ICE-SURFACE CHEMISTRY OF MgNC AND OTHER METAL-CONTAINING COMPOUNDS

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Density function theory calculations in $17H_2O$ and $24H_2O$ clusters were used to study the deposition and subsequent chemistry of MgNC, the first metal-containing molecule identified in interstellar space. MgNC is a reactive radical with a mixture of covalent and ionic bonding between the Mg and NC. We found that H can react facilely with adsorbed MgNC to form HMgNC, a known astromolecule; there is sufficient energy to eject HMgNC into the gas phase. Acetylene (HCCH) and hydrogen cyanide (HCN) reactions with adsorbed MgNC were also characterized. While there are barriers to forming complexes in both cases, they appear to be submerged below the reactant asymptote. Among the outcomes of these reactions are the formation of the vinyl radical (C_2H_3) from HCCH and the methaniminyl radical (H_2CN) from HCN. Deposition of compounds containing Na and Al will also be summarized.