

REACTION MECHANISM OF OLEFIN METATHESIS WITH A NOVEL MOLYBDENUM CATALYST

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Synthesis of highly functionalized polymers is an ultimate goal in chemistry because it allows for design of materials with tailored properties. Molybdenum catalysts (e.g. of the Schrock type) have successfully been used for polymerization of olefins but these catalysts are very sensitive to functional groups at the monomers. However recently, an *N*-heterocyclic carbene Mo-alkylidene catalyst has been reported that does tolerate functional groups and polymerizes olefins with hydroxyl or carbonyl functionalities.¹

Density functional theory investigations were used in combination with experimental studies to unravel the reaction mechanism of this new catalyst generation and to explore the origin of its functional group tolerance. Regioselectivity of the polymerization was studied at the example of bicyclo[2.2.1]hept-5-en-2-carbaldehyd monomer. Energetics of the polymerization reaction as well as of the deactivation reaction are presented and regioselectivity of the polymer formation is explained. Compared to Schrock type catalysts, this novel Mo-alkylidene catalyst shows significantly reduced reactivity towards carbonyl coordination.²

References

1) M. R. Buchmeiser, S. Sen, J. Unold, W. Fey, *Angew. Chem Int. Ed.* **2014**, 53, 9384.

2) *Manuscript in preparation*