QUANTUM CHEMICAL MODELING OF ASTROCHEMICAL REACTIONS OF C ATOM AND C^+ CATION WITH NH_3 BOUND TO AMORPHOUS WATER ICE

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Reactions of C atoms and C^+ cations with NH_3 on water ice were characterized with density function theory using modestly sized water clusters. Both reactions are expected to occur in dense interstellar clouds and in protostellar sources. The neutral C(^{3}P) + NH_3 reaction on ice begins with the formation of triplet CNH_3 via dative bonding involving the $2s^2$ lone pair on nitrogen. Assuming it is not ejected into the gas phase, CNH_3 can subsequently react with one or two H atoms to yield CH_2NH_2 and then CH_3NH_2. The ion-molecule C^+(^{2}P) + NH_3 reaction on ice begins with charge transfer so that C(^{3}P) reacts with NH_3^+. The short-lived CNH_3^+ intermediate, which has a covalent C-N bond, deprotonates to yield the H_2NC radical, which was detected in 2021 toward the dark cloud L483 and other sources. Doublet H_2NC can react with H atoms to yield several different products. The vibrational spectrum of NH_3 on amorphous ice will also be presented.