

Direct Alkylation of Toluene with Ethane

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The activation of small alkanes is among the great challenges of modern catalysis research. By far the most work in this area has been devoted to the oxidative rather than the non-oxidative pathway, even though CO and CO₂ are formed as by-products in the oxidative route. One example of non-oxidative activation is the direct alkylation of aromatics with alkanes. Some researchers have investigated the reaction of *benzene* with ethane and propane [1-3]. Due to the higher reactivity of propane, its cracking products alkylate benzene forming mainly ethylbenzene and toluene. The direct alkylation products cumene and n-propylbenzene are only favored at low temperatures and contact times. The less reactive ethane molecule is much less prone to cracking and therefore gives the direct alkylation product ethylbenzene, but only at higher temperatures. In this work, the direct alkylation of *toluene* with ethane to the isomeric ethyltoluenes and hydrogen was chosen as a model reaction for the non-oxidative activation of alkanes. The reason for this choice is twofold: Firstly, this reaction has not been investigated so far. Secondly, the product of direct alkylation contains an ethyl group on the aromatic ring and can hence easily be discerned from the toluene disproportionation products benzene and xylenes.

The alkylation of toluene with ethane can be catalyzed by zeolite Pd/H-ZSM-5 with relatively high selectivities under certain conditions. Besides the isomeric ethyltoluenes and hydrogen, the main products are benzene and xylenes formed by disproportionation of toluene. In addition, small amounts of ethene and ethylbenzene are produced, also some propane and C₄ hydrocarbons. Using just toluene as reactant, the products were only benzene and xylenes, i.e., ethyltoluenes cannot be formed from toluene under these conditions. Using just ethane as reactant, only dehydrogenation to ethene is observed, i.e., ethyltoluenes cannot be produced by aromatization of ethane at these conditions. Thus, the non-oxidative activation of ethane for the direct alkylation of toluene is clearly feasible on Pd/H-ZSM-5 zeolite under the reaction conditions chosen. Further experiments will aim at increasing the conversion and at a further enhancement of the selectivity to ethyltoluenes.

References

- [1] A.V. Smirnov, E.V. Mazin, V.V. Yuschenko, E.E. Knyazeva, S.N. Nesterenko, I.I. Ivanova, L. Galperin, R. Jensen, S. Bradley, *J. Catal.* 194 (2000) 266.
- [2] C. Bigey, B.-L. Su, *J. Mol. Catal. A: Chemical* 209 (2004) 179.
- [3] S. Kato, K. Nakagawa, N. Ikenaga, T. Suzuki, *Catal. Lett.* 73 (2001) 175.