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Low energy electron scattering by polar molecules H_2S, NH_3 and C_2H_6

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ABSTRACT

In this work we present theoretical study on electron collision with polar molecules in the low energy range, we report, the rotational excitation Differential scattering cross sections (DCS) calculated for electron scattering by polar molecules H_2S, NH_3 and C_2H_6 in the low energy range (5.0-10 eV.). The Born Eikonal Series (BES) approximation method and the hard sphere dipole interaction potential model are used to present electron-molecule interaction. The results obtained are compared with experiment and theoretical data available in the literature.

INTRODUCTION

The study of electron collision with the polar molecules is a very wide field of research. In particular, the collisions of electrons with polar molecules such as H_2S, NH_3, and C_2H_6 among others play an important role in several areas of investigation, mainly in atmospheric Physics, plasma physics, radiation biology, chemistry, astrophysics, biophysics, gaseous electronics, solar and planetary atmospheres, stellar –interstellar clouds and cometary bodies etc. Many of these molecules are plasma processing gases and some of there are also of environmental interest for being green house gases, or stratospheric ozone depleting gases. The importance is recognized as atmospheric pollutants and in connection with ozone depletion processes. Because of their industrial and environmental importance, the study of electron interactions with polyatomic molecules is very useful in the areas mentioned above.

We present a theoretical study of electron scattering by polar molecules in the low – energy range. The calculations are done for electrons scattering by polar molecules such as H_2S (Three atoms-polar molecule), NH_3 (Four atoms-polar molecule) and C_2H_6 (Eight atoms polar molecules). The rotational excitation Differential Scattering Cross Sections (DCS) of these molecules are calculated employing Born Eikonal Series (BES) approximation method and the hard sphere dipole interaction potential model is used for present calculation. The hard sphere cut-off parameter "a" is taken as "D/2", where "D" is dipole moment of the molecule[1,2].

FORMULATION

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 collision (Gerjuoy et-al). In the present investigations an attempt is made to

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employ Born Eikonal Series (BES) method for the cross sectional calculations for the low energy electron polyatomic molecule collision[2].

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

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

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[2].

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

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

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

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

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

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

A series expansion of scattering amplitude as given by,

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

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

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

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,

$$\frac{d\sigma}{d\Omega}(j_0 m_{j0} \rightarrow j m_j;\theta) = \frac{kf}{ki}\left|f_{E1}+f_{E2}+f_{E3}\right|^2 \quad (8)$$

Summing over m_j and averaging over m_{j0} one gets the DCS for the rotational transition $j_0 \rightarrow j_o + 1$. Differential Scattering cross-section (DCS):

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

Where $A = mDe / h^2$

RESULTS AND DISCUSSION

The main interest of the present work is to discuss rotational excitation differential scattering cross-section (DCS) for electron collision with polar molecules like H_2S, NH_3, and C_2H_6. 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. Present results are compared with theoretical results of Gianturco et al[3], Machado et al[5], Varella et al[6,7] and available experimental results. The differential scattering cross section (DCS) for each of these molecules is discussed separately below.

e-H_2S scattering

Figures 1 and 2 show present DCS results calculated for e-H_2S at energy 5.0 and 7.5 eV respectively, using BES hard sphere dipole potential model. The present results are compared with the results obtained using FBA point, finite dipole potential methods, Gianturco et al.[3] and Jain Thompson et al.[4], Machado et al.[5]. It is found that results of FBA point, finite dipole potential methods do not show appreciable difference. They are overlapping at lower angle. At higher angle, the results of FBA finite dipole potential are slightly lower than those of FBA point dipole potential. The FBA point, finite dipole potential results from 20° to 180° are in good agreement with the theoretical results of Gainturco et al.[3] and Jain & Thompson et al.[4] as compared with and Machado et al.[5]. But below 40°, the present BES results are in better agreement with the results of Gianturco et al.[3] and Jain & Thompson et al.[4], FBA results and Machado et al.[5]. Above 120°, the present BES results are in better agreement with

the results of Machado et al.[5]. In general, qualitative agreement is observed between the present and those of compared results.

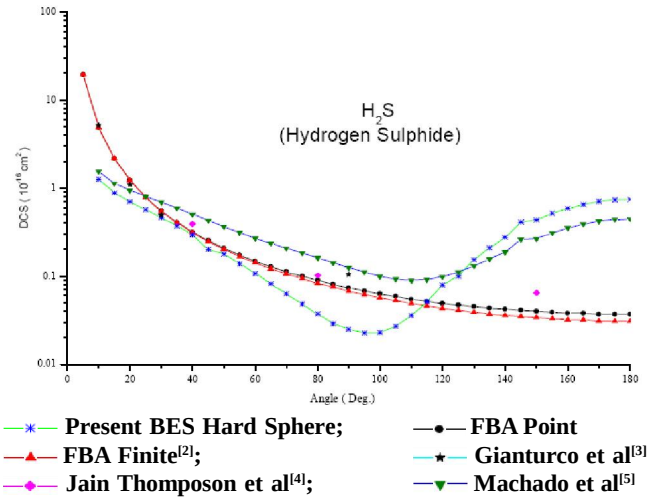

Figure 1 : DCS (0-1) for e-H_2S at energy 5.0 eV.

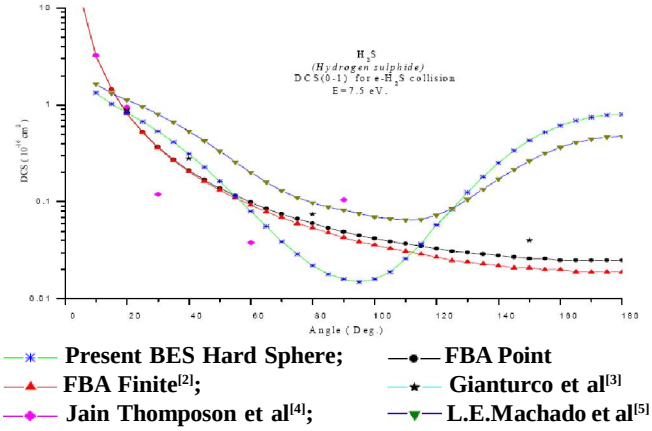

Figure 2 : DCS for electron scattering from H_2S at energy 7.5 eV.

e-NH_3 scattering

The present DCS results calculated for e-NH_3 collision at energy 10 eV, using BES hard sphere dipole potential method are shown in the figure 3. The present results are compared with the results obtained using FBA point, finite dipole potential methods and theoretical results of Machado et al.[5]. It is observed that present BES hard sphere dipole potential results are in good agreement with the theoretical results of Machado et al.[5].

e-C_2H_6 scattering

Figure 4 show our calculated DCS results for e-C_2H_6 at energy 10.0 eV., using BES hard sphere dipole potential method. The present results are compared with the theoretical results of Varella et al.[6,7]. It is found that the present results at smaller ($\theta < 40^o$) and higher ($\theta > 120^o$) scattering angles shows good agreement with results of Varella et al.[6,7].

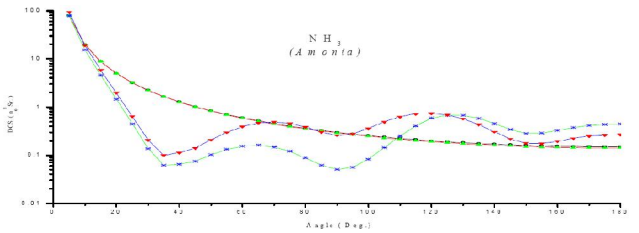

Figure 3 : DCS (0-1) for NH_3 at energy E = 10.0 eV.

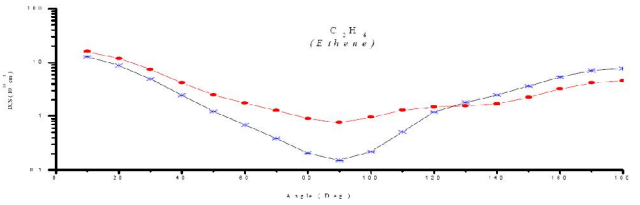

Figure 4 : DCS (0-1) for C_2H_6 at energy 10.0 eV.

Considering three, four and eight atoms polar molecules, the present results are in better agreement with the results of Gianturco et al.[3], Jain & Thompson et al.[4], Machado et al.[5] and Varella et al.[6,7]. Thus it indicates that as the number of atoms increases in the molecule, the results are not diverted in present method.

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