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

JAY C. AMICANGELO, DYLAN JOHNSON, CATHERINE KAISER, YUDHISHTARA PAYAGALA, JACOB OSLOSKY, LIA TOTLEBEN, *School of Science (Chemistry), Penn State Erie, Erie, PA, USA*.

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 H_2O_2-C_6H_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 H_2O_2-C_6H_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 using isotopically labeled hydrogen peroxide (D_2O_2 and HDO_2) and benzene (C_6D_6) in argon were also performed and the analogous peaks for the isotopically labelled complexes were observed. A series of co-deposition experiments with H_2O_2 and C_6H_6 was also performed using nitrogen as the matrix gas. Quantum chemical calculations were performed for the H_2O_2-C_6H_6 complex at the MP2/aug-cc-pVDZ and M06-2X/aug-cc-pVDZ levels of theory in order to obtain optimized complex geometries and predicted vibrational frequencies of the complex, which were compared to the experimental infrared spectra.