

THE PFI-ZEKE PHOTOELECTRON SPECTROSCOPY OF C₂H₂ AND C₂D₂ NEAR ITS IONIZATION THRESHOLD

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The 1+1' two-color pulsed-field induced zero-kinetic-energy (PFI-ZEKE) photoelectron spectra of C₂H₂ 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 C₂H₂ and C₂D₂ 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 C₂H₂⁺ obtained from the best fit are in good agreement with those reported by Jagod et al.^b: B=1.098±0.002 cm⁻¹, A_{so}(spin-orbit constant)=-30.84±0.05 cm⁻¹, and IP₀=91967.06±0.03 cm⁻¹. Those of C₂D₂⁺ are B=0.82±0.03 cm⁻¹, A_{so}=-31.1±0.3 cm⁻¹, and IP₀=92004.7±0.3 cm⁻¹. IP₀ 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 IP₀ to denote the ionization potential of the molecule, of which the cation belongs to the Hund's case (b) coupling.

^aS.T. Pratt, P. M. Dehmer, and J. L. Dehmer, *J. Chem. Phys.* **99**, 6233(1993).

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