# Fragmentation of water molecules by $He^{2+}$ and $Li^{3+}$ impact

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**Synopsis** We employ the Continuum Distorted Wave-Eikonal Initial State approximation for impact of $He^{2+}$ and $Li^{3+}$ ions on water molecule to study the production of fragmentation patterns resulting from multiple electron removal processes at the intermediate to high projectile energy range. Results were compared with previous calculations.

Investigation of single and multiple-electron removal processes occurring between fully stripped ions and simple molecules is of fundamental interest in many areas such as nuclear fusion [1], plasma physics [2] and others. In particular, collisions of ions with $H_2O$ are of principal interest in biology and medicine [3]. The ionization of water molecules produce different charged species, which can damage the surrounding cells. Therefore, it is important to calculate cross sections of pure ionization, capture and transfer-ionization reactions to determine their contributions to the fragmentation processes.

The aim of the present investigation is focused on theoretical calculations of fragmentation cross sections for water molecules interacting with $He^{2+}$ and $Li^{3+}$ ions, based on the model proposed in the work [4]. We use the three-body Continuum Distorted Wave-Eikonal Initial State approximation (3B-CDW-EIS) [5] to obtain the cross sections. 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.

We compare our results just with previous calculations, because to our knowledge no experimental data exist for these systems. Fragmentation cross sections for the case of $He^{2+}$ on $H_2O$ collisions are shown in Figure 1.

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

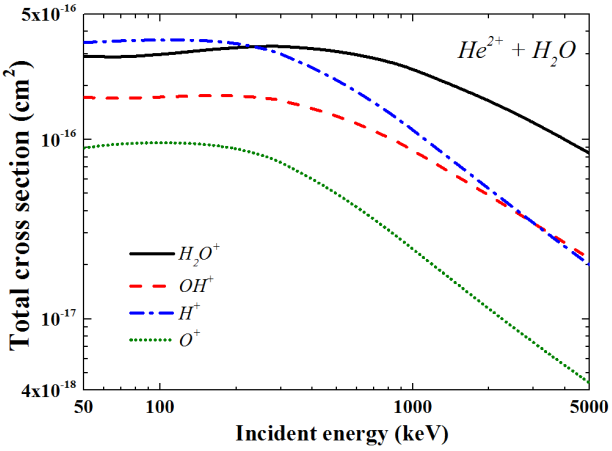


**Figure 1.** Fragmentation cross sections as a function of the incident energy for $He^{2+}$ impacting on water target.

## References

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