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Agilent CP-Al_2O_3/Na_2SO_4

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Energy and chemicals

Effects of Si/Al ratio on the distribution of framework Al and on the rates of alkane monomolecular cracking and dehydrogenation in H-MFI

Journal of the American Chemical Society, **135**, 19193–19207 (2013)
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Tags
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Abstract
The aim of this study was to identify the influence of Si/Al ratio on the location of Brønsted-acid sites within the framework of zeolite MFI and on the rates and selectivities of monomolecular cracking and dehydrogenation of n-butane. Based on UV-visible spectroscopic analysis of Co(II) cations exchanged into MFI, it was inferred that the fraction of Brønsted-acid centers located in channel intersections relative to straight and sinusoidal channels increases with increasing Al content. The turnover frequencies for all monomolecular processes, and the selectivities to dehydrogenation versus cracking and to terminal cracking versus central cracking, also increased with increasing Al content. Higher turnover frequencies for dehydrogenation and terminal cracking were observed despite similar or increasing activation energies and are attributed in part to increases in the intrinsic activation entropies. The increasing selectivity to dehydrogenation at higher Al content is consistent with the finding that the transition-state geometry for dehydrogenation is loose and resembles a product state, and should, therefore, be best accommodated in the channel intersections. The transition states for cracking are earlier, more compact and have a weaker preference for less confining locations. It is also observed that the presence of isobutene inhibits the rate of n-butane dehydrogenation. In summary, we conclude that monomolecular cracking and dehydrogenation of n-butane in H-MFI occur preferentially at Brønsted protons located in the intersections of MFI and that the fraction of such sites increases with increasing concentration of Al for the samples investigated.

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