SPECTRAL ANALYSIS OF THE BENDING LEVELS OF ACETYLENE CATION

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Twenty-seven vibronic levels (v_4=0-6, v_5=0-2, K=0-3) of the ground electronic state of acetylene cation have been previously studied by 1+1' two-color pulsed-electric field induced zero-kinetic energy (PFI-ZEKE) photoelectron spectroscopy[a]. These levels, rotationally resolved, are about 0-3520 cm^{-1} above the zero-point energy level. Previously, only the Renner-Teller effects of the trans- and cis-bending vibration and the vibrational anharmonicity were included in the effective Hamiltonian[b]; one standard deviation of the fit was 4.1 cm^{-1}, about six times of the measurement uncertainties. Large discrepancies between the observed and calculated frequencies were identified at combination levels. In this fit, effects such as vibrational $\ell-$type doubling and second-order anharmonic interaction were also considered due to the near degeneracy of the trans- and cis-bending vibration. The results of the fit are satisfactory; most of the vibronic bands can be fitted within one standard deviation of 1.0 cm^{-1}, except the lower component of (v_4=0, v_5=1, K=0). The results of the fit will be presented and few observed vibronic levels, yet unassigned, will be discussed.

[a] Shuenn-Jiun Tang, *Ph. D. thesis*, Chemistry Department, National Taiwan University, Taiwan, R. O. C., 1999.
[b] J. M. Brown, *J. Mol. Spectrosc.* **68**, 412(1977).