International Journal of Engineering and Management Research
www.ijemr.net
e-ISSN: 2250-0758 | p-ISSN: 2394-6962
Volume-12, Issue-3 (June 2022)
https://doi.org/10.31033/ijemr.12.3.29

Total Ionization Cross Sections due to Electron Impact of Ammonia from Threshold to 10 MeV

Pramod Kumar[1], Amrita[2], Yogesh Kumar[3], Lalit Kumar[4] and Kiran Pal[5]
[1]Department of Physics, Vardhman College, Bijnor, INDIA
[2]Department of Physics, D.A.V. College, Muzaffarnagar, INDIA
[3]Department of Physics, D.A.V. College, Muzaffarnagar, INDIA
[4]Department of Physics, D.A.V. College, Muzaffarnagar, INDIA
[5]Department of Physics, D.A.V. College, Muzaffarnagar, INDIA

[2]Corresponding Author: amritaiitd@yahoo.com

ABSTRACT

In the present paper, we have employed modified Khare-BEB method [Atoms, (2019)] to evaluate total ionization cross sections by the electron impact for ammonia in energy range from the ionization threshold to 10 MeV. The theoretical ionization cross sections have been compared to the available previous theoretical and experimental results. The collision parameters dipole matrix squared M_j^2 and C_{RP} also have been calculated. The present calculations were found in remarkable agreement with the available experimental results.

PACS: 34.50

Keywords-- Collision, Cross Section, Electron-Impact Ionization

I. INTRODUCTION

The total ionization cross sections of molecules due to electron impact are not only important to understand the basic collision mechanism but also in wide range of practical applications, for example the modelling of semi conduction manufacturing by plasma processing needs ionization cross sections of molecules used as the ideal gas. Furthermore, the ionization cross sections are needed in various research areas such as atmospheric physics, astrophysics, radiation physics etc. As we know conventional technologies are powered by fossil fuel exploitation that creates expensive environmental concerns, hydrogen may be replacement of fossil fuels which is also a carbon free energy carrier but its storage for long distance transportation remains a challenge. Ammonia may be used as indirect hydrogen storage and transportation links to make it an accessible fuel source. Furthermore, ammonia is identified as a promising sustainable fuel for solid oxide fuel cells. These fuels release less toxic gas on burning in the internal combustion engine, during combustion of fuel in car engine, plasma is produced. The ionization cross section is needed for modelling of car engine. In industries, ammonia is required as source of nitrogen to fabricate nitride films and also used to create the $N_2 - H_2$ plasma. This molecule is detected in the interstellar space medium and also in the atmosphere of planets in the solar system, where it plays important role in the chemistry of environments. Thus electron impact ionization cross sections of ammonia have an importance and needed in various fields [1-6].

Bederski et al. [7] have reported experimentally the partial ionization cross sections for production of ions NH_3^+, NH_2^+, NH^+, H^+ and N^+ from NH_3 and get the total cross sections by summing all partial ionization cross sections. Rao & Srivastava [8] have measured the cross sections by using crossed electron beam-molecular beam collision geometry with 15% uncertainty in their experiment. Mark et al. [9] measured the ionization cross sections by using double focussing spectrometer.

Rejoub et al. [10] have measured the partial ionization cross sections in group of ions. They have used a time-of-flight mass spectrometer and detected with a position-sensitive detector whose output shows that all product ion species are collected with equal efficiency irrespective of their initial kinetic energies. At relativistic energies, we have only one experimental data set, which was measured by Reike and Prepejchal [11] in terms of two collision parameters, dipole matrix squared M_j^2 and $C_{RP,}$ in energy range .1-27 MeV. Recently Kumar and Kumar [12] calculated the ionization cross sections for considered molecule.

II. THEORY

In the modified Khare-BEB model [12], the electron impact ionization cross section of a molecule for j_{th} molecular orbital is given by

$$\sigma_{jT} = \sigma_{jM} + \sigma_{jB} + \sigma_{tj} \qquad (1)$$

where, Mott term (the ionization cross section due to the hard collision) σ_{jM} is given by

$$\sigma_{jM} = \frac{AN}{[E+I+U]I} \times \left[1 - \frac{2}{t+1} + \frac{t-1}{2t^2} + \frac{5-t^2}{2(t+1)^2} - \frac{1}{t(t+1)} - \frac{t+1}{t^2}\ln(\frac{t+1}{2}) \right] \qquad (2)$$

e-ISSN: 2250-0758 | p-ISSN: 2394-6962
Volume-12, Issue-3 (June 2022)
https://doi.org/10.31033/ijemr.12.3.29

where $t = E/I$, $E = \frac{1}{2}mc^2\left[1 - \frac{1}{1+\frac{T}{mc^2}}\right]$, $A = 4\pi a_0^2 R^2$.

The notations U, a_0, I, N, T, m, c and R represent the average kinetic energy of bound electron, the first Bohr radius, the ionization energy, the occupation number of molecular orbital, the kinetic energy of the incident electron, rest mass of electron, velocity of light and Rydberg energy, respectively. The Bethe cross-section σ_{jB} is

$$\sigma_{jB} = \frac{AN}{2[E+I+U]I}\left[\frac{1}{2}\left(1-\frac{1}{t^2}\right) - X\right] \quad (3)$$

where the term X is given by

$$X = 2ln\left(\sqrt{t} - \sqrt{(t-1)}\right) + \frac{1}{2t^2}\left\{\begin{array}{c} 1 - \frac{1}{2}\left(\frac{t}{t-\sqrt{t(t-1)}}\right)^2 \\ + \frac{1}{2}\left(\frac{t}{t+\sqrt{t(t-1)}}\right) - \left(\frac{t}{t-\sqrt{t(t-1)}}\right) \\ -\frac{3}{4}ln\left(\frac{t+\sqrt{t(t-1)}}{t-\sqrt{t(t-1)}}\right)\end{array}\right\}$$

and the cross section due to the transverse interaction is

$$\sigma_{tj} = -\frac{4\pi a_0^2 R}{E} M_j^2[\ln(1-\beta^2)+\beta^2] \quad (4)$$

where β is the ratio of the incident velocity v and the velocity of light c, M_j^2 represents the total dipole matrix squared measured in units of a_0^2 and given by

$$M_j^2 = \int_{I_j}^{E} \frac{R}{w}\frac{df_j(w,0)}{dw}dw \quad (5)$$

where the continuum optical oscillator strength (COOS)

per unit energy range $\frac{df_j(w,0)}{dw}$ is

$$\frac{df_j(w,0)}{dw} = \frac{NI_j}{w^2} \quad (6)$$

The expression of collision parameter for jth molecular orbit C_{jRP} is given by [9]

$$C_{jRP} = \frac{RE}{A}\sum_j(\sigma_{jB}+\sigma_{jM}) - {M_j}^2 ln\beta^2 \quad (7)$$

To evaluate total ionization cross section and collision parameters of molecule, the contributions come from all molecular orbital are added.

III. RESULTS AND DISCUSSION

The theoretical methods described in above section are employed to calculate the total ionization cross sections of ammonia. The required molecular parameters binding energies I, kinetic energies of bound electrons U and occupation numbers N are taken from reference [14].

The figure (1) depicts total ionization cross action due to electron impact of ammonia from ionization threshold to 10 keV along with available previous experimental data. A good agreement is found among the present calculation and experimental data those measured by Rejoub et al. [10] and Roa & Srivastava[8] over whole range of incident energy studied by them. The experimental results of Mark et al. [9] and Bedeski et al. [7] are lower than present values as well as other previous experimental and theoretical results and do not agree them. Our cross section and Kim-BEB calculations [14] are slightly greater then calculated values of Kumar-Kumar [12].

In the figure (2), depicts the present cross section along with the experimental data measured by of Reike and Prapejchal [11] have been shown. In energy range .1 MeV to 10 MeV. The present calculations are found in good agreement with the experimental data. The values of our calculated collision parameters C_{RP} and dipole matrix squared M_j^2 are 39.9 and 3.31 (in unit of a_0^2), respectively. On increasing the kinetic energy of incident electron this value remains nearly constant, which is according to expectation?

e-ISSN: 2250-0758 | p-ISSN: 2394-6962
Volume-12, Issue-3 (June 2022)
https://doi.org/10.31033/ijemr.12.3.29

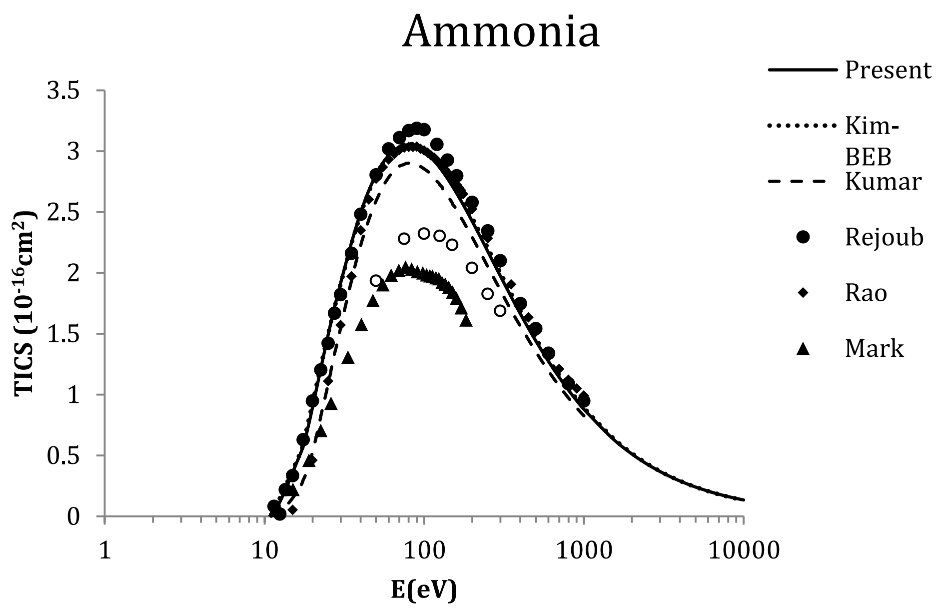

Figure 1: Total ionization cross sections (TICS) for ammonia in 10^{-16} cm^2. Solid line, dashed line, and dotted line are present results, theoretical results of Kumar & Kumar [12], and Kim-BEB calculations [14], respectively. Filled circles, filled rhombus, filled triangles and open circles are the experimental results of Rejoub et al. [10]. Rao and Srivastava [8], Mark et al. [9] and Bederski et al. [7] respectively

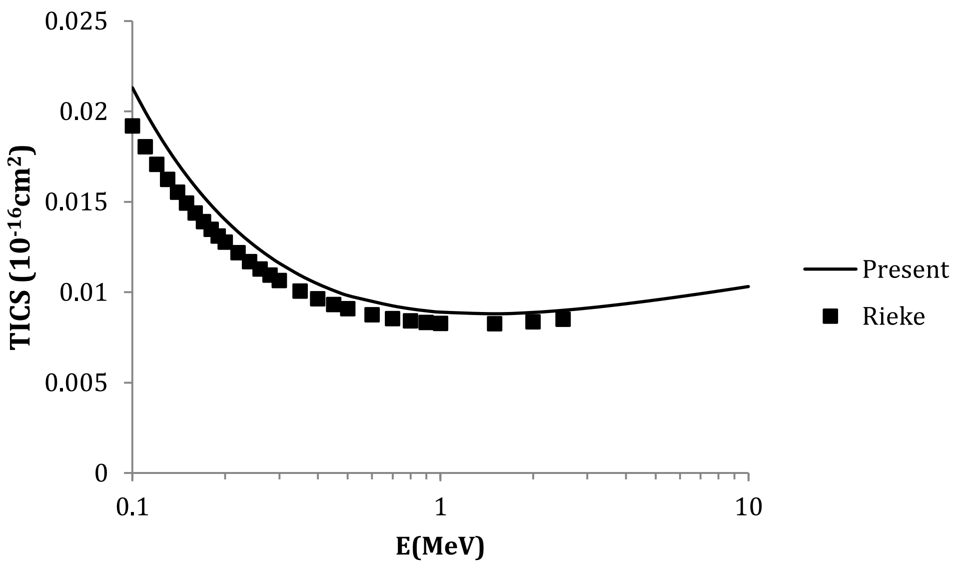

Figure 2: In this figure we compare the present total ionization cross sections in 10^{-16} cm^2 to experimental results of Rieke and Prepejchal (filled rectangles) [11] for ammonia at high energy range .1 MeV to 10 MeV

The calculated value of C_{RP} is greater that the experimental value (34.86) by 14.4 %, however present value of dipole matrix squared M_j^2 is lower than the experimental value (3.58) of Reike and Prapejchal [11] by 7.5%.

IV. CONCLUSION

Khare-BEB model is used to calculate the ionization cross action of ammonia from ionization threshold to 10 MeV. The present cross sections are found in the good agreement with available experimental data over most of incident energy range. The calculated

e-ISSN: 2250-0758 | p-ISSN: 2394-6962
Volume-12, Issue-3 (June 2022)
https://doi.org/10.31033/ijemr.12.3.29

values of parameters are also found in good agreement with the experimental values.

ACKNOWLEDGMENT

We are grateful to Dr Manoj Kumar, Meerut college, Meerut (India) for fruitful discussion and also thankful to principal, D.A.V. College, Muzaffarnagar, (India) for providing the facilities for research work.

REFERENCES

[1] W. Lindinger & F. Howorka. (1985). *Electron impact ionization*. eds. T. D. Mark, and Dunn, G. H. Berlin: Springer.
[2] G. Jeerh, M. Zhang & S. Tao. (2021). Recent progress in ammonia fuel cells and their potential applications. *J. Mater. Chem. A, 9*, 727-752.
[3] A. C. Cheung, D. M. Rank, C. H. Townes, D. D. Thornton, & W. J.Welch. (1968). *Phys. Rev. Lett. 21*, 1701.
[4] C. F. Mueller-Wodarg, D. F. Strobel, J. J. Moses, J. H.Waite, J. Crovisier, R. V. Yelle, S. W. Bougher & R. G. Roble. (2008). *Space Sci. Rev. 139*, 191.
[5] S. R. Federman & D. L. Lambert. (2002). *J. Electron Spectrosc. Relat. Phenom. 123*, 161.
[6] M. Sode, W. Jacob, T. Schwarz-Selinger & H. Kersten. (2015). *J. Appl. Phys. 4117*, 83303.
[7] K. Bederski, L. Wdjcik & B. Adamczyk. (1980). *International Journal of Mass Spcctrometry and Ion Physics*, *35*, 171.
[8] M. V. V. S. Rao & S. K. Srivastava. (1991). *Journal of Geophysical Research, 96*(17), 563.
[9] T. D. Märk, F. Egger & M. Cheret. (1977). *The Journal of Chemical Physics*, *67*, 3795.
[10] R. Rejoub, B. G. Lindsay & R. F. Stebbings. (2001). *J. Chem. Phys. 115*, 5053.
[11] F. R. Rieke & W, Prepejchal. (1972). *Phy. Rev. A 6*, 1507.
[12] Y. Kumar & M. Kumar. (2020). *Chem. Phys. Letter*, *740*, 137071.
[13] Y. Kumar, M. Kumar, S. Kumar & R. Kumar. (2019). *Atoms*, *7*, 60.
[14] https/www.nist.gov.