Fast beam experiments on XUV and soft-X-ray photofragmentation of molecules

C. Domesle[a], L. S. Harbo[b], O. Heber[c], B. Jordon-Thaden[a], L. Lammich[b], M. Förstel[d], T. Arion[d], U. Hergenhahn[d], S. Dziarzhytski[e], N. Gerassimova[e], R. Treusch[e], H. B. Pedersen[b], and A. Wolf[a]

[a]*Max-Planck-Institut für Kernphysik, 69117 Heidelberg, Germany*
[b]*Department of Physics and Astronomy, Aarhus University, 8000 Aarhus C, Denmark*
[c]*Department of Particle Physics, Weizmann Institute of Science, 76100 Rehovot, Israel*
[d]*Max-Planck-Institut für Plasmaphysik, EURATOM Association, 85748 Garching, Germany*
[e]*HASYLAB / DESY, 22603 Hamburg, Germany*

Abstract. In harsh radiative environments, molecules can be broken following the production of valence or inner-shell vacancies. For polyatomic structures, the molecular breakup patterns generated by photofragmentation comprise smaller, charged and neutral molecules and atoms, which are characteristic for the specific potential surfaces created by the initial photoexcitation or ionization step. Beside the initial electronic transition, the molecular breakup pattern in particular reflects the propagation of the nuclei or molecular sub-units on the relevant potential surfaces (as well as the ones becoming relevant by dynamical couplings to other electronic states on the fragmentation pathway). While such unimolecular reaction data are required in various fields – astrochemistry, planetary and atmospheric research, radiation biochemistry, and others – experimental results, especially for neutral fragments and fragment radicals, are often not available and reliable theoretical predictions often not in reach.

At the free electron laser FLASH (HASYLAB, DESY, Hamburg) [1], we have developed the ion beam infrastructure TIFF [2,3] to study molecular photofragmentation by XUV and soft-X-ray photons in multi-fragment coincidence measurements in the crossed-beams geometry. In recent measurements, we obtained the main fragmentation channels triggered by ~30–100 eV photons for protonated water [3,4], protonated water clusters [4,5], the water (H_2O^+) cation [6], and others. The fragmentation momenta were used to obtain kinetic energy releases, fragmentation angular distributions, and angular geometries for three-body fragmentation channels. Moreover, we identified the photofragmentation channels, determined their branching ratios, and the absolute photofragmentation cross section. Recently, also first results were obtained for photoelectron energies which reveal the molecular vacancy states created by the incident XUV and soft-X-ray radiation. Further measurements are planned to study polyatomic photofragmentation and molecular structures of interest in astrochemistry and other fields.

This work was partly supported by the Max-Planck Working Group (ASG) at the Centre for Free Electron Lasers, Hamburg, Germany, and the Lundbeck Foundation.

References

[1] W. Ackermann *et al.*, Nature Photonics **1**, 336 (2007); K. Tiedtke et al., New J. Phys. **11**, 023029 (2009).
[2] H. B. Pedersen *et al.*, Phys. Rev. Lett. **98**, 223202 (2007).
[3] H. B. Pedersen *et al.*, Phys. Rev. A **80**, 012707 (2009).
[4] C. Domesle *et al.,* in preparation.
[5] L. Lammich *et al.*, Phys. Rev. Lett. **105**, 253003 (2010).
[6] H. B. Pedersen *et al.*, in preparation.