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LETTER TO THE EDITOR

Reply to Zoltán Paál, "Hydrogen Effects in *n*-Hexane Isomerization on Pt/Sulfated Zirconia. A Comment on the Paper by Duchet *et al.* (*J. Catal*. **198**, 328 (2001))"

We thank Z. Paál for his comments on our recent work on the isomerization of *n*-hexane over Pt/sulfated zirconia catalysts. He puts it in the perspective of maximum rate phenomenon. It is indeed well known that various hydrocarbon reactions on metal, acid, or metal–acid catalysts display a maximum rate with hydrogen partial pressure. Many rate equations with a squared hydrogen term in the denominator will automatically give rise to such a maximum. So a large number of equations can fit the influence of hydrogen at one given hydrocarbon pressure. However, the validity of the equation must be tested at various reactant pressures and care should be taken to use few and chemically meaningful kinetic parameters. These criteria are fulfilled in our paper (1).

Our systematic study of the influence of hydrogen encompasses industrially relevant conditions (pressure and temperature) for isomerization of *n*-hexane. Highly active and stable catalysts were prepared for this purpose.

We account for both hydrogen and hexane reaction orders, from a sequence of elementary steps in a mechanism based on Lewis sites and hydride species. This mechanism is very different from the classical bifunctional pathway encountered on Pt/zeolite catalysts operating at higher temperature, but incorporates some features of the work of Iglesia *et al.* (2). The work of Iglesia was, however, performed at much lower pressures. Our equation fits simultaneously the rate at various hexane pressure (1–5 bar) in a wide range of hydrogen pressures (0–49 bar). To the best of our knowledge, this equation and therefore its parameters (k, α, β) have never been proposed for hexane isomerization. More important than the equation itself is the chemical significance of the kinetic parameters. Besides the rate constant (k), we established that the two other parameters characterize *independently* the acid sequence (β) and the platinum–hydrogen couple (α) and show a consistent variation with the platinum content. These two parameters (α, β) are a powerful tool in the design of better catalysts because of the following:

—they allow a rationalization of the effect of poisons (basic molecules, H_2O, S compounds);

—they guide the research through "what if ?" experiments such as the effects of other hydrocarbons (aromatics and naphthenes) and catalyst properties (acidity, Pt loading, and accessibility)... on these independent parameters.

As Z. Paál states, much work remains to be done to understand and improve this family of catalysts, already used commercially in light (C_5–C_6) alkane isomerization. They are in a position to displace both zeolite (high temperature required) and chlorinated alumina (corrosiveness and environmental problems) based catalysts if further and significant improvements are made.

We are continuing our approach of rational catalyst design and new results are forthcoming on the aspects not described in our *J. Catal*. paper. In future work we will interpret the variation of the platinum efficiency with loading.

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