Zeolites are a group of aluminosilicate minerals with catalytic properties. They may be used for many industrial applications such as catalytic cracking of oil. Zeolites are also capable of converting ethanol to diethylether and ethylen. This reaction is known as dehydration of ethanol. The reaction is potentially interesting as a way of converting ethanol to more valuable molecules.

An experimental study (Shashikant A. Kadam, Mariya V. Shamzhy, 2018) has proven that diethylether is the preferred product when the temperatures are low and the partial pressure of ethanol is high. Ethylen is more significant product with higher temperature and lower partial pressure of ethanol. Aim of this thesis is to determine the mechanism of dehydration of ethanol. Furthermore it was attempted to explain the behavior of the reaction under different circumstances.

The research was done *in silico* using the methods of computational chemistry. Such methods give information on the geometry and the energy of systems of molecules. Thus computational chemistry can be used to investigate the relational path and activation energy of the studied reaction. This thesis is a theoretical study of dehydration of ethanol catalysed by a zeolite.