THE ULTRAVIOLET SPECTROSCOPY OF PHENYLCYCLOPENTENE AND PHENYLCYCLOPENTADIENE

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Recent studies of the effluents of an electric discharge of benzene, 1,3-butadiene, and vinylacetylene independently observed a resonant two-photon ionization (R2PI) spectrum with mass $\frac{m}{z} = 142$ whose carrier was unidentified. Based on the similarity of its low frequency vibronic structure to that of α-methylstyrene, we have synthesized phenylcyclopentadiene, recorded its R2PI spectrum, and found it to be the carrier of the discharge-produced $\frac{m}{z} = 142$ spectrum. The molecule exists in two isomeric forms: phenylcyclopentadi-1,3-ene and phenylcyclopentadi-1,4-ene. UV-UV holeburning spectroscopy was used to record the UV spectra of the two possible isomers. The suspected origin transitions of the two isomers are found at 31738 and 31687 cm^{-1}, respectively. Using similar reasoning, an analogous spectrum observed in a butadiene discharge at m/z 144 is ascribed to phenylcyclopentene, with an S_0-S_1 origin at 34646 cm^{-1}. In addition to recording the R2PI spectrum, LIF excitation and single vibronic level dispersed fluorescence scans of phenylcyclopentene and phenylcyclopentadiene have been recorded. In phenylcyclopentene, a progression involving the out-of-plane torsion of the two rings was identified, with a vibrational frequency of 44 cm^{-1} in S_0 and 72 cm^{-1} in S_1. An analysis of this torsional vibronic structure and its underlying torsional potential will be described and compared with ab initio predictions.