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Charge exchange in proton collisions with the water dimer

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Synopsis We calculate the electron capture cross sections in collisions of protons with water dimers, using a simple *ab initio* approach. The formalism involves one-electron scattering wave functions and a statistical interpretation to evaluate many-particle cross sections. By comparing with proton-water collisions, we aim at identifying aggregation effects in the electron capture cross sections.

Proton-water collisions have been studied in both numerous experimental and theoretical works (see references in [1]) motivated by their interest in cellular damage by ionizing radiations [2] and their relevance in the production of cometary X-rays [4, 3]. In this work, we consider proton collisions with the water dimer in order to identify the importance of molecular interactions in the electron capture and ionization cross sections; this is the first step to establish the applicability of the theoretical data obtained in gas phase to the cellular environment.

Following our previous work [1], our method relies on using a one-electron scattering wave function expanded over asymptotically frozen molecular orbitals, from which cross sections are derived by means of the independent particle model. The interaction of the active electron with the molecule is described by means of a six-center pseudo potential. With this method, one avoids the need of regularizing conical intersections between electronic states, regions where dynamical couplings diverge (see, e.g. [5] and references therein), and where non-adiabatic transitions predominantly take place at low energies.

Within the semiclassical eikonal approach, we assume that the projectile follows straight-line trajectories ($\boldsymbol{R} = \boldsymbol{b} + \boldsymbol{v}t$) with impact parameter $\boldsymbol{b}$ and velocity $\boldsymbol{v}$; generally, this is adequate for $E > 100$ eV/amu, where most of the experiments are carried out. We also assume that the nuclear geometry of $(H_2O)_2$ is kept fixed during the collision, with the nuclei at their equilibrium positions in the electronic ground state (Franck-Condon approximation). We have considered a set of 16 different projectile trajectory orientations. As an illustration, we plot in Fig. 1 the single-electron-loss (single electron capture + single ionization) cross sections for the trajectory orientations shown in Fig. 2.

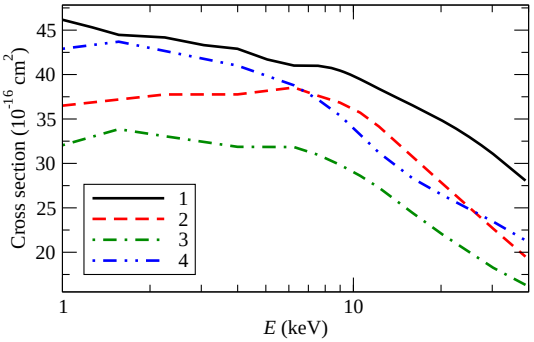

Figure 1. Total cross section for electron-loss in H^+ collisions with the water dimer for the trajectory orientations indicated in Fig. 2.

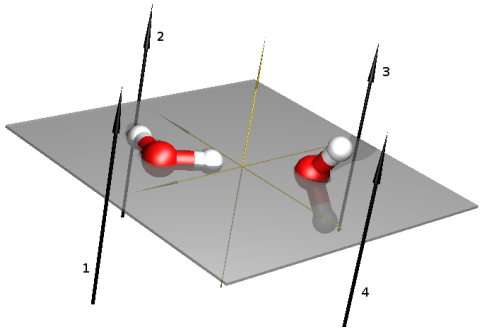

Figure 2. Trajectory orientations employed in Fig. 1.

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