STUDY OF PHENYLACETYLENE BY CAVITY RING-DOWN SPECTROSCOPY

GARY V. LOPEZ, PHILIP M. JOHNSON, TREVOR J. SEARS[a] , *Department of Chemistry, Stony Brook University, Stony Brook, New York 11794*; and CHIH-HSUAN CHANG, *Department of Chemistry, Brookhaven National Laboratory, Upton, New York 11973.*

Cavity ring-down (CRD) measurements have been made on the $S_1(\tilde{A}\ ^1B_2) \leftarrow S_0(\tilde{X}\ ^1A_1)$ absorption spectrum of slit jet-cooled phenylacetylene (PA) in the 279 nm region as a further investigation of the photophysical properties of PA reported by Hosftein et al.[b] The intensities in the new CRD data are compared with those obtained in the old REMPI experiments, and computational models.[c] The results show that the strong bands in the REMPI spectrum are attenuated while the weak bands (a_1 modes) remained the same when compared to CRD spectra. The comparison of the simulated spectrum to the CRD and REMPI spectra were satisfactory for most part when the a_1 modes were scaled up by a factor of 3.24 and 3.55, respectively, giving evidence of some possible theoretical artifacts.[c] The temperature of the slit jet-cooled PA was found to be in the range of 30 ± 5K by comparison with simulations of the rotational structure of the band origin of the $S_1 \leftarrow S_0$ transition. Additionally, many hot bands located near the band origin of the this transition have been assigned.

Acknowledgments: Work at Brookhaven National Laboratory was carried out under Contract No. DE-AC02-98CH10886 with the U.S. Department of Energy and supported by its Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences and Biosciences.

[a] also: *Department of Chemistry, Brookhaven National Laboratory, Upton, New York 11973*

[b] J. Hofstein, H. Xu, T. J. Sears and P. M. Johnson, J. Phys. Chem. A **112**, 1195 (2008)

[c] C. Chang , G. V. Lopez, T. J. Sears, and P. M. Johnson, J. Phys. Chem. A **114**, 8262 (2010)