INFRARED SPECTROSCOPY OF THE Ge AND Si + HCN SYSTEMS IN HELIUM NANODROPLETS

<u>C. MICHAEL LINDSAY</u>, PETER T. LAKE, Jr., and ROGER E. MILLER, *Department of Chemistry, The University of North Carolina, Chapel Hill, NC*, 27599.

High resolution infrared spectroscopy and *ab initio* theory are used to study the association of silicon and germanium atoms with HCN in superfluid helium nanodroplets. Møller-Plesset, density functional, and coupled-cluster calculations of these "reactions" predict that both weakly bound van der Waals complexes and chemically bound molecules can be produced along completely barrierless reaction pathways. A high-temperature oven has been developed to dope germanium and silicon atoms into helium droplets. After the subsequent pick-up of an HCN molecule, both field free and Stark spectra are reported for the associated system and analyzed using standard gas phase Hamiltonians. The experimental results are compared to theory and used to draw conclusions about the nature of chemical reactions in the low temperature, superfluid helium bath.