THE PFI-ZEKE PHOTOELECTRON SPECTROSCOPY OF C_2H_2 AND C_2D_2 NEAR ITS IONIZATION THRESHOLD

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The 1+1' two-color pulsed-field induced zero-kinetic-energy (PFI-ZEKE) photoelectron spectra of C_2H_2 via a single rovibronic level of the $\tilde{A}^1A_u$ state of acetylene were previously reported by Pratt et al [a]. In this work, with similar approach the effects of the pulsed-field strengths and the rovibronic symmetries of the intermediate states of C_2H_2 and C_2D_2 on the PFI-ZEKE photoelectron spectra near the ionization threshold were investigated and will be reported. Although the number of observed transitions was limited, the spectroscopic constants of the zero-point energy levels of $C_2H_2^+$ obtained from the best fit are in good agreement with those reported by Jagod et al [b]: B=1.098$\pm$ 0.002 cm^{-1}, A_{so}(spin-orbit constant)=-30.84$\pm$0.05 cm^{-1}, and IP_0=91967.06$\pm$0.03 cm^{-1}. Those of $C_2D_2^+$ are B=0.82$\pm$ 0.03 cm^{-1}, A_{so}=-31.1$\pm$0.3 cm^{-1}, and IP_0=92004.7$\pm$ 0.3 cm^{-1}. IP_0 is defined as the energy difference between the zero-point levels of the ground states of the neutral and its cation. We propose to use IP_0 to denote the ionization potential of the molecule, of which the cation belongs to the Hund's case (b) coupling.

[a] S.T. Pratt, P. M. Dehmer, and J. L. Dehmer, J. Chem. Phys. **99**, 6233(1993).

[b] .M.-F. Jagod, M. Rösslein, C. M. Gabrys, B. D. Rehfuss, F. Scappini, M. W. Crofton, and T. Oka, J. Chem. Phys. **97**, 7111(1992).