

## **DFT study on alkene metathesis proceeding on molybdena-alumina cat:**

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Alkene metathesis proceeds according to the carbene mechanism. Metal complex reacts with alkene molecule, giving the metallacyclobutane intermediate, which decomposes to a new alkene molecule and another metal-alkylidene complex.

In the work DFT study on alkene metathesis proceeding on monomeric Mo<sup>VI</sup> centre of molybdena-alumina catalyst was done. The Mo sites were mounted on alumina cluster, whose correctness was previously verified [1]. B3LYP functional and LANL2DZ basis set were employed. The GAUSSIAN 98 program was applied.

Mechanisms of ethene metathesis, productive propene metathesis and the non-productive one were compared. In the case of the non-productive metathesis, the predicted activation enthalpy of propene addition to the Mo-methylidene centre is higher by 10 kJ·mol<sup>-1</sup> than the activation enthalpy of the ethene addition. Where the productive metathesis is depending on position of the attacking propene molecule, the predicted energy is higher by 3 or 10 kJ·mol<sup>-1</sup> than in the case of the non-productive one. In all the initial trigonal bipyramidal molybdacyclobutane can rearrange to the square pyramidal one.

[1] J. Handzlik, J. Ogonowski, J. Mol. Catal. A, 175 (2001) 215.

