HIGH RESOLUTION INFRARED SPECTROSCOPY OF JET-COOLED PHENYL RADICAL IN THE GAS PHASE

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Phenyl radical (C_6H_5) is one of the most important reactive intermediates, as it is formed from the homolytic cleavage of a CH bond in benzene (C_6H_6), and hence it plays a central role in the combustion of fossil fuels that are typically rich in aromatics. We recently recorded the first high resolution infrared spectra of jet-cooled phenyl radical in the gas phase. This was obtained by direct absorption laser spectroscopy in a slit-jet discharge supersonic expansion of a phenyl halide precursor (C_6H_5X, $i.e.$ C_6H_5I and C_6H_5Br) diluted in a Neon/Helium gas mixture. We observed an A-type band, which arises from a fundamental excitation of the out-of-phase symmetric CH stretch (ν_{19}). The unambiguous assignment of the rotational structure in this band to C_6H_5 is facilitated by comparing 2-line combination differences with the Fourier transform microwave (FTM) and direct absorption millimeter-wave (mm-wave) measurements of the ground state by McMahon $et\ al.$[a]. A least-squares fit to an asymmetric top Hamiltonian of the rotationally-resolved vibrational band is done to determine upper-state rotational constants and a gas-phase band origin (ν_0) of 3071.8904 (10) cm^{-1}. This is in very good agreement with the value of 3071 cm^{-1} for the out-of-phase symmetric CH stretch of phenyl reported by Friderichsen $et\ al.$[b] from matrix isolation studies, which indicates a surprisingly small red shift due to the low-temperature argon environment.

[a] R. J. McMahon, M. C. McCarthy, C. A. Gottlieb, J. B. Dudek, J. F. Stanton and P. Thaddeus, *Ap. J.* **590**, L61 (2003).

[b] A. V. Friderichsen, J. G. Radziszewski, M. R. Nimlos, P. R. Winter, D. C. Dayton, D. E. David and G. B. Ellison, *J. Am. Chem. Soc.* **123**, 1977 (2001).