Laboratory astrophysics at FLASH: XUV photofragmentation of the water cation H_2O^+

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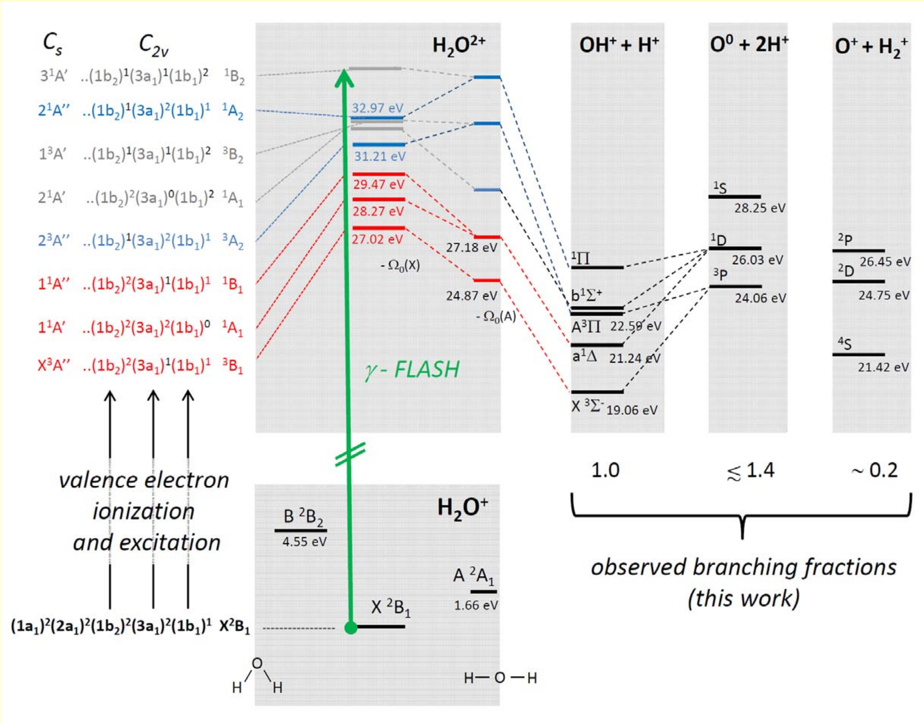
XUV photofragmentation of H_2O^+

The water cation H_2O^+ occurs in several natural environments where molecular gas is exposed to ionizing radiation. Its has been directly observed in the upper atmosphere [1] and in the tails of several comets [2–7] though its visible emission spectrum. These observations have been used to indirectly identify the presence of neutral water in comets, since H_2O molecules themselves do not show a visible emission spectrum. Recently, the astrophysical importance of H_2O^+ has been highlighted by several observations of both H_2O^+ as well as other oxygen hydride ions (OH^+ and H_3O^+) using the Herschel Space Observatory [8–11].

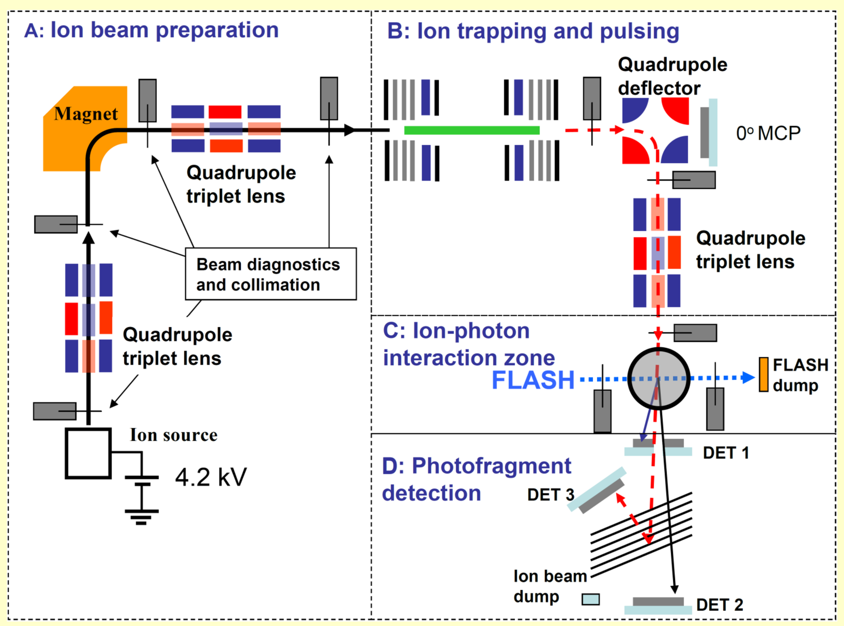
Reactions of oxygen and its smaller hydrides are part of models of the interstellar chemistry in various environments [12–15], where in particular H_2O^+ ions are formed in reaction of H_2 and OH^+, while being depleted by further reactions with H_2 to form H_3O^+ and by dissociative recombination. The fragmentation of water cations under *ionizing radiation* is not considered in present models.

Using FLASH in combination with techniques based on accelerated ion beams we have investigated the fragmentation of isolated H_2O^+ ions under ionizing radiation in the form of mono-energetic photons for two wavelengths, 35.0 nm and 21.8 nm, in the extreme ultraviolet (XUV) regime.

In a molecular physics perspective, we here make the first investigation of the potential energy surfaces of the water di-cation starting from the mono-cation [16].



TIFF experiment with new analyzing system for charged photofragments



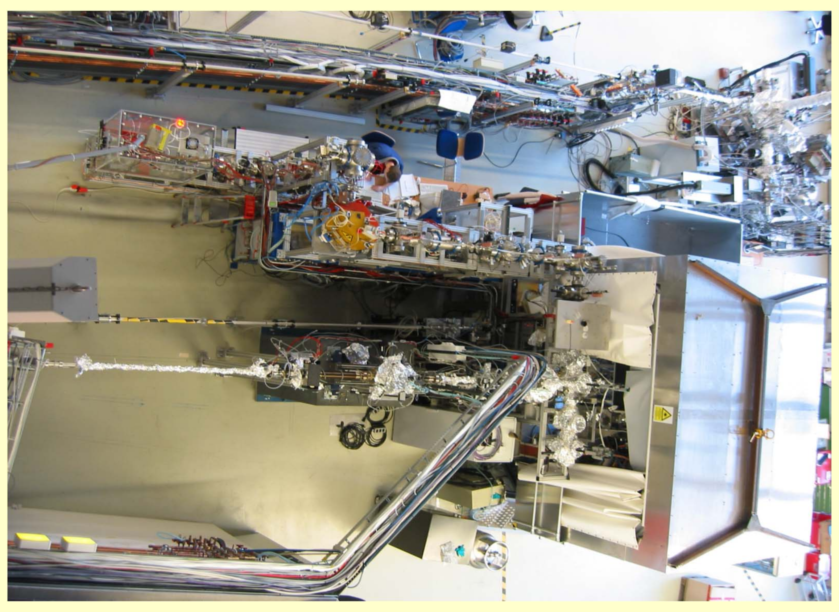
TIFF

Trapped

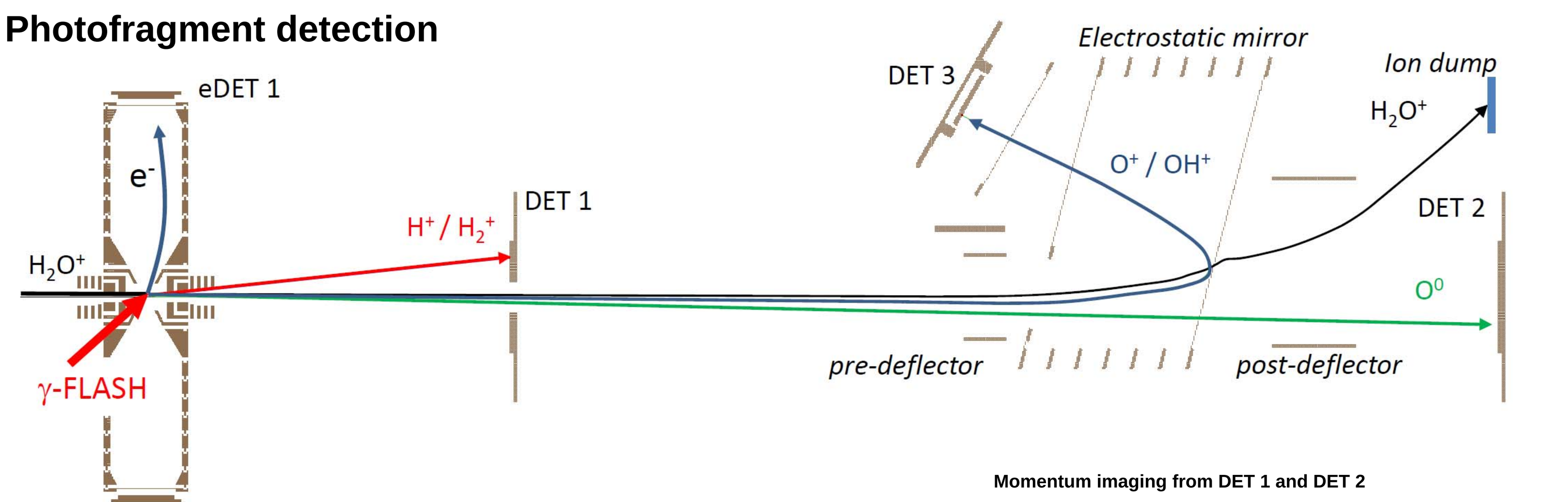
Ion

Fragmentation at

FLASH



Photofragment detection

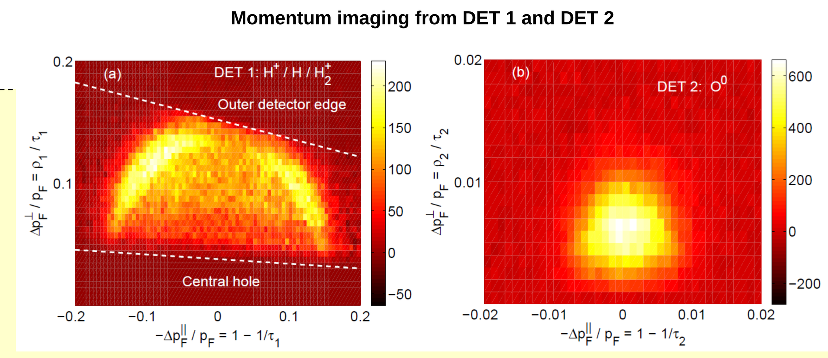


FLASH
- λ = 21.8 nm / 35.0 nm
- E = 30-40µJ/pulse
- 50 pulses at 200kHz (5µs)

TIFF
- E_I = 4.2 keV
- I = 20 nA
- 50 pulses of 1.5µs

Total ion-photon reaction rate = 250 Hz

Momentum imaging from DET 1 and DET 2



Momentum imaging from DET 1-3

Position and time

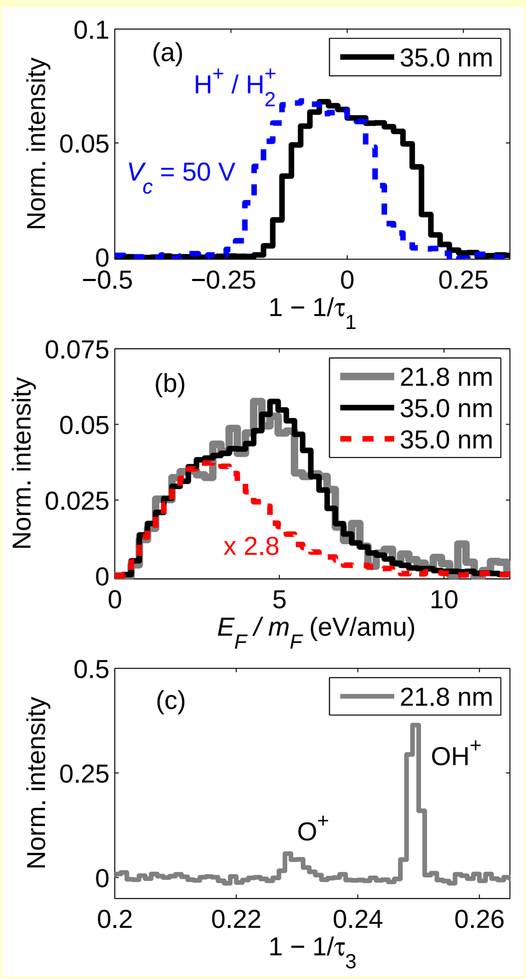
$\rho_i = r_i / L_i$ $\tau_i = t_i / (v_I L_i)$

$p_F = m_F v_I$

$\frac{\Delta p_F^{\parallel}}{p_F} = \frac{1}{\tau_i} - 1$ $\frac{\Delta p_F^{\perp}}{p_F} = \frac{\rho_i}{\tau_i}$

Relative momenta

Fragmentation channel identification



Relative longitudinal momentum on DET 1
- All light fragments are charged, i.e. H^+ or H_2^+

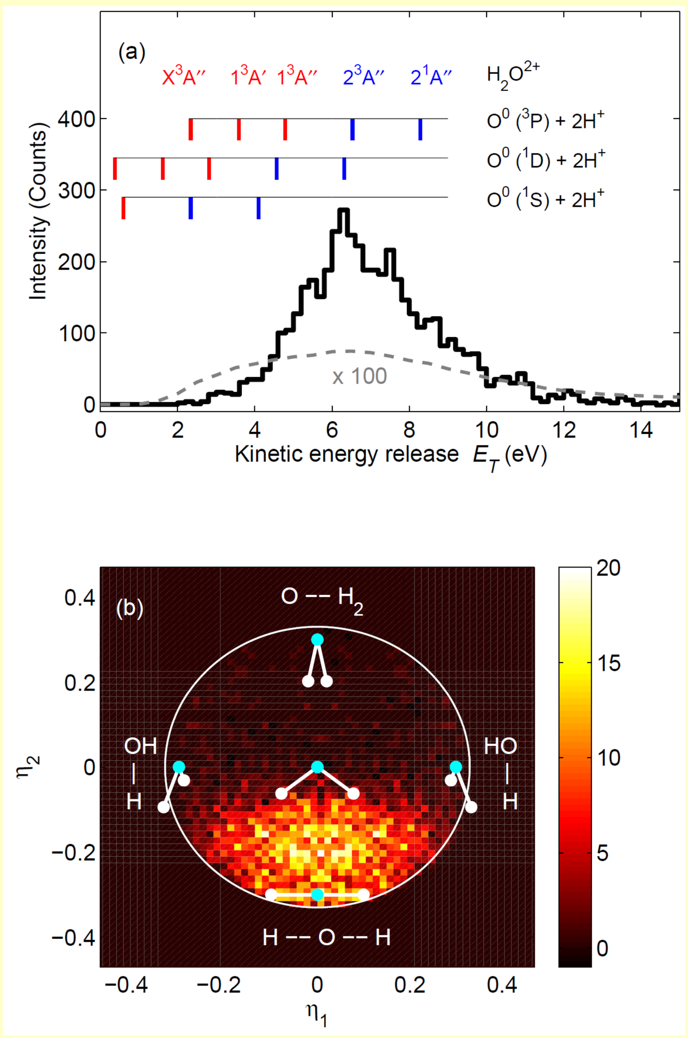
Energy per mass on DET 1
- Different wavelength - same break-up dynamics
- Coincidence with O^0 (red curve)

Three-body	< 1.4
Two-body	1.0

Relative longitudinal momentum on DET 3 (new)
- Two-body channel

$OH^+ + H^+$	1.0
$O^+ + H_2^+$	0.2

$\gamma + H_2O^+ \rightarrow H_2O^{2+} \rightarrow O^0 + H^+ + H^+$



Total kinetic energy release

$$E_F = \left[\left(\frac{1}{\tau_i}-1\right)^2 + \left(\frac{\rho_i}{\tau_i}\right)^2\right] \times \frac{m_F}{m_I} E_I$$

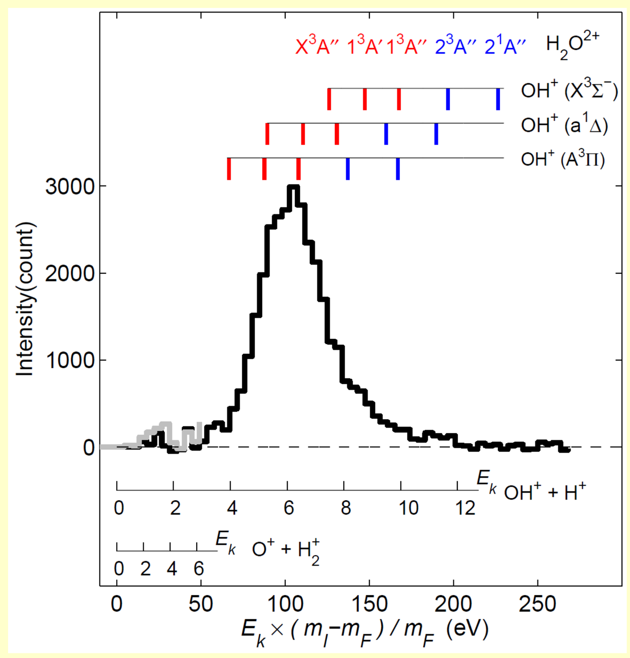
$$E_T = E_{O^0} + E_{H^+} + E_{H^+}$$

3-body break-up dynamics - Dalitz plot [17]

$$\eta_1 = \sqrt{\frac{m_I}{3m_O}} \frac{E_{H1^+} - E_{H2^+}}{\sqrt{3}E_T}$$

$$\eta_2 = \frac{m_I}{3m_H} \frac{E_{O^0}}{E_T} - \frac{1}{3}$$

$\gamma + H_2O^+ \rightarrow H_2O^{2+} \rightarrow OH^+ + H^+$



Two-body kinetic energy release

$$E_k = \left[\left(\frac{1}{\tau_i}-1\right)^2 + \left(\frac{\rho_i}{\tau_i}\right)^2\right] \times \frac{m_F}{m_I - m_F} \times E_I$$

Future directions with TIFF at FLASH

- **For H_2O^+**
  - High statistics measurement with the new fragment analyzer to enable full charaterization of the two-body channels
  - Photoelectron-photofragment spectroscopy to experimentally completely specify the photofragmentation pathways (photoelectronspectroscopy has been demonstrated for anions and larger water clusters)
- **Larger molecular systems under study/proposal**
  - Water clusters ions $H^+(H_2O)_n$ - Astrophysics / atmospheric physics
  - Small molecular cations: HeH^+, He_2^+, O_2^+, N_2^+, … - Non-adiabatic interactions / competition between ionization and excitation
  - Atomic anions He^-, Li^-, O^-, … - full characterization of processes dominated by electron correlation
  - Molecular anions: $H^+(N_2)$, $C_2H_2^-$, C_n^-, PAH⁻, … - Astrophysics / atmospheric physics
- **Collaborations are welcome !**

Present conclusions on H_2O^+

- Photofragmentation dynamics similar at 35.0 nm and 21.8 nm. XUV induced process: ionization followed by fragmentation.
- Major fragmentation channels of H_2O^+ under ionizing radiation
  - $O + H^+ + H^+$ 1.0
  - $OH^+ + H^+$ < 1.4
  - $O^+ + H_2^+$ 0.2
- Three-body-channel ($O^0 + H^+ + H^+$)
  - Wide distribution of energy release around 6 eV Consistent with predictions of Gervais *et al.* [16]
  - Break-up dynamics: *"the protons carries the momentum"*
- Two-body-channel ($OH^+ + H^+$ / $O^+ + H_2^+$)
  - Major kinetic energy release around 5 eV
  - Future measurements can distinguish channels and clarify angular distributions
- Further interpretation of fragmentation mechanisms from theory would be very interesting !

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