THE GAS-PHASE SPECTRA OF THE 1-INDANYL RADICAL

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The gas-phase resonant two color two photon ionization (R2C2PI) spectrum of the 1-indanyl radical (*m/z*=117) has been identified in the region 20800 — 22600 cm^{-1} in a molecular beam. The radical was produced from the discharge of ∼1 % indene in Argon . Laser induced fluorescence (LIF) spectra were recorded in the same region revealing those features observed in R2C2PI. Other precursor molecules were investigated and it was found that the indane precursor resulted in the strongest signal. The fluorescence of the 1-indanyl radical origin band (21158 cm^{-1}) was dispersed in order to determine the ground state vibrational energies. The dispersed fluorescence (DF) spectrum is consistent with the previously observed condensed-phase emission spectrum of the 1-indanyl radical[a]. The DF values were compared with those ground state energies determined by DFT. Franck-Condon factors computed based on the *ab initio* results showed good agreement with the observed spectrum. Based on the theoretical results we assigned the observed bands. The LIF spectrum contained other bands inconsistent with the 1-indanyl radical. These have been determined to be carried by 1-phenylpropargyl radical[b] and another currently unknown radical determined by R2C2PI to have *m/z*=133.

[a] T. Izumida, K. Inoue, S. Noda, and H. Yoshida, *Bull. Chem. Soc. Jpn.* **54**, 2517 (1981).

[b] N. J. Reilly, D. L. Kokkin, M. Nakajima, K. Nauta, S. H. Kable, and T. W. Schmidt, *J. Am. Chem. Soc.* **130**, 3137 (2009).