

BERKELEY CATALYSIS CENTER

Distinguished Lecture Series

Seminar

Friday April 11, 2008

The McCollum Room

775-A & B Tan Hall

8:30-10:00 a.m.

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“Hydrodesulfurization of 4,6-dimethyl-dibenzothiophene and its hydrogenated intermediates over metal sulfide and metal catalysts”

ABSTRACT

To reduce the sulfur content in gasoline and diesel fuel to 10 ppm, as required in many countries by 2010, even refractory molecules such as 4,6-dimethyl-dibenzothiophene (DMDBT) must be desulfurized. To reach that goal, the mechanism of hydrodesulfurization (HDS) must be studied and better catalysts must be developed. Therefore, two hydrogenated intermediates of dibenzothiophene (DBT), tetrahydro- and hexahydro-DBT (TH- and HH-DBT), were synthesized, and their HDS was investigated over sulfided Mo/ γ -Al₂O₃ at 300 °C and 5 MPa H₂. These molecules interconverted fast and reached equilibrium. The C-S bond breaking in TH-DBT was faster than in HH-DBT and H₂S strongly inhibited desulfurization of DBT, TH-DBT and HH-DBT. The breaking of the two C-S bonds occurs by hydrogenolysis, as in the DDS route in the HDS of DMDBT. DFT calculations indicate that the aliphatic C-S bond breaks first.

Noble metal catalysts are much better hydrogenation catalysts than metal sulfides, but are sulfur sensitive. This can be improved by alloying and by using an acid support. Bimetallic Pt-Pd supported on mesoporous ZSM-5 was much more active in the HDS of DMDBT than Pt and Pd catalysts and than Pt-Pd supported on other supports. The superior HDS activity is attributed to the catalytically active sites of the alloy catalyst particles in the mesopores of the mesoporous ZSM-5, which are not only accessible to DMDBT, but also promoted by the strong acidity of the zeolitic support.