Direct and Dissociative Ionization Cross Section of Oxygen Molecule from Threshold to 10 KeV

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Abstract---Due to abundant applications of ionization in various fields of applied sciences, it's desirable to calculate absolute ionization cross sections of various atoms or molecules. In this literature, we have calculated the absolute direct and dissociative ionization cross sections of the oxygen molecule from threshold energy to 10,000 eV by using revisited Jain-Khare semi-empirical approach.

In this literature, the total direct and absolute ionization cross section data have compared with easily available experimental and/or theoretical data. The present results give a better account for the ionization cross sections up to higher incident electron energies.

Keywords: Direct and dissociative ionization, Electron impact ionization, Ionization cross section.

I. INTRODUCTION

Oxygen is an interesting molecule to study. However, many work have been done on the O₂ molecule. As the wide significant properties of the O₂ molecule, we have determined the direct and dissociative ionization cross sections of the oxygen molecule. There are many applications in the field of plasma processes; vacuum technology, ionosphere, gas discharges, planetary atmospheres and others [1], [2].

Since the 1930s, many experimental and theoretical ionization cross sections have been carried out for the O₂ molecule and the techniques are improved from time to time. James A. R. Samson [3], Krishan Kumar and Srivastava [4] and B.VanZyl [5] studied the ionization cross sections of the O₂ molecule experimentally. And the same work had been analyzed by Straub and co-worker theoretically and determines the cross section up to 1000 eV [6].

Donald Rapp [1], S. P. Khare [7], D. Margreiter [8], H. Deutsch [9], Ashok Jain [10], VandanaSaksena [11], K. N. Joshipura [2] used the different theoretical methods and gave the total ionization cross sections for the O₂ and other molecules. Recently, Stefan E.Huber et al. [12] derived the partial and total ionization cross sections for the O₂ and other fusion –relevant diatomic molecules from threshold to 10 KeV using the binary –encounter-Bethe and the Deutsch-Mark formalisms. So, there are several cross sections for the O₂ molecule, only a few are discussed here. There are various theoretical formalisms to determine the ionization cross sections of molecules[8], [14]. For better accuracy and less mechanical computations, we use the revisited Jain-Khare semi-empirical formalism [7],[15]-[20] to determine

direct and dissociative ionization cross sections of the O₂ molecule.

II. THEORETICAL METHODOLOGY

We developed the MATLAB programming codes to calculate the ionization cross sections of the O₂ molecule for the given equations. This gives ionization cross section to the production of an ith type of cation of the molecule by an incident electron of energy 'E' solving the following equations:

$$Q_i(E) = \frac{4\pi a_0^2 R}{E} \left[\frac{E}{E - I_i} \left(M_i^2 - \frac{R}{E} S_i \right) \ln[1 + C_i(E - I_i)] + \frac{R(E - I_i)}{E} S_i \right. \\ \left. \times \int_0^{(E - I_i)/2} \frac{1}{\varepsilon^3 + \varepsilon_0^3} \left(\varepsilon - \frac{\varepsilon^2}{(E - \varepsilon)} + \frac{\varepsilon^3}{(E - \varepsilon)^2} \right) d\varepsilon \right] \quad (1)$$

(1)

Where

$$M_i^2 = \int_{I_i}^{(E+I_i)} \frac{R}{w} \frac{df_i(w,0)}{dw} dw \quad (2)$$

$$S_i = \int_{I_i}^{(E+I_i)} \frac{df_i(w,0)}{dw} dw \quad (3)$$

$$C_i = C_T \exp \left[n \left(\frac{\sum_{i>1} M_i^2 \ln S_i}{\sum_{i>1} M_i^2} - \ln S_i \right) \right] \quad (4)$$

Where, ε_0 , ε , S_i , C_i , I_i , W , a_0 , and R are the mixing parameter, secondary electron energy, number of ionizable electrons, collision parameter, ionization potential, energy loss suffered by the incident electron, Bohr radius, and Rydberg energy, respectively [20]. And df_i/dw is an oscillator strength that is a key parameter to calculate the ionization cross section (ICS). The oscillator strength can be calculated theoretically if the experimental data is not available as it is directly proportional to the photoionization cross section [17]. We have used the experimental values of absolute dipole oscillator strengths for dissociative ionization of O₂ derived by C.E. Brion using (e, e+ ion) spectroscopy [21]. But the partial oscillator strengths of O₂⁺, O⁺ ions are available up to 75 eV. Thus, for $W > 75$ eV, we extrapolate the same data by the TRK sum rule, within 5-10% error bars [22]. The ionization potentials for of O₂⁺, O⁺ are taken 12.07 eV and 18.59 eV respectively [12]. The values derived for the total collision parameter and mixing parameter are ($C_T=0.04714$) and ($\varepsilon_0=50$) respectively. Summation of partial ionization cross sections (PICS) over the system gives the total ionization cross sections (TICS) as:

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$$Q'_i(E) = \sum_i Q_i(E). \quad (5)$$

We calculated the ICS by varying the secondary electron energy from 0 to $(E-I_i)/2$ using equations (1) because the results are more accurate and precise at this energy. However, Satyendra Pal [17] varying this energy from 0 to $(E-I_i)$ for partial differential cross sections. In partial ionization cross sections, if we varying secondary electron energy from 0 to $(E-I_i)$, then results at low incident energies are more as compared experimental and all other theoretical data.

III. RESULTS AND DISCUSSION

In this literature, we calculate the ionization cross sections of O_2 by electron impact using Equations (1) to (5)

with the help of MATLAB programming codes. The calculated results for partial and total ionization cross sections are tabulated in Table 1 and the partial ionization cross sections graphically presented in Fig. I. We compare our results for the total ionization cross sections with some easily available theoretical and/or experimental data [1],[4],[6],[7], [12],[13] shown in Fig. II. All these give excellent agreement from threshold up to high energies. Here, the total ionization cross sections data are collected as the mentioned referred journals. But the TICS data of S.P. Khare [7] and Stefan E. Huber et al. [12] is extracted from the graphs with some error bars.

Table 1
Present Result for Dissociative Ionization cross-section of O_2 molecule (10^{-16} cm^2)

Energy (eV)	Fragmented ions		Total	Energy (eV)	Fragmented ions		Total
	O_2^+	O^+			O_2^+	O^+	
25	0.2929	0.0654	0.3583	500	0.9955	0.3980	1.3935
30	0.7127	0.0224	0.7351	550	0.9347	0.3728	1.3076
35	1.0232	0.0457	1.0689	600	0.8815	0.3509	1.2323
40	1.2561	0.2269	1.4831	650	0.8344	0.3314	1.1658
45	1.4326	0.3535	1.7860	700	0.7924	0.3142	1.1066
50	1.5666	0.4434	2.0100	750	0.7548	0.2987	1.0535
55	1.6683	0.5106	2.1789	800	0.7209	0.2848	1.0057
60	1.7455	0.5580	2.3035	850	0.6901	0.2722	0.9623
65	1.8040	0.5921	2.3961	900	0.6621	0.2607	0.9228
70	1.8479	0.6193	2.4673	950	0.6364	0.2503	0.8867
75	1.8806	0.6418	2.5224	1000	0.6129	0.2407	0.8535
80	1.9046	0.6604	2.5650	1100	0.5710	0.2236	0.7946
85	1.9217	0.6849	2.6066	1200	0.5349	0.2090	0.7438
90	1.9329	0.7072	2.6401	1300	0.5034	0.1962	0.6996
95	1.9379	0.7185	2.6564	1400	0.4757	0.1851	0.6608
100	1.9387	0.7295	2.6682	1500	0.4511	0.1752	0.6263
110	1.9294	0.7396	2.6690	1600	0.4292	0.1664	0.5955
120	1.9102	0.7418	2.6520	1700	0.4094	0.1584	0.5678
130	1.8845	0.7387	2.6232	1800	0.3915	0.1513	0.5428
140	1.8546	0.7320	2.5866	1900	0.3752	0.1448	0.5200
150	1.8221	0.7229	2.5451	2000	0.3604	0.1389	0.4992
160	1.7881	0.7123	2.5004	2100	0.3467	0.1334	0.4802
170	1.7533	0.7006	2.4539	2200	0.3342	0.1284	0.4626
180	1.7184	0.6883	2.4067	2300	0.3226	0.1238	0.4464
190	1.6837	0.6756	2.3593	2400	0.3118	0.1196	0.4313
200	1.6493	0.6629	2.3121	2500	0.3018	0.1156	0.4174
210	1.6158	0.6501	2.2659	3000	0.2605	0.0993	0.3599
220	1.5829	0.6374	2.2203	4000	0.2060	0.0780	0.2840
230	1.5512	0.6250	2.1762	5000	0.1713	0.0645	0.2358
240	1.5202	0.6128	2.1330	6000	0.1471	0.0552	0.2023
250	1.4904	0.6009	2.0913	7000	0.1293	0.0483	0.1776
300	1.3554	0.5463	1.9016	8000	0.1155	0.0431	0.1586
350	1.2422	0.4999	1.7420	9000	0.1045	0.0389	0.1434
400	1.1467	0.4605	1.6071	10000	0.0956	0.0355	0.1311
450	1.0654	0.4269	1.4923	-	-	-	-

Fig. I: O₂ Dissociative Partial Ionization Cross Section

Fig. II: O₂ TICS in Å². Solid line, Present result; Pentagon, NIST [13].; Triangle, Krishan Kumar[4]; Circle, H.C.Straub [6]; Square, Donald Rapp[1]; Rectangle, S. P.Khare [7]; Solid star, Stefan (BEB) and star, Stefan (DM) [12].

Direct Ionization Cross Sections:

There are many channels for ionization of atoms/molecules. Here, the electron impact ionization technique is used for dissociation of O₂ molecule as the mechanism for direct ionization of O₂ molecule is given below:

The calculated direct ionization cross section is also compared to the experimental data [2]-[3] shown in Fig.III. This also gives good agreement. There is double ionization for further fragmentation of O₂ molecule as given in detail [4], [6].

Fig.III: O₂ Direct Ionization Cross Section (O₂⁺). Solid line, Present result; Star, Krishan Kumar [4]; Square, H. C. Straub [6];

IV. CONCLUSION

We calculate absolute partial and total ICS for O₂ molecule and the results are also compared with theoretical and experimental available data from threshold energy to high energies. These comparisons have a very good agreement with H.C. Straub [6], Stefan E.Huber et al. (BEB) [12] and NIST (BEB). But there are some higher Peak values of cross sections of Donald Rapp [1], Krishan Kumar [4] and S.P.Khare [7] while Stefan E.Huber et al. (DM) [12] have low peak values. Thus, from the compared data and graphs, we can say that the developed programming can produce reliable cross sections even for complex molecules also. And the present data could be used in the plasma process, modeling systems, and other applications.

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