Kinematically complete imaging of H_2O^+ after XUV photodissociation at FLASH

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The photodissociation of the H_2O^+ ion after irradiation at 35 nm was studied in a crossed-beams experiment at the ion beam apparatus TIFF (Trapped Ion Fragmentation at an FEL) installed in the PG2 beamline at FLASH. A set of two time-resolving imaging detectors was used to identify dissociation channels and to determine energy releases and fragmentation geometries through event-by-event coincidence measurements.

Fragmentation processes of molecular ions after XUV excitation or ionization play an important role in the chemistry of interstellar clouds and planetary atmospheres. Moreover, organic compounds and in particular water-based structures are crucial for the understanding of radiation induced processes in living organisms. The species studied here, H_2O^+, has attracted additional interest due to its role as a transition state in the double ionization of neutral water [1].

The TIFF setup is a dedicated instrument designed for the study of interactions between molecular ions and high-energy photons as provided by a free electron laser. The use of a fast (keV) ion beam allows for an efficient detection of both charged and neutral photofragments [2, 3]. The common problem of low target density in gas-phase ion experiments is here overcome by the use of short, collimated ion bunches synchronized with intense photon pulses. Both the large pulse energy and the high repetition rate of FLASH are exploited, making particular use of the strongly upgraded performance available after the 2009 upgrade of this machine [4].

In the present case, ions were created in a plasma discharge ion source operated with pure water vapor, accelerated to 4.2 keV kinetic energy and mass selected in a magnetic field, resulting in a 22 nA beam of H_2O^+. Ion pulses of 1 μs width were guided to the interaction point and overlapped with the FLASH pulses (wavelength 35 nm, pulse energy 40 μJ, repetition rate 500 Hz).

The emerging photofragments are registered on a set of two imaging detectors (see Fig. 1). The first one, DET1, is mounted close to the interaction point and thus sensitive to small fragments with large transversal velocities (here: protons). Heavier fragments and undissociated parent ions pass through a hole in this detector. Charged particles are then directed to a beam dump using an electrostatic deflector, while neutral fragments (here: oxygen atoms) are recorded on a second

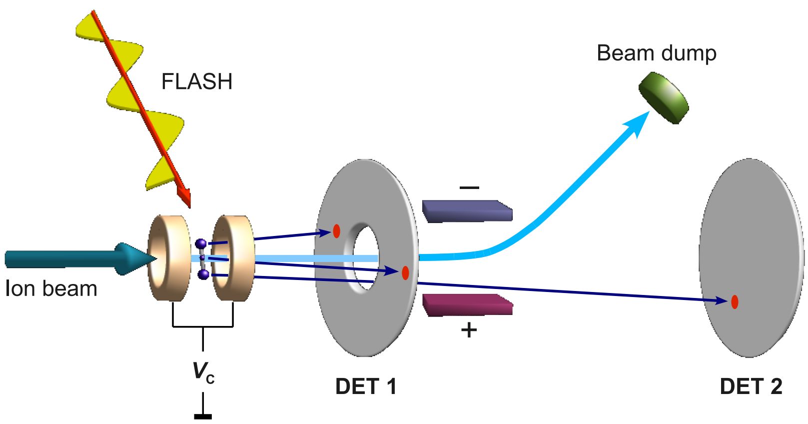

Figure 1: Schematic illustration of the ion-photon interaction point and the fragment detection system at TIFF.

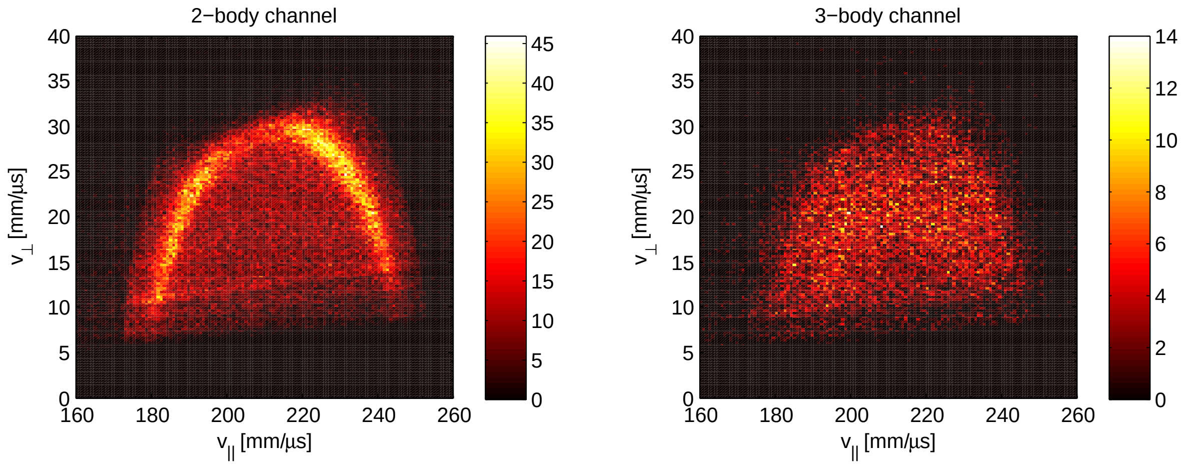

Figure 2: Proton velocities measured after the XUV photodissociation of H_2O^+. Left: single protons without accompanying neutral particles, right: events where two protons and one neutral oxygen atom were detected in coincidence. The plots show the velocity components transversal and parallel to the direction of the parent ion beam, which had a velocity of 213 mm/μs.

imaging detector, DET2. By means of a coincidence analysis, two fragmentation channels could be identified in the recorded data:

$$H_2O^+ + \gamma \rightarrow \begin{cases} OH^+ + H^+ + e^- \\ O + 2H^+ + e^- \end{cases}$$

Figure 2 shows the proton velocity distributions recorded for the two channels. For events where a single proton and no neutral fragment was recorded, the data show a rather sharp ring structure, a signature of a two-body breakup with well-defined kinetic energy release. Events composed of two protons and one neutral fragment in coincidence show a rather broad distribution of single-proton energies, as expected for a multi-fragment breakup.

To identify the fragments recorded on DET1 as protons, rather than neutral hydrogen atoms, H_2^+ or heavier fragments, the effect of an accelerating voltage applied to electrodes around the interaction point on the fragment velocities was studied in a separate measurement.

The three-body channel involving a neutral O product was newly discovered for this system. It was found with a considerable branching ratio and a set of fully detected triple-coincidence events has been measured. The complete reconstruction of each recorded dissociation event in terms of kinetic energy release, spatial orientation and breakup geometry is currently in progress.

In future experiments it is foreseen to record and characterize also the photoelectrons emerging from the initial ionization process in coincidence with the atomic and molecular fragments using a newly designed electron spectrometer. To facilitate the detection of photoelectrons, an upgrade of the infrastructure at the PG2 beamline is under way, aiming at improved collimation and suppression of stray light in the photon beam path.

Support by the Max-Planck Advanced Study Group at the Centre for Free Electron Laser Physics (CFEL) is gratefully acknowledged.

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