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Conformational properties of monosubstituted cyclohexane guest molecules constrained within zeolitic host materials. A solid-state NMR investigation

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Abstract

The conformational properties of monosubstituted cyclohexane guest molecules ($C_6H_{11}X$ with $X = CH_3, OH, Cl, Br$ and I) included within microporous solid host materials (silicalite-I, H-ZSM-5, NH_4 -mordenite and zeolite NH_4 -Y) have been elucidated *via* high-resolution solid-state ^{13}C NMR spectroscopy. For all of the inclusion compounds investigated, the fraction of monosubstituted cyclohexane molecules in the equatorial conformation is similar to that in solution, suggesting that these host materials do not impose any significant constraints upon the conformational properties of the monosubstituted cyclohexane guest molecules. For the monohalogenocyclohexane guest molecules ($C_6H_{11}X$ with $X = Cl, Br$ and I), this result is in marked contrast to the situation for the same guest molecules in the thiourea host structure, for which the conformational properties of the guest molecules are substantially different from those of the same molecules in solution. For cyclohexanol ($C_6H_{11}OH$) in H-ZSM-5, some amount of dicyclohexyl ether ($C_6H_{11}OC_6H_{11}$) is observed, and is analogous to the proposed production of dimethyl ether in the first stage of methanol-to-gasoline conversion on this zeolite. The comparatively low temperature (ambient temperature) at which this conversion from cyclohexanol to dicyclohexyl ether occurs is noteworthy. In addition to our high-resolution solid-state ^{13}C NMR studies of these materials, 1H MAS and ^{27}Al MAS NMR spectra have also been recorded, and are discussed.

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