

FORMATION OF THE ALMA MOLECULE HOCH₂CN AND RELATED SPECIES FROM THE REACTION OF C⁺ WITH HCN AND HNC IN ICY GRAIN MANTLES

DAVID E. WOON, *Department of Chemistry, University of Illinois at Urbana-Champaign, Urbana, IL, USA.*

Density functional theory cluster calculations indicate that the intermediate HOCHNC readily forms when C⁺ reacts with HCN embedded in the surface of an icy grain mantle. Subsequent H addition to HOCHNC yields the iscyano compound HOCH₂NC. There is enough energy from the H addition for HOCH₂NC to isomerize to HOCH₂CN (glycolonitrile), an important prebiotic molecule that was recently detected with ALMA observations toward the solar-type protostellar source IRAS 16293-2422 B by Zeng et al. [MNRAS 2019, 484, L43]. It was found that H can also add to HOCHNC to form HOCHNCH without a barrier. The analogous reactions of C⁺ with HNC in ice will also be discussed. Vibrational spectra of the various ice-bound reactants, intermediates, and products will be presented. The calculations were performed with B3LYP using aug-cc-pVDZ sets on C, N, and O and cc-pVDZ sets on H.