Hydrogenation of alkylaromatics over Rh/silica

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- Abstract

The hydrogenation, and competitive hydrogenation, of toluene, ethylbenzene, propylbenzene and the xylenes has been studied over a rhodium catalyst in the liquid phase at 323 K and 3 bar(g). The reactivity of the aromatics gave an order of *para*-xylene > *ortho*-xylene > *meta*-xylene > toluene > ethylbenzene ≫ propylbenzene. Kinetic analysis revealed that the order of reaction in hydrogen was typically first order while the reaction order in toluene was zero order and negative half order for ethylbenzene. The reaction order for propylbenzene and the xylenes was negative first order. Apparent activation energies were calculated and all were in the range 26–46 kJ mol^{-1}. Competitive hydrogenation between toluene, ethylbenzene and propylbenzene revealed that the propylbenzene was the most strongly adsorbed aromatic in agreement with the strongly negative reaction order. The xylenes gave an order of reactivity of *para* > *ortho* > *meta* following the increasing negative reaction order. Reactions with deuterium revealed an inverse kinetic isotope effect, most likely related to the change in hybridization of the carbon from sp^2 to sp^3, for all reactions, except that of *ortho*-xylene. Rapid exchange of the methyl group hydrogens was observed with all the xylenes, whereas total exchange was noted with toluene. The generation of *trans*-1,2-dimethylcyclohexane was explained by the formation of two intermediates, 1,2-dimethylcyclohexene and 1,6-dimethylcyclohexene, which give the *cis*-1,2-dimethylcyclohexane and *trans*-1,2-dimethylcyclohexane, respectively.