

CHARACTERIZATION OF A HYDROGEN PEROXIDE-BENZENE COMPLEX USING MATRIX ISOLATION INFRARED SPECTROSCOPY

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Matrix isolation infrared spectroscopy was used to characterize a 1:1 complex of hydrogen peroxide (H_2O_2) with benzene (C_6H_6). Co-deposition experiments with H_2O_2 and C_6H_6 were performed at 20 K using argon as the matrix gas. New infrared peaks attributable to the $\text{H}_2\text{O}_2\text{-C}_6\text{H}_6$ complex were observed near the O-H stretching vibrations and the OH bending vibrations of the H_2O_2 monomer and near the hydrogen out-of-plane bending vibration of the C_6H_6 monomer. The initial identification of the newly observed infrared peaks to those of a $\text{H}_2\text{O}_2\text{-C}_6\text{H}_6$ 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 hydrogen peroxide (D_2O_2 and HDO_2) and benzene (C_6D_6) and the analogous peaks for the isotopically labelled complexes were observed. Quantum chemical calculations were performed for the $\text{H}_2\text{O}_2\text{-C}_6\text{H}_6$ 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, which were compared to the experimental infrared spectra.