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Ab initio treatment of ion-water molecule collisions with a three-center pseudo potential

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Synopsis We calculate electron capture cross sections in collisions of protons with water molecules, using two simple *ab initio* approaches. The formalism involves the calculation of one-electron scattering wave functions and the use of three-center pseudo potential to represent the electron H_2O^+ interaction. Several methods to obtain many-electron cross sections are considered.

Ion-water molecule collisions play an important role in processes of interest in several areas such as plasma physics, astrophysics, atmospheric physics and medicine. These applications motivated several experiments [1, 2, 3, 4, 5] that measured charge transfer, ionization and fragmentation cross sections.

Following our work in Ref. [6], we extend some computational techniques, previously applied to ion-H_2 collisions [7], to the treatment of ion collisions with H_2O using a three-center pseudo potential to represent the interaction of the active electron with the molecular ion H_2O^+, and the use of asymptotically frozen molecular orbitals. We explore the workings of two methods:

- In the first one (IPEM), the collision event is described by means of a one-electron scattering wave function, from which cross sections are derived using the independent particle model (IPM) approximation.
- In the second one (IPM-SEC), a multi-electronic scattering wave function is obtained by considering single and double excitations from the ground state configuration, while the IPM is used to evaluate the hamiltonian integrals.

Calculations of H^+ and He^{2+} with H_2O are carried out within the semiclassical eikonal approach, which assumes that the projectile follows straight-line trajectories ($\boldsymbol{R} = \boldsymbol{b} + \boldsymbol{v}t$) with impact parameter $\boldsymbol{b}$ and velocity $\boldsymbol{v}$; this naturally accounts for the anisotropy of the target and the orientation averaged cross sections are obtained by considering ten different trajectory orientations.

As an illustration, we plot in Fig. 1 the orientation averaged electron capture cross sections in H^++H_2O collisions.

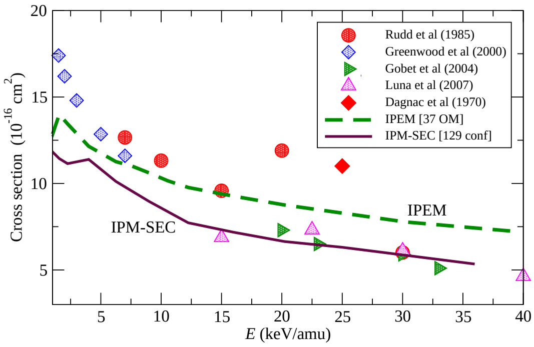

Figure 1. Single electron capture cross sections in proton-water collisions. Our calculations (lines) are compared with experimental data (symbols).

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