Theoretical investigation of water ionization by electron impact at low energies

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Synopsis Triple differential cross sections (TDCS) are calculated for the ionization of water by electron impact. The TDCSs are determined in the scattering plane and in the plane perpendicular to the incident beam direction. The obtained theoretical cross sections are compared with very recent experimental measurements and other theoretical calculations.

The ionization of water molecules has been studied intensely in the last years [1, 2, 3, 4, 5, 6, 7, 8]. This process is of interest for several research fields, like medicine or astrophysics. One possible application is related to radiative treatment methods, since organic tissue consists of a large percentage of water. It has been shown that low energy electrons have a particularly damaging effect on DNA strands.

Previously we have studied the ionization of water for different kinematical and geometrical conditions. We have calculated [7] TDCSs in the scattering plane for electron impact energies of 250 eV for the asymmetric ejection of the final state electrons. Further, the $3a_1$ orbital has been investigated [8] at low impact energies both in the scattering and the perpendicular planes and also for some geometrical arrangements between these two extreme configurations. In this case only symmetric ejection of electrons was considered.

In the current work we extend our investigation of water ionization for a different set of kinematical conditions and geometrical arrangements in order to further test the validity of our calculation method. The TDCSs are determined for a relatively low impact energy (81 eV) both in the scattering and perpendicular planes. The calculated cross sections represent the sum of the $1b_1$ and $3a_1$ TDCSs in order to compare with the experimental data [1]. In the experiment, these orbitals were not resolved, due to the limited binding-energy resolution of the experimental setup. Nevertheless, the cross sections are also calculated separately for the above mentioned orbitals. We investigate the asymmetric ejection of the final state electrons, the scattering angle of the projectile being set at -6° and -10°, respectively, relative to the incident beam direction. For both scattering angles, we consider ejected electrons at 5 eV and 10 eV, respectively. The ejected electron is the slower one. Beside the experimental data [1], the obtained results are compared with other theoretical calculations presented in the same paper.

In the calculations we use a distorted-wave approach for the description of the free states in the system, while the molecular orbitals are described by multi-center Gaussian-type orbitals. The distorted waves are calculated in the spherically averaged potential of the molecule or the molecular ion. Two schemes are considered for the final state particles. In the first one the ejected electron moves in the averaged field of the nuclei and residual electrons, while the faster electron experiences a potential which is totally screened by the slower one. In the second configuration we neglect this screening and both electrons move in the same potential of the molecular ion.

In the calculations we take into account the post collision interaction (PCI) effects between the final continuum electrons using the Coulomb distortion factor of [9]. Although the two electrons have different energies, these are relatively low values, therefore PCI effects may still be important for the correct description of the process.

Further details about the theoretical models and results will be presented at the conference.

References

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