H2O double ionization induced by electron impact

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Double ionization of water molecules remains, still today, rarely investigated on both the experimental and the theoretical side. In this context, the present work reports on a quantum mechanical approach providing a quantitative description of the electron-induced double ionization process on isolated water molecules for impact energies ranging from the target ionization threshold up to about 10 keV. The cross section calculations are here performed within the first Born approximation framework in which the initial state of the system includes a molecular ground-state wave function expressed as a single-center linear combination of atomic orbitals [1] while the final state of the system is characterized by two independent Coulomb wave functions used for describing the two ejected electrons coupled by a Gamov factor used for modeling the electron-electron repulsion. In comparison with the rare available experiments [2], the double vs single ionization cross section ratio shows an overall good agreement. Besides, in absence of measurement of absolute total cross sections in water vapor, the current theoretical predictions are compared with isoelectronic neon data. A very good agreement is observed over the whole incident energy range investigated. Finally, we report an average energy transfer of the double ionization process and clearly demonstrate the absolute necessity of considering the double ionization process in particular in a radiobiological context.

References

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