The impact of the multichannel coupling effects on the description of electron scattering by isoprene molecules

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In this work we report on integral, differential and momentum transfer cross sections for elastic and electronically inelastic scattering of electrons by the isoprene molecule. The scattering amplitudes were obtained by means of the Schwinger multichannel method [1] implemented with norm-conserving pseudopotentials [2] for energies ranging from 0 to 50 eV. These calculations were performed according to the minimal orbital basis for single configuration interactions strategy [3] within a level of channel coupling from 1-channel up to 147-channels and were carried out with the aim of investigating the influence of the multichannel coupling effects upon the description of elastic and electronically inelastic electron collisions by the isoprene molecule. From our results we found that as the level of channel coupling through which the calculations were performed increases, a drastic reduction in the magnitude of the cross sections is observed. We also present the total ionization cross section obtained according to the binary-encounter-Bethe model [4]. By summing the binary-encounter-Bethe ionization cross section with present elastic and electronically inelastic cross sections we provide an estimate to the total cross section for electron scattering by the isoprene molecule. Whenever possible, these results are critically compared to the data available in the literature.

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[1] Takatsuka, K. and McKoy, V. *Phys. Rev.* A, **1981** 24, 2473; *ibid.*, **1984** 30, 1734.

[2] Bettega, M. H. F.; Ferreira, L. G. and Lima, M. A. P. *Phys. Rev.* A, **1993** 47, 1111.

[3] da Costa, R. F.; da Paixão, F. J. and Lima, M. A. P. *J. Phys.* B, **2004** 37, L129; *ibid.*, **2005** 38, 4363.

[4] Kim, Y. K. and Rudd, M. E. *Phys. Rev.* A, **1994** 50, 3954.