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Double ionization of water molecule induced by swift H^+.

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Synopsis Experimental cross sections for single and double ionization of H_2O by swift H^+ with energy ranging from 0.5 to 2.0 MeV are reported. In this energy range the ionization is the dominant collision process and charge transfer reactions can be disregarded. A multi-hit coincidence technique was used to measure the $H^+ + OH^+$ and $H^+ + O^+$ fragmentation channels. A model calculation allowed us to separate the post collisional contribution from the direct double ionization process, whenever an electron vacancy occurs in the 2a1 molecular orbital.

The ionization process leading to a multiple electron emission can be generated by various mechanisms, related to the strength of the collision dynamics, i.e. a hard or soft collision, or post-collisional ionization (PCI), i.e. Auger and Coster Kronig processes, electron shake-off, excitation followed by double Auger [1].

For the case of water molecule, the removal of one or more electrons from most of it molecular orbitals can be followed by fragmentation. The yields for the various possible molecular fragments depend in which one of the molecular orbitals the vacancies were produced. A key point in this whole process is the link between the population of vacancies and the branching ratios of the fragmentation products. These branching ratios are very difficult to calculate because the ejection of fragments occurs in conjunction with an equally fast rearrangement of the electrons in the orbitals.

For vacancies occurring in inner valence molecular orbital (eg. $2a_1$ in water), the Auger-like de-excitation channel can be open and competes with a prompt single-vacancy fragmentation. The relative yields of these two alternatives are unknown and difficult to be estimated. One of the reasons is because the Auger-like de-excitation results into two ionized species which can also be produced via dynamical two-step vacancies by the impinging projectile.

In this work double ionization cross sections leading to $H^+ + OH^+$ and $H^+ + O^+$ were measured using a multi-hit coincidence set-up. The experimental arrangement was previously described in reference

[2] for the atomic target case. For a molecular target, opposite to the atomic ones, multiple ionization leads to the formation of multiple ionic fragments. In this case, the efficiencies related to ion collection (due to coulomb explosion) and double hit detection, have to be taken into account carefully. The procedures used in this work to obtain such efficiencies will be discussed in detail at the conference.

The comparison involving the measured ratios between double ionization cross sections and the single ionization channel (H_2O^+) with a model calculation based on first Born approximation allowed us to obtain the population of vacancies of the inner valence molecular orbitals. The contribution of an Auger like post collisional de-excitation from the $2a_1$ valence orbital to the double ionization was obtained. From the velocity dependence of the above ratios for proton and electron [3] impact it was possible to estimate the contributions from both the Auger-like and direct process (two-step ionization) to the total double ionization channel. It was found that Auger like process dominates for proton energies above 1.5 MeV while two-step process competes for lower energies.

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