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Electron Impact Single Ionization of Al^+, Cd^+ and Hg^+

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ABSTRACT Electron Impact single ionization cross sections of Al^+ , Cd^+ and Hg^+ ions have been calculated in the Modified Binary Encounter Approximation. Accurate expression of $\sigma_{\Delta E}$ (cross section for energy transfer ΔE) and Hatree-Fock velocity distributions for the target electrons have been used throughout the calculations. For positive ions the focusing effects of the target ion on the incident electron have been incorporated in the calculations. The present results of single ionization cross sections are in excellent agreement with the experimental observations in the intermediate energy range. The calculated cross sections differs from the experimental results in the low energy regions because the present approximation not exhibit better result in the low energy regions, while the over-estimations of experimental results in the high energy regions shows that more theoretical calculations is required to understand the dynamics of the system.

KEYWORDS Electron, Ionization, Cross-section, Ions

INTRODUCTION

Electron Impact single and multiple ionization of atoms and ions plays an important role to understand the dynamics of the system as well as its nature. Electronic collision processes is one of the most fundamental problem in atomic and molecular physics. The study of these processes finds important applications in various field of current interest and important for both the theoretical and experimental point of view. The absolute cross sections for charged particle impact are important for several fields ranging from thermonuclear fusion to astrophysics. Due to broad range of applications of ion-atom interaction processes, rigorous studies of these processes are required. The vibrant and interesting field of atomic collision physics attracted many workers for theoretical and experimental investigations of single and multiple ionization processes by the impact of charged particles. Several experimentalists investigated single and multiple ionization by impact of bare ions, but the theoretical explanations and the rigorous calculations for the cross sections of such processes is very few and limited.

Recently several experimental works have been carried out [1-5]. Due to mathematical complexicities and extremely heavy computation work, sophisticated theoretical calculations are not available in the literature [6]. Keeping in view, the difficulties in carrying out rigorous quantal calculations, the Modified Binary Encounter Approximation is considered to provide suitable theoretical description of direct double ionization process for multi-electron system [7]. In recent past, Binary Encounter Approximation has been used in the calculations of charged particle impact ionization [8]. The computed results have been found in the satisfactory agreement with the experimental observations [9]. The revival of interest in Binary Encounter Model becomes possible due to the early work of Gryzinski [10]. Later on, many workers used this model to investigate ionization process for atoms and ions. Roy and Rai [11] & Kumar and Roy [12] have used the expression of Vriens [13] in the symmetrical model to calculate electron impact single ionization cross section of alkali atoms and ions respectively. Thomas and Garcia [14] extended the Binary Encounter Approximation to incorporate the effects of residual ionic field of the target ion on the incident particle and the same model has been successfully applied to calculate electron impact ionization cross section for several ions.

Kumari and Jha [15] applied the method adopted by Thomas and Garcia [14] with suitable modification in the case of double ionization of Mg (Magnesium) by electron impact and found good agreement of calculated results with experimental measurements. After that, they have also applied this method in the case of several atoms and ions by electron impact [16-18].

With the success of the above model to find the cross sections of several atoms and ions by electron impact in case of single and multiple ionizations, we encourage to adopt this model in case of electron impact single ionization of Al^+ , Cd^+ and Hg^+ , and compare the calculated results with the experimental measurements of Belic et.al [19]. With the close observations, we found that the calculated results are in fare agreement with the experimental measurements and in excellent agreement in the intermediate energy regions.

METHODS OF CALCULATIONS

When the negatively charged incident particles (electron) approach the ionic target, it experiences Columbic force. It causes the projectile to change its velocity discussed by Thomas and Garcia [14]. This causes an appreciable increase in its kinetic energy and substantial decrease in impact parameter of the incident electron. The expression for the increased kinetic energy of the incident electron at a distance ξ from the nucleus of the ion can be given by

$$E_1^{'} = E_1 + \frac{Z^{'} e^2}{\xi} \qquad (1)$$

where, E_1 is the initial K.E of the incident electron and $Z'e$ is the net nuclear charge of the target ion.
The resulting expression for the ionization cross section can be related as

$$\sigma_1(E_1) = \sigma_1(E_1^{'}) \left[\frac{1}{2} + \frac{1}{2} \left\{ 1 + \frac{2z^{'} e^2 \Pi}{E_1 \sigma_1(E_1^{'})} \times \left[\xi - \left(\xi^2 - \frac{\sigma_1(E_1^{'})}{\Pi} \right)^{1/2} \right] \right\}^{1/2} \right]^2 \qquad (2)$$

Where $\sigma_1(E_1^{'})$ is the expression for cross section at increased electron energy $(E_1^{'})$ given by relation (1) and ξ is the collision radius whose value depends upon the ionic radius and electron-electron separation δ .The expression (2) can be further approximated for $\sigma_1 < \Pi \xi^2$ to

$$\sigma_1(E_1) = \sigma_1(E_1^{'}) \left[\frac{1}{2} + \frac{1}{2}\left(1 + \frac{z^{'}e^2}{E_1\xi}\right)^{1/2}\right]^2 \qquad (3)$$

Subsequently, the ionization cross section at increased electron energy $E_1^{'}$ multiplied by a factor

$$f = \left[\frac{1}{2} + \frac{1}{2}\left(1 + \frac{Z^{'}e^2}{E_1\xi}\right)^{1/2}\right]^2$$

gives the desired expression of ionization cross section for the positive ions.

In this work, we start from Vriens [13] expression for electron impact ionization cross section including exchange and interference which is given by

$$\sigma_1 = \frac{\Pi e^4}{(E_1+E_2+U)}\left[\left(\frac{1}{U} - \frac{1}{E_1}\right) + \frac{2}{3}E_2\left(\frac{1}{U^2} - \frac{1}{E_1^2}\right) - \frac{\phi^{'}}{(E_1+U)}\ln\left(\frac{E_1}{U}\right)\right] \qquad (4)$$

where $\Phi^{'} = cos\left[\left(\frac{R}{E_1+U}\right)^{1/2}\ln\left(\frac{E_1}{U}\right)\right]$.

Here E_2 and R are the kinetic energy and Rydberg constant of the target electron and Rydberg respectively.

Following Catlow and McDowell [20], we have introduced two dimensionless quantities s and t defined as

$$s^2 = v_1^2/v_0^2 \quad \text{and} \quad t^2 = v_2^2/v_0^2$$

Where U = v_0^2 is the ionization potential of the shells under consideration, expressed in Rydbergs and v_1 and v_2 are the velocities of the incident and the bound electrons respectively, in atomic units. All other energies have also been expressed in Rydbergs. In term of these dimensionless quantities, Vriens [13] expression for electron impact ionization cross section takes the form

$$\sigma_1(s,t) = \frac{4}{(s^2+t^2+1)}\left[\frac{(s^2-1)}{U^2s^2} + \frac{2t^2}{3}\frac{(s^4-1)}{U^2s^4} - \frac{\Phi^{'}}{U^2(s^2+1)}\ln s^2\right] \qquad (5)$$

where $\Phi^{'} = cos\left[\left(\frac{1}{s^2\,U+U}\right)^{1/2}\ln s^2\right]$.

We also defines a dimensionless quantity $s^{'}$ corresponding to increased electron energy $E_1^{'}$ and hence from equation (1)

$$s^{'2} = s^2 + \frac{2z^{'}}{\xi U} \qquad (6)$$

where ξ has been expressed in atomic units and energy in Rydbergs. Using the same variables, the factor f can be given by :-

$$f = \frac{(s+s^{'})^2}{4s^2} \quad . \qquad (7)$$

The expression for ionization cross section of ion can be obtained by multiplying the ionization cross section at increased energy $E_1^{'}$ by the factor f . Thus $\sigma_1(s,t)$ takes the form

$$\sigma_1(s,t) = \frac{(s+s')^2}{s^2(s'^2+t^2+1)}\left[\frac{(s'^2-1)}{U^2 s'^2} + \frac{2t^2}{3}\frac{(s'^4-1)}{U^2 s'^4} - \frac{\phi' \ln s'^2}{U^2(s'^2+1)}\right]\pi a_o^2 \qquad (8)$$

where $\Phi' = cos\left[\frac{\ln s'^2}{(s'^2 U+U)^{1/2}}\right]$.

The expression (8) has been integrated over Hartree-Fock velocity distribution for the bound electron of the target ion and the corresponding expressions for ionization and excitation cross section is given by

$$\sigma_1(s) = n_e \int_0^\infty \sigma_1(s,t)\, f(t) U^{1/2} dt \qquad (9)$$

where n_e is the number of equivalent electrons in the shell under consideration and f (t) is the momentum distribution factor for the bound electron which is defined as

$$f(t) = 4\pi t^2 U \rho_{nl}(tU^{\frac{1}{2}}) \qquad (10)$$

where $\rho_{nl} = \frac{1}{(2l+1)}\sum_{m=-1}^{m=+1} |\psi_{nlm}(\boldsymbol{\chi})|^2$

and $\psi_{nlm}(\boldsymbol{\chi}) = \frac{1}{(2\pi)^{\frac{3}{2}}}\int \emptyset_{nlm}(r) e^{\boldsymbol{ik.r}} dr$

is the Fourier transform of the one electron orbital.

$$\emptyset_{nlm}(r) = N_{nl} R_{nl}(r) Y_{lm}(\boldsymbol{\Omega})$$

in which $R_{nl}(r)$ is the analytical Hartree-Fock radial function. In the present calculations, momentum distribution function for the bound electron has been constructed using Hartree-Fock radial functions reported by Clementi and Roetti [21]. The binding energies of the shells have been taken from the Clementi and Roetti [21]. The ionic radii have been taken from the hand book of Chemistry and Physics [22] and from the table of Fraga et al. [23].

RESULTS AND DISCUSSION

In order to obtain electron impact single ionization cross sections of atoms and ions using the Binary Encounter Method, we know that the present method has a usual tendency to over-estimates ionization cross sections at low energy and to under-estimates them at high energy. Such trend has also been observed in the present work. Therefore, the calculations of single ionization cross sections at low energy for comparison with earlier experimental investigations and theoretical work are not meaningful. When we closely observed the results of the experimental measurements by Belic et.al [19] in the case of Al^+, Cd^+ and Hg^+ we found that these results also exhibits same kind of fluctuations at different impact energies. Confirming our attention to the calculations of above mention positive ions, we have also compared our calculated results by the Lotz [24,25] formula and other theoretical and experimental investigations. This consideration is based on the following physical reasoning. First the calculated data of Lotz have some reasonable agreement with the experimental measurement, but due to lacking of the wave functions, the Lotz formula is physically not justified. Due to acute shortage of quantal calculations, it is not possible to verify the authenticity of the results in low, intermediate and high energy regions. McGuire [26-28] calculated the extension of the 2p electrons of Al^+ using SPWB method. However, the SPWB method does not give rise to the finite cross section at threshold characteristic of the Coulomb potential, and the feature is completely washed out. His results can, however, be used to obtain the oscillator strength by looking at his data at high energies.

In the present work we have used Modified Binary Encounter Method to calculate electron impact single ionization of above mentioned positive ions.

Single ionization of Al^+

In this work we have carried out theoretical calculations of electron impact single ionization cross sections for Al^+ , we have considered ionization from 3s , 2p , and 2s shells only. Ionization from deeper inner shells has not been included in the present calculations because the magnitude of the calculated results is so small hence it is meaningless. The contributions from 3s, 2p and 2s shells have been shown separately in the Table 1(a) as well as in the Figure 1(a). Firstly, we would like to compare our calculated results with the experimental measurements of Belic et al. [19]. At low impact energies , the present results over-estimates the experimental cross sections by 17 , 10, 5.2 , 3.3 and 2.2 times at impact energies 20.0 eV , 20.9 eV , 22.8 eV , 25.8 eV and 28.6 eV respectively. Beyond this energy range the calculated cross sections comes closer to the experimental results with the increase of the energy range. At impact energy 34.3 eV the magnitudes of calculated results are 133.64x10^{-8} cm^2 and 71.2x10^{-18} cm^2 respectively. At this impact energy the ratio of the calculated cross sections to the experimental observations is 1.8 times larger. Beyond this energy region both the results come closer to each other and at impact energy 63.2 eV the ratio of calculated to the experimental results is 1.1 times greater than the experimental results. Between energy range 57.4 eV and 72.7 eV the ratios are almost equals to unity and at 72.7 eV the magnitude of cross sections of calculated results and experimental measurements are 66.74x10^{-18} cm^2 and 66.3x10^{-18} cm^2 respectively. It means at this energy both the results coalesce to each other. Besides this, between impact energy 74.6 eV to 165.3 eV the situation is completely in the reverse order. It means the calculated results unde- estimates the experimental measurements. At the highest energy regions at 990.0 eV the experimental result is almost 3 times greater than the calculated results.

Table 1(a): Electron Impact Single Ionization of Al^+ in units of 10^{-18} cm^2

Energy	3s	2p	2s	Total	Expt.[19]
19.0	96.79	101.69	25.24	223.72	3.8
20.0	92.20	97.69	24.33	214.22	12.6
20.9	88.42	94.35	23.56	206.33	20.0
22.8	81.39	88.01	22.10	191.50	36.8
23.8	78.12	85.00	21.40	184.52	40.8
24.7	75.40	82.47	20.81	178.68	49.5
25.8	72.31	79.57	20.13	172.01	51.2
26.7	69.97	77.35	19.60	166.92	52.8
27.7	67.54	75.02	19.05	161.61	56.6
28.6	65.49	73.05	18.58	157.12	61.3
30.4	61.75	69.39	17.71	148.85	67.2
34.3	54.95	62.61	16.08	133.64	71.2
36.2	52.15	59.76	15.39	127.30	70.7
38.2	49.49	57.04	14.73	121.20	72.2

40.0	47.33	54.79	14.18	116.30	73.1
42.0	45.13	52.49	13.61	111.23	73.1
43.9	43.22	50.48	13.11	106.81	72.0
45.8	41.47	48.61	12.65	102.73	74.5
47.8	39.78	46.80	12.20	98.78	73.1
49.8	38.29	45.19	11.80	95.28	72.4
51.6	36.91	43.70	11.43	92.04	72.9
53.5	35.62	42.29	11.08	88.99	72.6
55.5	34.37	40.91	10.73	86.01	71.4
57.4	33.25	39.68	10.42	83.35	70.8
59.4	32.15	38.46	10.11	80.72	69.9
61.2	31.22	37.43	9.85	78.50	69.5
63.2	30.25	36.34	9.57	76.16	68.8
65.1	29.38	35.37	9.33	74.08	68.0
66.9	28.60	34.49	9.10	72.19	67.6
68.9	27.79	33.57	8.87	70.23	66.5
70.7	27.09	32.78	8.66	68.53	67.2
72.7	26.36	31.94	8.45	66.74	66.3
74.6	25.69	31.19	8.26	65.14	66.1
76.6	25.03	30.43	8.06	63.52	67.2
78.5	24.44	29.75	7.89	62.08	67.0
80.4	23.87	24.09	7.72	60.68	67.8
82.2	23.35	28.50	7.56	59.41	67.8
84.2	22.80	27.86	7.40	58.06	65.9
86.1	22.31	27.29	7.25	56.85	65.5
106.5	18.08	22.33	5.97	46.38	58.8
125.9	15.32	19.04	5.10	39.46	54.8
145.6	13.26	16.57	4.45	34.28	51.4
165.3	11.69	14.66	3.95	30.30	48.8
185.0	10.45	13.15	3.54	27.14	45.1
204.5	9.46	11.93	3.22	24.61	41.5
223.6	8.65	10.93	2.95	22.53	38.3
243.1	7.96	10.08	2.73	20.77	35.8
262.5	7.38	9.35	2.53	19.26	33.5
281.8	6.87	8.72	2.36	17.95	31.8
301.3	6.43	8.17	2.21	16.81	30.9
320.8	6.04	7.68	2.08	15.8	29.9
340.3	5.69	7.25	1.97	14.91	28.8
359.8	5.39	6.86	1.86	14.11	27.8
378.8	5.12	6.52	1.77	13.41	27.0
588.0	3.30	4.22	1.15	8.67	21.7
787.0	2.46	3.16	0.86	6.48	18.0
990.0	1.96	2.52	0.68	5.16	15.0

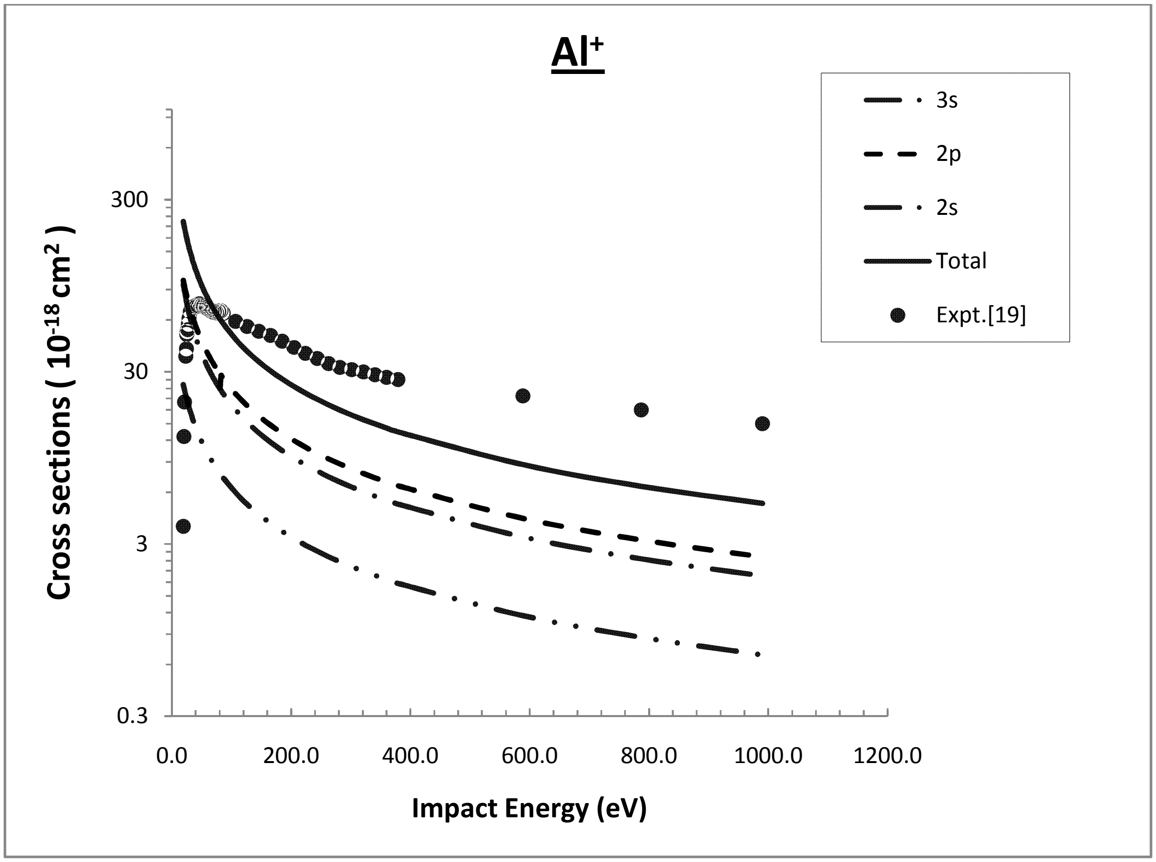

Figure 1(a): Electron Impact Single Ionization of Al^+ in units of 10^{-18} cm^2

Now, we compare the results of present calculations, calculated results of Lotz [24, 25] and experimental results of Harrison et.al [29] which is shown in Table 1(b) and Figure 1(b). From the close observations of these results we find that the ratios of experiment to the experimental results of Harrison et al. [29], Lotz [24, 25] and present calculations are 1.12, 0.8 and 1.0 at impact energy 70 eV. At 80 eV and 200 eV these ratios are 1.18, 0.82 and 0.89 & 1.18, 0.75 and 0.59 respectively. Since Binary Encounter Method is valid for intermediate and high energy regions, hence in the intermediate energy region our calculated results are in excellent agreement with the experimental measurements, while in the low energy regions it is not upto mark. The discrepancies in the results at the high energy regions are due to lack of some physical process in this region.

Table 1(b): Compared Data Table for Al^+

Energy(eV)	Expt.[29]	Lotz [25]	Total Cal.	Expt. [19]
20.0	12.0	12.0	214.22	12.6
30.0	70.0	65.0	148.85	67.2
40.0	75.0	80.0	116.3	73.1
50.0	69.0	85.0	95.28	72.40
60.0	65.0	87.0	80.72	69.9
70.0	60.0	84.0	68.53	67.2

80.0	57.0	82.0	60.68	67.8
90.0	55.0	79.0	56.85	65.5
100.0	53.0	77.0	46.38	58.8
200.0	35.0	55.0	24.61	41.5
300.0	29.0	49.0	16.81	30.9
400.0	28.0	42.0		
500.0	22.0	36.0		
600.0	20.0	30.0		
700.0	18.0	27.0		
800.0	16.0	22.0		
900.0	13.0	21.0		
1000.0	11.0	20.0	5.16	15.0

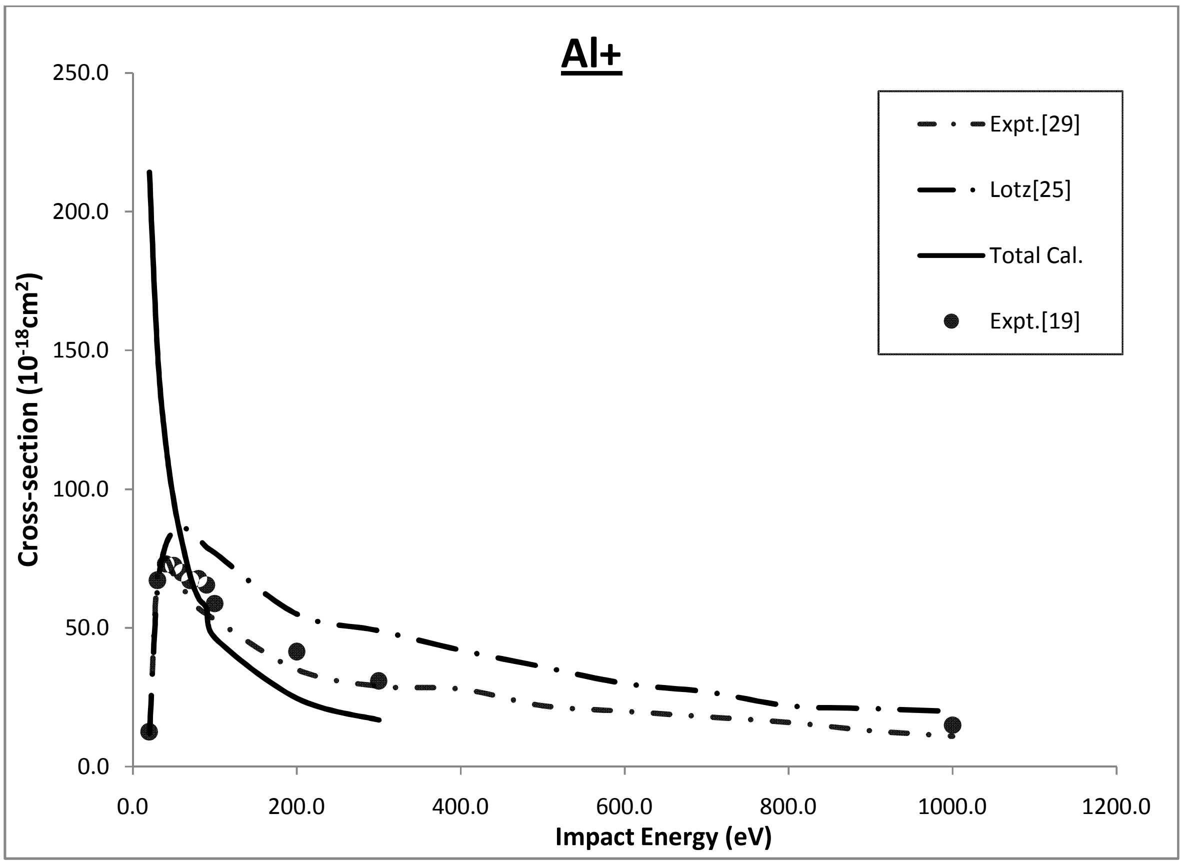

Figure 1 (b): Electron Impact Single Ionization of Al^+ in units of 10^{-18} cm^2

Single ionization of Cd^+

We have compared our calculated cross sections with experimental measurements of Belic et al. [19] in the energy ranges from 19.8 eV to 1991.0 eV for electron impact single ionization of Cd^+. In the case of Cd^+ we have taken the contributions of 5s, 4d, 4p and 4s shells only. Our calculated results of Cd^+ are shown in Table 2(a) and Figure 2(a) along with the experimental data. The present result over-estimates the experimental measurements from threshold energy to 43.8 eV. Beyond this energy range the theoretical results come closer to the experimental data and it is almost similar at impact energies 73.5 eV, 75.5 eV , 77.5 eV and 79.5 eV respectively. From energies range 63.7 eV to 87.5 eV, the theoretical and experimental curves are completely flat. After this, the experimental results over-estimate the theoretical calculations from energy 79.5 eV to 186.5 eV. During this region the ratio of the results are always within the factor of 2. Between energies value 234.4 eV to 1991.0 eV the experimental results dominates over the theoretical calculations and at the highest energy level, these results are 5 to 6 times greater than the calculated results. The similar trend we have also found in the case of Al^{+}. Although the results obtained by semi-empirical predictions from Darwin [30] and Lotz [24,25] which is shown in Table 2(b) and Figure 2(b) are closer to the experimental results at the highest energy region but in the intermediate energy region our calculated results are in excellent agreement with the experimental results.

Table 2(a): Electron Impact Single Ionization of Cd^{+} in units of 10^{-18} cm^{2}

Energy	5s	4d	4p	4s	Total	Expt.[19]
16.8	59.84	409.01	115.93	29.67	614.45	3.8
17.8	56.64	388.10	110.87	28.48	584.09	8.2
18.8	53.77	369.23	106.24	27.37	556.61	11.3
19.8	51.17	352.11	101.98	26.35	531.61	21.9
20.8	48.82	336.51	98.05	25.41	508.79	29.8
21.8	46.67	322.24	94.42	24.53	487.86	39.3
22.8	44.70	309.13	91.05	23.71	468.59	44.4
23.8	42.89	297.04	87.91	22.94	450.78	48.7
24.8	41.22	285.87	84.99	22.23	434.31	53.4
25.8	39.68	275.50	82.25	21.55	418.98	57.1
26.8	38.25	265.86	79.69	20.92	404.72	60.8
27.8	36.92	256.88	77.28	20.32	391.40	64.0
28.8	35.68	248.48	75.01	19.76	378.93	66.8
29.8	34.51	240.62	72.87	19.23	367.23	69.7
30.8	33.43	233.23	70.85	18.72	356.23	72.1
31.8	32.41	226.29	68.94	18.25	345.89	75.9
32.8	31.44	219.75	67.14	17.79	336.12	80.0
33.8	30.54	213.57	65.42	17.36	326.89	83.3
34.8	29.68	207.74	63.79	16.95	318.16	87.3
35.8	28.88	202.21	62.24	16.56	309.89	90.5
37.8	27.38	192.00	59.36	15.82	294.56	96.8
39.8	26.04	182.77	56.73	15.15	280.69	102.6
41.8	24.82	174.39	54.33	14.54	268.08	106.7
43.8	23.71	166.74	52.12	13.97	256.54	111.9
45.8	22.70	159.73	50.08	13.45	245.96	116.2
47.7	21.81	153.60	48.29	12.98	236.68	119.1
49.7	20.95	147.64	46.54	12.53	227.66	123.5
51.7	20.15	142.12	44.91	12.11	219.29	126.2

53.7	19.41	137.00	43.39	11.71	211.51	130.9
55.7	18.73	132.24	41.97	11.34	204.28	134.6
57.7	18.09	137.79	40.64	10.99	197.51	136.0
59.7	17.49	123.64	39.40	10.67	191.20	138.6
61.6	16.96	119.93	38.28	10.37	185.54	140.5
63.7	16.41	116.09	37.12	10.07	179.69	142.2
65.6	15.94	112.82	36.13	9.81	174.70	141.6
67.6	15.48	109.57	35.14	9.55	169.74	142.2
69.6	15.04	106.50	34.20	9.30	165.04	142.9
71.5	14.64	103.74	33.36	9.08	160.82	143.8
73.5	14.25	100.98	32.51	8.85	156.59	143.4
75.5	13.88	98.37	31.71	8.64	152.60	144.6
77.5	13.52	95.89	30.95	8.44	148.80	145.0
79.5	13.19	93.53	30.22	8.24	145.18	146.1
81.5	12.87	91.29	29.52	8.06	141.74	145.4
83.4	12.58	89.25	28.89	7.89	138.61	145.6
85.4	12.28	87.21	28.26	7.72	135.47	145.5
87.4	12.01	85.25	27.65	7.56	132.47	145.4
89.4	11.74	83.38	27.07	7.40	129.59	146.3
91.4	11.49	81.59	26.51	7.25	126.84	146.3
93.4	11.24	79.88	25.97	7.11	124.20	147.3
119.9	8.78	62.49	20.49	5.63	97.39	141.5
140.3	7.51	53.52	17.62	4.86	83.51	135.6
167.6	6.29	44.90	14.84	4.10	70.13	130.6
186.5	5.66	40.39	13.38	3.70	63.13	123.0
234.4	4.50	32.20	10.71	2.97	50.38	119.9
281.3	3.75	26.87	8.96	2.49	42.07	113.5
375.2	2.82	20.17	6.75	1.88	31.62	105.9
474.2	2.23	15.98	5.36	1.49	25.06	100.3
580.0	1.82	13.07	4.39	1.22	20.50	92.9
782.0	1.35	9.70	3.26	0.91	15.22	75.7
980.0	1.08	7.74	2.61	0.72	12.15	62.4
1490.0	0.71	5.10	1.72	0.48	8.01	39.5
1991.0	0.53	3.81	1.28	0.36	5.98	31.5

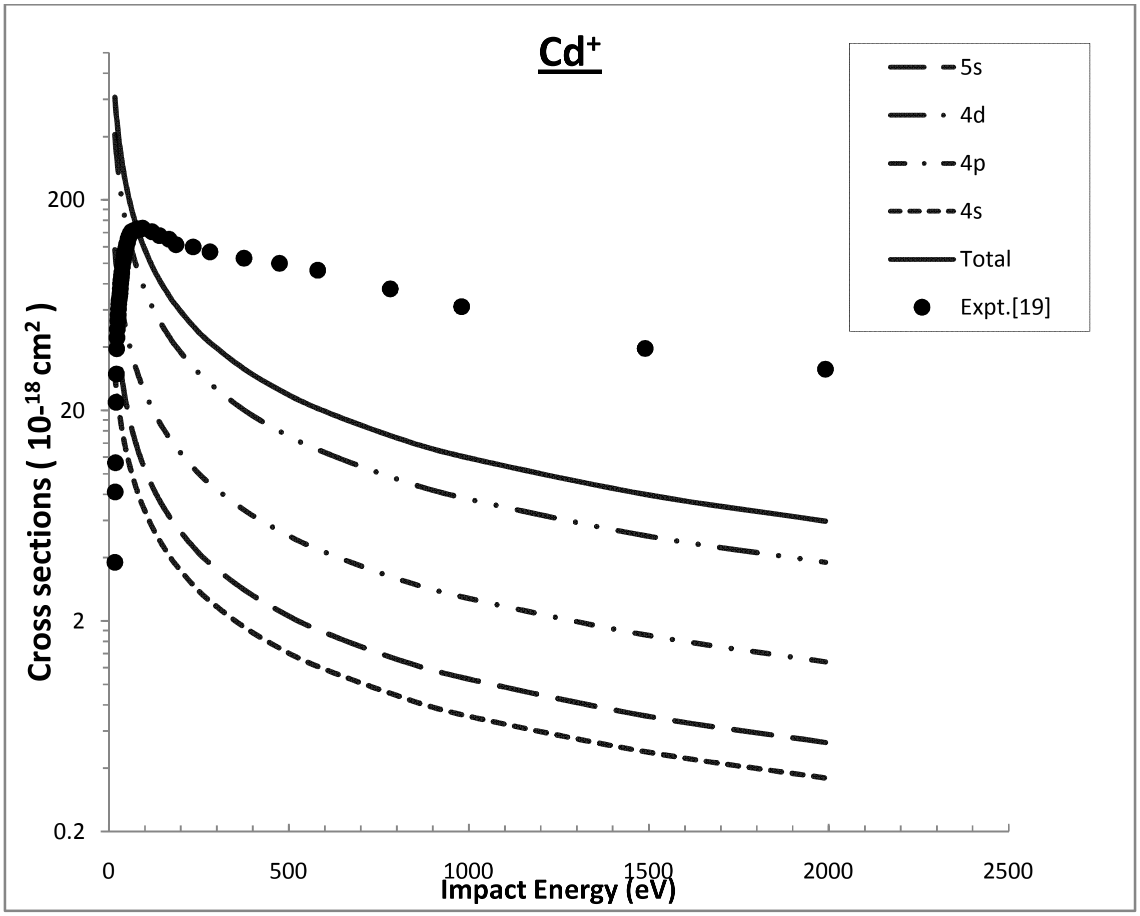

Figure 2(a): Electron Impact Single Ionization of Cd^+ in units of 10^{-18} cm^2

Table 2(b): Compared Data Table for Cd^+

E (in eV)	Lotz [25]	Darwin [30]	total calc.	expt.[19]
20.0	35.0	20.0	531.61	21.9
30.0	120.0	50.0	367.23	69.7
40.0	175.0	70.0	280.69	102.6
50.0	200.0	105.0	227.66	123.5
60.0	210.0	145.0	191.2	138.6
70.0	215.0	185.0	165.04	142.9
80.0	210.0	210.0	145.18	146.1
90.0	205.0	220.0	129.59	146.3
100.0	205.0	225.0		
200.0	160.0	195.0		
300.0	130.0	160.0		
400.0	105.0	130.0		
500.0	90.0	110.0		
600.0	80.0	100.0		
700.0	75.0	90.0		

800.0	70.0	85.0		
900.0	65.0	80.0		
1000.0	60.0	70.0		
2000.0	40.0	50.0	5.98	31.5

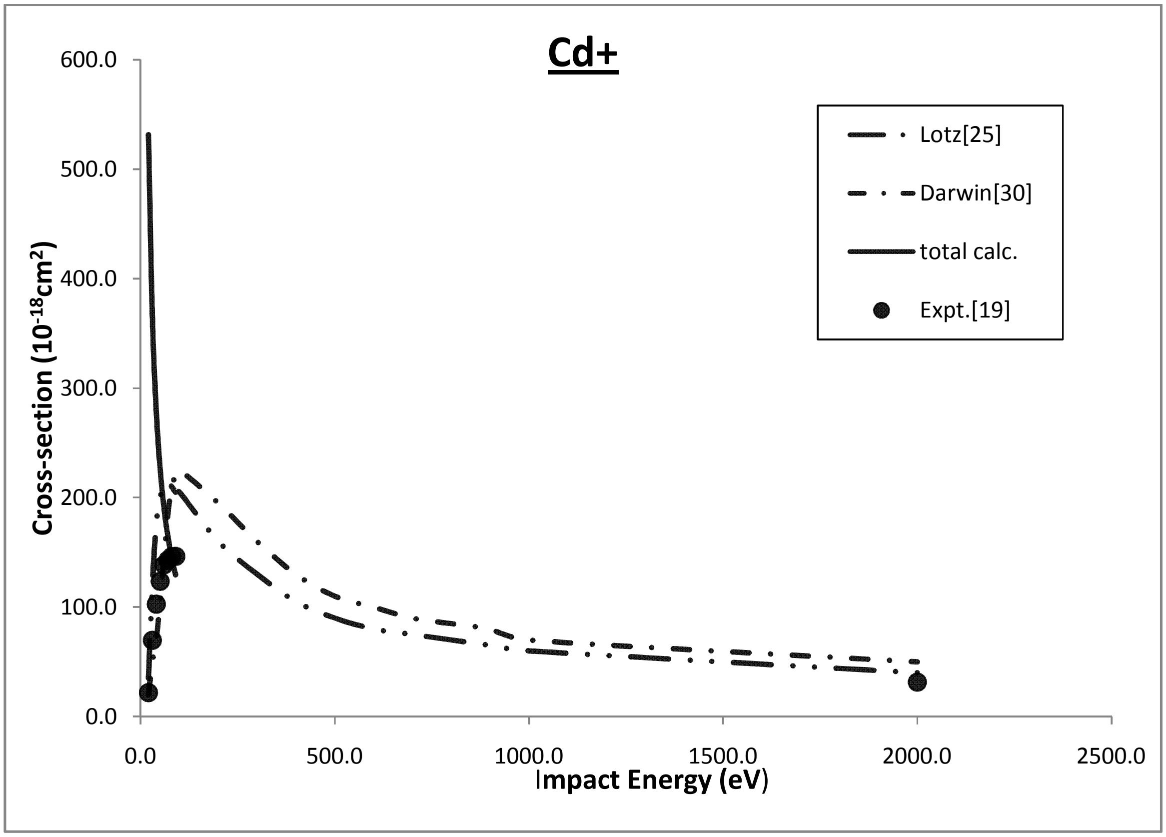

Figure 2(b): Electron Impact Single Ionization of Cd^+ in units of 10^{-18} cm^2

Single ionization of Hg^+

The calculated cross sections of single ionization of Hg^+ along with the experimental data have been shown in Table 3(a) and Figure 3(a). The contributions of 6s, 5d, 5p and 5s shells to single ionization of the target have also been shown separately in the Table and Figure. The calculated cross sections clearly indicate that the lowest energies region at which the calculated results is higher than the experimental observations. The calculated cross sections are found to decrease gradually with the increase in energy region 19.0 eV to 1980.0 eV. The experimental observations also show the similar trend. At low energy region, the ratio of theoretical results to the experimental cross sections is very high. With the increase in energy, the calculated results come closer to the experimental data and they are found to be nearly equal at impact energy 72.0 eV. At this energy the magnitudes of calculated cross sections and experimental observations are 164.8×10^{-18} cm^2 and 164.4×10^{-18} cm^2. Between the energy region 42.0 eV to 120.0 eV the ratio of both the results are very close to each other and it lies between factors 2 to 0.61. At impact energies 46.0 eV, 60.0 eV, 66.0 eV, 70.0 eV and 72.0 eV the ratios of the calculated cross sections to the experimental measurements are 1.8, 1.2, 1.1, 1.0 and 1.0 respectively. Beyond the energy 72.0 eV the magnitude of the experimental cross sections over-estimates the theoretical cross sections upto the highest energy considered. From the close inspection of the results we found that our calculated results are in excellent agreement between the energy regions 44.0 eV to 120.0 eV respectively. In the higher region, the calculated cross sections are in reasonable agreement with the experiment.

Table 3(a): Electron Impact Single Ionization of Hg^+ in units of 10^{-18} cm^2

Energy	6s	5d	5p	5s	Total	Expt.[19]
19.0	53.94	378.81	110.48	28.48	571.71	10.8
20.0	51.36	361.32	106.03	27.41	546.12	21.7
21.0	49.02	345.38	101.93	26.42	522.75	32.5
22.0	46.88	330.78	98.13	25.50	501.29	39.7
23.0	44.91	317.37	94.61	24.64	481.53	45.9
24.0	43.11	305.01	91.34	23.84	463.30	51.2
25.0	41.45	293.57	88.29	23.09	446.40	58.9
26.0	39.91	282.96	85.43	22.39	430.69	64.3
27.0	38.48	273.09	82.76	21.73	416.06	70.2
28.0	37.14	263.89	80.24	21.10	402.37	74.9
29.0	35.90	255.29	77.88	20.51	389.50	80.3
30.0	34.74	247.23	75.65	19.96	377.58	85.1
31.0	33.65	239.66	73.55	19.43	366.29	89.6
32.0	32.63	232.55	71.56	18.93	355.67	92.8
33.0	31.67	225.84	69.68	18.46	345.65	97.6
34.0	30.76	219.51	67.89	18.01	336.17	100.9
35.0	29.90	213.53	66.19	17.58	327.20	102.2
36.0	29.09	207.86	64.58	17.17	318.70	105.6
38.0	27.60	197.39	61.58	16.41	298.98	112.6
40.0	26.25	187.92	58.84	15.71	288.72	118.9
42.0	25.02	179.31	56.34	15.07	275.74	123.9
44.0	23.91	171.47	54.04	14.48	263.90	128.9
46.0	22.89	164.28	51.93	13.93	253.03	134.0
48.0	21.95	157.66	49.97	13.43	243.01	137.4
50.0	21.09	151.56	48.16	12.95	233.76	142.7
52.0	20.29	145.92	46.47	12.52	225.20	145.9
54.0	19.55	140.68	44.90	12.11	217.24	148.4
56.0	18.87	135.80	43.43	11.72	209.82	151.2
58.0	18.23	131.25	42.05	11.36	202.89	154.3
60.0	17.63	127	40.76	11.02	196.41	157.1
62.0	17.07	123.01	39.54	10.71	190.33	156.3
64.0	16.54	119.27	38.4	10.4	184.61	160.3
66.0	16.05	115.74	37.32	10.12	179.23	161.8
68.0	15.58	112.42	36.3	9.85	174.15	165.5

70.0	15.14	109.29	35.33	9.60	169.36	162.4
72.0	14.73	106.32	34.42	9.35	164.82	164.4
74.0	14.33	103.51	33.55	9.12	160.51	160.8
76.0	13.96	100.85	32.72	8.90	156.43	167.4
78.0	13.61	98.32	31.93	8.69	152.55	165.6
80.0	13.27	95.91	31.18	8.50	148.86	166.3
82.0	12.95	93.62	30.47	8.31	145.35	167.1
84.0	12.64	91.43	29.78	8.12	141.97	167.8
86.0	12.35	89.35	29.13	7.95	138.78	167.4
88.0	12.07	87.36	28.51	7.78	135.72	166.1
90.0	11.81	85.45	27.91	7.62	132.79	169.0
92.0	11.55	83.63	27.33	7.47	129.98	168.3
94.0	11.31	81.88	26.78	7.32	127.29	167.6
120.0	8.88	64.39	21.22	5.82	100.31	161.8
158.0	6.75	49.07	16.28	4.49	76.59	156.0
186.0	5.74	41.75	13.89	3.84	65.22	149.6
233.0	4.59	33.39	11.15	3.08	52.21	139.5
280.0	3.82	27.82	9.31	2.58	43.53	131.4
385.0	2.78	20.26	6.81	1.89	31.74	115.6
484.0	2.21	16.13	5.43	1.51	25.28	106.8
584.0	1.83	13.38	4.51	1.25	20.97	100.1
785.0	1.36	9.96	3.36	0.93	15.61	78.2
982.0	1.09	7.96	2.69	0.75	12.49	62.0
1474.0	0.72	5.31	1.79	0.50	8.32	43.6
1980.0	0.54	3.95	1.33	0.37	6.19	36.3

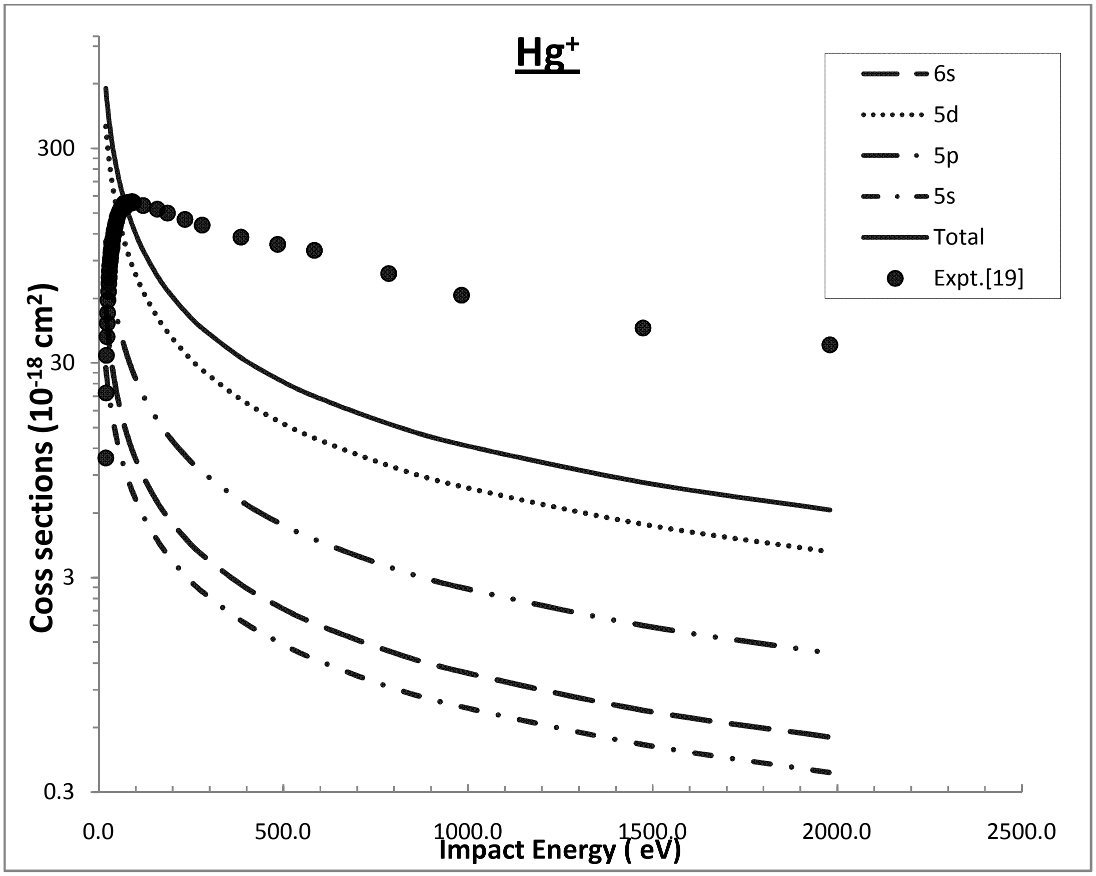

Figure 3(a): Electron Impact Single Ionization of Hg^+ in units of 10^{-18} cm^2

Now, we would like to compare the experimental observations with the results of semi-empirical prediction [30] and results obtained by Lotz [24, 25] which is shown in the Table 3(b) and and Figure 3(b). From the comparison of the above mention results, we found that the results obtained by Lotz [24,25] and Darwin [30] are in reasonable agreement in the low and high energy, while our calculated results are in excellent agreement with the experimental cross section in the intermediate energy region.

Table 3(b): Compared Data Table for Hg^+

E (in eV)	Lotz [25]	Darwin [30]	total calc.	expt.[19]
20.0	10.0	10.0	546.12	21.7
50.0	190.0	140.0	233.76	142.7
100.0	200.0	280.0	127.29	167.6
200.0	150.0	270.0	65.22	149.6
500.0	90.0	160.0	25.28	106.8
1000.0	60.0	100.0	12.49	62.0
2000.0	40.0	70.0	6.19	36.3

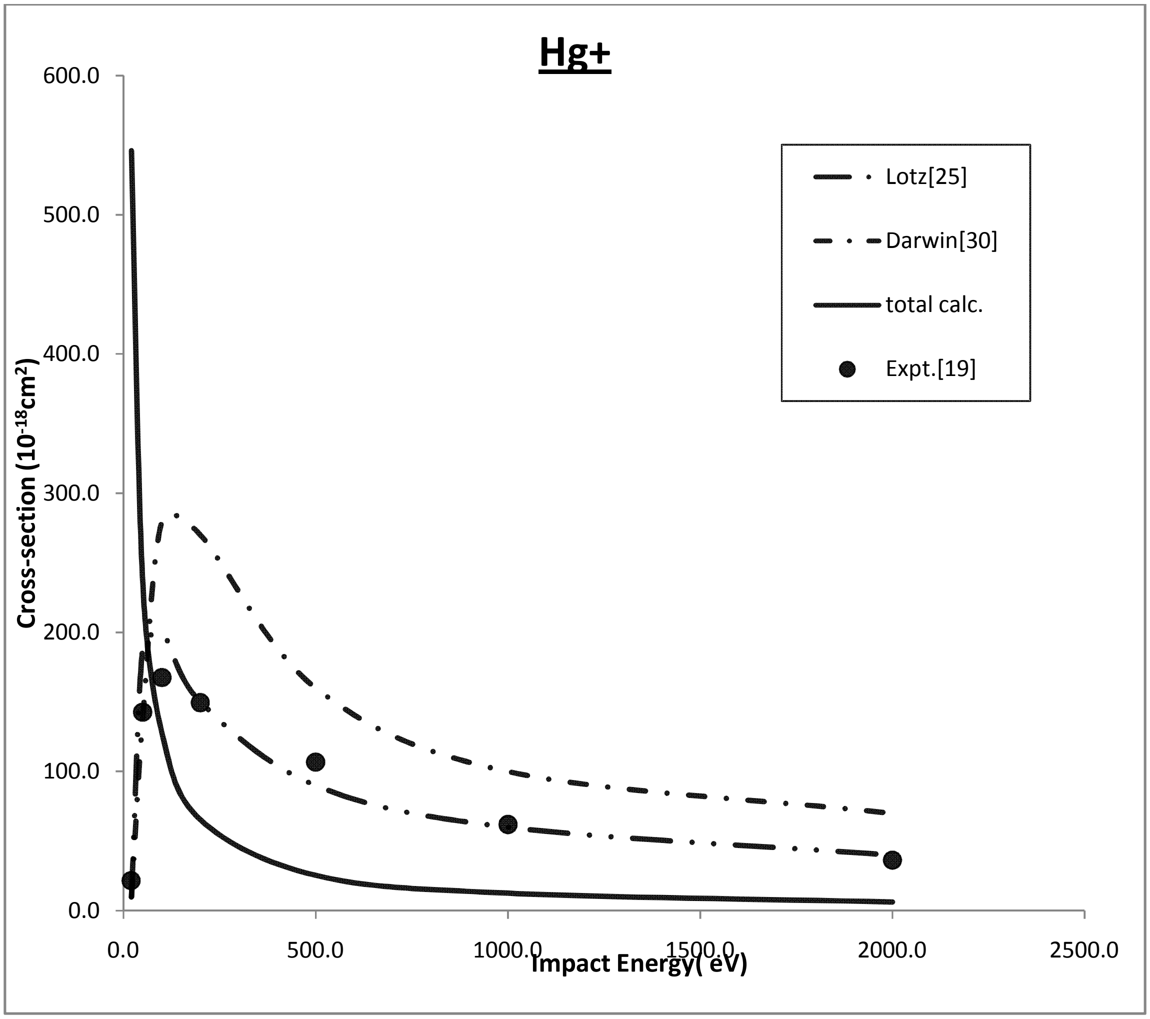

Figure 3(b): Electron Impact Single Ionization of Hg^+ in units of 10^{-18} cm^2

As we discussed earlier, the present model is valid for intermediate and high energy regions which is properly justified.

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