

Differential Scattering Cross Section Calculations for Low Energy Electron Interaction with Polyatomic Methyl chloride (CH_3Cl) and Methyl fluoride (CH_3F) Molecules

Jayantilal G. Raiyani¹

Associate Professor, Department of Physics, Shri M. M. Science College, Morbi, Gujarat, India¹

ABSTRACT: In this paper, we report the differential scattering cross section for low energy electron interaction with polyatomic Methyl chloride (CH_3Cl) and Methyl fluoride (CH_3F) molecules. The rotational excitation electron impact differential cross sections (DCS) for polyatomic Methyl chloride (CH_3Cl) and Methyl fluoride (CH_3F) molecules are calculated, at low energy 5.0 eV and 7.0 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° to 180°) are compared with experimental and other theoretically calculated results. The present results are found to be quite remarkable agreement with those of compared results.

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

I. INTRODUCTION

Methyl chloride is used mainly in the production of silicones. CH_3Cl is also used in the production of agricultural chemicals, methyl cellulose, quaternary amines, butyl rubber and starting material in the manufacture of such chemicals as methyl mercaptan, methylene chloride, chloroform, carbon tetrafluoride. Due to concerns about its ozone-depleting potential, it is no longer present in refrigerators. Low levels of methyl chloride occur naturally in the environment. Higher levels may occur at chemical plants where it is made or used. Acute (short-term) exposure to high concentrations of methyl chloride in humans has caused severe neurological effects. Methyl chloride has also caused effects on the heart rate, blood pressure, liver, and kidneys in humans. Chronic (long-term) animal studies have shown liver, kidney, spleen, and central nervous system (CNS) effects. Inhalation studies have demonstrated that methyl chloride causes reproductive effects in male rats, with effects such as testicular lesions and decreased sperm production. Human cancer data are limited. It has classified methyl chloride as a Group D carcinogen. In semiconductor manufacturing, methyl fluoride (CH_3F) is used in plasma etching of silicon compound films. Methyl fluoride CH_3F and methyl chloride CH_3Cl molecules play a potential role in the depletion of the Earth's protective ozone layer and all are active greenhouse gases. In addition they are also important in the chemical industry, for example, in semiconductor etching, as refrigerants, and as methylating agents.

The low energy 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 The 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.[1,2].

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The main goal in this work is to provide absolute values rotational excitation differential cross section (DCS) for electron- interaction with polyatomic for polyatomic methyl chloride (CH₃Cl) and methyl fluoride (CH₃F) molecules at low energy 5 eV. and 7.0 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 [8,9] calculated using the Schwinger multichannel method with norm-conserving pseudo potentials.and available experiment data. 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 [4]). 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 [5,6,7].

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

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

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 K₀(a Δ) - 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,

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

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):-

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

Where $A = mDe/h^2$

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 methyl chloride (CH_3Cl) and methyl fluoride (CH_3F) molecules at energy 5.0 eV. and 7.0 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 Varrela M.T. et-al [8,9] calculated using the Schwinger multichannel method with norm-conserving pseudo potentials.

Figure-1 shows the angular distribution curve of present DCS results, calculated for electron scattering by polyatomic methyl chloride (CH_3Cl) 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 Varrela M.T. et-al [8,9] calculated using the Schwinger multichannel method with norm-conserving pseudo potentials. . As shown in the figure-1, the present DCS results are found sharply decreases at scattering angle from 10° to 70° and above from 70° to 110° the present DCS are decreases smoothly, Than, these become minimum around the scattering angle $\theta = 90^\circ$ afterward they are increases slowly up to scattering angle 180° . The present results are found slightly lower than as compare with the results of Varrela M.T. et-al [8,9] in the angular range between 5° to 110° , the present results become minimum at angle 90° and they are found comparable agreement with the results of Varrela M.T. et-al [8,9] in angle between 10° to 120° , but at higher scattering angle from 120° to 180° , the present results are slightly higher than those of Varrela 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 Varrela M.T. et-al [8,9].

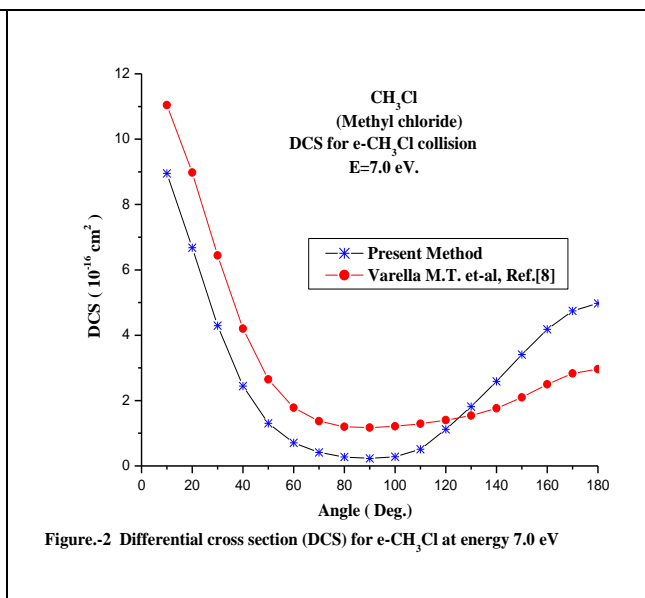
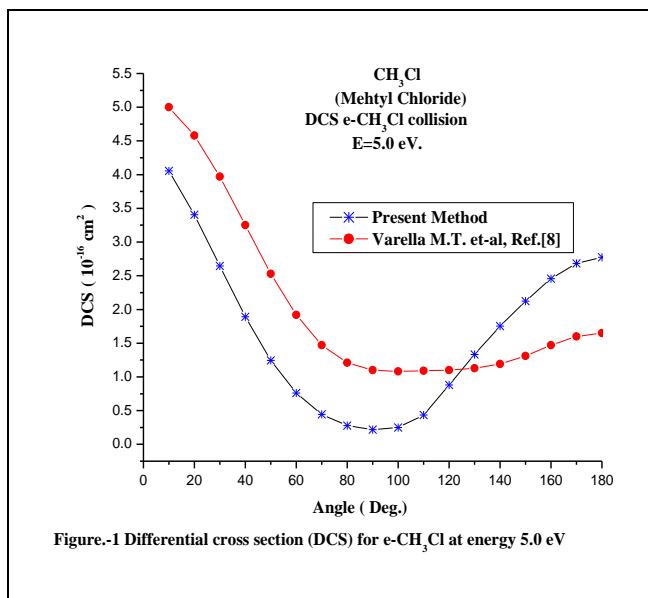


Figure-2 shows the angular distribution curve of DCS results, calculated for electron scattering by polyatomic methyl chloride (CH₃Cl) molecule at energy 7.0 eV, using present method. The present results are compared with theoretical results of Varrella M.T. et-al [8,9]. As shown in the figure-2, present DCS results are found sharply decreases at scattering angle from 10° to 50° and above from 50° to 110° 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°. 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 120°, the present results are found quite comparable agreement with the results of Varrella M.T. et-al [8,9] in angular range between 10° to 120°, but at higher scattering angle from 120° 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].

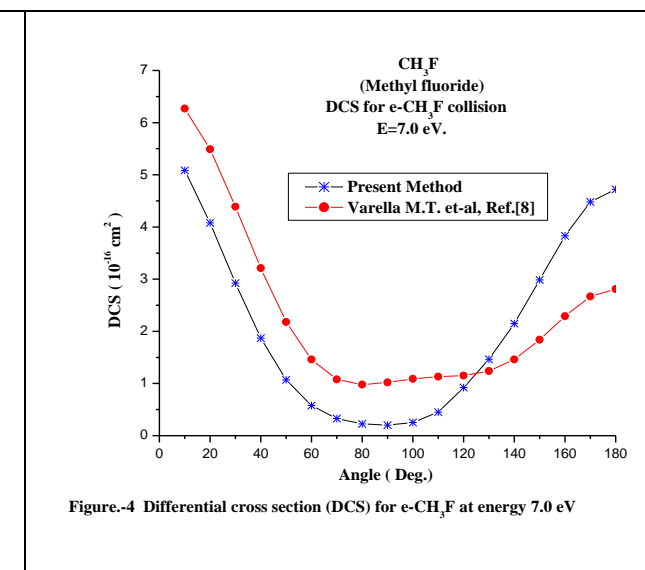
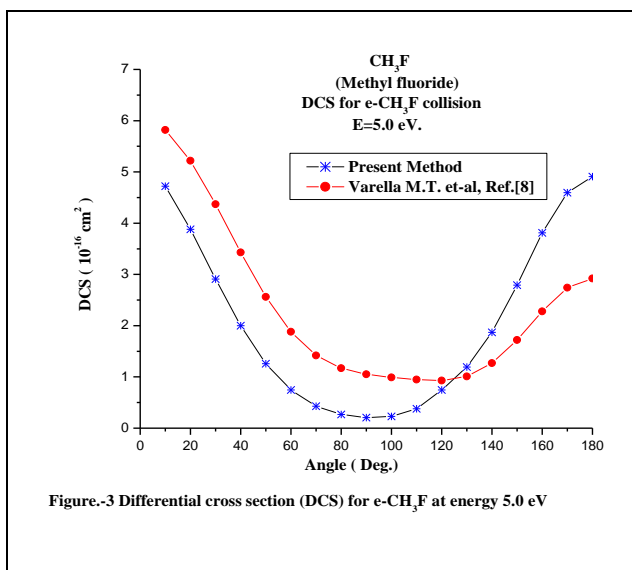


Figure-3 shows the angular distribution curve of DCS results, calculated for electron scattering by polyatomic methyl fluoride (CH₃F) molecule at energy 5.0 eV, using BES method. The present results are compared with

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theoretical results of Varrela 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 Varrela 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 Varrela M.T. et-al [8,9]. In general, qualitative agreement is observed between the present and those of compared results.

Figure-4 shows the angular distribution curve of DCS results, calculated for electron scattering by polyatomic methyl fluoride (CH_3F) molecule at energy 7.0 eV, using present method.. The present results are compared with theoretically calculated results of Varrela M.T. et-al [8,9]. The present DCS results are found sharply decreases at scattering angle from 10° to 60° and above from 60° to 110° the present DCS are decreases smoothly, Than, they become minimum at scattering angle $\theta = 80^\circ$ afterward they are rapidly increases up to scattering angle 180° . 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°) for electron impact, rotational transitions ($0 \rightarrow 1$) for polyatomic methyl chloride (CH_3Cl) and Methyl fluoride (CH_3F) molecules at low energy 5.0 eV and 7.0 eV respectively. We have employed the Born Eikonal Series (BES) approximation method and the hard sphere dipole interaction potential model for present electron-molecule collision. The electron collisions with those molecules play an important role, for many applications in plasma physics, atmospheric and interstellar models, stellar atmospheres, radiation physics, biophysics and chemistry. These DCS data can be helpful to provide understanding and behaviour of methyl chloride (CH_3Cl) and Methyl fluoride (CH_3F) molecules. 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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