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THEORETICAL CALCULATION OF ELECTRON IMPACT TOTAL CROSS SECTIONS FOR HCl MOLECULE OVER A WIDE RANGE OF IMPACT ENERGIES (0.1 eV – 2000 eV)

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ABSTRACT

Total cross sections Q_T for electron impact on hydrocholoric acid molecule is reported over a wide energy range from circa 0.1 eV through 2 keV. An *ab initio* calculation method, R-Matrix is employed using Quantemol- N software below the ionization threshold of the target and beyond which Spherical Complex Optical Potential (SCOP) calculations are performed. The two methods show consistency at the transition energy and in general good agreement is observed with the available data.

Key Words: *Spherical Complex Optical Potential, R matrix method, Total cross section*

INTRODUCTION

Electron impact collision data are in ever increasing demand for many decades. This is the consequence of their utility in various fields of applied physics. Hence considerable progress has been made on electron- atom/molecule collision studies both theoretically as well as experimentally. Looking to the theoretical side, with the availability of high performing computers and development of more accurate theories like R-matrix, computation of reliable cross sections are now possible. The accurate method e.g. R-matrix [1, 2] is feasible for low impact energies (energy insufficient to ionize the target), whereas beyond this energy the cross sectional data is obtained using theories like Spherical Complex Optical Potential formalism (SCOP) [3, 4]. SCOP formalism is used by many research groups [5, 6, 7] across the world and has been successfully utilized for varieties of targets [8, 9, 10]. The total cross section data is important at low, intermediate and high energy for their appropriate usage in various applications. Hence in the present work our attempt is to compute the total cross sections over wide range of impact energies from meV to keV for HCl.

Owing to enormous applications of HCl, it is highly attended molecule both by experimentalists as well as theoreticians. The first measurement of electron impact total cross sections was done by Bruche in 1926 [11] on a Ramsauer type apparatus for impact energies 4 - 30 eV. Radle et al [12] indirectly obtained the total cross sections from differential cross sections for impact energies 0.5 - 10 eV. Very recently Hamada and Sueoka [13] measured total cross sections using linear transmission type time of flight apparatus. On the theoretical front Itikawa and Takayanagi [14], Padial et al [15, 16], Pfingst et al [17] and Jain and Baluja [18] performed computation of electron impact total cross section for HCl in different energy regimes.

In this paper we present electron impact total cross sections, Q_T for HCl over a wide range of impact energies from 0.1 eV to 2 keV. Below the ionization threshold of the target the total cross section, Q_T, is obtained as a sum of the elastic and electronic excitation cross sections and in this energy regime we have employed UK molecular R-Matrix code through the Quantemol--N software package, while cross sections at energies beyond the ionization threshold are determined using the SCOP formalism. The two methods are found to be consistent at the transition energy. The present results are, in general, found to be in good agreement with previous experimental and theoretical results (wherever available) and thus the present results can serve as a benchmark for the cross sections over a wide range of energy.

THEORETICAL METHODOLOGY

This paper reports low energy (0.1eV to about 15 eV) ab-initio calculations using Quantemol- N [19] employing UK molecular R-matrix code [20] while the SCOP method is used for calculating total (elastic plus inelastic) cross sections beyond ionization threshold up to 2 keV [21]. These two (SCOP & R-matrix) being different approaches, we will discuss them separately in two subsections. Before going to the details of theoretical methods we discuss the target model employed for the present systems.

Target Model

HCl is a linear molecule with bond length of 2.409 atomic units (au). We have used a double zeta plus polarization (DZP) Gaussian basis set for target wave function representation. The double zeta basis set is important as it allows us to treat each orbital separately when we conduct the Hartee-Fock calculation. This gives us more accurate representation of each orbital. HCl has $C_{\infty v}$ point group symmetry but we have considered C_{2V} point group symmetry of the order 4. We have chosen C_{2V} point group because it reduces the computational efforts that are required to generate the target wave function. The ground state Hartree-Fock electronic configuration is $1a_1^2$, $2a_1^2$, $3a_1^2$, $1b_1^2$,$1b_2^2$, $4a_1^2$, $5a_1^2$, $1b_2^2$, $2b_2^2$. Out of 18 electrons we have frozen 10 electrons in $1a_1$, $2a_1$, $3a_1$, $1b_1$, $1b_2$ molecular orbitals while remaining 8 electrons are kept free in active space of $4a_1$, $5a_1$, $6a_1$, $7a_1$, $2b_1$, $2b_2$ molecular orbitals. Total 14 target states are represented by 298 configuration state functions (CSF's) for the ground state. A channel is a possible mode of fragmentation of the composite system (target + projectile) during the collision process and here the number of channels included in the calculation is 46. The R-matrix radius is taken as 10 a_0 while R- matrix calculation is propagated up to 100.1 a_0. The GAUSPROP and DENPROP modules of Quantemol-N generate target properties. DENPROP constructs the transition density matrix from the target eigenvectors obtained from the CI calculation. From this it then computes the multipole transition moments required for solving the outer region coupled equations, the dipole polarisability α_0 and where possible the diagonalised tensor components α_{xx} , α_{yy} and α_{zz}. These are computed using second-order perturbation theory and the property integrals evaluated by GUASPROP. Only multipole moments up to and including l=2 are computed.

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The GAUSPROP and DENPROP modules [22] yield the ground state energy of HCl as – 460.07 Hartree. There is no theoretical or experimental data available for comparison to best of our knowledge. The first electronic excitation energy is 8.168 eV which is probably reported here for first time. The present computed dipole moment is 0.544 au which is good agreement with theoretical value of 0.478 au [17]. The present rotational constant of 10.592 cm^{-1} is in very good agreement with theoretical value 10.593 cm^{-1} reported in [23].

All the computed target parameters for this system are reported in Table 1 with available comparisons. Notably there is no experimental data available for comparison for various target parameters.

TABLE-1 Target Properties: Ground state energy (Hartree), Dipole moment (au), First electronic excitation energy (eV) and Rotational constant (cm^{-1}).

Target	Ground state energy (Hartree)		Dipole moment (au)		First excitation energy E_1 (eV)			Rotational Constant (B) (cm^{-1})	
	Present	Theo	Present	Theo	Present	Theo	Exp	Present	Theo
HCl	-460.72	---	0.5438	0.4782 [17]	8.1684	---	8.317[24] 8.318[25]	10.592	10.59 [23]

The electronic excitation thresholds for HCl are listed in Table 2. HCl has 14 electronic excitation states.

Table - 2 Vertical excitation energies in eV.

HCL	
State	Energy(eV)
$^1A_1$	0.0
$^3B_1$	8.168
$^3B_2$	8.168
$^1B_1$	8.884
$^1B_2$	8.884
$^3A_1$	10.859
$^1A_1$	15.028
$^3B_1$	20.965
$^3B_2$	20.965
$^3A_2$	21.308
$^1B_1$	22.167
$^1B_2$	22.167
$^1A_2$	22.987
$^3A_1$	23.329

Low energy formalism (0.01 ~ 15 eV)

The crux idea behind the R-matrix formulation [22] lies in dividing the complete configuration space into two regions called inner region having R-matrix radius 'a' which is usually 10 au and the outer region extending to the radius of 100 au The splitting of R-matrix configuration space into these two regions relies mostly on the size of the target and also on the stability of the results obtained in the inner region and outer region calculations. This distribution is the consequence of electronic charge distribution around the centre of mass of the system. Presently we have considered R-matrix radius as 10 au for HCl which was found to give consistent results.

In the inner region the total wave function for the system is written as [20],

$$\psi_k^{N+1} = A\sum_I \psi_I^N (x_1,\cdots,x_N) \sum_j \zeta_j (x_{N+1}) a_{Ijk} + \sum_m \chi_m (x_1,\cdots,x_{N+1}) b_{mk} \quad (1)$$

where A is the anti-symmetrization operator, x_N is the spatial and spin coordinate of the n^{th} electron, ξj is a continuum orbital spin-coupled with the scattering electron and aIjk and bmk are variational coefficients determined in the calculation. The first summation runs over the target states used in the close-coupled expansion. The second summation runs over configurations χ_m, where all electrons are placed in target molecular orbitals. The number of these configurations varies considerably with the model employed. With the wavefunction given by eqn (1), a static exchange calculation has a single Hartree-Fock target state in the first sum. The second sum runs over the minimal number of configurations usually 3 or fewer, required to relax orthogonality constraints between the target molecular orbitals and the functions used to represent the configuration. Our fully close-coupled calculation uses the lowest number of target states, represented by a configuration interaction (CI) expansion in the first expansion and over a hundred configurations in the second. These configurations allow for both orthogonality relaxation and short-range polarization effects.

The complete molecular orbital representation in terms of the target and the continuum orbitals is done by using the Gaussian Type Orbitals (GTOs) and the continuum orbitals of Faure et al [26] and include up to g (l = 4) orbitals. For non-polar targets, the calculations performed up to g orbitals do not affect the accuracy of calculation [27] and this has an added advantage that it will allow us to see the resonance structures which are prominent at low energies. However for molecules with a permanent dipole moment, the dipole potential leads to strong coupling between channels which differ in 'l' values and also, due to the long range nature of the dipole potential which requires a large number of partial waves for convergence [27]. In practice, instead of including large number of partial waves in the expansion, the procedure is developed based on a frame transformation and the adiabatic nuclear rotation (ANR) approximation to account for rotational motion and the finite dipole Born approximation to account for the contribution of higher partial waves. We have performed the calculations with and without a dipole Born correction. The R-matrix provides the link between the inner region and outer region, the inner region is propagated to the outer region potential until its solutions match with the asymptotic functions given by the Gailitis expansion [20]. Thus by generating the wave functions, using equation 1, their eigen values are determined. These coupled single centre equations describing the scattering in the outer region are integrated to identify the K-matrix elements. Consequently the resonance positions, widths and various cross sections can be evaluated using the T-matrix obtained from S-matrix which is in turn obtained by the K-matrix elements.

Higher energy formalism (15 eV – 2 keV)

High energy electron scattering is modeled using the well established SCOP formalism [28, 29] which employs partial wave analysis to solve the Schrödinger equation with various model potentials as its input. The interaction of incoming electron with the target molecule can be represented by a complex potential comprising of real and imaginary parts as,

$$V_{opt}(r, E_i) = V_R(r) + iV_I(r, E_i) \quad (2)$$

such that

$$V_R(r, E_i) = V_{st}(r) + V_{ex}(r, E_i) + V_p(r, E_i) \quad (3)$$

where, Ei is the incident energy. Equation (3) corresponds to various real potentials to account for the electron target interaction namely, static, exchange and the polarization potentials respectively. These potentials are obtained using the molecular charge density of the target, the ionization potential and the polarizability as inputs. The molecular charge density may be derived from the atomic charge density by expanding it to the center of mass of the system. Our calculation for these TCSs is based on complex scattering potentials, generated from spherically averaged charge densities of the target. The charge density of lighter hydrogen atoms is expanded at the center of heavier atom (Chlorine) by employing the Bessel function expansion as in Gradshetyn and Ryzhik [30]. This is a good approximation since hydrogen atoms do not significantly act as scattering centers and the cross sections are dominated by the central atom size. Thus, the single-center molecular charge density is obtained by a linear combination of constituent atomic charge densities, renormalized to account for covalent molecular bonding. The atomic charge densities and static potentials (V_{st}) are formulated from the parameterized Hartree-Fock wave functions given by Cox and Bonham [31]. The parameter free Hara's 'free electron gas exchange model' [32] is used for the exchange potential (V_{ex}). The polarization potential (V_p) constructed from the parameter free model of correlation-polarization potential given by Zhang et al. [33]. Here, various multipole non-adiabatic corrections are incorporated in the intermediate region which will approach the correct asymptotic form at large 'r' smoothly. The target parameters like ionization potential (IP) and dipole polarizability (α_0) of the target used here are the best available from the literature [34].

Ionization potential (IP) of HCl is 12.74 eV and Dipole polarizability of HCl is 2.63 x 10^{-24} cm^3.

The imaginary part in Vopt called the absorption potential V_{abs} will account for the total loss of flux scattered into the allowed electronic excitation or ionization channels. The equation (2) is vibrationally and rotationally elastic. We have used here fixed nuclei approximation where the nuclear rotational and vibrational motions are not considered. This is due to the fact that these non spherical terms do not contribute much to the total potential at the present high energy range.

The well-known quasi-free model form of Staszeweska et al. [35] is employed for the absorption part given by,

$$V_{abs}(r,E_i) = -\rho(r)\sqrt{\frac{T_{loc}}{2}}\left(\frac{8\pi}{10k_F^3 E_i}\right)\theta(p^2 - k_F^2 - 2\Delta)(A_1 + A_2 + A_3) \qquad (4)$$

Where the local kinetic energy of the incident electron is

$$T_{loc} = E_i - (V_{st} + V_{ex} + V_p) \qquad (5)$$

Where $p^2 = 2E_i$, $k_F = [3\pi^2\ \rho(r)]^{1/3}$ is the Fermi wave vector and A_1, A_2 and A_3 are dynamic functions that depends differently on I, $\theta(x)$, Δ and E_i. Here, I is the ionization threshold of the target, is the Heaviside unit step-function and Δ is an energy parameter below which $V_{abs} = 0$. Hence, $\theta(x)$ is the principal factor which decides the values of total inelastic cross section, since below this value, ionization or excitation is not permissible. This is one of the main characteristics of Staszewska model [35]. This has been modified by us by considering Δ as a slowly varying function of E_i around I. Such an approximation is meaningful since fixed at I would not allow excitation at energies $Ei \le I$ However, if Δ is much less than the ionization threshold, then V_{abs} becomes unexpectedly high near the peak position. The amendment introduced is to give a reasonable minimum value $0.8I$ to Δ [36] and also to express the parameter as a function of E_i around I, i.e.,

$$\Delta(E_i) = 0.8I + \beta(E_i - 1) \qquad (6)$$

Here the value of the parameter β is obtained by requiring that $\Delta = I$(eV) at $E_i = E_p$, the value of incident energy at which present Q_{inel} reaches its peak. E_p can be found by calculating Q_{inel} by keeping $\Delta = I$, Beyond E_p Δ is kept constant and is equal to I. The expression given in eqn (6) is meaningful since if Δ is fixed at the ionization potential it would not allow any inelastic channel to open below I. Also, if it is very much less than I, then V_{abs} becomes significantly high close to the peak position of Q_{inel}.

The complex potential thus formulated is used to solve the Schrödinger equation numerically through partial wave analysis. This calculation will produce complex phase shifts for each partial wave which carrioes the signature of interaction f the incoming projectile with the target. At low impact energies only a few partial waves are significant, but as the incident energy increases more partial waves are needed for convergence. The phase shifts (δ_l) thus obtained are employed to find the relevant cross sections, total elastic (Q_{el}) and the total inelastic cross sections (Q_{inel}) using the scattering matrix $S_l(k) = \exp(2\,i\,\delta_l)$ [37]. Then the total scattering cross section (TCS), Q_T [38] is found by adding these two cross sections together.

RESULTS AND DISCUSSION

The present work reports total cross section for e –HCl scattering. We have employed the ab initio R matrix code below the ionization threshold of the target. In this energy regime the total cross section is sum of vibrationally and rotationally total elastic and total electronic excitation cross sections. Above the ionization threshold of the target we have computed the total cross section as the sum of total elastic and total inelastic cross section using the SCOP formalism [39, 40, 41]. The data sets produced by two formalisms are consistent at the transition energy (~ 15 eV). All the numerical results of total cross section (in $Å^2$) for both the targets from 0.1 eV to 2000 eV are presented in Table III and are also represented graphically along with the available comparisons in Figure1.

Table III: Total Cross Section Q_T ($Å^2$)

E_i (eV)	HCl	E_i (eV)	HCl
0.1	588.73	14	27.54
0.2	325.98	15	26.96
0.4	194.85	20	23.01
0.6	134.58	30	16.64
0.8	104.97	40	15.27
1.0	87.41	80	11.43
1.5	64.69	100	10.32
2.0	48.91	200	07.37
3.0	42.10	300	04.48
4.0	39.30	400	03.71
5.0	37.27	500	03.19
6.0	33.96	600	02.81
7.0	33.70	700	02.55
8.0	34.60	800	02.30
9.0	34.75	900	02.11
10	34.70	1000	01.96
11	33.72	1500	01.65
12	28.74	2000	01.16
13	27.65		

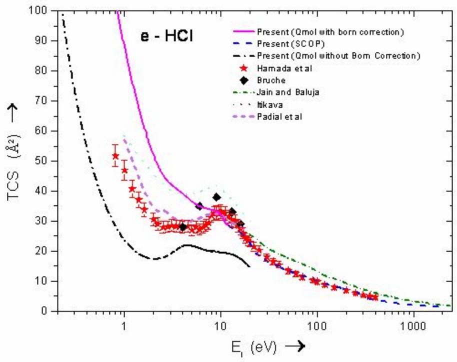

Fig.1 Total cross sections, Q_T, for e –HCl scattering

Solid line: Present results (Quantemol with Born correction); Dashed line: Present (SCOP); Dashed Dot line: Present (Quantemol without born correction); Short Dash Dotted line: Jain and Baluja [18]; Short Dash line: Padial et al [15]; Dotted Line: Itikava and Takayanagi [14]; Stars: Hamada and Seuoka [13]; Squares: Bruche [11].

Figure 1 shows comparison of e – HCl scattering with available comparisons. Looking to its importance in varied fields of applied interest, good amount of work is done at low energies. There are only two measurement data reported for total cross sections. Measurement results of Bruche [11] are very old and there is recent measurement by Hamada and Sueoka [13]. They have measured total cross sections using linear transmission type time of flight method for incident energies 0.8 – 400 eV. Their data were corrected for the effects of forward scattering using the differential cross section (DCS). The magnitude of the correction was very large in the low energy region. It could be easily seen from the graph that present data are in excellent agreement with data of Hamada and Sueoka [13] beyond 10 eV, below which the present data is higher due to Born approximation. A small hump in the total cross section is also observed in the present data without Born correction which is in accordance with the same observed by Hamada and Sueoka [13]. This structure disappears when Born correction is done. The experimental data of Bruche [11] are also in good agreement with present data except the one at 3 eV which is lower. On theoretical side there are relatively more comparisons. The low energy calculations are carried out by Itikawa and Takayanagi [14] and Padial et al [15]. Itikawa and Takayanagi [14] performed close coupling calculations in the energy from 0 to 10 eV. Peak appearing at 10 eV which could be easily observed in all experimental as well as theoretical data including present data is a consequence of shape resonance at this position [14]. Padial and Norcross have also performed ab initio calculation for very low energy (1 to 20 eV). Their results are lower than present results below 10 eV again due to Born approximation. Jain and Baluja [18] have calculated total cross sections from 10 eV to 5000 eV and their values are in good agreement with present results above 100 eV below which they are higher by small amount and this is attributed to the fact that they have considered the contribution of rotational excitation also which is significant for energies below 100 eV.

CONCLUSION

The main impetus of present work is to compute total cross sections over a wide range of impact energies starting from very low (0.1 eV) to high energy (2 keV) for HCl on electron impact. Since a single formalism cannot be employed over such a wide range, we have used UK molecular R-matrix code using Quantemol-N at low impact energies to yield ab initio results while at high energies SCOP formalism is used. We have illustrated earlier this methodology for three simple polyatomic molecular targets NH_3, H_2S and PH_3 [39] for which there exists a good database against which we can benchmark our results. The method has been extended to simple biomolecules [41] and in the present work for HCl. The results are promising since the two methods are consistent at the transition energy (15 eV) and show good agreement with available data throughout the energy range. Therefore now we have confidence that the methodology we propose may be used to calculate such cross sections in other molecular systems where experiments are difficult (e.g. exotic system and radicals). Such data set is needed in a variety of applications from aeronomy to plasma modeling which is the thrust area of research in the present era. Accordingly such a methodology maybe built into the design of on-line databases to provide a 'data user' with the opportunity to request their own set of cross sections for use in their own research. Such a prospect will be explored by the emerging Virtual Atomic and Molecular Data Centre (VAMDC) http :// batz.lpma.jussieu.fr/ www_ VAMDC/.

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