ISOMERS OF HYDROGEN FLUORIDE CLUSTERS $(HF)_N$ (N=4-6) FORMED IN HELIUM NANODROPLETS

G. E. DOUBERLY , and R. E. MILLER, *Department of Chemistry, The University of North Carolina at Chapel Hill, Chapel Hill, NC 27599*.

The infrared spectra (in the spectral region 3100 cm^{-1} to 3900 cm^{-1}) are reported for hydrogen fluoride clusters formed in helium nanodroplets. Comparisons with previous gas phase spectra reveal new isomeric forms of $(HF)_n$ (n=4-6), corresponding to tailed ring structures (i.e. trimer to pentamer rings to which an HF monomer is attached). Pendular state spectroscopy (in the presence of a large DC electric field) is used to establish that these isomers are polar. In addition, comparisons between the experimental and calculated transistion dipole moment directions provide further support for the assignments of the various vibrational bands. The ab initio calculatations (at the MP2 / 6-311++G(3df,3pd) level of theory) support the assignment of various spectral features to the (3+1) and the (4+1) HF complexes. Data of this type provides insights into the barriers associated with the insertion of an HF molecule into a preexisting cyclic complex.