

CHARACTERIZATION OF A CARBON DIOXIDE-HEXAFLOUROBENZENE COMPLEX USING MATRIX ISOLATION INFRARED SPECTROSCOPY

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Matrix isolation infrared spectroscopy was used to characterize a 1:1 complex of carbon dioxide (CO_2) with hexafluorobenzene (C_6F_6). Co-deposition experiments with CO_2 and C_6F_6 were performed at 20 K using argon as the matrix gas. New infrared peaks attributable to the CO_2 - C_6F_6 complex were observed near the O-C-O antisymmetric stretching vibration of the CO_2 monomer and near the C-F stretching vibration of the C_6F_6 monomer. The initial identification of the newly observed infrared peaks to those of a CO_2 - C_6F_6 complex was established by performing several concentration studies in which the sample-to-matrix ratios of the monomers were varied between 1:100 to 1:1600, by comparing the resulting co-deposition spectra with the spectra of the individual monomers, and by matrix annealing experiments (30 – 35 K). Co-deposition experiments were also performed using isotopically labeled carbon dioxide ($^{13}\text{CO}_2$) and the analogous peaks for the $^{13}\text{CO}_2$ - C_6F_6 complex were observed. Quantum chemical calculations were performed for the CO_2 - C_6F_6 complex at the MP2/aug-cc-pVDZ level of theory in order to explore the intermolecular potential energy surface of the complex and to obtain optimized complex geometries and predicted vibrational frequencies of the complex. The calculations for the exploration of the potential energy surface involved rigid scans along the intermolecular distance and various angle coordinates for several general orientations of the two monomers. Based on these calculations, full geometry optimizations were then performed and two stable complex minima were found: one in which the CO_2 is perpendicular and centered to the C_6F_6 ring ($\Delta E_{int} = -7.9$ kJ/mol) and one in which the CO_2 is parallel to the C_6F_6 ring but displaced from the center ($\Delta E_{int} = -6.0$ kJ/mol). Comparing the predicted vibrational spectra for both complexes to the observed experimental spectra, particularly for the O-C-O antisymmetric stretching region, it is concluded that both structures are present in the solid argon matrices.