Proton impact fragmentation of water molecules

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Synopsis The Continuum Distorted Wave-Eikonal Initial State approximation for impact of H^+ on H_2O molecules is used to calculate absolute cross sections for multiple electron removal processes at intermediate and high collision energies. Resulting fragmentation patterns are also matter of study. Results are compared with previous calculations and available experimental data.

Interaction of charged particles with molecular targets is of great interest in a number of areas of research such as nuclear fusion [1], plasma physics [2] and others. Particularly, collisions of ions with H_2O are of great importance in radiotherapy [3]. The ionization of water molecules produce different charged species, which can damage the surrounding cells. Therefore, it is important to analyze pure ionization, capture and transfer-ionization reactions to study fragmentation processes.

We present theoretical calculations of fragmentation cross sections based on the model proposed in the work [4] for water molecules interacting with H^+ impact. In the present work, cross sections are obtained in the framework of the three-body Continuum Distorted Wave-Eikonal Initial State approximation (3B-CDW-EIS) [5]. The initial wavefunctions of the active electrons bound to a particular water molecular orbital are described employing the complete neglect of the differential overlap (CNDO) approximation [6]. A trinomial distribution analysis has been employed to compute exclusive probabilities using the independent electron (IEL) model. A unitarization procedure is employed to avoid overestimations of 3B-CDW-EIS impact parameter probabilities.

From the comparison with the available theoretical and recent experimental results, we conclude that exclusive probabilities are required for a reliable description of the fragmentation yields (see Figure 1).

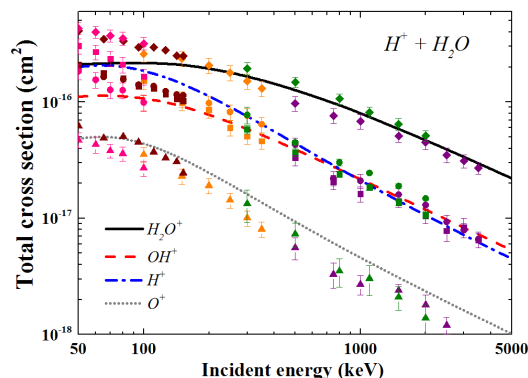The developed approach may be used to investigate fragmentation patterns of more complex molecules.

Figure 1. Fragmentation cross sections as a function of the incident energy for H^+ impacting on H_2O.

References

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