CHARACTERIZATION OF A 1:1 METHANOL-BENZENE COMPLEX USING MATRIX ISOLATION INFRARED SPECTROSCOPY

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Matrix isolation infrared spectroscopy was used to characterize a 1:1 complex of methanol (CH_3OH) with benzene (C_6H_6). Co-deposition experiments with CH_3OH and C_6H_6 were performed at 17 - 20 K using nitrogen and argon as the matrix gases. New infrared bands attributable to the CH_3OH-C_6H_6 complex were observed near the O-H and C-O stretching vibrations of CH_3OH and near the hydrogen out-of-plane bending vibration of C_6H_6. The initial identification of the new infrared bands observed was established by performing a conentration study (1:200 to 1:2000 S:M ratios), by comparing the co-deposition spectra with the spectra of the individual monomers, by matrix annealing experiments, and by performing experiments using isotopically labeled methanol (CD_3OD) and benzene (C_6D_6). Quantum chemical calculations were also performed for the CH_3OH-C_6H_6 complex using density functional theory and ab initio methods. Two stable minima were found for the complex: one in which the CH_3OH is above the C_6H_6 ring with the hydroxyl hydrogen interacting with the π cloud of the ring (H-π complex) and the other in which the CH_3OH is in the plane of the C_6H_6 ring with the hydroxyl oxygen interacting with one of the C-H bonds of the ring (CH-O complex). Comparing the calculated shifts of the vibrational frequencies for both complexes to the observed experimental frequency shifts, it is found that the H-π complex is in best agreement with the experimental shifts in both magnitude and direction. Therefore, it is concluded that the geometry of the CH_3OH-C_6H_6 complex observed in the matrix isolation experiments is the H-π complex.