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# Dissociative multiple ionization of the H<sub>2</sub>O molecule induced by ion impact: experimental and theoretical results

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# Dissociative multiple ionization of the H<sub>2</sub>O molecule induced by ion impact: experimental and theoretical results

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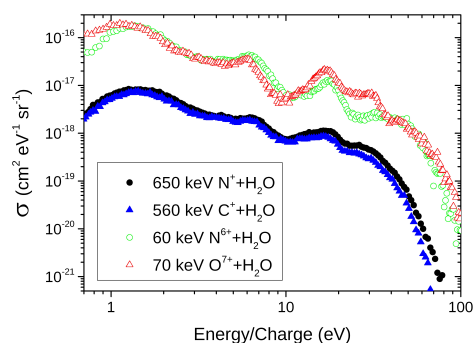
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**Synopsis** Fragment energy spectra of the water molecule impacted by singly charged (SCI) and highly charged (HCI) ions have been measured in crossed beam experiments. Double differential fragmentation cross sections (DDCS) have been determined. Similarities and differences of the measured DDCSs induced by the medium- and low-energy projectiles have been analyzed. Multiple target ionization cross sections have been deduced and they were further analyzed through the results of the CTMC and CDW-EIS models.

We present experimental results on the Coulomb explosion of H<sub>2</sub>O molecules, bombarded by different types of projectile ions. The initial multiple vacancy production in the target molecule is further analyzed through the results of CTMC and CDW-EIS calculations.

Gas phase water molecules were impacted by medium-energy singly charged (560 keV C<sup>+</sup> and 650 keV N<sup>+</sup>) and low-energy highly charged (60 keV N<sup>6+</sup> and 70 keV O<sup>7+</sup>) ions [1, 2]. The energy and angular distributions of the charged fragments were measured by single-stage electrostatic spectrometers. Double differential fragmentation cross sections have been deduced.



**Figure 1.** Measured fragmentation cross sections for the four different projectiles at 45° observation angle.

The shape of the spectra is found to be very similar for C<sup>+</sup>, N<sup>+</sup> and N<sup>6+</sup> impact (see Figure 1.). Though the dominant ionization mechanism and the average perturbation

strength is different for SCIs and HCIs, the similarity indicates that the same fragmentation channels appear in the collisions. While the SCI induced spectra are almost identical, slight differences in the relative intensities of the structures were found between the SCI and HCI induced spectra, as well as between the spectra induced by the two HCIs. It was attributed to the selectivity of the electron capture process compared to the direct ionization.

From the fragment ion spectra multiple ionization (MI) cross sections have been deduced. We found that the highest degrees of ionizations for the two SCIs approach those for the HCIs with non-negligible yields. The MI cross sections were further analyzed through the results of classical (CTMC) and quantum mechanical (CDW-EIS) model calculations [1, 3]. The calculated MI cross sections almost coincide with the experimental data for C<sup>+</sup> and N<sup>+</sup> impact, and are only in qualitative agreement with the measured HCI results. Further analysis have been performed through the calculated impact parameter dependent MI probabilities.

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