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Theoretical and experimental study on electron interactions with chlorobenzene: Shape resonances and differential cross sections

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ABSTRACT

In this work, we report theoretical and experimental cross sections for elastic scattering of electrons by chlorobenzene (ClB). The theoretical integral and differential cross sections (DCSs) were obtained with the Schwinger multichannel method implemented with pseudopotentials (SMCPP) and the independent atom method with screening corrected additivity rule (IAM-SCAR). The calculations with the SMCPP method were done in the static-exchange (SE) approximation, for energies above 12 eV, and in the static-exchange plus polarization approximation, for energies up to 12 eV. The calculations with the IAM-SCAR method covered energies up to 500 eV. The experimental differential cross sections were obtained in the high resolution electron energy loss spectrometer VG-SEELS 400, in Lisbon, for electron energies from 8.0 eV to 50 eV and angular range from 7° to 110°. From the present theoretical integral cross section (ICS) we discuss the low-energy shape-resonances present in chlorobenzene and compare our computed resonance spectra with available electron transmission spectroscopy data present in the literature. Since there is no other work in the literature reporting differential cross sections for this molecule, we compare our theoretical and experimental DCSs with experimental data available for the parent molecule benzene.

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