SPECTROSCOPIC STUDY OF CYANOACETYLENE CATION: SLOW PHOTO-ELECTRON SPECTROSCOPY AND AB-INITIO INVESTIGATIONS

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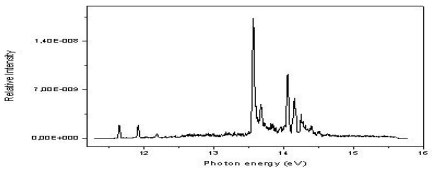

Cyanoacetylene is one of the key minor constituents in the atmosphere of Titan. The ion HCCCN+ has been detected in this atmosphere and it is supposed to be formed by the reaction between C3H2+ and atomic nitrogen[a]. We present here a spectroscopic investigation of the cyanoacetylene cation using photoexcitation of the neutral by vacuum-ultraviolet (VUV) synchrotron radiation coupled to a velocity map imaging electron/ion coincidence spectrometer[b]. The cation spectroscopy is studied by the Slow Photoelectron Spectroscopy technique (SPES) (figure below) and the Total Ion Yield (TIY). The TIY has been calibrated to absolute units using the known propane absolute cross-section. Quantum chemical calculations are performed in order to interpret these spectra. These calculations deal with the equilibrium geometries, electronic-state patterns and evolutions, and harmonic and anharmonic wavenumbers. Through this study, we observe, in the auto-ionization region above the ionization energy, a number of Rydberg series of neutral cyanoacetylene. These Rydberg series converge to the first and second excited states of the cation.

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[a] C. Barrientos, P. Redondo and A. Largo *J. Chem. Phys. A* **104**(49), 11541-11548. 2000

[b] L. Nahon, N. De Oliveria,J. F. Gil,B. Pilette,O. Marcouill, B. La garde and F. Polack *Journal of Synchrotron Radiation* **19**(4), 508-520; 2012