OBSERVATION OF THE C_6H_7 RADICAL IN AN ARGON MATRIX USING MATRIX ISOLATION INFRARED SPECTROSCOPY

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The cyclohexadienyl radical (C_6H_7) was observed in a low temperature argon matrix with matrix isolation infrared spectroscopy. The C_6H_7 radical was produced from the reaction of H atoms with benzene (C_6H_6) in the argon matrices. The H atoms were produced by vacuum ultraviolet (VUV) photolysis of H_2S, which was co-deposited with the C_6H_6 in the argon matrices. The most intense peak of the C_6H_7 radical was observed at 621.0 cm^{-1}, with several other weaker peaks observed at 865.9, 910.9, 961.2, 973.7, 1290.3, 1390.2, 1394.9, 1425.9, 2758.7, and 2781.3 cm^{-1}. The experiments were performed with various concentrations of H_2S and C_6H_6 and at deposition temperatures of 10 K, 15 K, and 20 K. The largest yield of the C_6H_7 radical was for VUV photolysis co-deposition of 1:200 H_2S:Ar with 1:200 C_6H_6:Ar at 15 K. The identification and assignment of the C_6H_7 radical peaks was accomplished by comparisons to spectra without VUV photolysis, the H_2S and C_6H_6 monomer spectra both with and without VUV photolysis, filtered (400 – 900 nm) Hg-Xe lamp photolysis, and 35 K annealing spectra. Experiments were also performed in which H atoms were reacted with C_6D_6 producing the C_6D_6H radical, with peaks observed at 460.0, 747.8, 759.3, 830.0, 1245.6, 1246.7, and 2791.9/2797.0 cm^{-1}. Quantum chemistry calculations for the C_6H_7 radical were also performed using density functional theory at the B3LYP/aug-cc-pVTZ level to obtain the theoretical structure and theoretical infrared spectrum to support the assignments. The peaks of the C_6H_7 radical observed in argon matrices are in good agreement with the values reported in xenon matrices[a] and *para*-hydrogen matrices[b].

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[a] V. I. Feldman, F. F. Sukhov, E. A. Logacheva, A. Y. Orlov, I. V. Tyulpina, and D. A. Tyurin, Chem. Phys. Lett. 437, 207 (2007)

[b] M. Bahou, Y. J. Wu, and Y. P. Lee, J. Chem. Phys. 136, 154304 (2012)