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Determination of partial single differential electron ionization cross sections of H_2

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Abstract

The partial single differential cross sections (PSDCS) for the ions H_2^+ and H^+ resulting from the direct and dissociative ionization of H_2 by electron impact have been calculated employing a semi-empirical approach. The calculations are made as a function of the secondary/ejected electron energy at 500 and 1000 eV incident electron energies. The partial ionization cross sections (PICS) for direct and dissociative ionization have also been calculated with incident electron energies varying from the ionization threshold to 10 keV. The results are compared with the available experimental data.

Keywords: Partial single differential, Cross sections, Electron, Hydrogen molecule

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1. Introduction

One of the most fundamental and ubiquitous processes occurring in nature is the collision of an electron with an atom or a molecule. An important process resulting from such collision is the ionization, with the ensuing loss of energy of the primary electron and the emission of one or more secondary electrons. The knowledge of this process has numerous applications in areas such as studies of the ionosphere, radiation damage, particle detector operations and in several other processes involving ionized gases or plasmas.

Early measurements and calculations of total integral cross sections for electron impact ionization have been supplemented in recent years by the determination of multifold differential cross sections [1]. Even today, the only measurements of single and/or double differential cross sections for the ionization of hydrogen molecule have been reported by Opal et al. [2] at 500 eV, Shyn et al. [3] at several energies ranging from 25 to 250 eV, DuBois and Rudd [4] at 100 eV, Rudd et al. [5] at several energies from 200 to 1500 eV and Ogurtsov [6] at energies from 100 to 1000 eV. The maximum secondary (ejected) electron energies in the experimental data [2,3] extended up to $(E-I)/2$, where E is the primary electron energy and I is the ionization threshold of H_2. On the other hand, Rudd and co-

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workers [4,5] extended this upper limit to $(E-I)$. A considerable body of experimental data for integral cross sections leading to direct and dissociative ionization for the hydrogen molecule by electron impact has been measured by Rapp et al. [7], Crowe and McConkey [8], Krishnakumar and Srivastava [9], Edwards et al. [10], Kossmann et al. [11], Van Zyl and Stephen [12], Adamczyk et al. [13] and Straub et al. [14] for various incident electron energies. ICRU report 55 [15] includes a compilation of experimental as well as theoretical status of ionization cross sections of H_2 molecule due to electron impact.

In the present investigation, we report the calculations of partial single differential cross sections (PSDCS) of ejected electrons from H_2 by electron impact at energies of 500 and 1000 eV, employing the modified Jain–Khare semi-empirical formula [16–20]. The calculations are made as a function of energy loss (sum of the secondary electron energy and the ionization threshold energy I) suffered by the incident electrons. The integral cross sections i.e. the partial ionization cross sections (PICS) have also been calculated by integration of the PSDCS over the secondary electron energy varying from 0 to $(E-I)$ (or energy loss W varying from I to E). The present calculations for the PSDCS and the integral cross sections distinguish the different modes of ionization, i.e. direct and dissociative ionization for the production of the H_2^+ and H^+ ions from H_2 by electron impact. Since no theoretical and/or experimental data for the PSDCS are available, we have made only a comparison of our calculated results for the single differential cross sections (SDCS), which is the sum of the PSDCS values, with available experimental data. However, the partial ionization cross sections (PICS) due to electron impact involving energies from the ionization threshold to 10 keV revealed a satisfactory agreement with a number of available experimental data [7–14] including those compiled in ICRU-55 [15].

2. Theory

The Jain–Khare semi-empirical formula [16,17] has yielded the results for SDCS in the secondary electrons energy range 0 to $(E-I)$12. Recently, we have extended this formula with the ejected primary or secondary electron energy varying from 0 to $(E-I)$, the maximum and applied it to the evaluation of partial single and double differential cross sections for molecules over a wide range of energies [19–21]. In the present evaluations, we have employed this modified approach to calculate the PSDCS for H_2. In brief, the PSDCS for the production of ith type of ion by the impact of an electron of energy E with a molecule leaving the secondary electrons of energy ϵ is given by

$$Q_i(E,\epsilon)=\frac{4\pi a_0^2 R}{E}\left[\left(1-\frac{\epsilon}{(E-I_i)}\right)\frac{R}{W}\times\frac{\mathrm{d}f_i(W,0)}{\mathrm{d}W}\ln\left[l+C_i(E-I_i)\right]+\frac{R}{E}S_i\frac{(E-I_i)}{(\epsilon_0^3+\epsilon^3)}\times\left(\epsilon-\frac{\epsilon^2}{(E-\epsilon)}+\frac{\epsilon^3}{(E-\epsilon)^2}\right)\right] \quad (1)$$

Where a_0, R, S_i, ϵ_0 and C, represent the first Bohr radius, Rydberg's constant, probability of ionizable electrons, mixing parameter and collision parameter, respectively. It is convenient to replace ϵ by $W-I_i$, where W is the energy loss suffered by the primary electron. So, we can easily calculate the total SDCS i.e., the sum of PSDCS values

$$Q_i^T(E,W)=\Sigma\, Q_i(E,W) \quad (2)$$

Further, integrating the PSDCS with respect to W within the limit I to E, we get the PICS.

$$Q_1(E)=\int Q_i(E,W)\,\mathrm{d}W \quad (3)$$

In order to evaluate $Q_i(E,W)$ and $Q_i(E)$ from the above equations, the required major input data are the oscillator strengths $\mathrm{d}f_i\ (W,0)/\mathrm{d}W$ for the production of ith type of ions, which were taken from the experimental data of Neil and Samson (see for instance Gallagher et al. [22]) for photon energies from threshold to 70 eV. For higher photon energies, we have used the total oscillator strengths calculated by Zeiss et al. [23] which were distributed among the various types of ions employing a constant branching ratio at the dipole breakdown ($W>50$ eV). The error introduced in the calculations of cross sections due to the utilization of the total oscillator strengths is about 10% which is of the order of the experimental error

in the measurements of the partial photo ionization cross sections. The mixing parameter ϵ_0 calculated by Jain and Khare [16,17] has been used and its value is taken to be 50 eV. In case of direct or non-dissociative ionization, where $i = 1$, C_1 is identical to C_T the total collision parameter. For dissociative ionization ($i = 2$), C_2 is calculated from the procedure of Khare et al. [18]. The value of C_T is obtained from the experimental data (~ 5% accurate) of Reike and Prepeichal [24]. For $E > 1$ keV, the relativistic corrections in the calculations of cross sections are taken into account. In the present evaluation estimated total error is not expected more than 10%.

3. Results and discussion

The present results for the PSDCS and SDCS are shown in Figs. 1 and 2 at the incident electron energies 500 and 1000 eV, respectively and summarized in Tables 1 and 2. In the figures, curves A and B represent the PSDCS values corresponding to the production of H_2^+ and H^+ ions, respectively. Curve C represents the single differential cross section

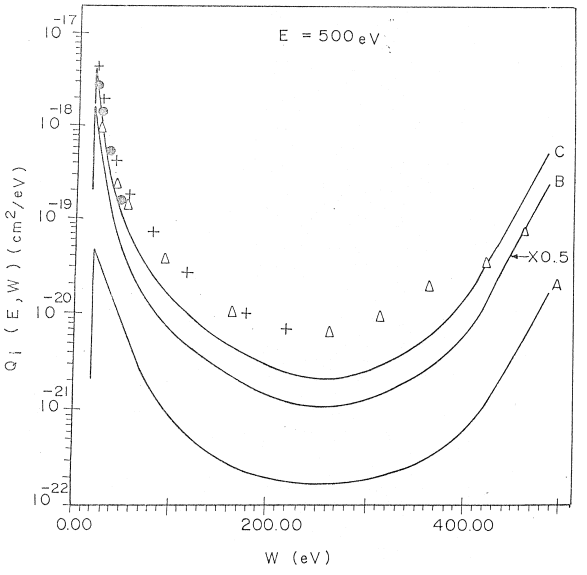

Fig. 1. Solid curves A, B and C represent the PSDCS and SDCS as a function of energy loss for H_2 by the impact of 500 eV electron, respectively. Experimental data: +, Opal et al. [4], △, Rudd et al. [5] and ●, Ogurtsov [6].

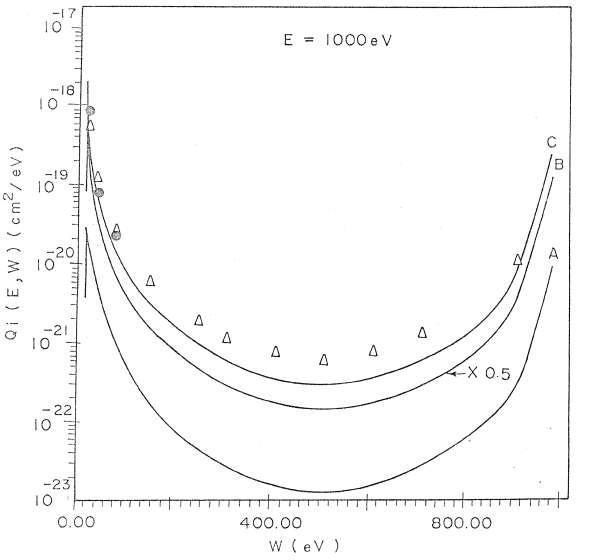

Fig. 2. As Fig. 1 but at $E = 1000$ eV.

(SDCS) values which is the sum of the PSDCS. Due to non-availability of any experimental and/or theoretical results for the PSDCS, the SDCS values via curve C are compared with the available experimental data [2,5,6].

We note that our calculated SDCS values (curves C) for $W < E/2$ are in reasonable agreement with the experimental data [2,5,6] in Figs. 1 and 2. At $W = E/$

Table 1
The PSDCS for H_2 by the impact of 500 eV electrons (10^{-22} cm^2/eV)

Energy loss W (eV)	PSDCS		SDCS
	H_2^+	H^+	
16	4600	–	4600
17	37 000	–	37 000
18	33 000	21	33 021
20	23 000	470	23 470
25	10 000	260	10 260
30	5200	320	5520
45	4800	380	5180
60	450	40	490
80	240	17	257
120	95	5.3	100.3
160	47	2.5	49.5
200	29	1.4	30.4
300	23	1.0	24
450	5300	170	5470

Table 2
The PSDCS for H_2 by the impact of 1000 eV electrons (10^{-23} cm^2/eV)

Energy loss W (eV)	PSDCS		SDCS
	H_2^+	H^+	
16	26 000	–	26 000
17	220 000	–	220 000
18	190 000	120	190 120
20	130 000	2700	132 700
30	29 000	1800	30 800
41	8200	850	9050
100	820	51	871
200	1600	8.3	1608
300	62	3.0	65
400	34	1.6	35.6
500	26	1.2	27.2
600	30	1.3	31.3
700	49	2.2	51.2
800	110	5.1	115.1

2, a significant deviation between the experimental data and the calculated results is noted. It may be due to the strong exchange effects at equal energies of the primary and secondary electrons. For $W > E/2$, the deviations reduce considerably. Regarding the PSDCS values (curves A and B in figures), the trends of the cross sections with ejected electron energy or energy loss function W is as expected [19–21]. It is noted that the differential cross sections are symmetric about $W/2$.

Figs. 3 and 4 show the PICS corresponding to the production of the H_2^+ and H^+ ions, respectively from H_2 by electron impact with incident electron energies varying from ionization threshold to 10 keV. The numerical values are also listed in Table 3. Fig. 3 clearly indicates that our calculated values of the PICS for the production of H_2^+ ions are in reasonably good agreement with most of the available experimental data [8–11,13,14] within the experimental uncertainties varying from 5% to 20% in different experiments. In case of dissociative ionization (Fig. 4) the presently calculated results are also generally in good agreement with the available experimental data [8,9,14]. The experimental data of Adamczyk et al. [13] for $Q_1(H^+)$ lie much lower than our results and other experimental results [9,12]. This may be due to the insufficient collection of H^+ ions with high kinetic energies [9]. The experimental data of Rapp et al. [7] for H^+ ions also lie lower than our

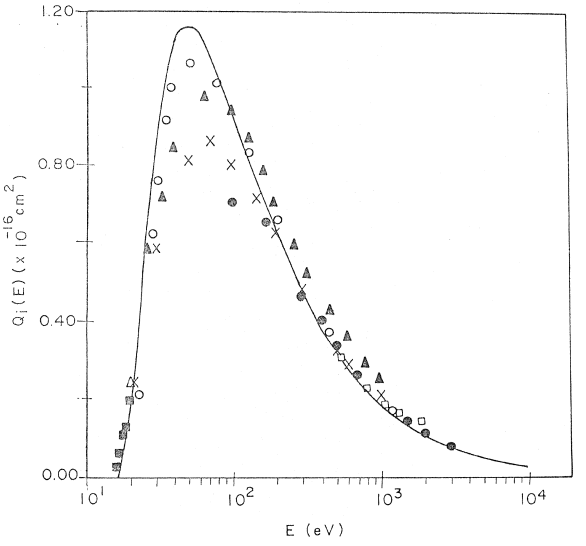

Fig. 3. The PICS as a function of impinging electron energy for the production of the H_2^+ ions from H_2. Experimental data: ■ Crowe and McConkey [8], ▲, Krishnakumar and Srivastava [9] □, Edwards et al. [10]. ●, Kossmann et al. [11], ×, Adamczyk et al. [13] and ○, Straub et al. [14].

calculated values and other experimental data [9,12]. Their measurement did not include H^+ ions formed with energies less than 2.5 eV. Recently, Van Zyl and

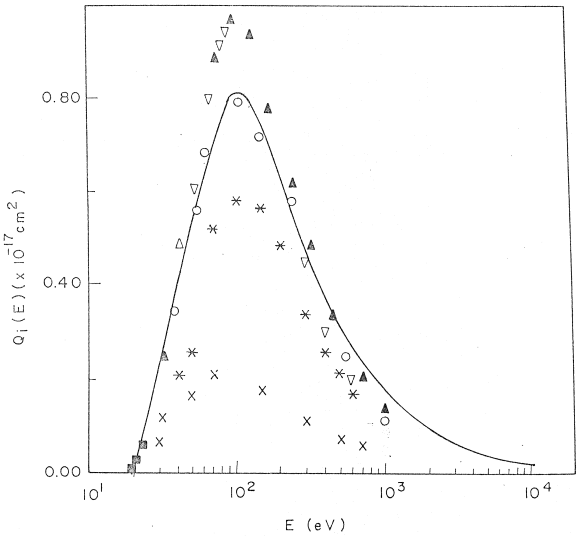

Fig. 4. As Fig. 3 but for the production of H^+ ions including the additional experimental data; *, Rapp et al. [7] and ▽, Van Zyl and Stephen [12].

Table 3
The PICS for H_2 by electron impact (10^{-18} cm^2)

E (eV)	H_2^+	H^+
16	0.2	–
18	7.2	–
20	23.3	0.14
25	63	1.46
30	89	2.16
35	103.7	2.90
40	115.9	3.27
50	116	4.25
60	113.3	4.35
70	109	4.90
80	104	5.65
90	99.1	6.65
100	943	7.33
110	90	8.10
150	75.5	8.17
200	63.1	7.53
250	54	6.61
300	47.2	5.83
500	32	5.18
1000	18.2	3.61
5000	4.6	0.54
10 000	2.5	0.29

Stephen [12] have reviewed the experiment of Rapp et al. [7] and found that the PICS for H^+ ions are about 70% larger than the previous measurements. The cross sections of Van Zyl and Stephen [12] are found to be in good agreement with the experimental data of Krishnakumar and Srivastava [8] and also with our results. The formation of H^+ is envisaged either as a direct dissociation (shake off process) or as a two step process via, double ionization of H_2. The contribution of two step process is about one third of that of the shake off process [1]. In the present investigation, we can not make any distinction between these two processes.

4. Conclusions

The PSDCS for the production of H_2^+ and H^+ ions via direct and dissociative ionization processes of the H_2 molecule by electron impact have been calculated at incident electron energies of 500 and 1000 eV using a modified semi-empirical formula [19–21]. It is difficult to comment on the accuracy of our calculations for PSDCS due to the lack of experimental data. However, the comparison of SDCS (sum of PSDCS) and the partial ionization cross-sections (integral of PSDCS) with the available experimental data shows a reasonably good agreement. It substantiates our approach to evaluate the PSDCS to a reasonable level of accuracy.

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