## VUV spectroscopy and photophysics of interstellar and prebiotic molecules

A. Bellili<sup>1</sup>, Y. Bénilan<sup>2</sup>, M.-C. Gazeau<sup>2</sup>, N. Fray<sup>2</sup>, S. Leach<sup>3</sup>, J.-C. Guillemin<sup>4</sup>, L. Poisson<sup>5</sup>, M. Hochlaf<sup>1</sup>, M. Schwell<sup>2</sup> <sup>1</sup> MSME, UMR 8208 du CNRS, Université Paris Est- Marne-La-Vallée, 1 rue Galilée, 77420 Champs-sur-Marne - France <sup>2</sup> LISA, UMR7583 du CNRS, Universités Paris Est-Créteil et Paris Diderot 61, Avenue du Général de Gaulle, 94010 Créteil - France <sup>3</sup> LERMA, UMR 8112 du CNRS, Observatoire de Paris-Meudon, 5 place Jules Janssen, 92195 Meudon - France <sup>4</sup> Institut des Sciences Chimiques de Rennes, UMR 6226 du CNRS, École Nationale Supérieure de Chimie de Rennes, 11 Allée de Beaulieu, 35708 Rennes Cedex 7 - France <sup>5</sup> Laboratoire Francis Perrin, CNRS URA 2453, CEA, IRAMIS, Service des Photons Atomes et Molécules, F-91191 Gif-sur-Yvette - France.

For many years, our group has been investigating the VUV spectroscopy and photophysics of large molecules of astrophysical and prebiotic interest. We have studied simple compounds like acetic acid, acetonitrile, acetamide, as well as molecules of more immediate biological importance such as nucleic acid bases [1]. Polyynes and cyano-polyynes have been investigated too since these linear carbon and nitrogen chain molecules are very important in the ISM and might act in prebiotic chemistry (see for example our recent work [2a,b]). An aerosol source for reactive and thermo-labile compounds has been developed since many bigger molecules of astrophysical or prebiotic importance are not easily vaporized [3]. We consider gas phase measurements as particularly necessary since they permit to measure the intrinsic photophysical properties of relevant molecules. Furthermore, comparison to quantum chemical calculations, where in most cases isolated molecules are studied, is straightforward. Complex molecules give us insight into the functioning of astrophysical objects because of their spectra which are highly instructive and the chemical network they constitute. Basic UV photophysical data are needed in order do understand and model the chemical evolution of such molecules.

We present here results from our last year's measurement campaigns at Soleil and Bessy where we studied especially aminoacetonitrile ( $H_2NCH_2CN$ ) and acetyl cyanide ( $H_3CCOCN$ ).  $H_2NCH_2CN$ , which is a direct precursor of glycine, has been detected in Sgr B2(N) in 2008. This detection has not been confirmed since, but this compound can be formed by Strecker-type reactions, pathways which are thought to be a solid scenario for the formation of amino acids in space.  $H_3CCOCN$  has not been detected yet in astrophysical objects. The formation of  $H_3CCOCN$  needs only bimolecular interaction of acetaldehyde and HCN (for example on grains). We also note that the lower homologue of acetyl cyanide, which is formyl cyanide (HCOCN) has been also detected in Sgr B2(N) in 2008.

At Soleil, we have measured photoelectron photoion coincidence (PEPICO) spectra from the IE up to 13.6 eV, which is the interstellar HI limit, using the newly developed DELICIOUS III

spectrometer available at the DESIRS beamline. This spectrometer allows for species selective spectroscopy which is of particular importance when studying unstable compounds. In Figure 1, we show the PEPICO photoionization efficiency spectrum (PEPICO-PIE) of  $H_3$ CCOCN where electrons with kinetic energies up to 3.36 eV are considered for the coincidence measurement.



**Figure 1.** PEPICO-PIE spectrum of acetyl cyanide  $H_3CCOCN$  (denoted AC). The intensity is normalized with respect to the incoming photon flux. The insert shows branching ratios of the three ions that can be formed ( $H_3CCOCN^+$ ,  $H_3CCO^+$ ,  $H_2CCO^+$ ) as a function of photo excitation energy.

In Figure 1, besides the parent ion yield curve, two dissociative ionization pathways are observed corresponding to loss of CN and HCN of the parent molecular cation. In order to interpret our experimental data obtained using synchrotron radiation, we explored the ground potential energy surface (PES) of acetyl cyanide and of its cation using standard and recent explicitly correlated methodologies [see for example ref. 4]. These calculations include the enol tautomers which can be formed at excitation energies covered in our study. This allowed us to deduce accurate thermochemical data. We will present these calculations and deduce that unimolecular decomposition of  $H_3CCOCN^+$  turns out to be very complex.

In this contribution, we will also present PEPICO-PIE spectra of aminoacetonitrile  $H_2NCH_2CN$  obtained using the same method. We will further present preliminary results from a campaign lead in June 2014 at Bessy II synchrotron radiation facility. There, the absolute VUV absorption spectra of  $H_3CCOCN$ ,  $H_2NCH_2CN$ , and also propynal (HCCCHO) and isoacetonitrile (CH<sub>3</sub>NC) have been studied for the first time at the U125/2 10m NIM beamline.

## References

[1] M. Schwell, M. Hochlaf, Top. Curr. Chem 2014, in press.

[2] (a) S. Leach, M. Schwell, G.A. Garcia, Y. Bénilan, N. Fray, M.-C. Gazeau, F. Gaie-Levrel, N. Champion, J.-C. Guillemin, *J. Chem. Phys.* **139**, 184304 (2013); (b) S. Leach, G.A. Garcia, A. Mahjoub, Y. Bénilan, N. Fray, M.-C. Gazeau, F. Gaie-Levrel, N. Champion, M. Schwell, *J. Chem. Phys.* **140**, 174305 (2014)

[3] D. Touboul, F. Gaie-Levrel, G. A. Garcia, L. Nahon, L. Poisson, M. Schwell, M. Hochlaf, *J. Chem. Phys.* **138**, 094203 (2013)

[4] Y. Pan, K.C. Lau, L. Poisson, G.A. Garcia, M. Hochlaf, J. Phys. Chem. A 117:8095 (2013).