Model potential calculations for the elastic positron scattering from hydrocarbons

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In some recent works of ours [1,2] we have provided some interesting results for the elastic positron scattering cross sections from a variety of small molecules, namely H_2 [1], N_2 [1], CH_4 [2], C_2H_2 [2] and C_2H_4 [2], with the Schwinger multichannel (SMC) method [3,4] in the static plus polarization (SP) approximation and in the static plus model potential ($S+V_{CP}$) approximation [1,2], with the model potential from the works of Swann and Gribakin [5].

In these works [1,2] we have chosen the cutting distances for each atom and each hybridization which best fitted the $S+V_{CP}$ approximation s-wave eigenphases to the ones from our more recent SP approximation calculations. It is important to check whether these chosen cutting distances would also provide reliable elastic positron scattering cross sections for other systems which also involve the atoms and hybridizations studied. To test these cutting distances, we have performed calculations with the SMC method in the $S+V_{CP}$ approximation for ethane (C_2H_6), propene (C_3H_6), cyclopropane (c-C_3H_6), propane (C_3H_8) and benzene (C_6H_6).

Our calculations provided some interesting elastic positron scattering cross sections for these systems, especially when compared to earlier calculations with the SMC method in the SP approximation for some of these systems [6-8].

References

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