



BERKELEY CATALYSIS CENTER

Distinguished Lecture Series Seminar

August 16, 2006 The McCollum Room
775A & B Tan Hall
10:00 - 12:00 Noon

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“Alkane activation by acid catalysts”

ABSTRACT:

The lecture addresses the elementary steps involved in acid catalyzed alkane activation and conversion, i.e., the interaction of alkanes with potential catalysts, the abstraction of hydrogen as initiating step, the surface reaction and finally the desorption of the products. The coupling of hydrogen abstraction with other acid catalyzed reactions and the hydride transfer to facilitate desorption are the key steps discussed. Only the subtle control of these steps leads to active and stable catalysts. Surface carbenium ions are the critical intermediates/transition states in the catalytic cycles.

The differences between such chemically coupled steps of alkane conversion will be discussed for three reactions on modified zeolites and sulfated oxides, including cracking, isomerization, and alkylation. Alkanes can be activated at temperatures below 100°C. With zeolites, activation is started in most instances alkane by carbenium ion formation from alkene impurities. Alternatively, it may also be started via low temperature hydrogen elimination and the generation of alkoxy groups through a direct polarization of the C-H bond. The rate of reaction depends subtly on the coverage of acid sites and the degree of pore filling suggesting hydride transfer to be crucial to proceed in the catalytic activity once the first C-H bond is broken. In contrast, alkane reactions on the anion-modified oxides are governed by stoichiometric oxidation and subsequent reaction on Brønsted acid sites. As with zeolites hydride transfer is needed to complete the catalytic cycle. With both materials, however, the chemistry seems to occur with paired electrons and not with radicals as has been suggested previously.