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## LETTERS TO THE EDITOR

# Isomerization of 1-Hexene into 2-Hexene, Catalyzed by the Product of Magnesium Oxidation with Molybdenum Pentachloride in Tetrahydrofuran

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It was found by Smirnov *et al*. [1] that compounds formed by cryocondensation of magnesium vapor with unsaturated hydrocarbons catalyze olefin isomerization, isotope exchange, polymerization, etc. Such transformations are not induced by magnesium halides, Grignard reagents, and highly dispersed metal but are catalyzed by transition metal complexes. Quantum-chemical calculations in [1] gave evidence showing that magnesium hydride clusters are stable as a compact metal frame (tetrahedron, trigonal bipyramid).

Compounds containing magnesium hydride clusters can be obtained by oxidation of magnesium with variable-valence metal halides in THF. Such complexes have first been reported in [2, 3]. Yamamoto *et al*. [2] detected the complex $[VHMg_2Cl_2 \cdot THF]$ in the postreaction mixture of vanadium trichloride and magnesium in THF. Later we showed [4, 5] that magnesium hydride complexes $[MH_nMg_mCl_l \cdot (TGF)_k]$ (**I**) are formed by oxidation of the metal taken in a considerable excess with higher chromium, molybdenum, niobium, tantalum, and tungsten halides.

Complexes **I** as dark solid amorphous materials are easily isolated from the reaction mixtures after removal of the solvent and excess magnesium. They are readily soluble in THF and sparingly soluble in benzene and toluene. Complexes **I** react with cyclopentadiene in THF, giving transition metal derivatives capable of catalyzing magnesium oxidation with this unsaturated compound to form $(C_5H_5)_2Mg$.

The magnesium hydride cluster formed by oxidation of excess metal with $MoCl_5$ in THF, $[MoHMg_{2.8}Cl_{2.0}THF]$ (**II**), catalyzes isomerization of 1-hexene into 2-hexene.

Reaction progress was followed by $^1H$ NMR spectroscopy. The ratio of *trans*- and *cis*-2-hexanes, determined by $^{13}C$ NMR spectroscopy, is 1 : 4.

The apparent activation energy of the reaction at 293–313 K is 30 kJ/mol, the reaction order in substrate is one, and the reaction order in catalyst is two. At 313 K and initial 1-hexene and complex **II** concentrations in THF of 3.2 and 0.03 M, respectively, about 60 catalytic cycles occur.

It should be noted that the isomerization of 1-hexene is also catalyzed by the products of magnesium oxidation with higher titanium, vanadium, niobium, tantalum, and tungsten in THF. At the same time, the compound formed by reaction of MoCl5 with sodium naphthalide in a 1 : 3 ratio in THF fails to catalyze the isomerization of 1-hexene.

Propene undergoes no polymerization at 293 K within 48 h when exposed gaseous at a pressure of 200 or 300 mm over a solution of complex **II** ($c_{\mathbf{II}}$ 0.05 M) in THF or toluene. The NMR spectra were measured on a Bruker DPX-200 solution in $CDCl_3$, internal reference TMS [working frequencies 200 ($^1H$) and 50 ($^{13}C$) MHz].

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