

Photofragmentation Study of the Acetaldehyde (CH_3CHO) at the Carbon and Oxygen K Edges

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Sinopse. In recent decades, due to the progress of astronomical observations, a lot of more complex organic molecules have been discovered in the interstellar medium, located millions of light years from Earth. One of these molecules is the acetaldehyde (CH_3CHO), which has great importance in astrophysics. It is considered a prebiotic molecule. According to some theories, these molecules have been formed in space and brought by comets and meteorites, giving rise to life on Earth. It would be related with the formation of biomolecules necessary for the generation and maintenance of life, like the nucleic acids (DNA and RNA) and proteins. Acetaldehyde was one of the molecules observed in Hale-Bopp comet using radio spectroscopic observations [1]. Other prebiotic molecules had also been studied by our group (see, for example, reference [2, 3]).

This work presents an experimental spectroscopic study of the acetaldehyde, also known as ethanal (CH_3CHO). Our main purpose was to investigate the possible ionization and dissociation routes of this molecule. Therefore, as the ionizing radiation it was used the Brazilian Synchrotron Radiation Facility (LNLS), in Campinas-SP. The experiment was performed with photons in the energy range of soft X-ray at the SGM beamline. We have used the time of flight mass spectroscopy technique to measure coincidence of electrons with one (PEPICO) or two (PEPIPICO) ions. Initially, we have obtained the Total Ion Yield (TIY) spectra to find the energy of the main electronic transitions. From the PEPICO spectra in this energy region, we identified the fragments produced according to their mass to charge ratio. We have also obtained Partial Ion Yield (PIY) spectra for each ionic fragmentation as a function of the incident radiation energy. Analyzing the PEPIPICO spectra, we have determined the relative yield of ionic fragment pairs measured in coincidence. Finally, we have found the most probable dissociation paths of the acetaldehyde

for the different photon energies. We observed at the TIY spectra, both at the lower energy of the C (carbonyl) edge as at the O edge, a more intense peak assigned to the transition to a π^* antibonding orbital. The other structures were assigned to excitations to Rydberg series orbitals. With the analysis of PIY spectra we identified the more produced fragments in each energy region. From the PEPIPICO spectra we assigned the delayed charge separation as the main fragmentation mechanism for most of the measured pairs.

Acknowledgments

CAPES, LNLS and UFBA.

References

- [1] J. Crovisier *et al.* 2004 *Astron. Astrophys.* **418**, 1141-1157.
- [2] M. S. Arruda, *et al* 2015 *J. Phys. Chem. A*, **119**, 10300-10308.
- [3] M. S. Arruda, *et al* 2016 *J. Phys. Chem. A*, **144**, 1441101.

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