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DISSOCIATION OF ATMOSPHERIC MOLECULES H_2 AND N_2 BY ELECTRON IMPACT - NEUTRAL ATOM PRODUCTION

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ABSTRACT

This paper aims at the estimation of neutral atom pair generation from abundant atmospheric molecules like H_2 and N_2 upon electron impact. Atmospheres of Jupiter and Titan (one of Saturn's moons) are largely comprised of H_2 and N_2 gases respectively. The relative atmospheric chemistry induced by neutral dissociation of H_2 and N_2 via energetic electrons or via photoelectrons plays an important role in these atmospheres. An attempt is made here to calculate this quantity using total dissociation cross sections for these molecules. The relevant cross sections are employed to estimate the rates for production of neutral atom pairs. While estimating productions of neutrals, cascading from higher states is considered duly, along with dissociative ionization generating a single atom per event.

Key words: *Electron impact, Excitation cross section, Neutral dissociation, Dissociative ionization*

INTRODUCTION

Molecular Hydrogen and Nitrogen are two of the most common species found in a large variety of natural and man-made systems. Hydrogen is the most abundant molecule in the universe, and also on the planet Jupiter. Nitrogen is also an important constituent in outer planets and satellites like Titan, as also in comets etc. The ground-state dissociation energies of H_2 and N_2 molecules are known to be 4.49 and 7.37 in eV [1]. Therefore these molecules are dissociated not by visible light, but by appropriate UV radiation. Our interest in the present paper is on electron impact neutral dissociation of each of these molecules into ground state atomic species, as follows.

$$e_i + H_2 \rightarrow H + H + e_s \quad (1)$$

$$e_i + N_2 \rightarrow N + N + e_s \quad (2)$$

Here the subscripts *i* and *s* refer to the incident and the scattered electron. The threshold energy in each case is the corresponding dissociation energy. For molecular hydrogen, the very first excited electronic state is $b^3\Sigma_u^+$, which is known, since the early days of quantum mechanics to be repulsive i. e. dissociative [2]. However, in (1) we must also include the contributions of higher electronic states cascading into the b-triplet state, thereby adding to the yield of the neutral H (1s). Complications arise in N_2 where there are several excited electronic states that decay into two neutral ground state nitrogen atoms, and these excited states, i.e. valence and Rydberg, have excitation energies in the range of 11.5 to 40 eV [3]. Nonetheless, theoretical [4] and experimental [5-8] work has been done to investigate the neutral dissociation of the title molecules by electron impact.

Electron impact processes including those resulting into uncharged fragmentations, have been a subject of study in view of their importance in various planetary and solar-system objects as well as in plasma environments. The neutrals generated through electron collisions themselves being reactive, give rise to their own chemistries in the concerned environment. Therefore a lot of importance is attached to these electron induced processes.

In an environment like the upper atmosphere of a planet or a satellite, the neutral dissociation must be examined from the bulk point of view, not just an isolated inelastic scattering event. Therefore in the present paper, we consider first the total cross sections of electron impact excitation to neutral fragments. Using these cross sections as an input along with number densities of target species, the collision frequency for neutral dissociation is obtained. As far as the impact electrons are concerned we have assumed Maxwellian energy distribution.

However, in addition to the direct dissociation processes mentioned above in (1) and (2), one must also consider the electron impact dissociative ionization of molecules, wherein a charged fragment is accompanied by a single neutral species, e.g. ,

$$e_i + H_2 \rightarrow H^+ + H(1s) + e_s + e_j \quad (3)$$

Here, subscript *j* refers to the electron ejected from the target molecule that is ionized. The ionization process of equation (3) occurs at energies higher than that in the previous cases vide equations (1) and (2). The latter must be properly included in any estimate of the number of neutral atom- pairs generated in a medium by electron impact. In section below we highlight our theoretical methodology for deriving electron impact neutral dissociation cross sections of the present two targets. Electron induced dissociative ionization is also included in the present calculations.

Presently our aim is to estimate the number of neutral atom pairs generated per second in a pure gas medium, as a function of incident electron energy E_i. This is done by calculating the respective electron collision frequencies from the relevant total cross sections of electron impact on a target.

THEORETICAL METHODOLOGY

In this paper we are primarily interested in the electron impact electronic excitations of the two molecules from their respective ground electronic states, vide equations (1) – (3). Our theoretical methodology is outlined separately for the two molecular targets as follows:

H_2 dissociation

Let us first consider the following electronic excitation of H_2, important at low incident energies,

$$e^-_i + H_2 (X^1\Sigma_g^+) \rightarrow H_2^*(b^3\Sigma_u^+) \rightarrow H(1s) + H(1s) + e^-_{sc} \quad (4)$$

Now, as mentioned by Yoon et al [9] that the only available experimental data in this regard are due to Corrigan [10] who had measured total dissociation cross sections of this triplet state.

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Corrigan's results included cross section for dissociative ionization of H_2. We could not resist quoting from Corrigan's paper [10] viz., "Cross *section for dissociation of molecular hydrogen into two ground-state atoms is in effect the cross section for excitation of all triplet states regardless of whether they are bound or repulsive*". This argument is supported by the absence of radiation for triplets to singlet inter-combinations, so that electron impact excitation to any triplet state must lead eventually to dissociation. Thus the formation of two H(1s) atoms by electron impact on H_2 results from direct excitation to $b^3\Sigma_u^+$, plus, excitation to higher triplet states followed by cascading down to $b^3\Sigma_u^+$ [4]. Near threshold, the excitation to $b^3\Sigma_u^+$ is expected to be the main contributor to the neutral dissociation [9]. Also, $a^3\Sigma_g^+$ (16%) and $c^3\prod_u$ (20%) are the two major cascading states to $b^3\Sigma_u^+$ while $e^3\Sigma_g^+$ (6%) and $d^3\prod_u$ states play only a minor (5%) role [4].

Based on the above discussion, we have presently made a comprehensive calculation for total cross sections of electron impact neutral dissociation of ground-state H_2 from 10.57 to ~200 eV. The cross section contribution of the direct excitation to $b^3\Sigma_u^+$ is calculated from the R-matrix theory by using the UK R-matrix package viz., Quantemol-N (SE) Version 3.6. In order to derive complete neutral dissociation cross sections for H_2 molecule, we have also considered the cascading from higher excited states $a^3\Sigma_g^+$ and $c^3\prod_u$ to the state $b^3\Sigma_u^+$. Also important for the production of single H (1s) atom is the dissociative ionization vide equation (3).

To calculate the excitation cross sections of H_2 into dissociative b-state as in (4), the *ab initio* R-matrix approach [11, 12] is adopted here through the Quantemol-N (SE) package Version 3.6 [13]. Experimental equilibrium geometries [14] are used for these calculations. Ground state electronic configuration of H_2 in $D_{\infty h}$ symmetry is $1\sigma^2$. However, the present calculations were performed in the reduced symmetry D_{2h} sub-group [15]. The Basis set is defined using EMSL Basis Set Exchange [16]. Full CI has been used for the calculation of this molecule with only 2 electrons. 12 target states were employed in the close-coupling expansion method for scattering calculations. R-matrix theory is based on the partition of coordinate space into an internal region and an external region separated by a spherical boundary of radius presently set to 10 a_0. This boundary is such that the molecular electron cloud is fully contained within the sphere. The short-range electron exchange and electron-electron correlation effects between the scattering electron and the target electrons are considered for this inner region. The said interactions are negligible in outer region and only long range interactions need to be considered there. The cross section for direct excitation to $b^3\Sigma_u^+$ is denoted by $Q_{exc}(b^3\Sigma_u^+)$.

Now, the excitation threshold for the very first state $b^3\Sigma_u^+$ is almost correctly reproduced in the package used by us, but the same is not reproduced accurately for the higher triplet states relevant to the present study. Therefore, the excitation cross sections to $a^3\Sigma_g^+$ and $c^3\prod_u$ states are adopted presently from Khakoo and Trajmar [17] and Khakoo et al [18]. These cross section data, involving errors of ~20% are added together, and the sum is referred as Q_{exc}'.

One more contributing process to the production of neutral Hydrogen H (1s) is *dissociative ionization* as shown by (3), which must be considered here. Recent calculations of total electron impact ionization of H_2 are due to Joshipura et al [19], but the quoted work does not spell out the contribution of dissociative ionization in the total ionization cross sections. Therefore, the required dissociative ionization cross section Q_{d-ion} corresponding to process (3) is adopted from the measured data of Straub et al [20].

It is thus possible to obtain overall or total neutral dissociation cross sections to be denoted by Q_{NDiss} in e^- - H_2 scattering. For this purpose the excitation cross sections to all the three above mentioned triplet states are added together to obtain total excitation to neutral dissociation Q_{Nexc}. The neutral dissociation via process (4) including cascading produces two H (1s) atoms whereas process (3) produces only one H (1s) atom per event. Thus, in order to obtain overall or total neutral dissociation cross section Q_{NDiss} for H_2 corresponding to production of a neutral atom *pair*, the half of the dissociative ionization cross section is added to Q_{Nexc}. We have finally,

$$Q_{NDiss} = Q_{Nexc} + \frac{1}{2} Q_{d\text{-}ion} \qquad (5)$$

where $$Q_{Nexc} = Q_{exc}(b^3\Sigma_u^+) + Q_{exc}' \qquad (6)$$

The factor 1/2 in the second term of equation (5) indicates that two ionization events are required to produce a neutral hydrogen atom pair.

N_2 dissociation

In the case of N_2 vide process (2) above, the situation is not so straightforward. Unlike H_2 there is no directly repulsive state, which upon de-excitation would result into neutral dissociation of N_2.The potential energy diagram for N_2 is much more complicated and few repulsive states, including $C^3\prod_u$ are available [21]. Even these states are not enough to account for total neutral dissociation of N_2. In fact any excitation to the lower-lying, non-dissociative excited states above their dissociation limits can also be taken as a contribution to direct dissociation. Thus the possible de-excitation will not only include radiative cascade to lower states, but also pre-dissociation to N atom at 12.137 and 13.329 eV energies [6]. It is seen that an important role is played by the family of $^1\Sigma_u^+$ and $^1\prod_u$ states lying above the dissociation limit, towards the neutral dissociation of N_2 molecule. Winters [5] had measured dissociation cross sections for N_2 by adsorption of N atoms on nickel and molybdenum surface and using pressure decrease relation. These data also include dissociative ionization [5, 6]. Neutral dissociation of N_2 was also investigated by Cosby [6], by directly detecting two N atoms, but the data of [6] are considerably lower than that of [5]. Thus Cosby [6] had recommended the weighted average of the two data sets after considering their stated error limits i.e. ±20 % for [5] and ±30 % for his data [6].

Now, our aim here is to determine overall or total cross sections for production of neural N-atom pair by the impact of electrons on N_2. In view of a large number of excited states involved here, it becomes necessary to consider a cumulative quantity viz., summed total excitation cross section denoted by $\sum Q_{exc}$, representing all accessible electronic excitations upon e^- - impact. In recent years, the cross section $\sum Q_{exc}$ has been obtained approximately as a contribution to total inelastic cross section Q_{inel} for e^- - impact on a large number of atomic and molecular targets in [22-24]. This theoretical method basically determines the contribution of ionization cross section Q_{ion}, but the quantity $\sum Q_{exc}$ is also obtained.

The method basically starts with simultaneous elastic and inelastic electron scattering treated in a complex potential $V(r, E_i) = V_R(r, E_i) + iV_I(r, E_i)$. Here, r is the radial distance from the mass-centre of the target. Further $V_R(r, E_i)$ is the real part and $V_I(r, E_i)$ is imaginary part of the total potential. The real part consists of the sum of static (V_{st}), exchange (V_{ex}) and polarization (V_{pol}) terms, and the imaginary term is the absorption potential V_{abs}. The basic input in constructing all these model potentials is the target electron charge density. The complex potential enables one to calculate total (complete) cross section Q_T defined by,

$$Q_T(E_i) = Q_{el}(E_i) + Q_{inel}(E_i) \tag{7}$$

where the first term on RHS is the total elastic cross section.

Further, we have

$$Q_{inel}(E_i) = \Sigma Q_{ion}(E_i) + \Sigma Q_{exc}(E_i) \tag{8}$$

The first term in equation (8) accounts for total of all ionization cross sections accessible energetically. The second term is of our present interest. If i is the initial molecular (ground) state and f is final state of electronic transition, and if $Q(i \rightarrow f)$ is the total cross section of this transition then,

$$\Sigma Q_{exc}(E_i) = \sum_f Q(i \rightarrow f) \tag{9}$$

The approach outlined above, called ‘complex potential ionization contribution’ (*CSP-ic*) method enables us to calculate the required quantity $\sum Q_{exc}$ for e^- - N_2 scattering [22-24]. This method also offers an estimate of the neutral dissociation cross section Q_{NDiss} for N_2. Specifically the idea is to subtract out total emission cross sections Q_{emiss} of major emission lines at 95.8, 337.1 and 135.4 nm [8, 25, 26] of N_2 from ΣQ_{exc} obtained by *CSP-ic* method. Finally as in the case of H_2, we also include dissociative ionization process resulting into single neutral N atom production per event. That is to say that we consider the dissociative ionization cross section $Q_{d\text{-}ion}$ representing

$$e_i + N_2 \rightarrow N + N^+ + e_s + e_j \tag{10}$$

The required cross sections $Q_{d\text{-}ion}$ are obtained from the experimental data of Lindsay and Mangan [27]. This leads us to the overall or total neutral dissociation cross section Q_{NDiss} for N_2 corresponding to production of a neutral atom *pair*.

$$Q_{NDiss} = (\sum Q_{exc} - Q_{emiss}) + Q_{d\text{-}ion}\tfrac{1}{2} \tag{11}$$

The errors in the measured data [8], [25] and [26] are ~13.5, 25 and 22 % respectively, while those in [27] are ~6%. The difference between equation (11) for N_2 and equation (5) for H_2 may be noted.

Neutral Dissociation Collision Frequency e^--H_2, e^--N_2

Our next task is to incorporate this microscopic quantity Q_{NDiss} to obtain macroscopic quantity i.e. effective collision frequency $<\nu_{NDiss}>$ for these molecules as in a realistic bulk medium.

If we assume incident electrons to be mono-energetic the neutral dissociation collision frequency ν_{NDiss} can be defined by,

$$\nu_{NDiss} = N.Q_{NDiss}(E_i).\upsilon \tag{12}$$

Where, N is the number density of target molecules per cc and υ is the velocity of the incident electron.

Actually the incident electrons are in the form of the flux of precipitated electrons or the photo-electrons. Hence, considering Shkarofsky [28] with notation of Itikawa [29], the effective collision frequency $<\nu_{NDiss}>$ for the production of neutral atom pair can be defined as,

$$<\nu_{NDiss}> = \frac{4}{3\sqrt{\pi}} \int_{I_p}^{\infty} \nu_{NDiss} \in^{\frac{3}{2}} e^{-\in} d\in \tag{13}$$

$\in = \dfrac{E_i}{kT_e}$; reduced kinetic energy of the electrons, where k = Boltzmann’s constant,

T_e = electron temperature 1.5 E+05 ^{0}K, m = mass of electrons and I_p = Ionization potential (in unit of kT_e) for the target molecule.

In equation (13), Maxwelllian distribution of energetic electrons is assumed as an approximation.

N_2 gas is dominant not only in Earth’s atmosphere but also the most abundant gaseous species in Titan’s atmosphere. Similarly H_2 gas is almost equally abundant in Jupiter’s atmosphere. The number density of H_2 in Jupiter atmosphere is derived from analysis of the α Leo occultation experiment on board *Voyager- 1* by Atreya et al [30]. They [30] had derived density profile for H_2 with altitude relative to Ammonia clouds located at pressure 600mb and temperature 150 ^{0}K in Jupiter’s atmosphere. The number density for N_2 in Titan’s atmosphere is obtained from globally averaged INMS (on board Cassini) profiles for N_2 for thermospheric temperature 154 ^{0}K in Jupiter’s atmosphere [31]. Respective number densities of H_2 and N_2 as shown in Table 1 are used in equation (12) to obtain the present calculations of $<\nu_{NDiss}>$, which indeed is a measure of the number of neutral fragment pairs of the concerned molecule. In our knowledge this is first attempt of its kind to estimate neutral atom pair production in planetary atmosphere of Jupiter and Titan.

Table – 1: H_2 and N_2 number density in Jupiter and Titan’s atmosphere respectively at different altitudes

Species	Altitude (km)	Number density (cm^{-3})
H_2 in Jupiter’s atmosphere	50	1.7 E+14
	200	8.3 E+11
N_2 in Titan’ atmosphere	1000	5.6 E+09
	1200	3.1 E+08

RESULTS AND DISCUSSION

The present paper aims at two-fold purpose. Firstly we calculate the neutral dissociation cross section Q_{NDiss} of simple diatomic species like H_2 and N_2. In case of H_2, Q_{NDiss} is calculated by adding up excitation cross sections to the states $b^3\Sigma_u^+$, $a^3\Sigma_g^+$ and $c^3\prod_u$ along with the consideration of dissociation ionization appropriately. While in the case of N_2 complicated potential energy diagram with many states contributing to neutral dissociation lead us to choose our *CSP-ic* method to extract out Q_{NDiss}. For N_2, Q_{NDiss} is obtained via subtraction of cross section for major emission lines from $\sum Q_{exc}$ and addition of $(1/2).Q_{d\text{-}ion}$. Secondly we have performed here the calculations on the rate of neutral atom pair production via electron impact on the H_2 and N_2 gases in the planetary atmosphere of Jupiter and Titan respectively. Finally the desired collision frequencies are obtained through equation (13) and thereby deriving the number of neutral atom pairs generated upon electron impact. The relative abundance of these extensively studied molecules in planetary atmospheres of

Jupiter and Saturn’s moon-Titan tempted us to perform these calculations.

Hydrogen Molecule

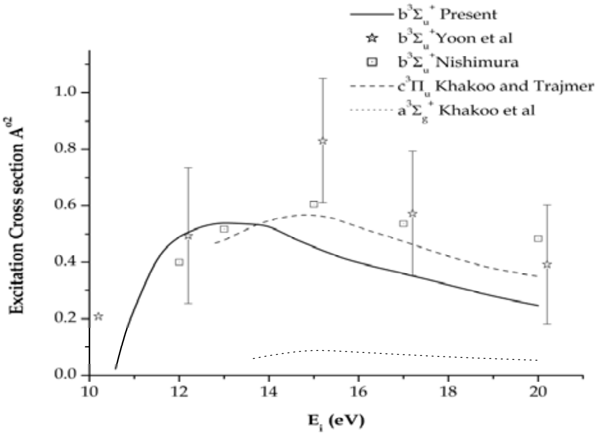

Fig. 1 Excitation cross sections to the states $b^3\Sigma_u^+$ (solid line), $c^3\Pi_u$ (dashed line) and $a^3\Sigma_g^+$ (dotted line): Yoon et al [9] (star); Nishimura and Danjo [32] (Square).

Excitation cross sections to be utilized for the neutral dissociation calculations are shown in Fig. 1. Solid curve indicates excitation to the $b^3\Sigma_u^+$ state extracted via Quantemol-N package. Comparison is made with available recommended experimental data by Yoon et al with an error of ~±25% [9] and Nishimura and Danjo [32]. Deviation of our calculated results from the available experimental data above 13 eV can be attributed partly to our theory i. e. Quantemol calculations, and partly to experimental errors. The experimental measurement of [9] and [32] are obtained through electron energy loss spectra via spectrum integration over concerned energy loss region. Present results match within experimental errors. Dashed curve in Fig. 1 shows cross sections for excitation to the state $c^3\Pi_u$ [17] and dotted curve shows that for excitation to $a^3\Sigma_g^+$ state [18]

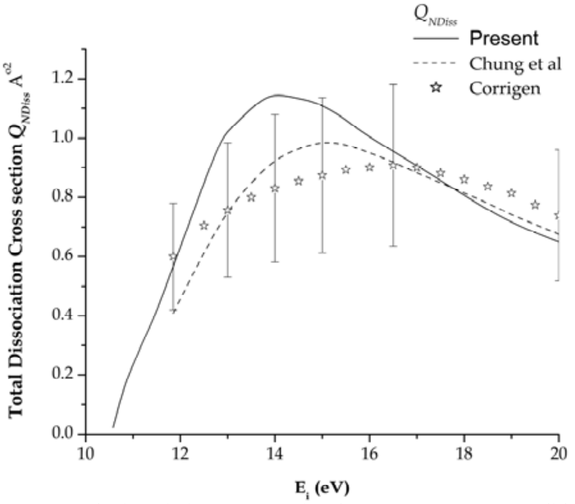

Fig. 2 Total Dissociation cross section for H_2: present Q_{NDiss} (solid line); Corrigan [10] (Star); Chung and Lin [4] (dash)

Cross section for excitation to $b^3\Sigma_u^+$, $c^3\Pi_u$ and $a^3\Sigma g^+$ states are added together [4] to derive total neutral dissociation cross section Q_{NDiss} as shown in Fig. 2. Present results are compared with available theoretical [4] and experimental [10] data. Overall good agreement can be seen with both the available data. Present results fall within the large error bars of Corrigan data.

H_2 is the most abundant molecule in Jupiter’s atmosphere. Dissociation of H_2 into a pair of neutral H atom via EUV or electron impact must be playing the most important role in the atmospheric chemistry of Jupiter. Based on this argument it is necessary to estimate the number of neutral atoms generated via electron impact to understand atmospheric chemistry. As an initiative we have tried to estimate this number approximately by mean of collision frequency, using equation (13).

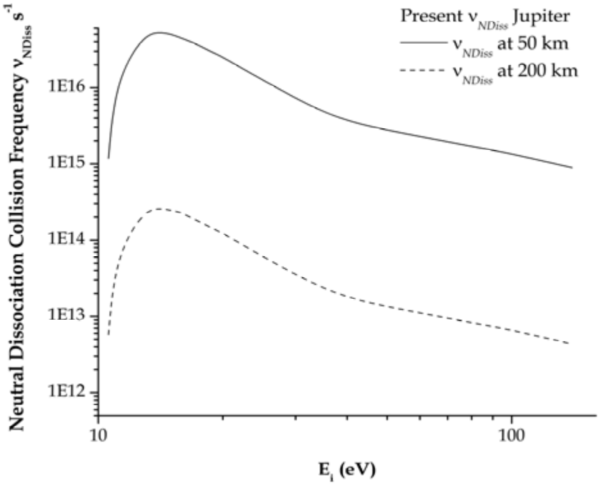

Fig. 3 Effective neutral dissociative collision frequency $<\nu_{NDiss}>$ for electron impact upon H_2 molecule in Jupiter's atmosphere: collision frequency at 50 km (solid line); collision frequency at 200 km (dashed line).

Fig. 3 shows the neutral dissociation collision frequency of electron impact upon H_2 molecule in Jupiter atmosphere. Effective $<\nu_{NDiss}>$, corresponding to two different altitudes of 50 and 200 km relative to ammonia clouds, is shown. Number densities of H_2 at respective altitudes are 1.7 E+14 per cc and 8.3 E+11 per cc [30]. The calculated frequency sharply peaks at about 14 eV at both altitudes.

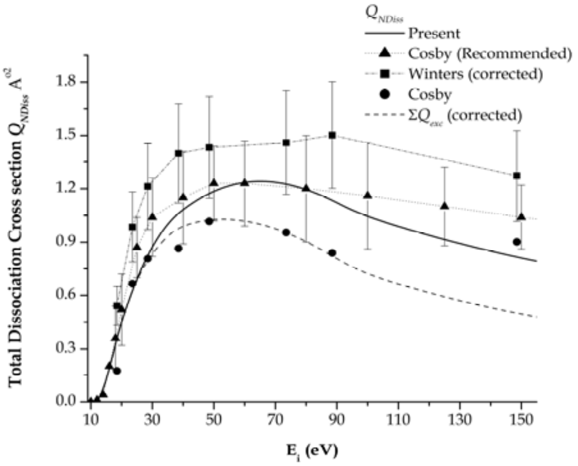

Fig. 4 Total Dissociation cross section for N_2: present Q_{NDiss} (solid line); Winters [5] (filled square); Cosby (recommended) [6] (filled triangle); Cosby (original) [6] (filled circle); ΣQ_{exc} (corrected) [dash].

Nitrogen Molecule

Now for electron impact on N_2, total dissociation cross sections Q_{NDiss} is calculated and obtained as mentioned in theoretical methodology section. Graphically these cross sections can be seen as is shown in Fig. 4. Solid line represents present values of Q_{NDiss}. Curve with dashed line indicate ΣQ_{exc}, obtained via *CSP-ic* method, corrected for emission cross sections. Winters' [5] original data contained ionization contribution and hence corrected for the dissociation cross section is shown by filled squares in Fig. 4. Cosby [6] has performed experiment for neutral dissociation of N_2. But owing to its lower values than winters'(filled circle) a recommended data set is given by Cosby [6] after considering the error involved in both the experiment is shown as filled triangle in Fig. 4.

N_2 molecule is the most profuse gaseous constituent not only in Earth's atmosphere but also in Saturn's satellite –Titan. N_2 is subjected to significant bombardment both by energetic electrons as in the case of aurora and by low energy photoelectrons produced in normal atmosphere [33, 34]. Thus role of neutral dissociation of N_2 cannot be neglected in the study of their atmospheric chemistry.

An estimate of number of neutral pair generated by electron impact having energy from excitation threshold to 140 eV is shown graphically in Fig. 5. Upper curve with solid line shows effective collision frequency of electrons with ~5.6E+9/cc N_2 molecule available at 1000 km altitudes of the Titan's atmosphere and dashed curve in the lower part shows similar profile for ~3.1E+8/cc N_2 molecules available at 1200 km altitudes of the Titan's atmosphere.

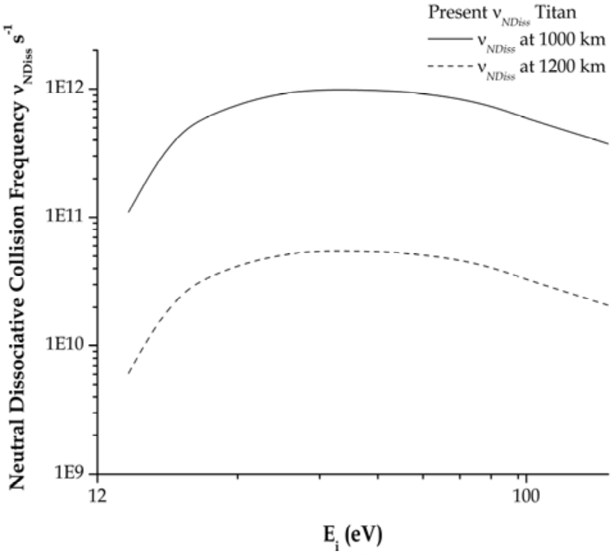

Fig. 5 Effective neutral dissociative collision frequency $<\nu_{NDiss}>$ for electron impact upon N_2 molecule in Titan's atmosphere: collision frequency at 1000 km (solid line); collision frequency at 1200 km (dashed line).

In case of effective collision frequency for N_2, a broad peak is observed as compared to a sharp profile for H_2 as shown in the Fig. 3. This difference arises due to the dissociative ionization. For H_2 the dissociative ionization has very small contribution in low energy region [9] where as for N_2 there is a significant contribution from dissociation ionization above 30 eV, which effectively broadens the distribution as seen from Fig. 5.

CONCLUSION

We conclude that the key finding of the present paper is neutral pair production rate via dissociation of atmospheric molecule H_2 and N_2 upon electron impact, either via externally precipitated electrons or photoelectrons. Maximum neutral pair production rate in Jupiter's atmosphere is 5.38E+16 pairs per sec at 50 km altitude and 2.6E+14 pairs per sec at 200 km altitude and it occurs for electrons having 14 eV energy. In case of the Titan, the corresponding values are 9.92E+11 pairs per sec at 1000 km altitude and 5.49E+10 pairs per sec at 1200 km altitude for electrons having 40 eV energy. These frequencies depend on the respective cross sections of electron impact and on the number density at respective altitudes. The errors involved in the present theoretical estimates in collision frequencies are at least of the order of respective experimental data employed in deducing the cross sections. Further we have not taken into account the recombination of H^+ giving neutral H, after dissociative ionization equation (3). A true picture of neutral atom production rate can emerge if one also considers the photo-dissociation of the molecules in the respective environments.

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REFERENCES

[1] Herzberg, G. (1950) *Molecular spectra and molecular structure*, *Spectra of Diatomic Molecules*, New York: Van Nostrand Reinhold.

[2] Chung,S. Lin, C. C. and Edward Lee, T. P. (1975) Dissociation of the hydrogen molecule by electron impact, *Phys. Rev.* A **12:** 1340.

[3] Zipf, E. C. (1984) *Dissociation of Molecules by electron impact, in Electron- Molecule interaction and their applications*, Vol. **1**, Edited by L. G. Chrostophorou, p.365, Academic Press.

[4] Chung, S. and Lin, C. C. (1978) Application of the close-coupling method to excitation of electronic states and dissociation of H_2 by electron impact, *Phys. Rev.* A **17:** 1874.

[5] Winters, H. F. (1966) Ionic adsorption and dissociation cross section for nitrogen, *J. Chem. Phys.* **44:** 1472.

[6] Cosby, P. C. (1993) Electron-impact dissociation of nitrogen, *J. Chem. Phys.* **98:** 9544

[7] Zipf E. C. and McLaughlin, R. W. (1978) On the dissociation of nitrogen by electron impact and by E.U.V. photo-absorption, *Planet. Space. Sci.* **26:** 449.

[8] Ajello, J. M. James, G. K. Frenklin, B. O. and Shemansky, D. E. (1989) Medium- resolution studies of extreme ultraviolet emission from N_2 by electron impact: vibrational perturbations and cross sections of the $c^1\Sigma_u^+$ and $b^1\Sigma_u^+$ states, *Phys. Rev.* A **40:** 3524.

[9] Yoon, J. Song, M. Han, J. Hwang, S. Chang, W. Lee, B. (2008) Cross sections for electron collision with hydrogen molecules, *J. Phys. Chem. Ref. Data* **37:**

[10] Corrigan, S. J. B. (1965) Dissociation of molecular hydrogen by electron impact, *J. Chem. Phys.* **43:** 4381.

[11] Burke, P. G. and Berrington, K. A. (1993) *Atomic and Molecular Processes- An R-matrix Approach,* Bristol Institute of physics publishing, Bristol.

[12] Burke, P. G. and Tennyson, J. (2005) R-matrix theory of electron molecule scattering, *Mol. Phys.* **103:** 2537.

[13] Tennyson,J. Brown, D. B. Munro, J. Rozum, I. Varambhia, H. and Vinci, N. (2007) Quantemol-N: an expert system

for performing electron molecule collision calculations using the R-matrix method *Journal of Physics:* Conference Series **86:** 012001 http;//www.quantemol.com.

[14] NIST Computational Chemistry Comparison and Benchmark Database, NIST Standard Reference Database Number 101 Editor: Russell D. Johnson III http://srdata.nist.gov/cccbdb/ and reference therein.

[15] Tennyson, L. A. J. and Gillan, C. J. (1998) The UK molecular R-matrix codes, *Comput. Phys. Commun.* **114:** 120.

[16] K. L. Schuchardt et al, (2007) Basis set exchange: A community database for computational sciences, *J. Chem. Inf. Model.* **47:** 1045.

[17] Khakoo, M. A. and Trajmar, S. (1986) Electron impact excitation of the $a^3\Sigma_g^+$, $B^1\Sigma_u^+$, $c^3\Pi_u$ and $C^1\Pi_u$ states of H_2, *Phys. Rev.* A **34:** 146.

[18] Khakoo, M. A. Trajmar, S. Mcadams, R. and Shyn, T. W. (1987) Electron excitation cross section for the $b^3\Sigma_u^+$ state of H_2, *Phys. Rev.* A **35:** 2832.

[19] Joshipura, K. N. Kothari, H. N. Shelat, F. A. Bhowmik P. and Mason, N. J. (2010) Electron scattering with metastable $H_2^*(c^3\Pi_u)$ molecules: ionization and other total cross sections, *J. Phys.* B **43:** 135207.

[20] Straub, H. C. Renault, P. Lindsay, B. G. Smith, K. A. and Stebbings, R. F. (1996) Absolute partial cross section for electron-impact ionization of H_2, N_2 and O_2 from threshold to 1000 eV, *Phys. Rev.* A **54:** 2146.

[21] Gillan, C. J. Tennyson, J. McLaughlin, B. M. and Burke, P. G. (1996) Low-energy electron impact excitation of nitrogen molecule- optically forbidden transitions, *J. Phys.* B **29:** 1531.

[22] Joshipura, K. N. Gangopadhyay, S. Kothari, H. N. and Shelat, F. A. (2009) Total electron scattering and ionization of N, N_2 and metastable excited $N_2^*(A^3\Sigma_u^+)$: Theoretical cross sections, *Phys. Lett.* A **373:** 2876.

[23] Joshipura, K. N. and Gangopadhyay, S. (2008) Electron collisions with sulfur compounds SO, SO_2 and SO_2AB (A, B = Cl, F): various total cross sections, *J. Phys.* B **41:** 215205.

[24] Joshipura, K. N. Vaishnav, B. G. and d Gangopadhyay, S. (2007) Electron impact ionization cross-sections of plasma relevant and astrophysical silicon compounds: SiH_4, Si_2H_6, $Si(CH_3)_4$, SiO, SiO_2, SiN and SiS, *Int. J. Mass. Spectrom* **261:** 146.

[25] Ajello, J. M. and Shemansky, D. E. (1985) A re-examination of important N_2 cross section by electron impact with application to the airglow: The Lyman-Birge-Hopfield band system, *J. Geophys. Res.* **90:** 9845.

[26] Shemansky, D. E. Ajello, J. M. and Kanik, I. (1995) Electron excitation function of the N_2 second positive system, *Astrophys. J.* **452:** 472.

[27] Lindsay, B. G. and Mangan, M. A. (2003) *Photon and electron interaction with atom molecules and Ions*, Landolt-Bornstein Vol **1**/17, Subvolume C, Edited by Y. Itikawa, Springer, New York.

[28] Shkarofsky, I. P. (1961) Values of the transport coefficients in a plasma for any degree of ionization based on a Maxwelllian distribution, *Can. J. Phys.* **39:** 1619.

[29] Itikawa, Y. (1971) Effective collision frequency of electrons in atmospheric gases, *Planet. Space Sci.***19:** 993.

[30] Atreya, S. K. Donahue, T. M. Festou, amd M. C. (1981) Jupiter: *Structure and composition of the upper atmosphere*, *The Astrophys. J.* **247:** L43.

[31] Brown, R. H. Lebreton, Hunter Waite, J. J. (2010) *Titan from Cassini-Huygens* Springer, Dordrecht, ISBN 978-1-4020-9214-5.

[32] Nishimura, H. and Danjo, A. (1986) Differential cross section of electron scattering from molecular Hydrogen.II. $B^3\Sigma_u^+$ excitation *J. Phys. Soc. Japan* **55:** 3031.

[33] Fox, J. L. and Victor, G. A. (1988) Electron energy deposition in N_2 gas, *Planet. Space Sci.* **36:** 329.

[34] Strobel, D. F. Meier, R. R. Summers, M. E. and Strikland, D. J. (1991) Nitrogen airglow sources: Comparison of Triton, Titan, and Earth, *Geophys. Res. Lett.* **18:** 689.

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