

# Low Energy Electron Impact Momentum Transfer Cross Section Calculations for Polyatomic Molecules Detected in Comets and their Atmosphere

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**ABSTRACT:** The rotational excitation momentum transfer cross section (MTCS) for low energy electron collision with polyatomic molecules detected in Comets and their atmosphere has been calculated. The polyatomic cometary's molecules groups like HCN, SO<sub>2</sub>, H<sub>2</sub>CO, HC<sub>3</sub>N, CH<sub>3</sub>OH and CH<sub>3</sub>CHO, CH<sub>3</sub>CN, NH<sub>2</sub>CHO, HCOOH, HOOCH<sub>3</sub> are consider for present study. The Born Eikonal Series Approximation method and the hard sphere dipole interaction potential model are employed in the present investigation. The electron impact rotational excitation momentum transfer cross sections are calculated for these molecules in the energy range (0.5-16eV.). The results obtained are compared with available data and to examine the effect of dipole moment on the momentum transfer cross section (MTCS) for low energy electron collision.

**KEYWORDS:** Ccomet's molecules, Dipole potential, Momentum transfer cross section

## I. INTRODUCTION

Comets contain some of the oldest and most pristine materials in our Solar System. Understanding their unique chemistry could reveal much about the birth of our planet and the origin of organic compounds that are the building blocks of life. ALMA's high-resolution observations provided a tantalizing 3D perspective of the distribution of the molecules within comets and their atmospheres.

Atacama Large Millimetre/submillimeter Array (ALMA) has made incredible 3D images of the ghostly atmospheres surrounding comets ISON and Lemmon. These new observations provided important insights into how and where comets forge new chemicals, including intriguing organic compounds A study of the comet's organic materials "will help us to understand whether organic molecules were brought by comets to the early earth," which could have kick-started life here, said Stephan Ulamec, the Philae lander manager and scientist at the German Aerospace Center. Researchers had to find organic molecules on the comet, known as 67P/Churyumov-Gerasimenko. But thanks to the probe, they are for the first time able to direct search for organic molecules in both the comet's gases and its surface material.

The most important exciting aspects of the astrophysics is the continued discovery of the wide range of molecular species. In the present study, we report on the polyatomic molecules detected in comet and their atmosphere. Infrared and microwave spectroscopic observation of comets Austin, Hale-Bopp, Hyakutake, Borrelly, Ikeya-Seki, Helley, Swift-tuttle, Temple-1&2 and Wild-2 detected diatomic, triatomic and polyatomic molecules. They are most considerable interest founded in different types of interstellar clouds and these molecules are of interest of Bioscientists. The study of electron collision with these molecules may provide important information on the formation of non-volatile grains, cooling gases of comet and physical properties of ices relevant to comets.[1-4]

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In the study of e-HCN collision under space condition, Saha et-al<sup>5</sup> calculated rotational excitation total cross-section in low energy range by using the Close-Coupling method and compared the results with those of due to First Born Approximation. In the above calculations they used the point dipole potential model .[5,6]

In present investigation rotational excitation momentum transfer cross-section (MTCS) for electron collisions with cometary molecules groups like HCN, SO<sub>2</sub>, H<sub>2</sub>CO, HC<sub>3</sub>N, C<sub>2</sub>H<sub>2</sub>, CH<sub>3</sub>OH and CH<sub>3</sub>CHO, CH<sub>3</sub>CN, NH<sub>2</sub>CHO, HCOOH, HOOCH<sub>3</sub> etc. are calculated, employing Born Eikonal series (BES) approximation method and using hard sphere dipole interaction potential model. For the present calculation, the energy range from 0.5 to 16.5 eV. are taken. The hard sphere cut-off parameter “a” is taken as “D/2”, where “D” is dipole moment of the molecule. [7,8]

## II. METHODOLOGY

In order to take into account some what higher terms of Born series, one can use Eikonal approximation. Ashihara et-al (1975) 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 collisions[9] (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 cometary molecule collision.

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

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

Where r<sub>></sub> and r<sub><</sub> are the larger and the smaller of r and P<sub>n</sub>(r,s) is the Legendre polynomial of the order n. “a” is the parameter which indicates finiteness of the dipole and it is related to the dipole moment by the relation D=2aq. Taking n = 1, one can get the expression for electron finite dipole interaction potential and it is formulated in cylindrical polar co-ordinate. Here it can be called a linear dipole model<sup>7</sup>.

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

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

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

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

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

Where, ‘γ’- is the direction cosine of the dipole axis with respect to the polar axis. A series expansion of scattering amplitude as give by,

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

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

$$f_{E3} = \frac{4}{3} \frac{D^9 \gamma^9}{ki} \frac{e^{-a\Delta}}{a} \quad (7)$$

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,

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

The expression for the momentum transfer cross section “ $Q^m$ ” (MTCS) for rotational transition  $j \rightarrow j_0+1$ , in atomic units is given by,

$$\begin{aligned} Q^m_{j_0, j_0+1} = & \frac{4D^2}{ki^3 kf} \left\{ \frac{j_0+1}{3(2j_0+1)} \right\} \left[ \frac{\exp[-2(ki+kf)a]}{4a^2} \{-2a(ki+kf)-1\} \right. \\ & - \frac{\exp[-2|ki-kf|a]}{4a^2} \{-2a|ki-kf|-1\} \left. \right] \\ & + \frac{16D^6}{9a^2 ki^7 kf} \left[ \frac{6(j_0+2)(j_0+1)j_0}{175(2j_0+5)(2j_0-1)(2j_0+1)} + \frac{3(j_0+1)}{25(2j_0+1)} \right] \\ & \left[ \frac{\exp[-2(ki+kf)a]}{16a^4} \{-8(ki+kf)^3 a^3 - 12(ki+kf)^2 a^2 \right. \\ & - 12(ki+kf)a - 6\} - \frac{\exp[-2|ki-kf|a]}{16a^4} \{-8|ki-kf|^3 a^3 \\ & - 12|ki-kf|^2 a^2 - 12|ki-kf|a - 6\} \left. \right] + \frac{16D^4}{3a ki^5 kf} \\ & \left\{ \frac{j_0+1}{5(2j_0+1)} \right\} \left[ \frac{\exp[-2(ki+kf)a]}{8a^3} \{4(ki+kf)^2 a^2 + 4(ki+kf)a + 2\} \right. \\ & - \frac{\exp[-2|ki-kf|a]}{8a^3} \{4|ki-kf|^2 a^2 + 4|ki-kf|a + 2\} \left. \right] \\ & - \frac{(ki-kf)^2}{2kikf} Q_{j_0, j_0+1} \end{aligned}$$

(In atomic unit) (9)

As  $a \rightarrow 0$ , the above equation reduces to that of point dipole potential.

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## III. RESULTS AND DISCUSSION

The aim of present study is that to obtain theoretical rotational excitation momentum transfer cross section (MTCS) for electron scattering by polyatomic molecules detected in comet and their atmosphere. The polyatomic molecules like HCN, SO<sub>2</sub>, H<sub>2</sub>CO, HC<sub>3</sub>N, CH<sub>3</sub>OH, CH<sub>3</sub>CHO, CH<sub>3</sub>CN, NH<sub>2</sub>CHO, HCOOH and HOOCH<sub>3</sub>. etc. are considered in present calculation. The Born Eikonal Series (BES) approximation method and hard sphere dipole interaction potential model is employed in low energy range from 0.5 to 16. eV. The hard sphere cut-off parameter “a” is considered as D/2, D-is the dipole moment of molecule.

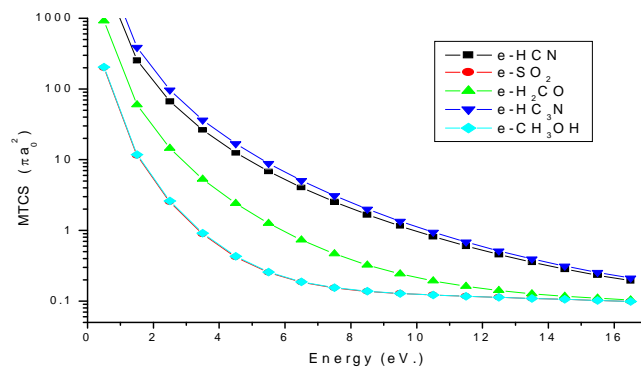


Figure 1. Momentum transfer cross section(MTCS) for e-HCN, SO<sub>2</sub>, H<sub>2</sub>CO, HC<sub>3</sub>N and CH<sub>3</sub>OH polyatomic cometary molecules collision

Figure.1 show the rotational excitation momentum transfer cross sections (MTCS) results for e-HCN, SO<sub>2</sub>, H<sub>2</sub>CO, HC<sub>3</sub>N and CH<sub>3</sub>OH scattering in the energy from 0.5 To16 eV. The present calculated MTCS results are shown graphically as in figure.-1. It is found that MTCS are sharply decreases at low energy from 0.5 to 4 eV, but at higher energy range from 4 to 16 eV, it decreases slowly. The magnitude of MTCS is shown significantly difference for polyatomic cometary molecules but the shape of energy distributed MTCS curve remains in same. The magnitude of momentum transfer cross section (MTCS) for cometary molecules are found in order of HC<sub>3</sub>N > HCN > H<sub>2</sub>CO > CH<sub>3</sub>OH > SO<sub>2</sub>

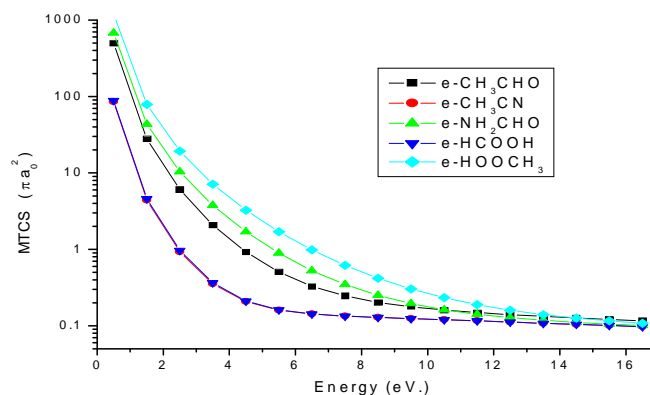


Figure 2. Momentum transfer cross section(MTCS) for e-CH<sub>3</sub>CHO,CH<sub>3</sub>CN, NH<sub>2</sub>CHO, HOOCH<sub>3</sub> and HCOOH<sub>3</sub> polyatomic cometary molecules collision

Figure.2 show the rotational excitation momentum transfer cross sections (MTCS) results for e-CH<sub>3</sub>CHO, CH<sub>3</sub>CN, NH<sub>2</sub>CHO, HCOOH and HOOCH<sub>3</sub> scattering in the energy from 0.5 To16 eV. The present calculated MTCS results are

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shown graphically as in figure.-2. It is found that MTCS are sharply decreases at low energy from 0.5 to 3.5 eV, but at higher energy range from 3.5 to 16 eV, it decreases slowly. The magnitude of MTCS is shown significantly difference for polyatomic molecules  $\text{CH}_3\text{CHO}$ ,  $\text{CH}_3\text{CN}$ ,  $\text{NH}_2\text{CHO}$ ,  $\text{HCOOH}$  and  $\text{HOOCH}_3$  are detected in comet and their atmosphere but the shape of energy distributed MTCS curve remains in same. The magnitude of momentum transfer cross section (MTCS) for cometary poly molecules are found in order of  $\text{CH}_3\text{CHO}$ ,  $\text{CH}_3\text{CN}$ ,  $\text{NH}_2\text{CHO}$ ,  $\text{HCOOH}$  and  $\text{HOOCH}_3$ .

As shown in figure.-1 and figure.-2, the magnitude of rotational excitation momentum transfer cross section (MTCS) for polyatomic comets molecules are found in order of  $\text{HC}_3\text{N} > \text{HCN} > \text{H}_2\text{CO} > \text{CH}_3\text{OH} > \text{SO}_2$  and  $\text{HOOCH}_3 > \text{NH}_2\text{CHO} > \text{CH}_3\text{CHO} > \text{HCOOH} > \text{HOOCH}_3$ . The same inequalities are found in the magnitudes of the dipole moments of the above molecules. So it can be shown that momentum transfer cross section (MTCS) increase with increase in dipole moment. So it can be concluded that MTCS increases with increase in dipole moment of the molecule. Hence it will be worthwhile to use hard sphere dipole potential model in Born Eikonal Series (BES) for better to study of electron-molecules collision process in low energy region

#### IV. CONCLUSION

The present work reports to calculated momentum transfer cross section (MTCS) for low energy electron impact, rotational transitions ( $0 \rightarrow 1$ ) for polyatomic molecules collision in the low energy range (0.5 to 16 eV.). 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. 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 MTCS 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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