EXPERIMENTAL AND THEORETICAL STUDY OF HCN COMPLEXED TO SMALL MAGNESIUM CLUSTERS

P. L. STILES, D. T. MOORE, and R. E. MILLER, *Department of Chemistry, The University of North Carolina at Chapel Hill, Chapel Hill, NC 27599*.

Infrared spectra, dipole moments, potential energy surfaces, and electron density difference plots are presented for two HCN-Mg isomers, HCN-Mg_3, and HCN-Mg_4. The magnesium clusters are first formed in the helium droplets by sequential pick-up of gas phase atoms. The HCN is then added to the droplets and the C-H stretch is measured with a color center laser. Stark spectroscopy is used to measure the dipole moments of each metal-adsorbate complex, which, along with rotational constants, are compared to the ab initio calculations. We also present the electron density difference plots of each complex in order to reveal the nature of the HCN-Mg_n bond.