



Differential Ionization Cross Sections of HCl Molecule

Ravinder Sharma^{a*}, Ritu Sharawat^b, Meenakshi^b & Rajeev Kumar^c

^aDepartment of Biomedical Engineering, Deenbandhu Chhotu Ram University of Science & Technology, Murthal, Sonapat, Haryana-131 039 India

^bDepartment of Physics, Baba Mast Nath University, Rohtak, Haryana-124 001 India

^cDepartment of Physics, D. J. College, Baraut, Baghpat, Uttar Pradesh-250 611 India

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In this article, the differential ionization cross-sections of the HCl molecule in the gas phase is investigated. The single differential ionization cross-section (SDCS) as a function of loss of incident electron energy and Double Differential Cross Section (DDCS) as a function of energy loss of incident electron and incident angle, is calculated. To reach exact values of differential ionization cross sections for HCl molecule, a modified semi-empirical approach of Jain and Khare is used. Partial and total absolute ionization cross-section of HCl is available but there is no data for differential ionization cross-sections. So, first time, the results for single and double differential ionization cross-sections for HCl molecule is investigated.

Keywords: Partial ionization; Single differential ionization; Double differential ionization; Electron impact ionization cross-section

1 Introduction

The data on the study of electron impact ionization of HCl molecule is not only important in mass spectrometry and scattering theory but also interesting for atmospheric physics, radiation chemistry, Plasma physics, gas discharges and other related phenomenon¹. There are also many industrial applications of gaseous hydrogen chloride, such as in pharmaceuticals, gasoline refining, chemicals, manufacture of rubber, metals processing, tanning leather, *etc.*¹ There are many other miscellaneous applications such as semiconductors etching, catalyst in chemical syntheses, mineral and rock processing, industrial water treatment, food processing *etc.*

HCl is a colourless, corrosive and non-flammable gas having a strong odour at room temperature. HCl gas is very soluble in water at 20 °C. HCl is not symmetrical because it is a polar molecule and the electronic configuration in the ground state can be written as: $KL(3s\sigma)2(3p\sigma)2(3p\pi)4$. There are many theoretical and experimental calculations for the determination of the absolute ionization cross-sections of HCl molecule²⁻⁶, but no data is available for differential ionization cross-section. For the determination of absolute results of differential cross

sections for HCl molecule, a modified Jain and Khare semi-empirical approach has been used⁷⁻¹⁵. We have determined single differential cross-sections (SDCS) as a function of energy loss of incident electron at constant incident electron energies (100, 200 and 500 eV). We have also investigated double differential cross-sections (DDCS) as a function of energy loss of incident electron and incident angles (30°, 60° and 90°) at the constant incident electron energies (100, 200 and 500eV).

2 Theoretical Methodology

We used here a modified Jain and Khare formulation for Single differential cross sections as a function of energy loss W of primary electron /or secondary electron energy ϵ corresponding to the production of the i^{th} type of ion in ionization of a molecule is given by¹⁶⁻²⁴.

$$Q_i(E, \epsilon) = \frac{4\pi a_0^2 R}{E} \left[\left(\frac{1}{1 + \frac{I_i}{E}} \right) \frac{R}{E} \frac{df}{dw} \ln[1 + C_i(E - I_i)] + \left[\frac{R(E - I_i)}{E} S_i \frac{1}{\epsilon^3 + \epsilon_0^3} \left(\epsilon - \frac{\epsilon^2}{(E - \epsilon)} + \frac{\epsilon^3}{(E - \epsilon)^2} \right) \right] \right] \quad \dots(1)$$

For the determination of double differential cross sections (DDCS) we have taken a formula derived by Kumar *et al.*¹⁵

*Corresponding author: (E-mail: ravindersharma591@gmail.com)

$$Q_i(E, W, \theta) = \frac{4\pi a_0^2 R^2}{E} \left[\frac{8R^2 Z^2}{W^2} \left(1 - \frac{\epsilon}{(E-\epsilon)}\right) \left(1 - \frac{W}{E}\right)^{1/2} \sin\theta \frac{df}{dW} \ln(1 + C_i(E - I_i)) \right. \\ \left. + S_i \frac{\epsilon^3}{\epsilon^3 + \epsilon_0^3} \left(\frac{E - I_i}{E}\right) \left(\epsilon - \frac{1}{(E-\epsilon)} + \frac{1}{(E-\epsilon)^2}\right) \frac{\sin\theta}{2} \right] \dots(2)$$

Here

$$C_i = C_T \exp \left[n \left(\frac{\sum_{j>1} M_j^2 - S_j}{\sum_{j>1} M_j} - \ln S_j \right) \right] \dots(3)$$

Where in above equations $W = (\epsilon + I_i)$, S_i , M_i^2 , I_i , a_0 , ϵ_0 , C_i and R is energy loss suffered by the incident electron, number of ionizing electrons, transition probabilities for various ionic species, ionization threshold for the production of the i th type of ion, first Bohr's radius, energy parameter, collision parameter and the Rydberg's constant, respectively

In the determination of ionization cross sections, oscillator strength (df/dw) is a key parameter. Here we have taken experimental results of oscillator strength from Daviel *et al.*²⁵ from 13 to 40 eV for the HCl molecule and its fragmented ions (HCl^+ , Cl^+ , and H^+) by using (e, e^+ ion) spectroscopy. For higher energies, oscillator strength is extrapolated up to the desired energy. Collision and energy parameters are 0.02124 and 80eV respectively¹.

3 Results and Discussion

Here first time we have calculated partial and total single differential cross-sections (SDCS) at constant incident electron energies i.e.100, 200 and 500 eV. The results are given in Tables 1 to 3 and graphically represented in Fig. 1.

Table 1 — SDCS (in cm^2/eV) of HCl molecule at fixed 100 eV incident energy.

W (eV)	HCl ⁺	Cl ⁺	H ⁺	Total
20	1.321E-17	1.299E-18	4.762E-19	1.498E-17
25	5.549E-18	2.215E-18	4.066E-19	8.171E-18
30	2.004E-18	1.331E-18	4.685E-19	3.804E-18
35	6.984E-19	5.982E-19	3.337E-19	1.630E-18
40	4.088E-19	3.434E-19	2.055E-19	9.577E-19
45	4.080E-19	2.482E-19	1.228E-19	7.790E-19
50	4.103E-19	1.859E-19	8.519E-20	6.814E-19
55	4.336E-19	1.411E-19	6.053E-20	6.352E-19
60	4.881E-19	1.097E-19	4.408E-20	6.419E-19
65	5.918E-19	8.888E-20	3.315E-20	7.139E-19
70	7.759E-19	7.727E-20	2.626E-20	8.794E-19
75	1.095E-18	7.498E-20	2.270E-20	1.192E-18
80	1.649E-18	8.406E-20	2.247E-20	1.755E-18
85	2.641E-18	1.098E-19	2.637E-20	2.777E-18
90	4.529E-18	1.642E-19	3.667E-20	4.730E-18
95	8.521E-18	2.761E-19	5.898E-20	8.856E-18
100	1.867E-17	5.257E-19	1.085E-19	1.930E-17

Table 2 — SDCS (in cm^2/eV) of HCl molecule at fixed 200 eV incident energy.

W (eV)	HCl ⁺	Cl ⁺	H ⁺	Total
20	1.057E-17	7.712E-19	2.690E-19	1.161E-17
25	4.582E-18	1.364E-18	2.382E-19	6.184E-18
30	1.686E-18	8.531E-19	2.857E-19	2.825E-18
35	5.667E-19	4.003E-19	2.126E-19	1.180E-18
40	3.032E-19	2.408E-19	1.375E-19	6.815E-19
45	2.970E-19	1.831E-19	8.665E-20	5.668E-19
50	2.839E-19	1.447E-19	6.374E-20	4.923E-19
55	2.743E-19	1.156E-19	4.817E-20	4.381E-19
60	2.664E-19	9.370E-20	3.727E-20	3.974E-19
65	2.591E-19	7.701E-20	2.943E-20	3.656E-19
70	2.520E-19	6.413E-20	2.366E-20	3.398E-19
75	2.448E-19	5.407E-20	1.933E-20	3.182E-19
80	2.380E-19	4.613E-20	1.602E-20	3.001E-19
85	2.318E-19	3.979E-20	1.345E-20	2.850E-19
90	2.267E-19	3.470E-20	1.143E-20	2.729E-19
95	2.235E-19	3.062E-20	9.835E-21	2.639E-19
100	2.225E-19	2.738E-20	8.573E-21	2.585E-19
120	2.552E-19	2.074E-20	5.834E-21	2.818E-19
140	3.948E-19	2.315E-20	5.841E-21	4.238E-19
160	8.169E-19	3.991E-20	9.382E-21	8.662E-19
180	2.408E-18	1.040E-19	2.353E-20	2.535E-18
200	1.775E-17	5.611E-19	1.191E-19	1.843E-17

Table 3 — SDCS (in cm^2/eV) of HCl molecule at fixed 500 eV incident energy.

W (eV)	HCl ⁺	Cl ⁺	H ⁺	Total
20	6.548E-18	3.662E-19	1.221E-19	7.036E-18
25	2.877E-18	6.593E-19	1.100E-19	3.647E-18
30	1.063E-18	4.198E-19	1.344E-19	1.617E-18
35	3.444E-19	2.006E-19	1.019E-19	6.470E-19
40	1.701E-19	1.229E-19	6.723E-20	3.602E-19
45	1.648E-19	9.522E-20	4.322E-20	3.033E-19
50	1.552E-19	7.669E-20	3.246E-20	2.643E-19
55	1.482E-19	6.250E-20	2.505E-20	2.357E-19
60	1.427E-19	5.163E-20	1.981E-20	2.142E-19
65	1.379E-19	4.324E-20	1.598E-20	1.971E-19
70	1.332E-19	3.667E-20	1.313E-20	1.830E-19
75	1.283E-19	3.145E-20	1.096E-20	1.707E-19
80	1.230E-19	2.724E-20	9.265E-21	1.595E-19
85	1.175E-19	2.379E-20	7.921E-21	1.492E-19
90	1.116E-19	2.092E-20	6.836E-21	1.394E-19
95	1.057E-19	1.851E-20	5.948E-21	1.301E-19
100	9.969E-20	1.645E-20	5.210E-21	1.213E-19
120	7.717E-20	1.068E-20	3.235E-21	9.109E-20
140	5.912E-20	7.273E-21	2.137E-21	6.853E-20
160	4.587E-20	5.154E-21	1.480E-21	5.251E-20
180	3.653E-20	3.792E-21	1.068E-21	4.139E-20
200	3.015E-20	2.900E-21	8.026E-22	3.385E-20
250	2.301E-20	1.810E-21	4.779E-22	2.529E-20
300	2.539E-20	1.640E-21	4.116E-22	2.744E-20
350	4.030E-20	2.285E-21	5.520E-22	4.314E-20
400	8.887E-20	4.712E-21	1.116E-21	9.470E-20
450	3.167E-19	1.574E-20	3.667E-21	3.361E-19
500	8.277E-18	2.718E-19	5.818E-20	8.607E-18

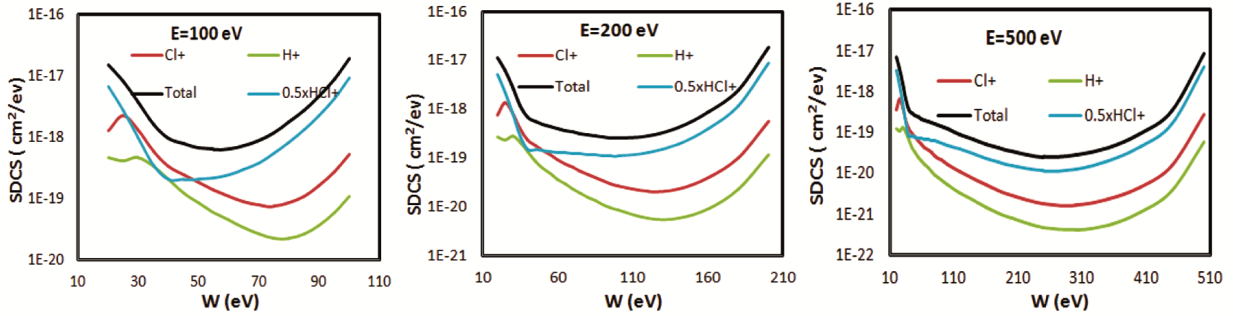


Fig. 1 — SDCS as a function of energy loss of incident electron at fixed incident energies 100, 200 and 500eV.

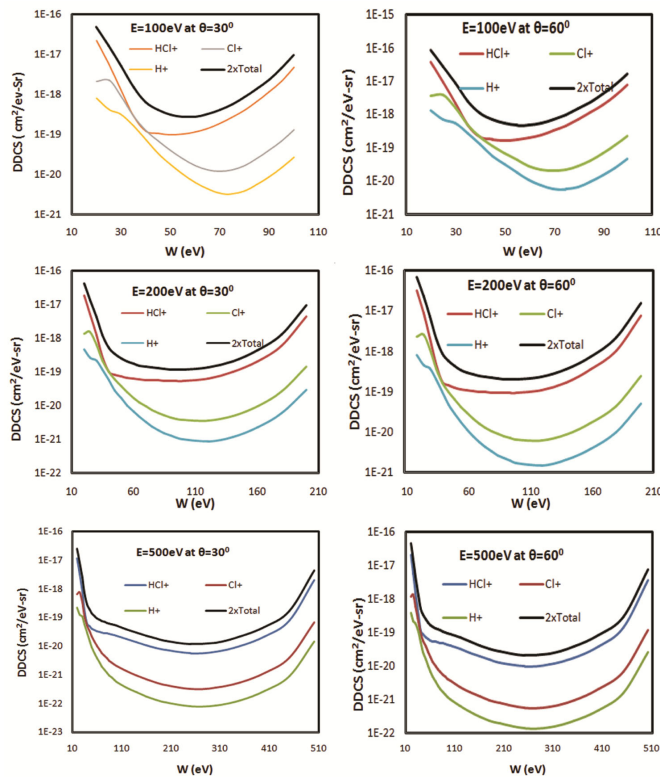


Fig. 2 — Double Differential Cross Sections (DDCS) at constant incident electron energies (100, 200 and 500 eV with fixed incident angles 30° and 60°)

We also calculated partial and total double differential cross-sections (DDCS) as a function of loss of incident electron energy W and incident angles (30° and 60°) at constant incident energies (100, 200 and 500 eV) are shown in Fig. 2. We have determined double differential cross-sections at constant secondary electron energy (20 eV) by varying the incident angle at fixed incident electron energies *i.e.* 100, 200 and 500 eV are presented graphically in Fig. 3. The 3D profiles (variation of DDCS with incident angle and secondary electron energy) of HCl are also presented in Fig. 4 at constant incident

energies *i.e.* 100 and 200 eV. At present time no other data of SDCS and DDCS are available for comparison. Although, the qualitative behaviour of the cross-sections are the same as for other molecules¹⁸⁻²⁴ investigated previously. The energy-dependent cross sections for SDCS and DDCS are symmetric at $W/2$ at which the energies of primary and the secondary electrons are almost equal, except for some irregular behaviour near the threshold values. The first part of the formulation explains the contribution of exchange effects and the second part of the formula explain resonances.

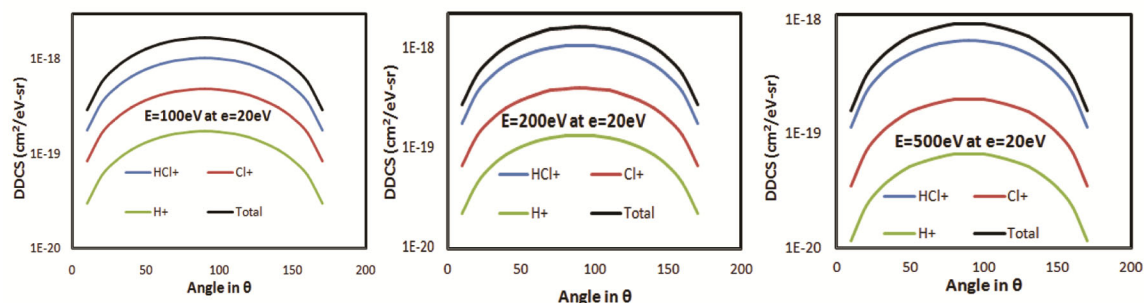


Fig. 3 — Double Differential Cross-Sections (DDCS) at constant secondary electron energy (20 eV) by varying the incident angle at fixed incident electron energies i.e.100, 200 and 500 eV

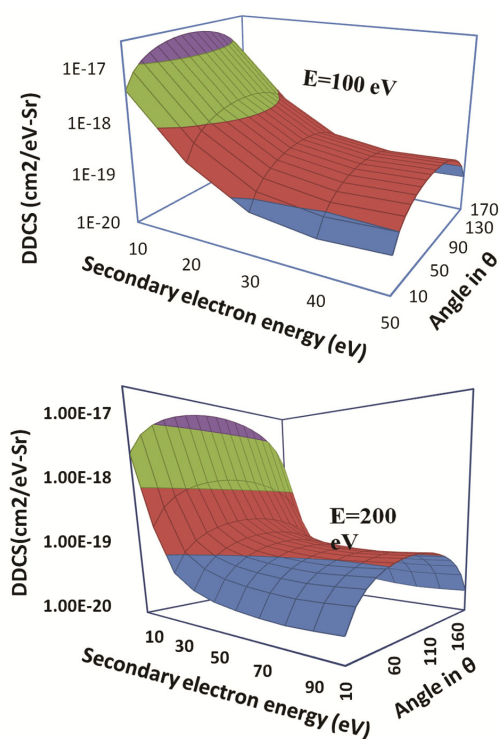


Fig. 4 — 3D profile of total DDCS at constant incident energies 100 and 200 eV.

4 Conclusion

In the present study, we have investigated partial and total SDCS & DDCS first time here for the HCl molecule. No other data was available till now. These are not only theoretical findings but also based on some major experimental inputs such as ionization potential, differential oscillator strength and other key parameters. Hence, our results evaluated by Semi-empirical formulation are more reliable. All investigated data are very much desirable in various fields of applied sciences such as gaseous fluxing in babbiting operations, metal etching, etc.

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