1+1′ PFI-ZEKE PHOTOELECTRON SPECTROSCOPY OF C2H2-THE RENNER-TELLER EFFECT OF C2H2+

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This paper presents the 1+1′ pulsed-field induced zero-kinetic energy (PFI-ZEKE) photoelectron spectrum of C2H2 recorded in the range of 91900-95600 cm⁻¹ via a single rovibrational level of Λ1Λu as the intermediate. The prominent spectral features were due to trans-bending vibration progression (ν₄+ν₅=0-6, K⁺=0-3) of the Λ2Πu state of C2H2⁺. Although transitions to levels of the cis-bending vibration and levels with combination of Λ0,0 and Λ2,0 vibrational excitation were generally much weaker, the combination levels of (0,0,0,1,1) were fairly easily detected. From the parities and symmetries of the nuclear spin of the observed rovibrational levels of the cations and the intermediate, we deduced that both odd and even partial waves were given off in the pulsed-field photoionization of the Λ state of acetylene. The spectroscopic parameters such as the trans-bending/cis-bending vibrational frequencies, anharmonicity constants, the gK corrections, and Renner-Teller parameters obtained from the best fit to the observed vibronic levels using a model for the Renner-Teller effect of molecule with two bending vibrational modes will be presented.