

# Differential Scattering Cross Section Calculations for Low Energy Electron Interaction with Polyatomic Nitrogen oxide ( $N_2O$ ) and Ozone ( $O_3$ ) Molecules

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**ABSTRACT:** In this paper, we calculated differential scattering cross section for low energy electron collision interaction with polyatomic Nitrogen oxide ( $N_2O$ ) and Ozone ( $O_3$ ) molecules. The rotational excitation electron impact differential cross sections (DCS) for polyatomic  $N_2O$  and  $O_3$  molecules are calculated, at low energy 5.0 eV, 7.5 eV and 10 eV. respectively. The Born Eikonal Series Approximation method and the hard sphere dipole interaction potential model are employed in the present investigation. The present DCS results obtained in angular range ( $0^\circ$  to  $180^\circ$ ) are compared with experimental and other theoretically calculated results. The present results are found better than as compared results.

**KEYWORDS:** Hard sphere dipole potential, Differential cross section, Born Eikonal Series Method.

## I. INTRODUCTION

The electron-molecule collisions are not only of fundamental interest but of immense importance for many applications. For example, a detailed knowledge of these processes is required for plasma physics, laser physics, atmospheric and interstellar models, stellar atmospheres, isotope separation, MHD power generation, electric discharges and radiation physics and chemistry. The increased interest in the subject has been stimulated experimentally by the availability of electron beams with milli volt energy and the need for data for plasma modelling, particularly in relation to plasma etching. Calculations of cross-sections and other parameters for electron collisions with polyatomic molecules are considerably more difficult than the analogous studies with atomic targets. This is due both to the loss of symmetry in molecular systems and the much greater difficulty in representing the target wave function. In addition molecules have vibrational and rotational degrees of freedom which can be excited by electron impacts. It is therefore not surprising that calculations of electron polyatomic-molecule impacts are often much cruder than their electron atom counterparts. However, many of the successes achieved in electron molecule scattering have used ideas originally developed for atoms. A comprehensive survey of computational methods for electron molecule collisions can be founded in Ref.[1]. The Ozone  $O_3$  is key species for atmospheric study. The  $N_2O$  is an important species in the upper atmosphere, which plays a role in ozone destruction.  $N_2O$  lasers are also of interest. In both cases, electron collisions play an important role, though data on the various collision processes remain fairly scarce.[2,3]

The main goal this work is to provide absolute values rotational excitation differential cross section (DCS) for electron- interaction with polyatomic for polyatomic  $N_2O$  and  $O_3$  molecules at low energy 5 eV, 7 eV, 7.5 eV and 10 eV. in angular range (0 to 180). The Born Eikonal Series (BES) Approximation method and hard sphere dipole interaction potential model is employed for present calculations. The hard sphere cut-off parameter "a" is considered as "D/2", where "D" is dipole moment of molecule.[6,7] The present DCS results are compared with the results of Varella M.T. et-al [7,8] and available experiment data. It is found that the present results are in good agreement with those of compared results.

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## II. METHODOLOGY

In order to take into account somewhat higher terms of Born series, one can use Eikonal approximation. Ashihara et-al [6] employed Glauber formulation in Eikonal approximation for electron dipole collisions. They calculated cross section for strongly polar molecules. Although this approximation is originally a high energy approximation, it has been applied successfully to the low energy electron atom collision (Gerjuoy et-al [5]). In the present investigations an attempt is made to employ Born Eikonal Series (BES) method for the cross sectional calculations for the low energy electron polyatomic molecule collision [6].

The interaction potential  $V(r)$  can be expressed in following form,

$$V(\underline{r}) = -2eq \sum_{n=odd} \frac{r_{<}^n}{r_{>}^{n+1}} P_n(\hat{r}, \hat{s}) \quad \text{--- (1)}$$

Where  $r_{>}$  and  $r_{<}$  are the larger and the smaller of  $r$  and  $P_n(\hat{r}, \hat{s})$  is the Legendre polynomial of the order- $n$ . "a" is the parameter which indicates finiteness of the dipole and related to the dipole moment by the relation  $D = 2aq$ . Taking  $n = 1$  only one can get the expression for electron finite dipole interaction potential and it is employed in cylindrical polar co-ordinate, one can name a linear dipole model. In the present investigation following form of the interaction dipole potential is employed [5,6].

$$V(\underline{r}, \hat{s}) = V(\underline{b}, z) = 0 \quad \text{for } z < a \quad \text{--- (2)}$$

$$V(\underline{r}, \hat{s}) = V(\underline{b}, z) = -\frac{D}{b^2 + z^2} P_1(\underline{r}, \hat{s}) \quad \text{for } z > a \quad \text{--- (3)}$$

Where, "a" - is the hard sphere parameter (cut-off parameter).

The formula for the Eikonal phase shift function  $\chi(b)$  is given by,

$$\chi(b) = \frac{2D\gamma}{ki} \int_a^\infty \frac{zdz}{(b^2 + z^2)^{3/2}} \quad \text{--- (4)}$$

' $\gamma$ ' - is the direction cosine of the dipole axis with respect to the polar axis. A series expansion of scattering amplitude as given by,

$$f_{E1} = \frac{2D\gamma}{\Delta \exp(a\Delta)} \quad \text{---- (5)}$$

$$f_{E2} = \frac{2iD^2\gamma^2}{ki} k_0(a\Delta) \quad \text{---- (6)}$$

$$f_{E3} = \frac{4}{3} \frac{D^3\gamma^3}{ki} \frac{e^{-a\Delta}}{a} \quad \text{---- (7)}$$

Where  $K_0(a\Delta)$  - is a Bessel function,  $\Delta = |ki - kf|$  is momentum transferred. The differential cross section (DCS) for three terms in Born Eikonal Series Approximation can be expressed as follow,

$$\frac{d\sigma}{d\Omega}(j_0 m_{j_0} \rightarrow j m_j; \theta) = \frac{kf}{ki} |f_{E1} + f_{E2} + f_{E3}|^2 \quad \text{--- (8)}$$

Summing over  $m_j$  and averaging over  $m_{j_0}$  one gets the DCS for the rotational transition  $j_0 \rightarrow j_0 + l$ . Differential Scattering cross-section (DCS):-

$$\frac{d\sigma}{d\theta} = \frac{ki}{kf} \left[ \frac{4A^2}{\Delta^2 e^{2a\Delta}} \left\{ \frac{j_0 + 1}{3(2j_0 + 1)} \right\} + \frac{16}{9} \frac{A^6}{ki^4} \frac{e^{-2a\Delta}}{a^2} * \left\{ \frac{6}{175} \frac{(j_0 + 2)(j_0 + 1)j_0}{(2j_0 + 5)(2j_0 - 1)(2j_0 + 1)} + \frac{3}{25} \frac{(j_0 + 1)}{(2j_0 + 1)} \right\} \right]$$

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$$-\frac{16}{3} \frac{A^4}{ki^2} \frac{e^{-2a\Delta}}{a\Delta} \left\{ \frac{(j_0 + 1)}{5(2j_0 + 1)} \right\} \quad \text{---- (9)}$$

Where  $A = mDe/h^2$

### III. RESULTS AND DISCUSSION

The main interest of the present work is to discuss rotational excitation differential scattering cross-section (DCS) for electron collision with polyatomic N<sub>2</sub>O molecules at energy 5 eV., 7.5 eV respectively and for O<sub>3</sub> molecule, the energy is taken as 7 eV., 10 eV. respectively. The rotational excitation differential cross-sections are calculated using Born Eikonal Series (BES) approximation method and employed hard sphere dipole interaction potential model. The hard sphere parameter is taken as “a” = D/2, where D-is dipole moment of respective molecules. The present results are compared with theoretical results of Varrella M.T. et-al [8,9]

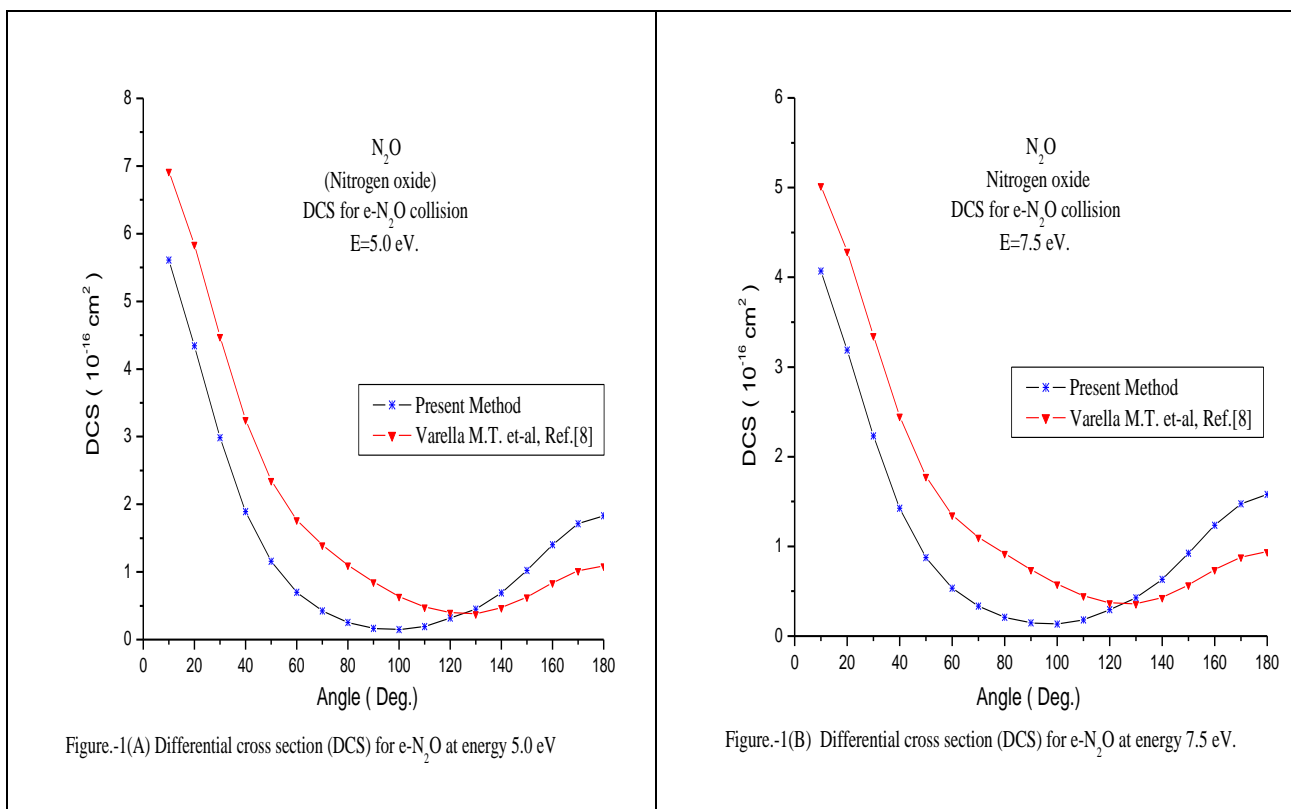


Figure-1(A) shows the angular distribution curve of DCS results, calculated for electron scattering by polyatomic N<sub>2</sub>O molecule at energy 5.0 eV, using BES method and considering hard sphere dipole interaction potential model. The hard sphere parameter “a” is considered as a= D/2, where D-is dipole moment of concerned molecule. The present results are compared with theoretical results of Varrella M.T. et-al [8,9]. As shown in the figure-1(A), present DCS results are found sharply decreases at scattering angle from 5° to 60° and above from 60° to 110° the present DCS are decreases smoothly, Than, they become minimum at scattering angle  $\theta = 110^\circ$  afterward they are increases slowly up to scattering angle 180°. The present results are found slightly lower than as compare with the results of Varrella M.T. et-al [8,9] in the angular range between 5° to 110°, the present results become minimum at angle 110° and they are found comparable agreement with the results of Varrella M.T. et-al [8,9] in angle between 110° to 140°,

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but at higher scattering angle from 140° to 180°, the present results are slightly higher than those of Varrella M.T. et-al [8,9]. The present DCS results using BES method for hard sphere dipole potential are overall in good agreement in with results of Varrella M.T. et-al [8,9].

Figure-1(B) shows the angular distribution curve of DCS results, calculated for electron scattering by polyatomic N<sub>2</sub>O molecule at energy 7.5 eV, using present method. The present results are compared with theoretical results of Varrella M.T. et-al [8,9]. As shown in the figure-1(B), present DCS results are found sharply decreases at scattering angle from 5° to 60° and above from 60° to 100° the present DCS are decreases smoothly, Than, they become minimum at scattering angle  $\theta = 100^\circ$  afterward they are increases slowly up to scattering angle 180°. The present results are found slightly lower than as compare with the results of Varrella M.T. et-al [8,9] in the angular range between 5° to 100°, the present results become minimum at angle 100° and they are found comparable agreement with the results of Varrella M.T. et-al [8,9] in angle between 90° to 130°, but at higher scattering angle from 130° to 180°, the present results are slightly higher than those of Varrella M.T. et-al [8,9]. In general, the present DCS results are found in good agreement in with Varrella M.T. et-al [8,9].

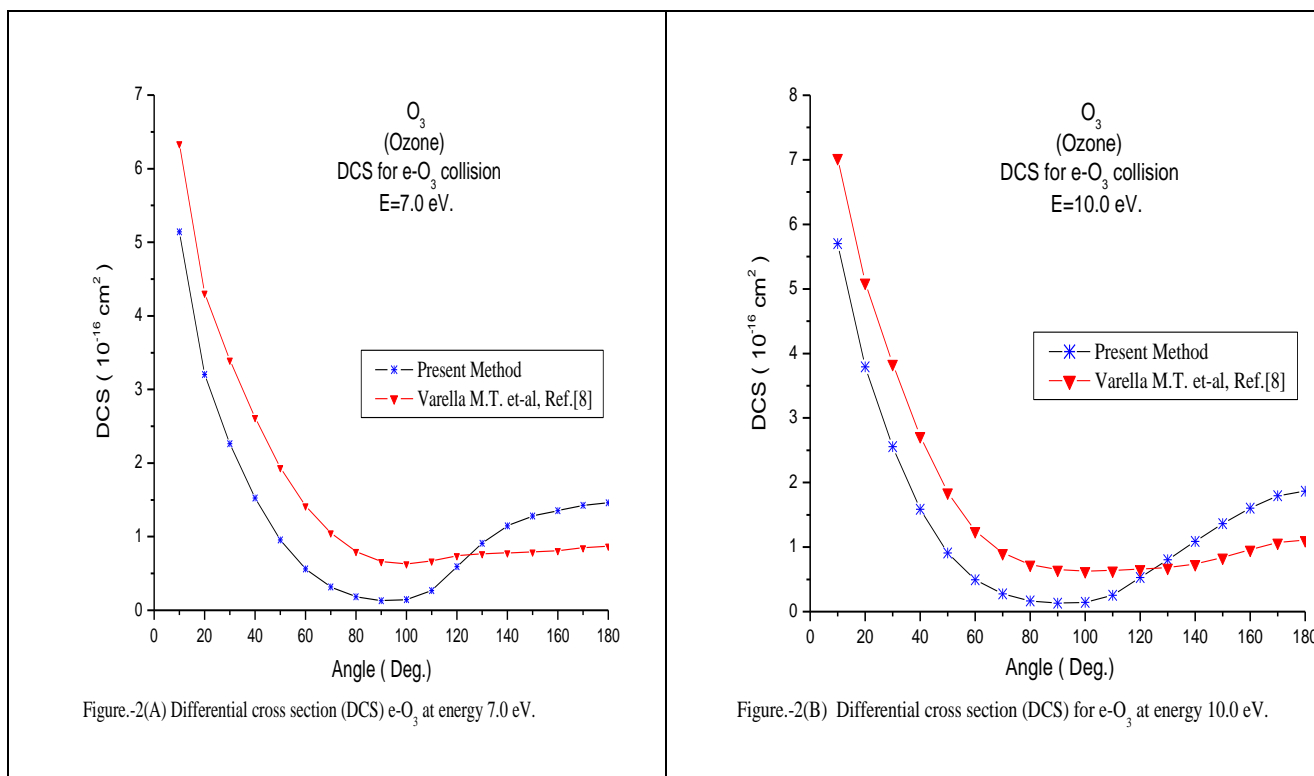


Figure-2(A) shows the angular distribution curve of DCS results, calculated for electron scattering by polyatomic O<sub>3</sub> molecule at energy 7.0 eV, using BES method. The present results are compared with theoretical results of Varrella M. T. et-al [8,9]. The present results are found to be decreasing at scattering angle from 5° to 90° than, they become minimum at scattering angle  $\theta = 95^\circ$  afterward they increase slowly up to scattering angle 180°. The present results are found comparable agreement with those of Varrella M.T. et-al [8,9] results at the angle between 5.0° to 140°. The present DCS results are in comparable agreement with the results of Varrella M.T. et-al [8,9]. In general, qualitative agreement is observed between the present and those of compared results.

Figure-2(B) shows the angular distribution curve of DCS results, calculated for electron scattering by polyatomic O<sub>3</sub> molecule at energy 10.0 eV, using present method.. The present results are compared with theoretically calculated

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results of Varrela M.T. et-al [8,9]. As shown in the figure-2(B), present DCS results are found sharply decreases at scattering angle from  $5^\circ$  to  $40^\circ$  and above from  $40^\circ$  to  $90^\circ$  the present DCS are decreases smoothly, Than, they become minimum at scattering angle  $\theta = 90^\circ$  afterward they are increases slowly up to scattering angle  $180^\circ$ . The present DCS results are found with good agreement with those of Varrela M.T. et-al [8,9] results

## IV. CONCLUSION

The present work reports on the calculations of differential cross section (DCS) in angular range (0 to  $180^\circ$ ) for electron impact, rotational transitions ( $0 \rightarrow 1$ ) for polyatomic  $N_2O$  molecules collision at low energy 5.0 eV and 7.5 eV respectively, whereas for  $O_3$  molecule at low energy 7.0 eV and 10.0 eV. respectively. We have employed the Born Eikonal Series (BES) Approximation method and the hard sphere dipole interaction potential model is taken for present electron-molecule collision. The Ozone  $O_3$  is key species for atmospheric study. The  $N_2O$  is an important species in the upper atmosphere which plays a role in ozone destruction.  $N_2O$  lasers are also of interest. In both cases, electron collisions play an important role, though data on the various collision processes These DCS data can be helpful to provide understanding and behaviour of  $N_2O$  &  $O_3$  in they used in manufacturing semiconductor devices and other application. This method is well established for obtaining cross section with reasonable accuracy. The present results may be improved by taking higher term of BES method. Using the present theory and assumption, one could find stability of concern polyatomic molecules from its DCS data. Therefore we have confidence that the methodology may be used to improve the molecular data base. Such data set is needed in a variety of applications in atomic & molecular physics and chemistry. We are quite sure that present work will be inspiring researchers in those fields.

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