

Electron Impact Total Cross Section for Polyatomic Molecules CH_3OH , CH_3CHO and CH_3CN Detected In Interstellar Space

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ABSTRACT: One of the most exciting aspects of the astrophysics is the continued discovery of the wide range of molecular species. The polyatomic molecules like as CH_3OH , CH_3CHO and CH_3CN detected in interstellar space matter have been covered in present study. In this paper, we report a theoretical study on electron scattering by polyatomic molecules in the low-energy range. The rotational excitation total cross sections (TCS) are calculated for electron scattering by polyatomic interstellar space molecules like as CH_3OH , CH_3CHO and CH_3CN at the energy from 0.5eV. to 16.5eV. The Born Eikonal Series (BES) Approximation method is employed for present calculation and using the hard sphere dipole interaction potential model for electron-molecule interaction. The results obtained for present calculation are compared with experiment and theoretical data available in the literature.

KEYWORDS: Hard sphere dipole potential, Born Eikonal Series method, Total cross section

I. INTRODUCTION

The space between two stars is known as the interstellar space and matter existing therein is called the interstellar matter. One of the most exciting aspects of the astrophysics is the continued discovery of the wide range of molecular species. The polyatomic interstellar gas molecules detected have been covered in present study. The study of these molecules may show that throw more light on the formation of star and the cooling of interstellar gas. If there are exist free electrons, then their collisions with interstellar gas molecules might be an important mechanism to cool the interstellar gas. Recently, polyatomic molecules like as CH_3OH , CH_3CHO and CH_3CN have been detected interstellar space from the interpretation of spectral data. So it is necessary to consider electron collision with polyatomic molecules like as CH_3OH , CH_3CHO and CH_3CN in present study. In the study of e-HCN collision under interstellar condition, Saha et-al calculated rotational excitation total cross section in low energy range by using the close coupling method and compared the results with those due to First Born Approximation in the above calculations they used the point dipole potential model.[1-4]

In present investigation, the rotational excitation total cross sections (TCS) are calculated for electron scattering by polyatomic molecules like as CH_3OH , CH_3CHO and CH_3CN detected interstellar space. The total cross sections (TCS) are calculated at the energy from 0.5 to 16.5eV. 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.[5-7] The present results are compared with theoretical the results of Desai H.S et-al.[7] using FBA finite dipole potential model. In general the present TCS results for polyatomic interstellar space molecules like as CH_3OH , CH_3CHO and CH_3CN at the energy range from 0.5 to 16.5eV. are found in good agreement with those of compared results.

II. METHODOLOGY

BORN EIKONAL SERIES METHOD (BES)

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

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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 collisions (Gerjuoy; 1971). In the present investigations an attempt is made to employ Born Eikonal Series method for the cross sectional calculations for the low energy electron interstellar gas molecule collision.

The interaction potential $V(r)$ can be expressed in following form,[7]

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

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.[7]

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

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

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

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

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

' γ ' is the direction cosine of the dipole axis with respect to the polar axis.

A series expansion of scattering amplitude as give by,

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

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

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

Where $K_0(a\Delta)$ - is a Bessel function, $\Delta=|k_i - k_f|$ 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 $j_0 \rightarrow j_0 + 1$. Therefore using the standard formula, one can calculate the expression for the TCS which will be as follows

$$\begin{aligned} Q_{j_0, j_0+1} &= \frac{2D^2}{ki^2} \left\{ \frac{4(j_0 + 1)}{3(2j_0 + 1)} \right\} \int_{|ki-kf|}^{|ki+kf|} \frac{e^{-2a\Delta}}{\Delta} d\Delta \\ &+ \frac{32D^6}{9ki^6 a^2} \left\{ \frac{6(j_0 + 2)(j_0 + 1)j_0}{175(2j_0 + 5)(2j_0 - 1)(2j_0 + 1)} \right. \\ &+ \left. \frac{3(j_0 + 1)}{25(2j_0 + 1)} \right\} \left[\frac{\exp[-2|ki+kf|a]}{4a^2} \{-2a(ki+kf) - 1\} \right. \\ &- \left. \frac{\exp[-2|ki-kf|a]}{4a^2} \{-2a|ki-kf| - 1\} \right] \\ &+ \frac{16D^4}{3ki^4 a^4} \left\{ \frac{j_0 + 1}{5(2j_0 + 1)} \right\} [\exp[-2|ki+kf|a] - \exp[-2|ki-kf|a]] \end{aligned} \quad \text{--- (9)}$$

III. RESULTS AND DISCUSSION

Aim of the present study is to obtain theoretical the rotational excitation total cross sections (TCS) are calculated for low energy electron scattering by polyatomic molecules like as CH_3OH , CH_3CHO and CH_3CN detected interstellar space. In the present calculations, the energy range of electron is taken from 0.5 to 16.5eV. The Born Eikonal Series (BES) Approximation method and hard sphere dipole interaction potential model is employed for present calculation. The hard sphere cut-off parameter "a" is considered as $D/2$, D-is the dipole moment of molecule.

Fig.-1: show the rotational excitation total cross sections (TCS) results for e- CH_3OH in the energy from 0.5 to 16.5eV. Due to non availability of experimental data, the present TCS results are compared with the results of Desai H.S et-al.[7] using FBA method for finite dipole potential model. As shown in fig.-1, it is found that present TCS results decrease sharply at low energy 0.5 to 3.0 eV. But at higher energy it decreases slowly. Present results are in good agreement in shape of curves, but differ in magnitude and slightly increasing in magnitude with results of Desai H.S et-al.[7] In general the present results are found better than in the agreement with the results of Desai H.S et-al.[7]

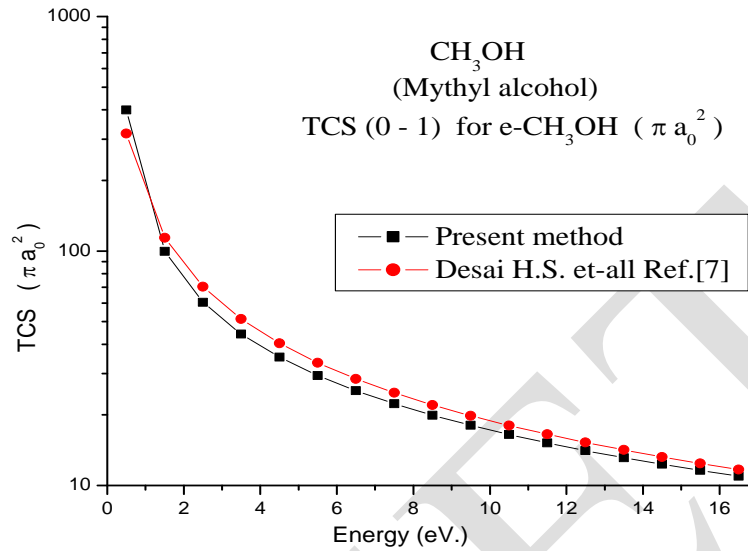


Fig:-1 Total cross section (TCS), for $e\text{-CH}_3\text{OH}$

Fig-2: show the rotational excitation total cross sections (TCS) results for $e\text{-CH}_3\text{CHO}$ in the energy range from 0.5 to 16.5eV. The present TCS results are found with sharp decrement at low energy (0.5 to 3.0eV) region and comparable with the results of Desia H.S. et-al.[7] At higher energy 3.0 to 16.5eV, it decreases slowly. The present TCS results for $e\text{-CH}_3\text{CHO}$ at energy range from 3.0 to 16.5 eV. are found higher than results of Desai H.S et-al.[7] In general the present TCS results for interstellar gas polyatomic molecules CH_3CHO at low energy range are found in good agreement with those of compared results.

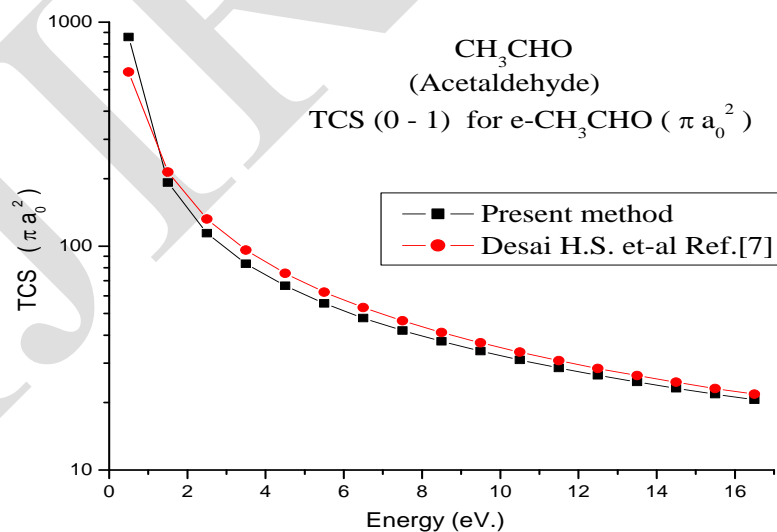


Fig:-2 Total cross section (TCS), for $e\text{-CH}_3\text{CO}$

Fig-3: show the rotational excitation total cross sections (TCS) results for $e\text{-CH}_3\text{CN}$ in the energy range from 0.5 to 16.5eV. The present TCS results are found with sharp decrement at low energy (0.5 to 3.0eV) region. At higher energy it decreases slowly. The present TCS results for $e\text{-CH}_3\text{CN}$ at energy range from 0.5 to 16.5 eV. are found

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better than results of Desai H.S et-al.[7] In general the present TCS results for interstellar gas polyatomic molecules like as CH_3OH , CH_3CHO and CH_3CN at low energy range are found in good agreement with those of compared results.

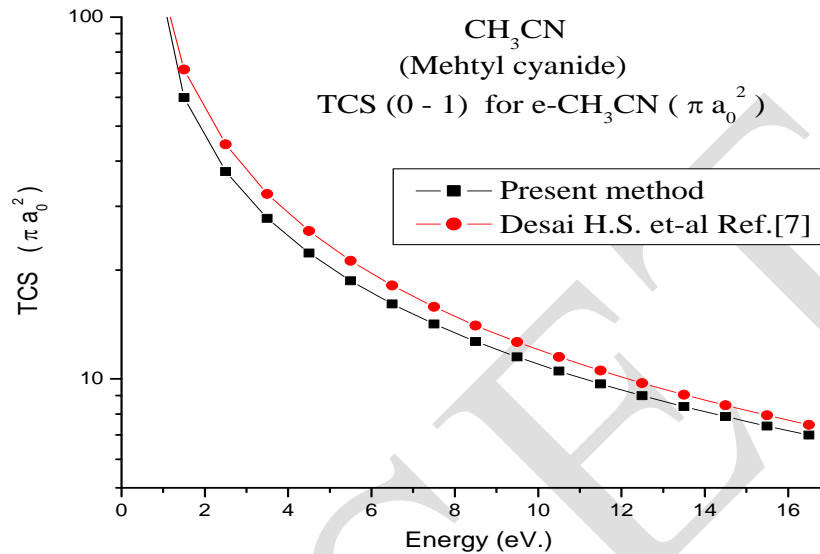


Fig:-3 Total cross section (TCS), for $e\text{-CH}_3\text{CN}$

IV. CONCLUSION

In this work, we have reported a theoretical study of low-energy electron collision with polyatomic molecules like as CH_3OH , CH_3CHO and CH_3CN are detected interstellar space. The total cross sections (TCS) are calculated using BES method and hard sphere dipole potential model. The rotational excitation total cross section (TCS) results are presented in comparison with some existing theoretical results.[7] The present results are in general good agreement with the measured data. This good agreement supports the description of the interaction dynamic considered in the present study and methods used for solving the scattering equations. Hence it will be worthwhile to use hard sphere dipole potential model in Born Eikonal Series (BES) for better to study of electron- interstellar gas molecules collision process in low energy region. The present results may be improved to consider higher terms in present method.

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