

CONFORMATION-SPECIFIC ELECTRONIC SPECTROSCOPY OF JET-COOLED 5-PHENYL-1-PENTENE

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The electronic spectroscopy of jet-cooled 5-phenyl-1-pentene was studied by resonant two photon ionization (R2PI). This molecule is of interest because intramolecular photochemistry occurs from intermediate conformations that bring the vinyl group up over the phenyl ring.^a Five conformations were confirmed by UV-UV hole-burning (UVHB) spectroscopy. The S_0 - S_1 origins of these conformations were found between 37507 and 37585 cm^{-1} . The origin transitions clearly separate into two groups split by about 50 cm^{-1} (three to the red and two to the blue). According to existing literature, the interaction of the methylene gamma hydrogen with the pi cloud of the ring in gauche conformations causes a red shift in their origins. Therefore, the three origins to the red are anticipated to be gauche conformations while the origins to the blue are anti conformations. Tentative structural assignments have been made by comparing rotational band contours with calculated contours based on transition moments and rotational constants from *ab initio* calculations. These assignments and experimental techniques will be discussed. A study was also conducted to look for conformation-specific lifetime shortening in vibronic levels above the origin, but no evidence of this was found.

^aChang-Dar D. Ho and Harry Morrison, *J. Am. Chem. Soc.*, **127**, 2114 (2003).