

OBSERVATION OF THE OH-C₆H₆ RADICAL COMPLEX IN AN ARGON MATRIX USING MATRIX ISOLATION INFRARED SPECTROSCOPY WITH A VACUUM ULTRAVIOLET PHOTOLYSIS SOURCE

JAY C. AMICANGELO, CATHERINE KAISER, TRACY JONES, DYLAN JOHNSON, *School of Science (Chemistry), Penn State Erie, Erie, PA, USA.*

Utilizing matrix isolation infrared spectroscopy with a vacuum ultraviolet (VUV) photolysis source (121 nm), a 1:1 complex of the hydroxyl radical (OH) with benzene (C₆H₆) was observed in low temperature argon matrices. Co-deposition experiments with simultaneous VUV photolysis of H₂O and C₆H₆ mixtures were conducted in an argon matrix at 15 K. The OH stretching peak for the OH-C₆H₆ complex was observed at 3502.3 cm⁻¹. Identification of the observed peak of the OH-C₆H₆ complex was established by performing experiments with varying concentrations of the H₂O and C₆H₆ relative to the argon matrix, comparing the co-deposition spectra to the individual monomer spectra of H₂O and C₆H₆ in argon matrices both with and without VUV photolysis, as well as matrix annealing experiments (30 - 35 K). Experiments were also performed using the D₂O isotopomer and the OD stretching peak for the OD-C₆H₆ complex was observed at 2584.1 cm⁻¹. Quantum chemical calculations were performed at the MP2, M06-2X, and ωB97X-D levels of theory with the aug-cc-pVDZ basis set to obtain the optimized geometry and simulated infrared spectrum for the OH-C₆H₆ complex. The observed OH and OD stretching peaks of the OH(D)-C₆H₆ radical complexes observed in argon matrices in the current experiments are in good agreement with the values previously reported in argon matrices using a different production method.^{a,b}

^aA. Mardyukov, E. Sanchez-Garcia, R. Crespo-Otero, and W. Sander, *Angew. Chem. Int. Ed.* **48**, 4804 (2009)

^bA. Mardyukov, R. Crespo-Otero, E. Sanchez-Garcia, and W. Sander, *Chem. Eur. J.* **16**, 8679 (2010)