Quantum Chemical Studies of Ice-Bound Reactions of Carbonyl-Containing Species (Formaldehyde, Acetaldehyde, and Acetone) with Ammonia

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Reactions between ammonia (NH_3) and carbonyl-containing organic species such as formaldehyde have been shown to possess very small reaction barriers when they occur in an ice matrix (D. E. Woon, Icarus 142, 550 1999), making them particularly promising pathways for chemistry leading to potential prebiotic molecules within icy grain mantles in dark interstellar clouds or on cold satellite surfaces. Small cluster MP2 molecular orbital studies (up to 4 waters) combined with IPCM solvation to describe bulk polarization provide a benchmark for larger cluster B3LYP density function theory (DFT) studies (over 10 waters) of reactions between ammonia, acetaldehyde, and acetone. All are known interstellar species. In addition to characterization of the reaction surfaces, the DFT cluster calculations allow us to predict the vibrational spectra of both reactant complexes and the product amine species, which should prove useful in interpreting Spitzer and other infrared observations of protostellar objects known to exhibit other molecular ice features. One of the intriguing features of the ammonia-acetaldehyde reaction is that it yields stereoisomers with slightly different reaction energies and thus a preference for one over the other.

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