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Effect of microsolvation in low-energy positron collisions with formaldehyde-water complexes.

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Abstract: The microsolvation's effect in formaldehyde water have been studied in scattering of electrons [1]. In this work, we report the integral cross sections for elastic collisions of low energy positrons with the $CH_2O...H_2O$ complex. In the scattering cross sections calculations we employed the Schwinger Multichannel Method (SMC) [2,3] in the static plus polarization (SP) approximation for energies from 0.1 to 10 eV. We also include the contribution of the permanent electric dipole moment of molecule through the *Born closure*. In this work, we considered four different hydrogen-bonded structures for the $CH_2O...H_2O$ complex that were generated by classical Monte Carlo simulation of formaldehyde in water environment at room temperature [4]. We also optimized the geometry of the four formaldehyde complexes, after the optimization we need to consider only one systems since all four complexes have the same optimized geometry. We also showed a comparison of the integral cross section for this optimized structure with the results for the other four structures. The aim of this work is to investigate the influence of microsolvation on the cross section of formaldehyde. The scattering of positrons by formaldehyde in gas phase (CH_2O) has been studied before [5] and we compared our results for CH_2O molecule with this previous experimental results in the literature.

Key-words: microsolvation, scattering, positrons
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