

Theoretical and experimental cross sections for elastic scattering of electrons by chlorobenzene

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Synopsis In this work we will present recent theoretical and experimental cross sections obtained for the elastic scattering of electrons by chlorobenzene.

The pioneer study of Boudaïffa *et al.* [1] indicated that single and double strand breaks can be induced in DNA by low energy electrons (LEEs). Later it was shown that the dissociation processes can be mediated by the formation of shape resonances in specific sites of the DNA chains [2]. Since then, intense theoretical and experimental activity has focused on better understanding the interactions of LEEs with biomolecules and their precursors, in particular the characterization of resonances and their role in the dissociation processes. More recently, halogenated DNA and RNA bases [3], as well their precursors [4], have also gained attention because their sensitizing effects in the radiotherapy of tumors.

In the present work we report theoretical and experimental cross sections for elastic scattering of electrons by chlorobenzene (ClB). ClB can be seen as a prototype for radiosensitizers and furthermore, ClB is a simple system with a peculiar spectrum of transient anion states. Besides the π^* shape resonances from the benzene ring, ClB also presents a σ^* resonance arising from the replacement of a H by a Cl atom. Furthermore, as in the closely related halopyrimidine molecules [4], the halogen substituent tend to stabilize the π^* anion states. Similar trends are expected in ClB, but interesting features also arise from the halogen-induced symmetry breaking, i.e., the lifting of the degeneracy of the first $\pi^*(E_{2u})$ anion state of benzene. The theoretical integral (ICS) and differential cross sections (DCS) were calculated with two different methodologies: the Schwinger multichannel method implemented with pseudopotentials (SMCPP) [5] for lower electron energies and the independent atom method with screening corrected additivity rule (IAM-SCAR) [6] for

higher energies. We compare our calculated ICS with total available total cross sections [7, 8]. And also, from our calculated SMCPP ICSs we could identify the shape resonances of ClB and compare the results with available experimental data [9, 10, 11]. We also report experimental differential cross sections (DCSs), 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° . Since, to our knowledge, DCSs have not been reported for electron-ClB collisions, it is desirable to compare the present data with DCSs for the parent molecule benzene [12].

References

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