CHARACTERIZATION OF A WATER-HEXAFLUOROBENZENE COMPLEX USING MATRIX ISOLATION INFRARED SPECTROSCOPY

JAY C. AMICANGELO, DANIEL G. IRWIN, CYNTHIA J. LEE, and NATALIE C. ROMANO, NANCY L. SAXTON, *School of Science, Penn State Erie, Erie, PA 16563*.

Matrix isolation infrared spectroscopy was used to characterize a 1:1 complex of water (H_2O) with hexafluorobenzene (C_6F_6). Co-deposition experiments with H_2O and C_6F_6 were performed at 17 K using nitrogen and argon as the matrix gases. New infrared bands attributable to the H_2O-C_6F_6 complex were observed near the asymmetric stretching, symmetric stretching, and bending vibrations of the water monomer and near the C-F and C-C stretching vibrations of the C_6F_6 monomer. Identification of the new infrared bands to those of the complex were established by comparing the co-deposition spectra with the spectra of the individual monomers, by performing experiments with isotopically labeled water (D_2O and HDO), and by matrix annealing experiments. Theoretical calculations were also performed for the H_2O-C_6F_6 complex using ab initio and density functional theory methods. In general, the calculations predict the H_2O and C_6F_6 vibrational frequencies in the H_2O-C_6F_6 complex to be shifted with respect to the H_2O and C_6F_6 monomers by similar magnitudes as to what we observe experimentally, lending support to our assignments.