

Dissociation Dynamics of Doubly Ionized Water Using 57 eV Photons

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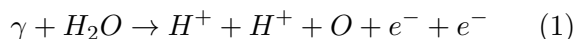
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Synopsis We have measured the photoelectron emission and dissociation of water in the gas phase following double photoionization by a 57 eV photon. The momenta of the resulting dication ion fragments and electrons were measured in coincidence with Cold Target Recoil Ion Momentum Spectroscopy (COLTRIMS) [1]. The dissociation dynamics following the photoionization process show a marked dependence on both bond angle and kinetic energy release distribution among the fragments.

We have focused our attention the following final state following the photionization of H₂O by 57 eV photons:



Because of the innate asymmetry of H₂O, fixing the molecular body frame to investigate electronic dynamics has proven to be a challenge. Because the kinetic energy release (KER) is not always equally partitioned between the two ions (in addition to the unmeasured neutral oxygen), the axial recoil approximation breaks down in general. Furthermore, because water has a vibrational mode that corresponds to the bending of the molecule, interpreting KER with a 1-dimensional potential model is inadequate.

For example, Figure 1a) shows the energy correlation between the two measured protons in the isolated dissociation channel above. The distribution of energy sharing as well as total ion energy is quite broad, demonstrating the challenge of isolating particular dissociation pathways from energy measurements alone.

Figure 1b) shows the momentum space histogram in a frame defined by the momentum sum P_{par} of the ion fragments (horizontal axis) vs. the corresponding perpendicular momentum. We note that the magnitude of the ion fragment momentum has a clear correlation with the relative angle between the two momentum vectors. This seems plausible, as one might expect a higher KER for smaller initial bond angles. Also evident in Figure 1b) is the presence of two yet

unidentified distinct dissociateve states.

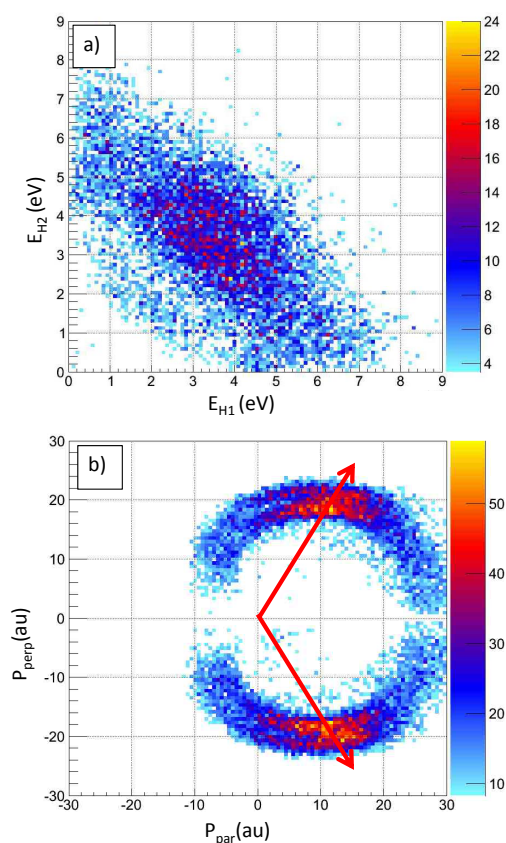


Figure 1. a) Energy correlation map for H⁺ ions. b) Molecular frame momenta for both hydrogen fragments, H1 top half, H2 bottom half. The red arrows indicate the average bond angle for neutral water.

Analysis is underway to isolate the fixed-body-frame of the molecule in order to investigate molecular frame electronic correlation effects.

References

- [1] T. Jahnke, *et al.*, J. Electron Spectrosc. Relat. Phenom. 141, 229 (2004).

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