



BERKELEY CATALYSIS CENTER

Seminar

Monday October 13

The McCollum Room

775 Tan Hall

9:00 am

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n-Hexane Isomerization on Pt/ZrO₂-SO₄: Roles of Acidity and Platinum

ABSTRACT:

The isomerization of light paraffins (C₅-C₇) is a key process to produce high quality components of the gasoline pool meeting the most demanding present and expected environmental regulations. The isomerization of heavier fractions (diesel, lube, synthetic FT paraffins, ...) is equally important to produce high quality transportation fuels and specialty chemicals. This presentation will be devoted to the isomerization of light paraffins, but the conclusions are partially applicable to the isomerization of heavier paraffinic feedstocks. It also illustrates the type of cooperation between industrial and academic catalysis laboratories.

A detailed spectroscopic characterization of the acidic and metallic functions of a bi-functional Pt/Sulfated Zirconia has been undertaken by IR spectroscopy. The catalyst was a prototype of an industrial catalyst shaped by extrusion with alumina. The catalytic assessment took place with two reactions :

Toluene Hydrogenation: measures the accessibility of the metallic function and correlates remarkably well with IR characterization of the Pt function.

n-C₆ Isomerization: the reaction of interest is studied over a wide range of (partial) pressures of hydrocarbon and H₂

The integration of these spectroscopic and catalytic informations is summarized in a model valid over a wide window of operating conditions and takes into account the roles of acidity (Lewis in our case) and some peculiarities of the Pt function (discussed in depth during the presentation). Moreover, and more importantly, the model is a tool to investigate "What if scenarios" likely to occur during the catalyst preparation, unit start-up and operation.