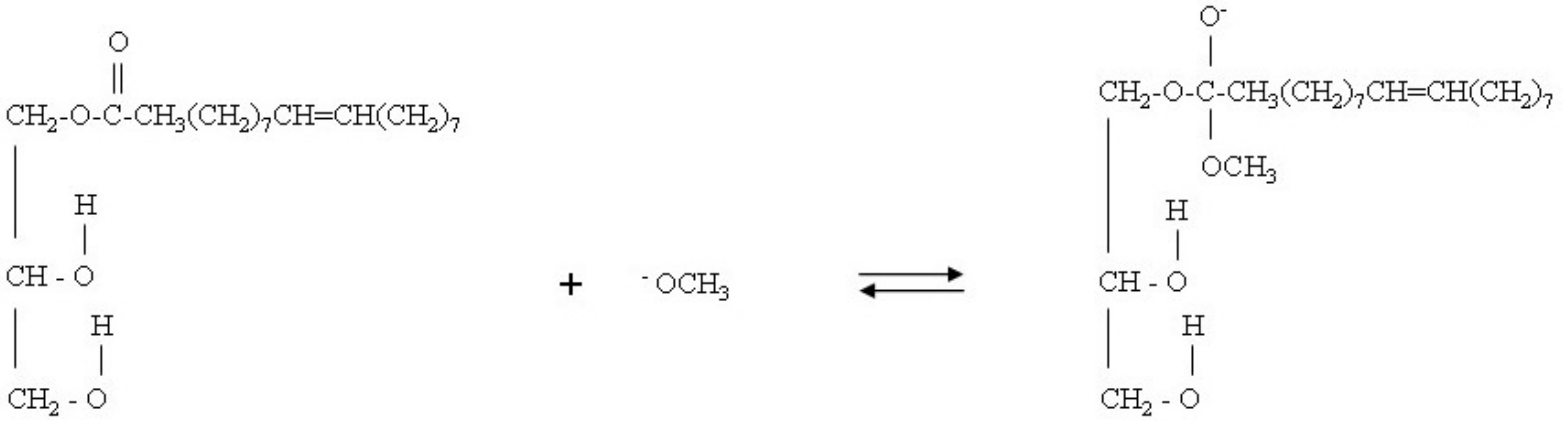

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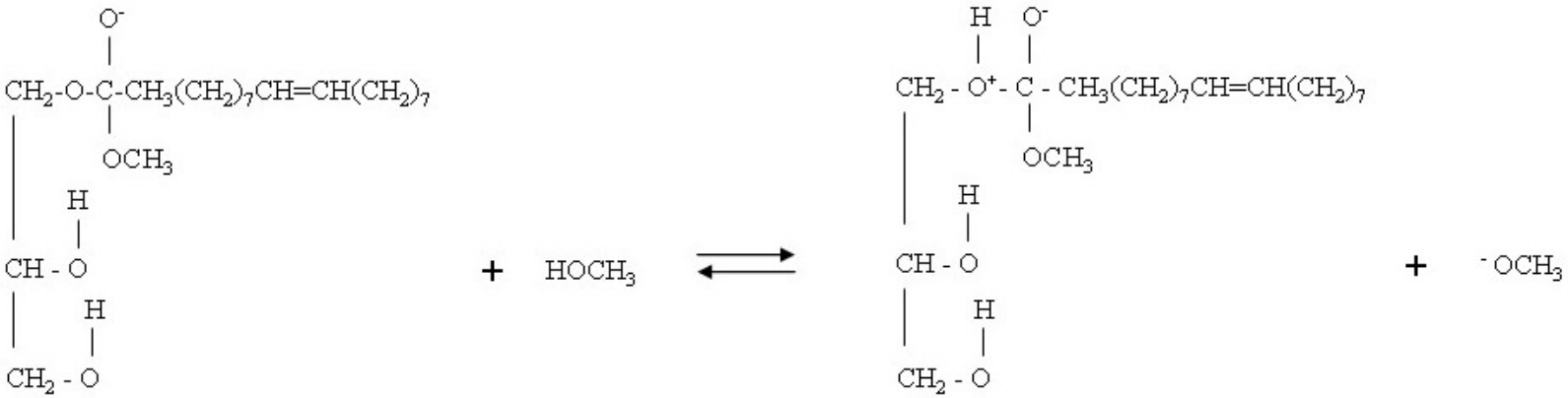
Figure 10 Transesterification mechanism type4. (Cont'd)



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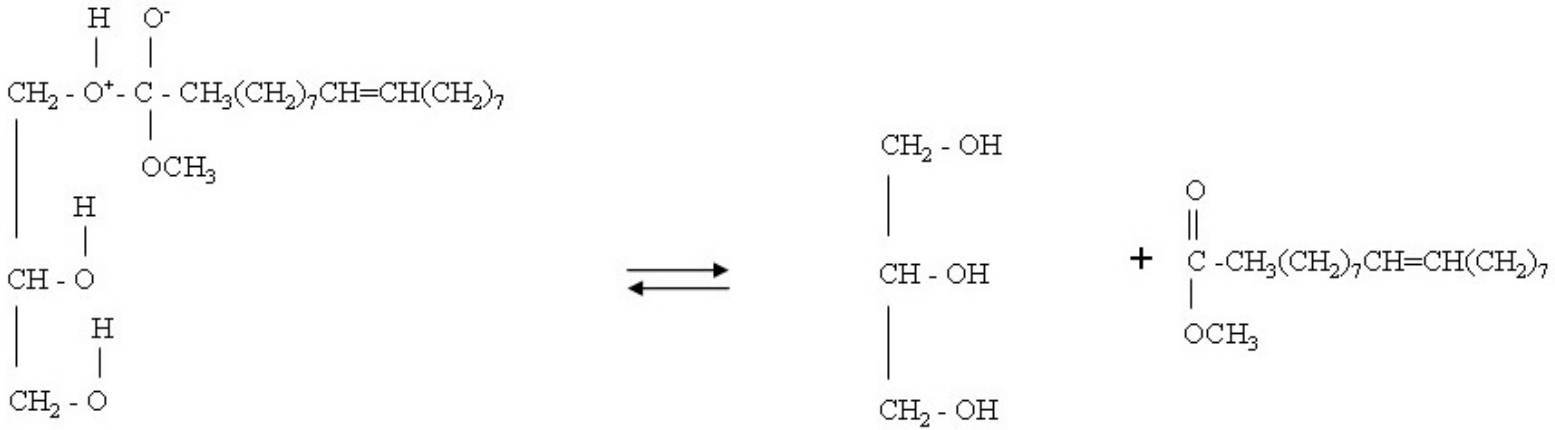

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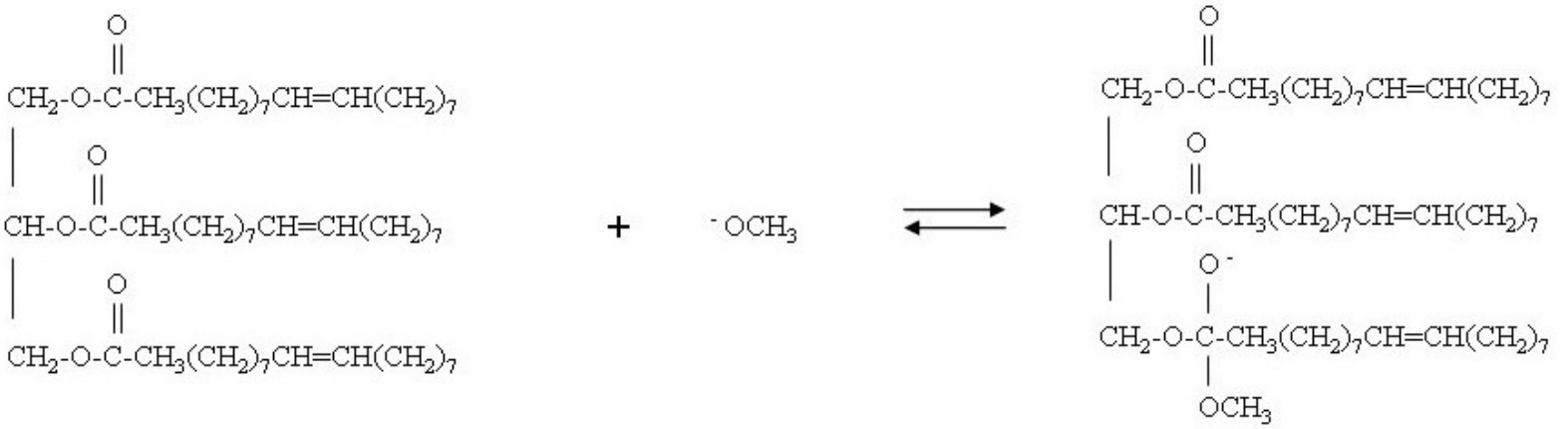
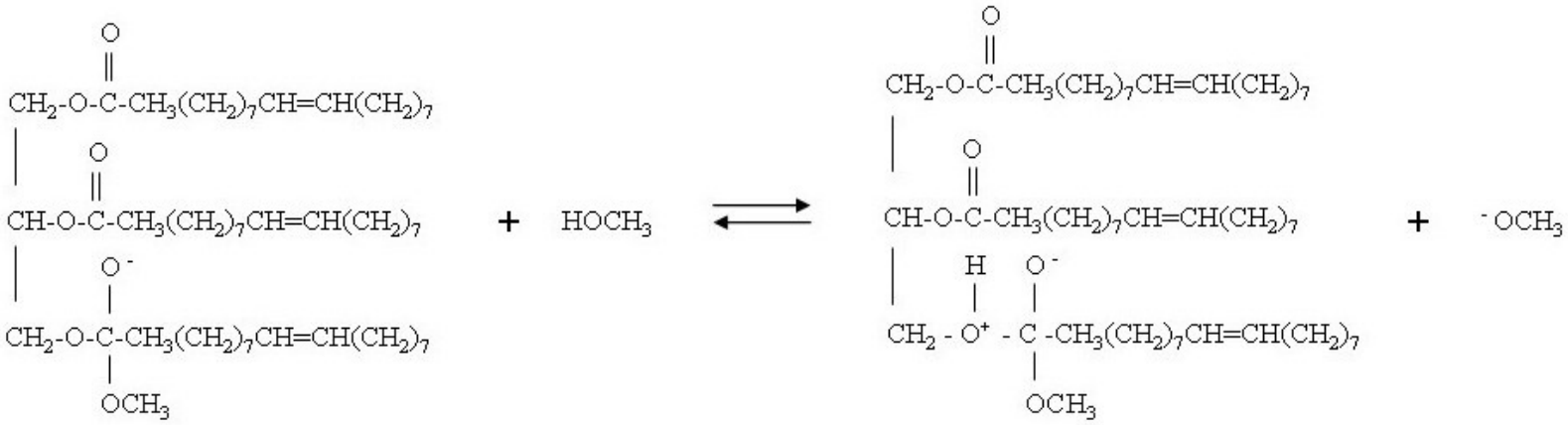
Figure 10 Transesterification mechanism type4. (Cont'd)

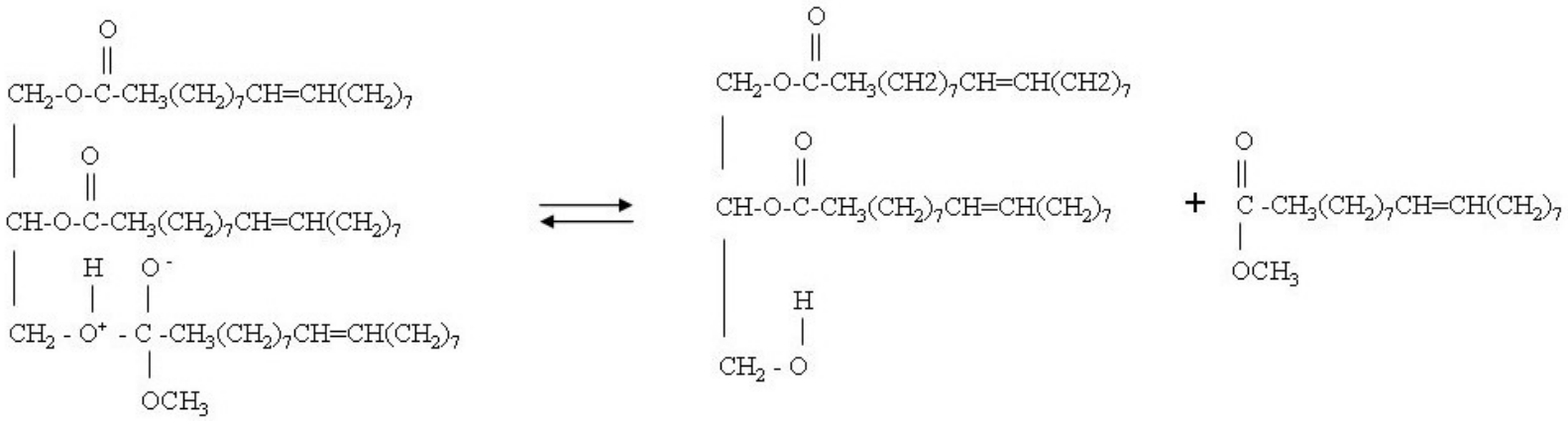


(a.1)



(a.2)

Figure 11 Transesterification mechanism type5.



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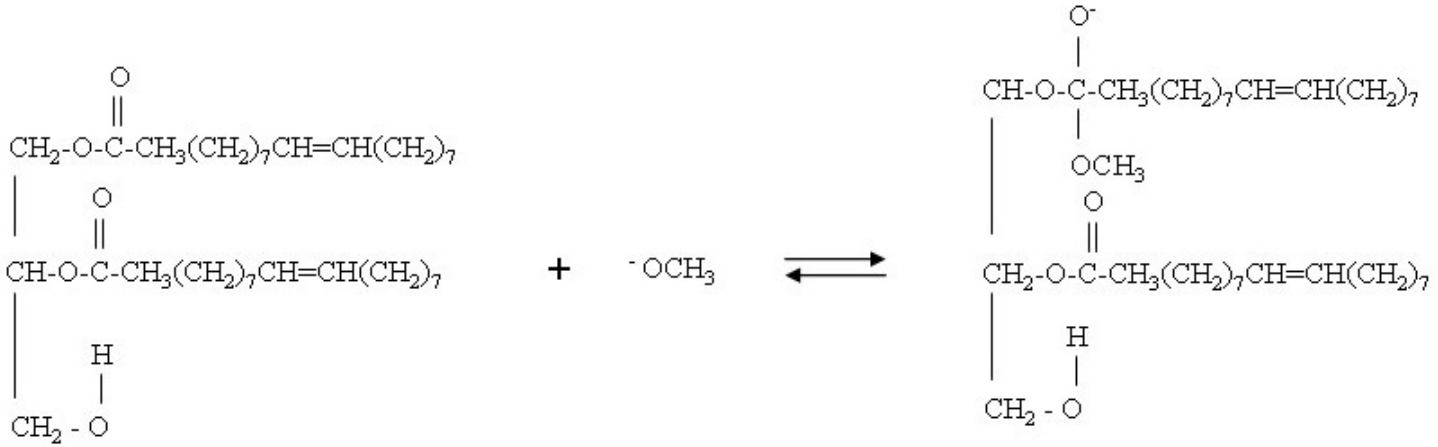

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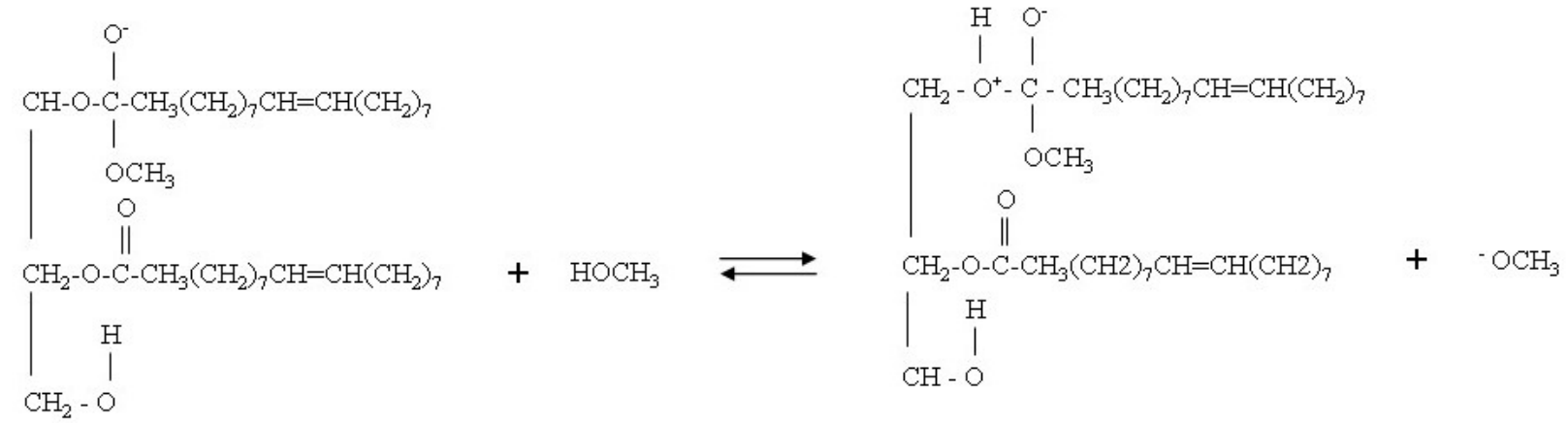
Figure 11 Transesterification mechanism type5. (Cont'd)



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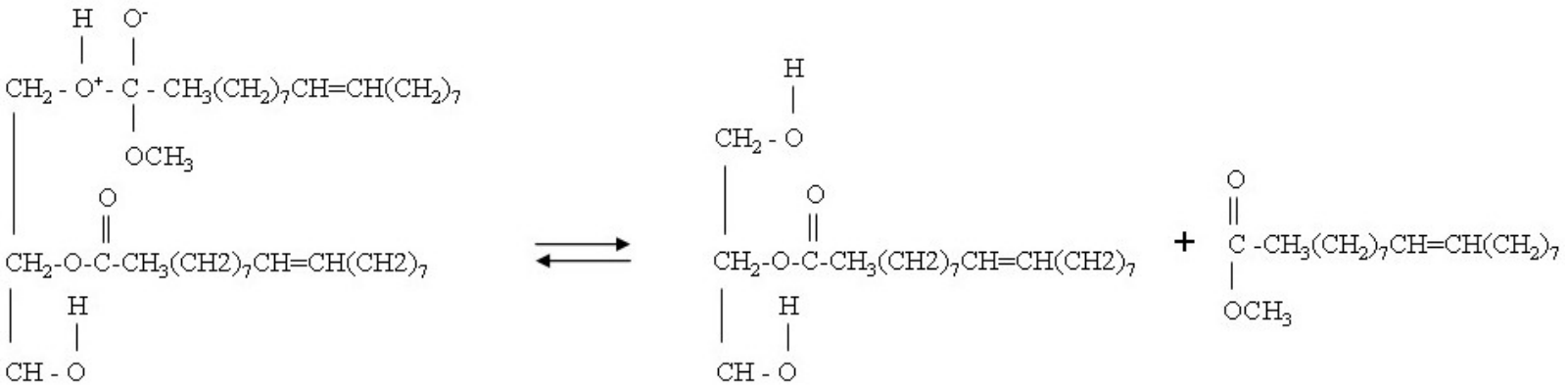

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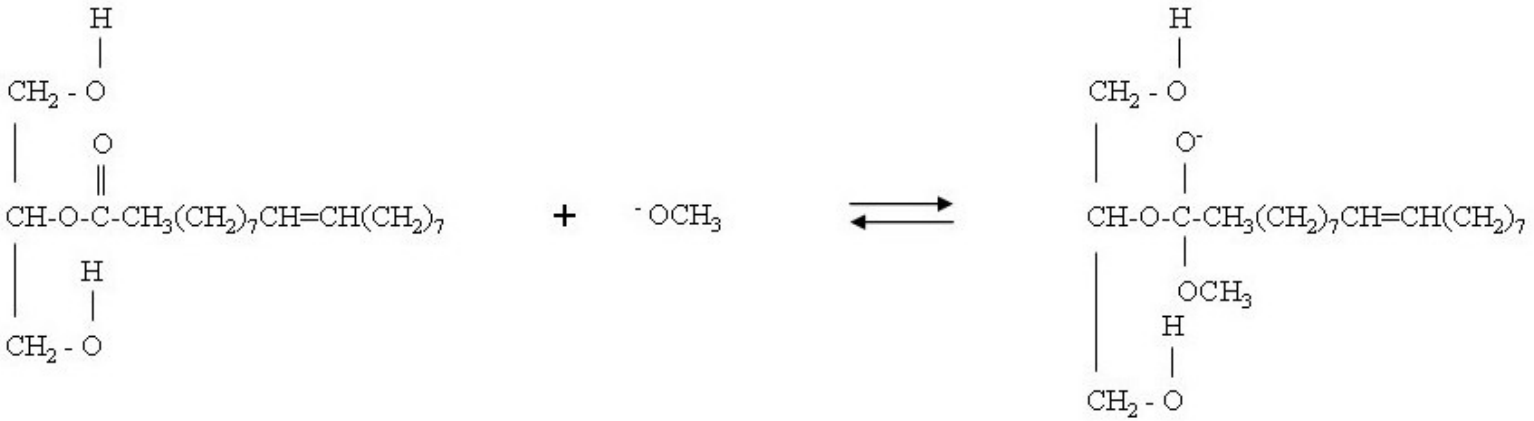
Figure 11 Transesterification mechanism type5. (Cont'd)



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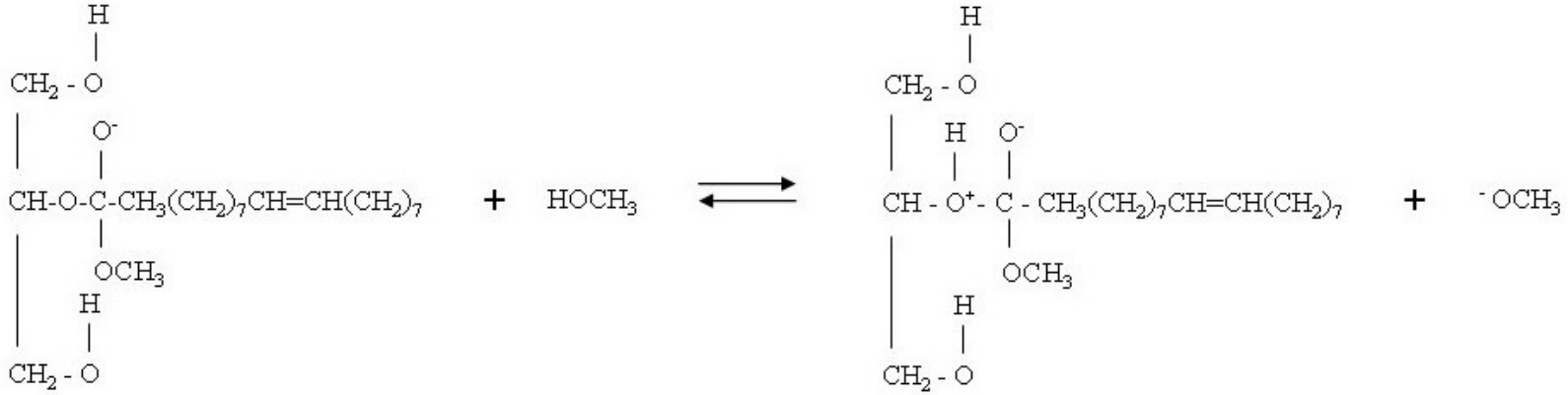

(c.2)

Figure 11 Transesterification mechanism type5. (Cont'd)

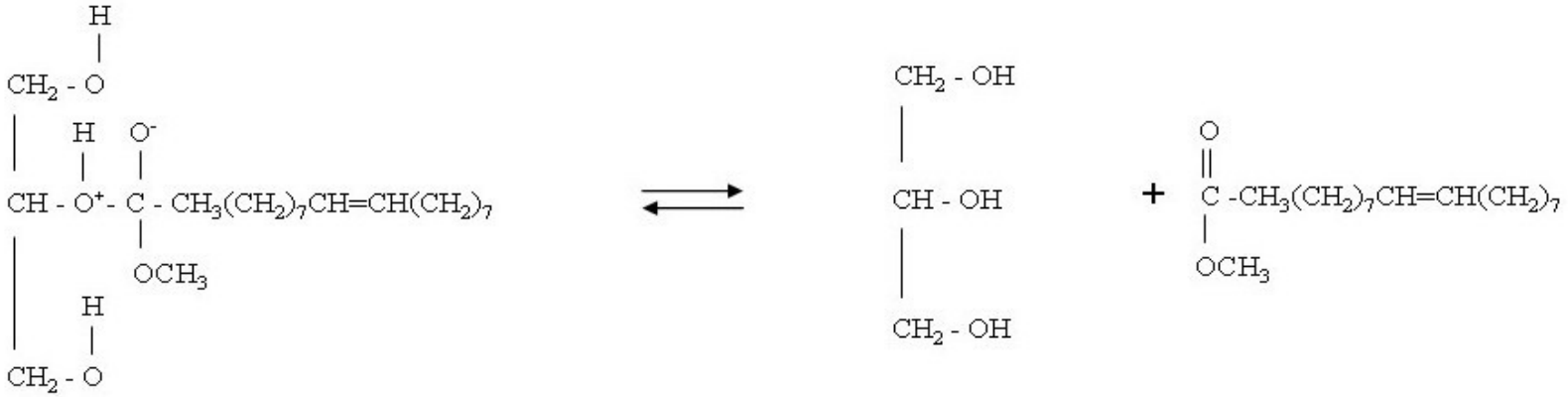

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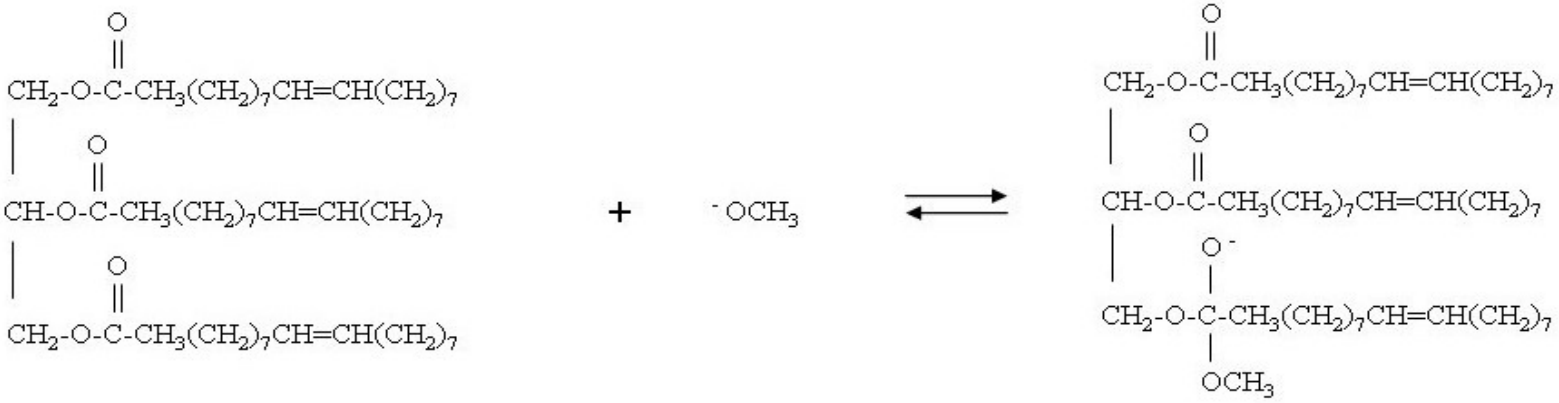
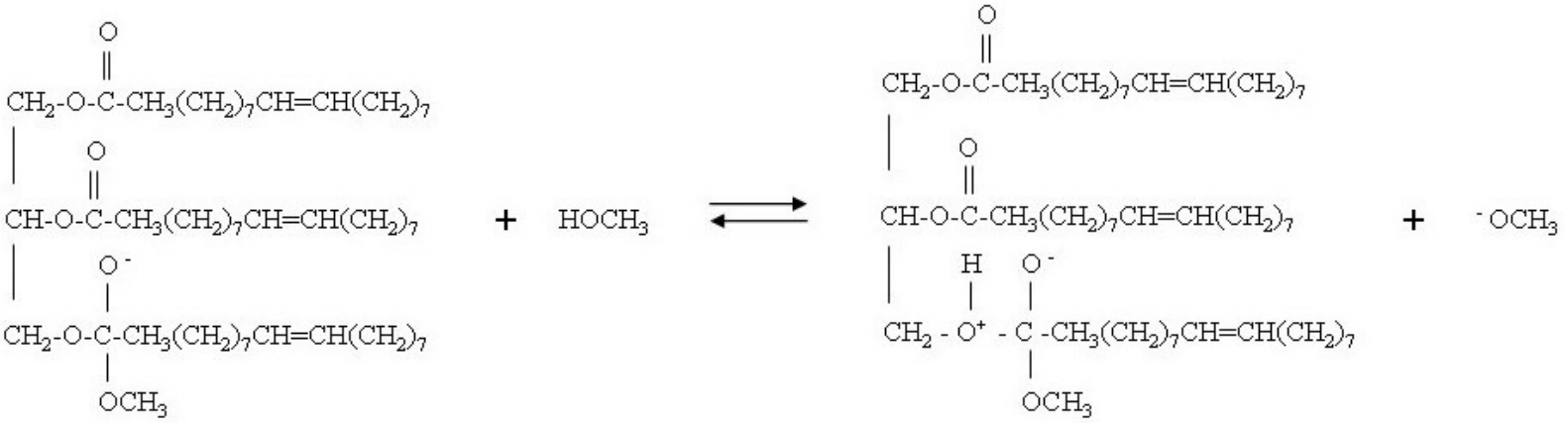
Figure 11 Transesterification mechanism type5. (Cont'd)



(a.1)

Figure 12 Transesterification mechanism type6.



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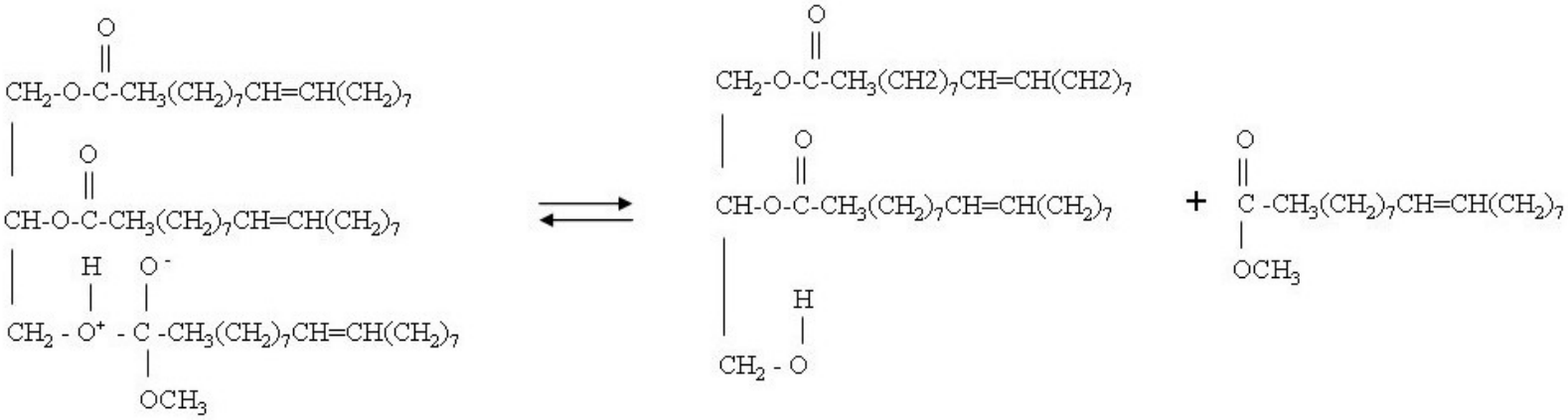
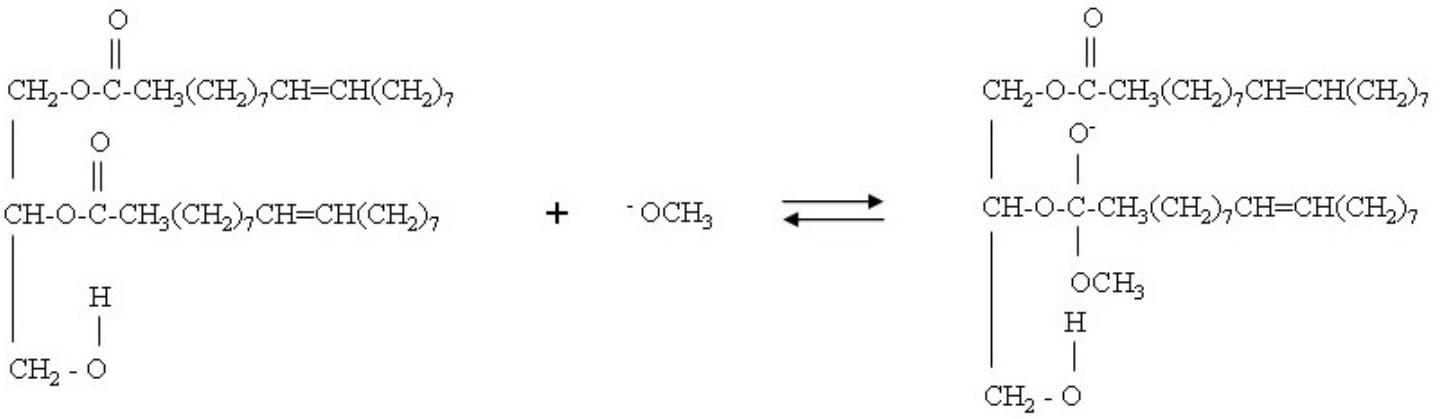
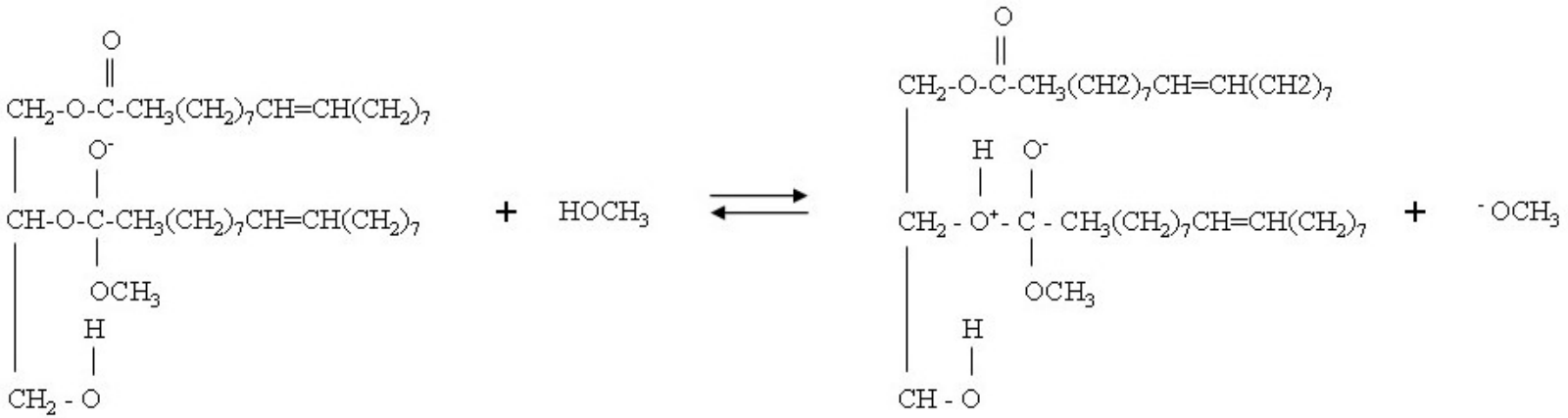


(a.3)

Figure 12 Transesterification mechanism type6. (Cont'd)

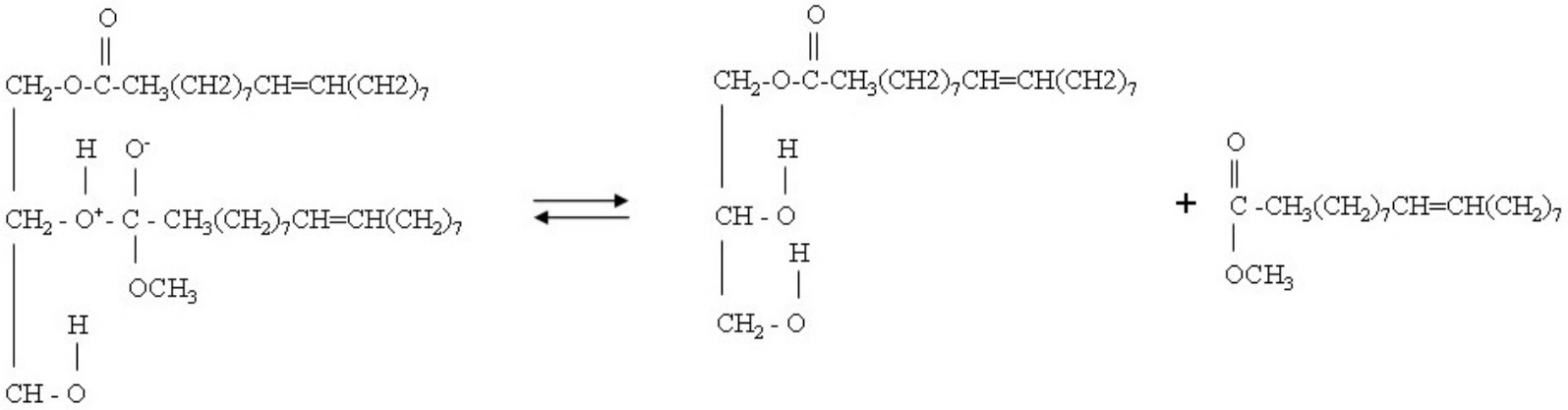


(b.1)

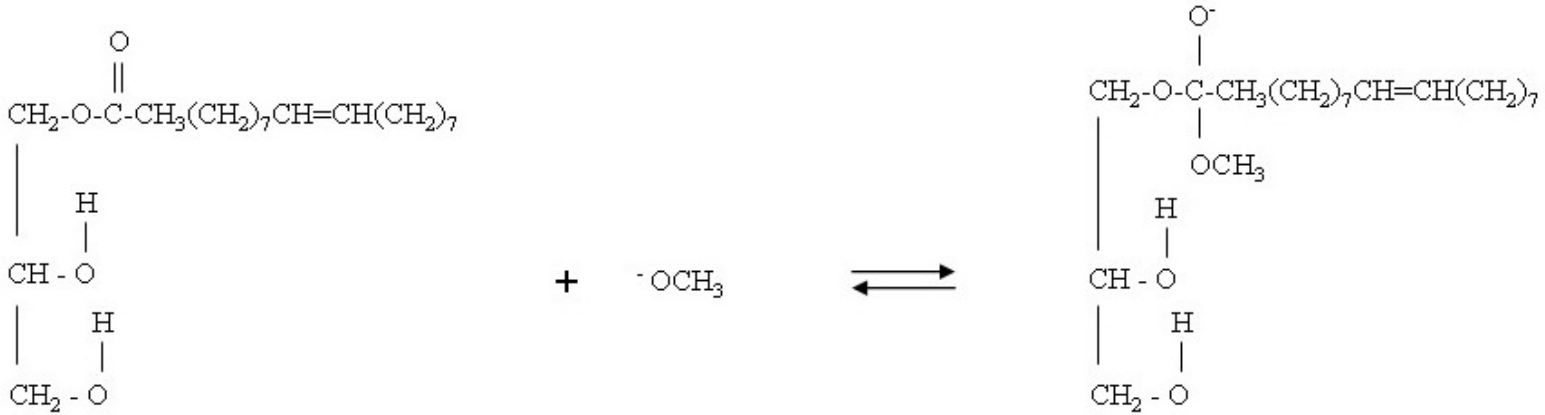


(b.2)

Figure 12 Transesterification mechanism type6. (Cont'd)

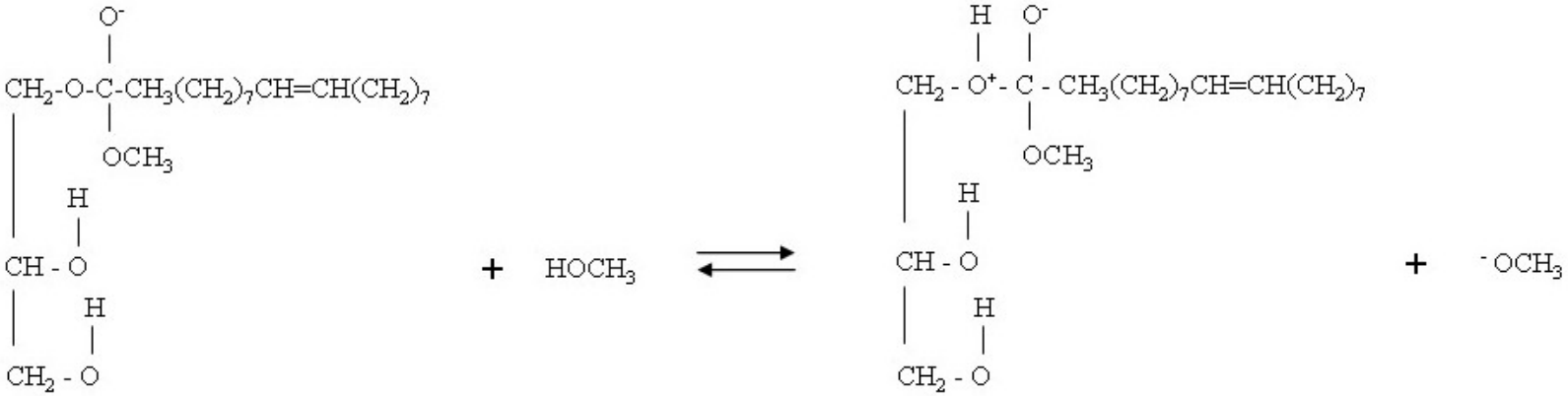


(b.3)

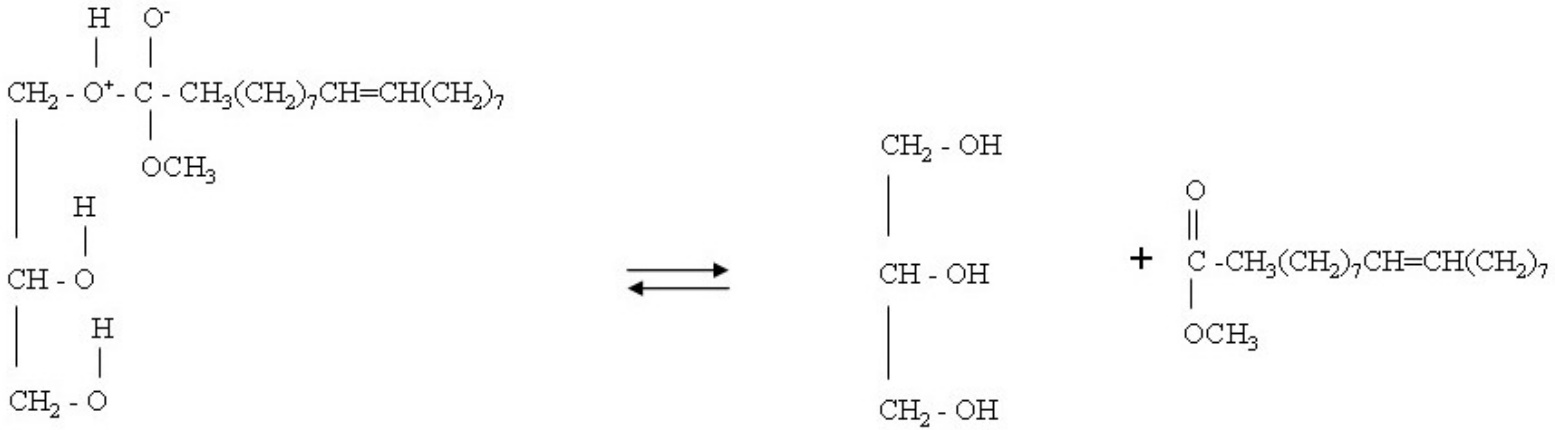


(c.1)

Figure 12 Transesterification mechanism type6. (Cont'd)



(c.2)



(c.3)

Figure 12 Transesterification mechanism type6. (Cont'd)

All of reactions mentioned above were determined to find possibility in the transesterification part way. First, for each mechanism such as in Fig. 7 (a.1) to Fig. 7 (a.3), the reaction of triolein of the transesterification mechanism type1, the three input files were proposed in a GaussViewW and was constructed by drawing reactants in each reaction step. The other inputs were constructed the same as the first one but the reactants were changed into the reactants in the following step. Then run the simulation of all input files with a semiempirical PM3 and an *ab initio* Hartree-Fock based on GAUSSAIN 03W.

The distance between a active site in transesterification mechanism was determined because of the input files are the reaction between two molecules which are the reaction between glyceride and methoxide and the reaction between product of the first reaction (intermediate1 or product in step 1) and methanol. The first active sites is a site between carbon atom in carbonyl group of glyceride (C=O) and oxygen atom of methoxide. The second active site is a site between oxygen atom that is next to the carbon atom in carbonyl group of glyceride (C=O) and hydrogen atom of methanol. These two active site were based on transesterification mechanism in Fig. 3. The distance between glyceride and methoxide was varying in a range of 1.430 to 1.600 and the distance between product of the first reaction (intermediate1 or product in step 1 and methanol was varying in a range of 0.9 to 1.2 to find the minimum distance. Next, all reactions were simulated based on semiempirical PM3 to find the minimum reaction distance. Fore more accuracy, the *ab initio* Hartree-Fock was simulated all of reactions again. All those possible reactions and molecules can be illustrated in simple diagram as follow.

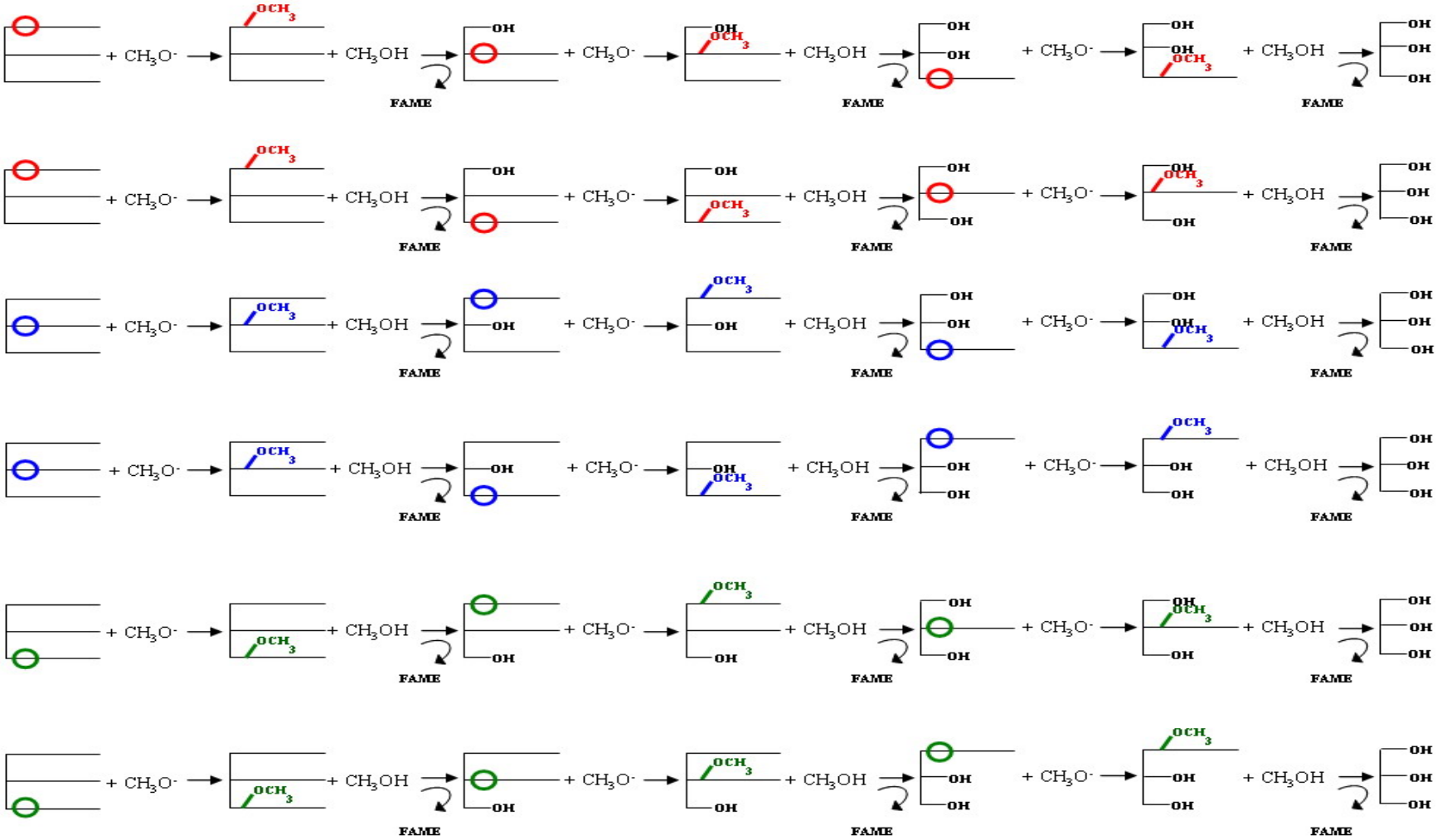


Figure13 A simple diagram of transesterification mechanism.