VUV PHOTOIONIZATION AND FRAGMENTATION OF CYANO-PAHs

M. Roy Chowdhury¹, G. A. Garcia¹, E. Rouquet¹, H. Hrodmarsson², J.C. Loison³ and L. Nahon¹

¹Synchrotron SOLEIL, L'Orme des Merisiers, 91192 Gif Sur Yvette, France E-mail : madhusree.roy-chowdhury@synchrotron-soleil.fr

²Laboratory for Astrophysics, Leiden Observatory, Leiden University, NL-2300 RA Leiden, The Netherlands

³ISM, Universite Bordeaux 1, CNRS, 351 cours de la Libération, 33405 Talence Cedex, France

Abstract. Polycyclic aromatic hydrocarbons (PAHs) are postulated to be present abundantly in the interstellar medium (ISM) and they constitute a major reservoir of carbon. Although their presence is widely acknowledged through the observation of the aromatic infrared emission bands (AIBs), the individual identification of the PAHs is hindered due to their highly symmetric molecular structures. The attention is shifted to detect less symmetric ones like the substituted PAHs. Recently, the two nitrile group functionalized PAHs, i.e., 1- and 2-cyanonaphthalenes and cyanobenzene have been detected in the TMC-1 molecular cloud, (McGuire et al. 2021 and 2018).

The detection of these molecular species has driven further interest in studying the photoionization and fragmentation of these molecules in the laboratory in the VUV spectral region. We have performed experimental investigations at the VUV DESIRS beamline at Synchrotron SOLEIL to study the photoelectron spectroscopy of 1- and 2-cyanonaphthalene and cyanobenzene using the double imaging electron/ion coincidence spectrometer, DELICIOUS 3. We have obtained the high resolution threshold photoelectron spectrum (TPES) over an extended binding energy range which will be compared with *ab initio* calculations. The state-selected fragmentation over a wide photon energy range have been obtained which when compared with the case of unsubstituted PAHs unravels the effect of cyano-substitution in terms of photostability. Theoretical investigations predict that PAHs contribute abundantly to the photoelectric heating of the ISM by thermalization of the emitted electrons, (Bakes et. al. 1994). The present measurements provide the KE distributions of the photoelectrons which can be employed to model the photoelectric heating for any incoming photon spectral distribution.

References

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