

International Journal of Innovative Research in Science, Engineering and Technology

(An ISO 3297: 2007 Certified Organization)

Vol. 4, Issue 8, August 2015

Low Energy Electron Impact Differential Scattering Cross Section Calculations for Polyatomic CHF₃ Molecule

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ABSTRACT: In this paper we calculated differential scattering cross section for low energy electron collision interaction with polyatomic Trifluoromethane (CHF₃). The electron collision processes will be helpful to understanding the behaviour of CHF₃ in its use in manufacturing semiconductor devices and other application. CHF₃ is used for plasma etching of silicon compounds for microelectronics fabrication, and so there is interest in developing computer models for plasmas sustained in CHF₃. Recent measured data have provided a sufficient basis to develop the electron impact differential cross section set for CHF₃. The rotational excitation electron impact differential cross sections (DCS) for polyatomic CHF₃ molecule are calculated, at low energy 1.5eV, 5.0eV and 7.0eV. 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 to 180) are compared with experimental and other theoretically calculated results. The present results are found better than as compared results.

KEYWORDS: Dipole potential, differential scattering cross section, Born Eikonal Series Method.

I. INTRODUCTION

Trifluoromethane, CHF₃, is plasma processing and greenhouse gas due to the global warming potential. CHF₃ is a gas extensively used in the microelectronics industry for etching of silicon compounds.[1–3] As a result, there is great interest in developing reaction mechanisms for gas mixtures containing CHF₃ for use in computer models of plasma processing reactors. Recent reviews and assessments of fundamental data [4] and recent measurements of electron swarm data in CHF₃ have provided sufficient background that a working low energy electron impact differential cross section (DCS) for polyatomic CHF₃ molecule. In this article, the rotational excitation electron impact differential cross sections (DCS) for polyatomic CHF₃ molecule are calculated, at low energy 1.5eV, 5.0eV and 7.0eV. in angular range (0 to 180). The cross section data will be used in a model of a plasma etching reactor and results for plasma densities.

The main goal this work is to provide absolute values rotational excitation differential cross section (DCS) for electron-CHF₃ at low energy 1.5eV, 5.0eV and 7.0eV. 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], Morgan W.L. et-al [8] and available experiment data (Varella M.T., phys. Rev.). It is found that the present results are in good agreement with those of compared results.

II. METHODOLOGY

In order to take into account somewhat higher terms of Born series, one can use Eikonal approximation. Ashihara et-al [5] 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). In the present investigations an

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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,

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

' γ ' - 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 $j_0 \rightarrow j_0 + 1$.

Differential Scattering cross-section (DCS):-

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

Where $A = mDe / \hbar^2$

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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 CHF_3 molecules at energy 1.5eV., 5.0eV and 7.0eV 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 Varrela M. T. et-al [10] and Morgan W. L. et-al [8] and experimental results of Ref.[9,11]

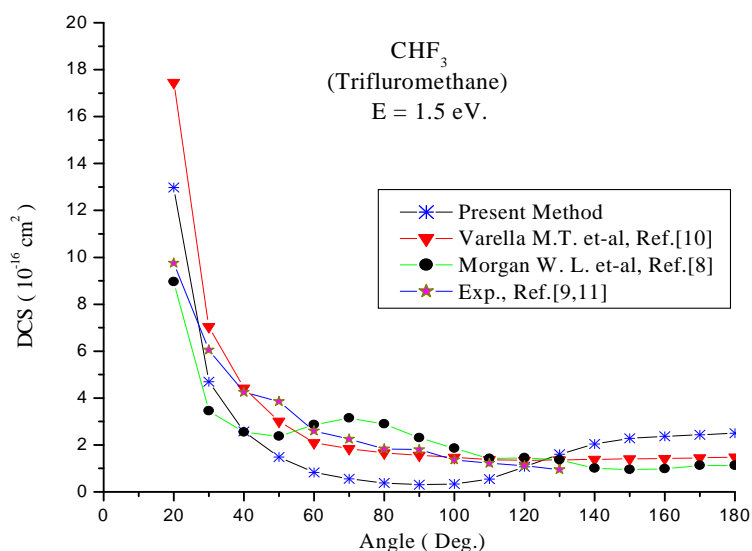


Figure:-1. Differential Cross Section(DCS) for e- CHF_3 collision at energy 1.5eV.

Figure-1 shows the angular distribution curve of DCS results, calculated for electron scattering by polyatomic CHF_3 molecule at energy 1.5 eV, using BES method and considering hard sphere dipole interaction potential model. The hard sphere parameter “a” is taken as $a = D/2$, where D-is dipole moment of concerned molecule. The present results are compared with theoretical results of Varrela M. T. et-al [10] and Morgan W. L. et-al [8] and experimental results of Ref.[9,11]. As shown in the figure-1, present DCS results are found sharply decreases at scattering angle from 5° to 40° and above from 40° to 90° the present DCS are decreases smoothly, Than, they become minimum at scattering angle $\theta = 95^\circ$ afterward they are increases slowly up to scattering angle 180° . The present results are in good agreement with those of Morgan W. L. et-al[8] results at the angle between 5° to 40° , but above 40° they differ appreciably. The present results are found comparable agreement with those of Varrela M. T. et-al [10] results at the angle between 40° to 110° but at higher scattering angle from 110° to 180° , the present results are slightly higher than those of Varrela M. T. et-al [10] and Morgan W. L. et-al [8] results. The present DCS results of BES method for hard sphere dipole potential are in good agreement in with Varrela M. T. et-al [10] and Morgan W. L. et-al [8] and experimental results of Ref.[9,11].

Figure-2 shows the angular distribution curve of DCS results, calculated for electron scattering by polyatomic CHF_3 molecule at energy 5.0 eV, using BES method and considering hard sphere dipole interaction potential model. The hard sphere parameter “a” is taken as $a = D/2$. The present results are compared with theoretical results of Varrela M. T. et-al [10] and Morgan W. L. et-al [8] and experimental results of Ref.[9,11]. The present BES 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° .

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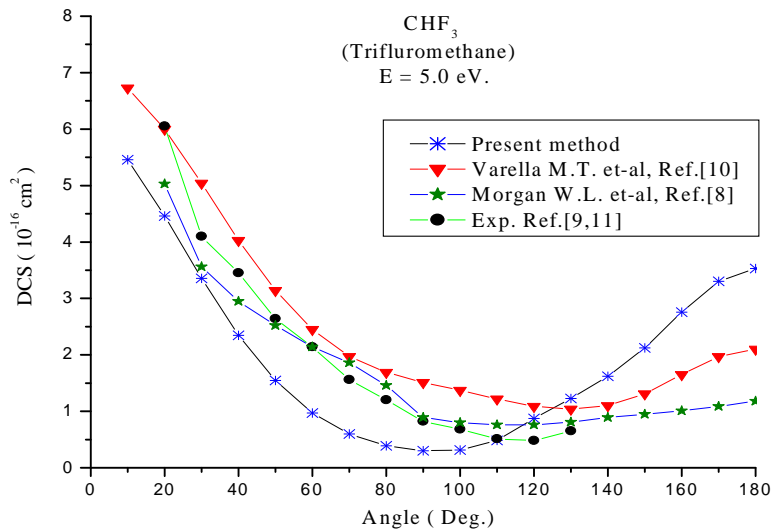


Figure:-2. Differential Cross Section(DCS) for e- CHF_3 collision at energy 5.0eV.

The present results are found comparable agreement with those of Varrela M. T. et-al[10] results at the angle between 5.0° to 40° but at higher scattering angle from 40° to 110° , the present results are slightly lower than those of Varrela M. T. et-al[10] and Morgan W. L. et-al[8] results. The present DCS results are in better agreement with the results of Varrela M. T. et-al[10] and Morgan W. L. et-al[8] and experimental results of Ref.[9,11]. In general, qualitative agreement is observed between the present and those of compared results.

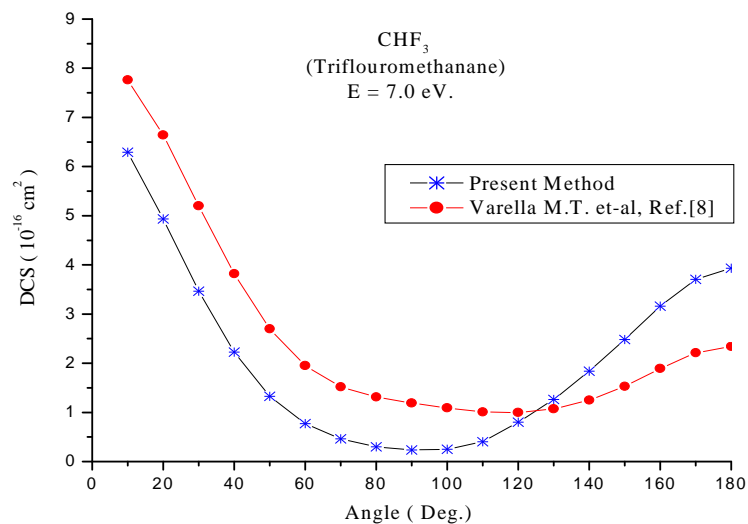


Figure:-3. Differential Cross Section(DCS) for e- CHF_3 collision at energy 7.0eV.

Figure-3 shows the angular distribution curve of DCS results, calculated for electron scattering by polyatomic CHF_3 molecule at energy 7.0 eV, using BES method and considering hard sphere dipole interaction potential model. The hard sphere parameter "a" is taken as $a = D/2$. The present results are compared with theoretically calculated results of Varrela M. T. et-al [10]. As shown in the figure-3, present DCS results are found sharply decreases at

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scattering angle from 5° to 40° and above from 40° to 90° the present DCS are decreases smoothly, Than, they become minimum at scattering angle $\theta = 95^\circ$ afterward they are increases slowly up to scattering angle 180° . The present DCS results are found with good agreement with those of Varrelá M. T. et-al [10] results

IV. CONCLUSION

The present work reports on the calculations of differential cross section (DCS) in angular range (0 to 180°) for electron impact, rotational transitions ($0 \rightarrow 1$) for polyatomic CHF_3 molecules collision at low energy 1.5eV, 5.0eV and 7.0eV. 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. These DCS data can be helpful to provide understanding and behaviour of CHF_3 in its use 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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