

Basis generator method study of electron removal from water molecules by multiply-charged ion impact

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Synopsis We apply the basis generator method for ion-molecule collisions to study He^{2+} and C^{6+} impact on H_2O in the energy range of 20–5000 keV/amu. Results are compared with experimental data and previous calculations where available.

In a recent series of publications we have described the adaptation of the basis generator method (BGM), originally developed for ion-atom collisions, to molecular targets and have reported on results for proton and He^+ -ion impact on H_2O molecules [1].

The main ideas of this approach are (i) to represent self-consistently generated molecular orbitals (MOs) in terms of a single-center atomic oxygen basis; (ii) to propagate these MOs using the BGM and an energy representation of the molecular Hamiltonian to avoid the computation of multi-center matrix elements; (iii) to analyze the propagated MOs on the level of the density matrix thereby respecting the Pauli principle; (iv) to perform a (somewhat restricted) orientation average and sum over impact parameter in order to calculate total cross sections.

The microscopic collision calculations were complemented with a semi-phenomenological fragmentation model, which in contrast to previous models takes multiple electron removal processes into account. This turned out to be crucial for obtaining reasonable agreement with experimental data for the production of the singly charged fragment ions H_2O^+ , OH^+ , H^+ , and O^+ .

In this contribution, we report on results obtained from the same methodology for bare helium and carbon ion impact on H_2O . Figure 1 shows our net ionization cross section for He^{2+} - H_2O collisions in comparison with the results of a three-center classical trajectory Monte Carlo (CTMC) calculation [2] and experimental data [3, 4]. Overall, we note the consistency of calculations and measurements. At projectile energies below 50 keV/amu our results are in better

agreement with experiment than the CTMC calculation.

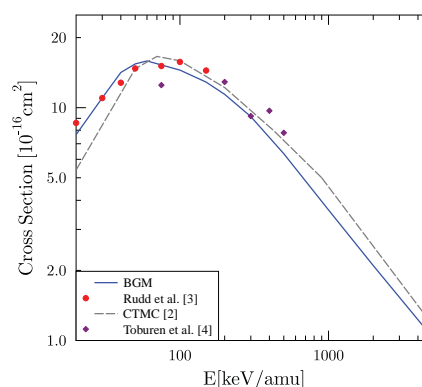


Figure 1. Net ionization cross section in He^{2+} - H_2O collisions as function of projectile energy.

The case of C^{6+} impact turns out to be more challenging. A large number of projectile states needs to be taken into account in order to obtain reasonably well-converged cross sections. This problem, as well as more details on the He^{2+} - H_2O collision system will be discussed at the conference.

References

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