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Low energy electron collisions with polyatomic pollutant molecules SO_2, NH_3 and CH_4

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ABSTRACT

In this work we present theoretical study on electron collision with polyatomic pollutant molecules in the low energy range, we report, the rotational excitation Differential and Total scattering cross sections are calculated for electron collision with polyatomic pollutant molecules SO_2, NH_3 and CH_4 in the low energy range. 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 given valuable information about polyatomic pollutant molecules.

KEYWORDS

Collision;
Cross section;
Interaction potential.

INTRODUCTION

Air pollution is cause harm, discomfort to humans and other living organisms. It damages the natural environment and the atmosphere. The atmosphere is a complex, dynamic natural gaseous system that is essential to support life on planet Earth. An air pollutant is known as a substance in the air that can cause harm to humans and the environment. Pollutants can be in the form of solid particles, liquid droplets, or gases. In addition, they may be natural or man-made[1]. Pollutants can be classified as either primary or secondary. Usually, primary pollutants are substances directly emitted from a process, secondary pollutants are not emitted directly. Rather, they form in the air when primary pollutants react or interact. SO_2 is produced by volcanoes, industrial processes and combustion of coal and petroleum. NH_3 - emitted from agricultural processes. CH_4 is an extremely efficient greenhouse gas which contributes to enhanced global warming. The study of electron collision with these molecules may be provided important information about the formation and its physical properties. In present study, reports on the rotational excitation Differential scattering cross sections (DCS) and Total scattering cross section (TCS) are calculated for electron collision with polyatomic pollutant molecules SO_2, NH_3 and CH_4 in the low energy range.

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 collisions. 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],

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

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].

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

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

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

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

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

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

A series expansion of scattering amplitude as give by,

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

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

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

Where $K_0(a\Delta)$ - is a Bessel function, $\Delta = {}^2 ki - kf^2$ is momentum transferred. The differential cross section (DCS) for three terms in Born Eikonal Series Approximation can be expressed as follow,

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

From the above expression, the Total cross sections (TCS) are calculated for rotational transition $j \to j_0 + 1$

RESULTS AND DISCUSSION

The present results reported for the study for electron collision with polyatomic pollutant molecules SO_2, NH_3 and CH_4 in the low energy range. The Differential scattering cross section (DCS) and Total scattering cross section (TCS) for electron scattering by polyatomic pollutant molecules SO_2, NH_3 and CH_4 are calculated. The Born Eikonal Series Approximation method (BES) method and hard sphere dipole interaction potential is used in present study. Figure 1 & 2, show our calculated "TCS" results for e-SO_2 and e-CH_4 collision process, in rotational excitation $(0 \to 1)$ using BES hard sphere potential model. As shown in figure 1 & 2, 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. Figure 3, show the DCS results calculated for e-NH_3 collision at energy 10 eV, using BES hard sphere dipole potential. Those results are compared with experimental and theoretical results. The present study of polyatomic pollutant molecules SO_2, NH_3 and CH_4

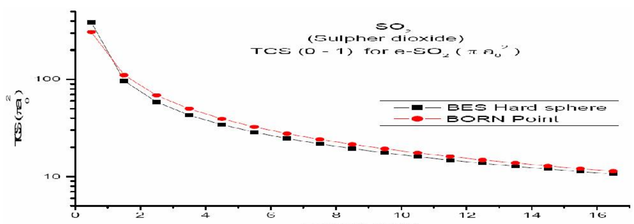

Figure 1 : TCS (0-1) for e-SO_2 collision

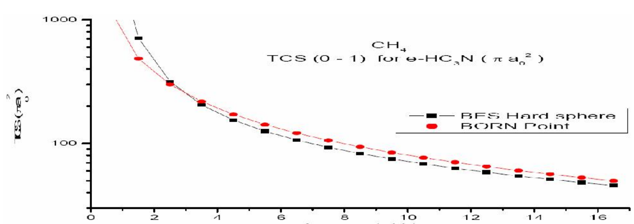

Figure 2 : TCS (0-1) for e-CH_4 collision

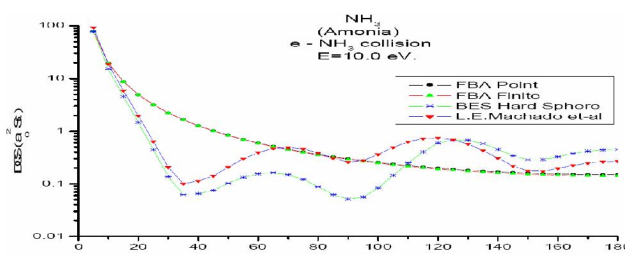

Figure 3 : DCS (0-1) for e-NH_3 collision

provided valuable information and knowledge about understand various phenomena in our Earth's atmosphere. Their importance is recognized as atmospheric pollutants and in connection with ozone depletion processes. Collision of these molecules with electron plays an important role in the study of earth's atmospheric environment and climate changes.

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