Electron Induced chemistry of Chlorobenzene

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Synopsis Electron interactions with aromatic molecule are important in many areas of applied physics. We compute target properties & electron scattering cross sections of chlorobenzene and discuss different phenomena and their importances.

Electron impact studies with organic targets gained prominence after the study, that secondary electrons produced by energetic radiations are responsible for single and double strand breaks in DNA. Moreover systematic and detailed knowledge of cross sections resulting from electron collisions with simple organic systems can help us to understand the behaviour of more complex biomolecules.

A detailed theoretical study is carried out for electron interactions with chlorobenzene (C_6H_5Cl) with impact energies ranging from 0.01 to 5000 eV. Owing to the wide energy range we have been able to investigate variety of processes and report data on dissociative electron attachment (DEA) through resonances, vertical electronic excitation energies, differential, momentum transfer, ionization and total cross sections (TCS) as well as scattering rate coefficients. In order to compute TCS we have employed ab initio R-matrix method (0.01 to 20 eV) [1, 2] and the spherical complex optical potential (SCOP) method (20 to 5000 eV) [3, 4]. The R-matrix calculations were performed using close coupling approximation employing a static exchange plus polarization (SEP) model. The target properties reported using quantum chemistry codes are in good agreement with earlier reported data as shown in Table 1.

Table 1. Target Properties of Chlorobenzene

Target property (unit)	Present	Other[5]
Ground State (Hartree)	-688.64	-689.99
Ionization Potential (eV)	9.200	9.080
Diapole Moment (Debye)	1.689	1.690

As a sample result we report here DCS data of e-C_6H_5Cl scattering at 20 eV in Figure 1. The present data finds overall good agreement with lone data of Barbosa et al.[6].

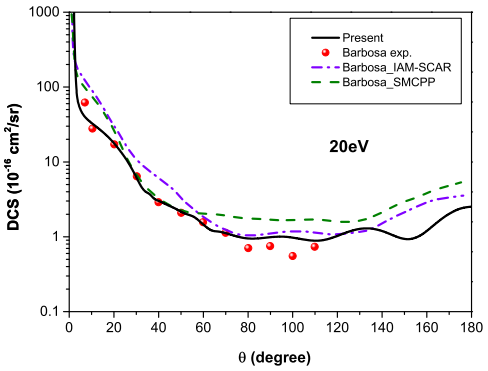

Figure 1. Differential Cross Section of chlorobenzene at 20eV

Minaxi Vinodkumar acknowledge DAE-BRNS, Mumbai for the Major research project [37(3)/14/44/BRNS-2014] for financial support under which part of this work is carried out.

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