

Elastic scattering of electrons from oxygen and ozone molecules at high energies

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Abstract. Elastic differential cross-sections for the e -O₂ and e -O₃ systems are obtained in the independent atom model at high energies ($E_i \geq 300$ eV). The basic atomic scattering amplitudes are obtained in the partial wave method through a sum of static exchange and polarization potentials. Our e -O₂ results agree with experiments except for small angles. No data are available for O₃, for comparison.

Keywords. Elastic scattering; static exchange; polarization; independent atom model.

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1. Introduction

This paper deals with theoretical calculations of the differential cross-sections (DCS) for the elastic scattering of fast electrons ($E_i \geq 300$ eV) by oxygen and ozone molecules, which are of interest in atmospheric and gas-discharge physics. Experimentally e -O₂ elastic scattering has been investigated by Bromberg (1974), Daimon *et al* (1982) and recently by Iga *et al* (1987), while the theoretical DCS for this system were obtained by Khare and Raj (1982) (see also references therein). Khare and Raj (1982) also compared their theoretical results with the experimental data of Bromberg (1974), which are for small scattering angles up to 40° and up to $E_i = 500$ eV only. Practically no data, either theoretical or experimental, exist for e -O₃ system (see, however, Joshipura 1987).

Electron-molecule problems, such as the present ones, may be studied in the framework of the independent atom model (IAM) given by Massey *et al* (1969) and later refined by many authors (e.g. Choi *et al* 1979; Jain and Tayal 1984). This model is quite successful at high energies above 100 eV for the light H₂ molecular target and has also provided a good estimate in other cases. The simple IAM can be employed for sufficiently fast electrons for which multiple atomic scattering in the molecule would not be appreciable. A reasonable estimate of the molecular DCS can be obtained in this model, by incorporating all possible atomic interactions of the projectile and by calculating the atomic scattering amplitudes accurately. In the present problem basically we are required to calculate the electron-oxygen atom scattering amplitudes. We have improved upon the earlier calculations (Khare and Raj 1982) by including the electron exchange effect in addition to the static and the polarization potentials. Different models for the static potential are also examined. Our DCS results are compared with very recent experiments on O₂, which enables us to make definite conclusions about our e -O₃ theoretical results.

2. Theory and calculations

The following well-known expression of the IAM (Massey *et al* 1969) for the average DCS of electron-molecule scattering is employed in the present work

$$\begin{aligned} \bar{I}(\theta, k_i) = & \sum_i |f_i|^2 + \sum_{i \neq j} |f_i| \times |f_j| \cos(n_i - n_j) \\ & \times \frac{\sin qr_{ij}}{qr_{ij}} \cdot \exp(-l_{ij}^2 q^2/2), \end{aligned} \quad (1)$$

where f_i , f_j and n_i , n_j are the scattering amplitudes and phases from the constituent atoms of the molecule and q is the elastic momentum transfer. Further, r_{ij} and l_{ij} are the internuclear equilibrium-distances and the mean vibrational amplitudes for the (i, j) th pair of atoms in the molecule (Herzberg 1966). Presently the task is to calculate the scattering amplitude for the electron-oxygen atom system. For this purpose we assume a real, spherically symmetric (atomic) optical potential V_{opt} constructed as follows:

$$V_{\text{opt}} = V_{\text{st}}(r) + V_{\text{Ex}}^{\text{FEG}}(r, k_i) + V_{\text{pol}}(r, k_i) \quad (2)$$

where the three terms denote the static, exchange and polarization potentials respectively. Suitable models are employed for all of them. Two principal models are attempted for the static potential. The Thomas-Fermi static potentials of Bonham and Strand (1963) and Reitan (1981) are parametrized in the Yukawa form. The Hartree-Fock potentials of Cox and Bonham (1967) are also of the same form, while those of Strand and Bonham (1964) are the sums of Yukawa and exponential terms. We have tried each of these potentials in equation (2).

Now, for the electron-atom polarization potential, the only long range potential of import to our problem, the following model is adopted:

$$V_{\text{pol}}(r, k_i) = -\frac{1}{2} \left[\frac{\alpha_d r^2}{(r^2 + r_c^2)^3} + \frac{\alpha_q r^4}{(r^2 + r_c^2)^5} \right] \quad (3)$$

with α_d and α_q as the dipole and the quadrupole polarizabilities. The energy dependent cut-off parameter r_c is expressed in terms of the average excitation energy Δ as, $r_c = (3/8)(k_i/\Delta)$, following Jhanwar and Khare (1976) and Jain (1988). Finally, the model potential $V_{\text{Ex}}^{\text{FEG}}(r, k_i)$ to account for the exchange effect is adopted from Hara (1967) and Sur and Ghosh (1985).

Starting with the optical potential as discussed in the foregoing, the atomic scattering amplitude is calculated in the partial wave method. The relevant Schrödinger equation is solved by the Numerov method for the first few dominant partial waves ($l \sim 25$) and the Born approximation is used for the rest of them. The scattering amplitudes of the e -O atom system are employed in the appropriate forms of equation (1) to obtain the averaged molecular DCS of the O_2 and the O_3 targets.

3. Results and discussion

Owing to the high energies ($E_i \geq 300$ eV) of our interest here the choice of the simple IAM, equation (1) is justified. Multiple scattering may be ignored at these energies,

since the incident wavelength is shorter than the internuclear equilibrium-distances of the target molecules. The aim of this paper is to obtain satisfactory theoretical cross-sections for e - O_2 elastic scattering and to extend the calculations to e - O_3 scattering which is not much explored as yet. The elastic DCS of O_2 and O_3 molecules obtained by us are exhibited in figures 1a and 1b at 300 and 500 eV respectively. The present results have been compared with the experimental works of Bromberg (1974), Daimon *et al* (1982) and Iga *et al* (1987), for the O_2 molecule. For calculating the oxygen atom scattering amplitudes we have employed several models for the static potential, as mentioned in §2. The static potential of Strand and Bonham (1964), found to be the most suitable one, has been employed in all our theoretical results shown in figures 1a and 1b.

Our results show fair agreement with the experimental ones at the high energies considered. However, the theory tends to overestimate the experimental DCS at small angles of scattering, broadly because in equation (1), we have not considered the effect of binding of the atoms in the target molecule. The effect of binding of atoms is to reduce the cross-section for the target molecule. We also note that with the inclusion of the exchange in the electron-atom optical potential, the cross-sections are enhanced to an extent depending on the incident energy. The DCS of atomic oxygen are enhanced by about 18% at $E_i = 100$ eV and $\theta = 5^\circ$, due to the exchange. At 300 eV the contribution of the exchange to the e - O_2 DCS is about 8%. Further, for both the O_2 and O_3 molecules, there are typical variations in the slopes of the theoretical DCS curves, especially at lower energies. These are supported by the experimental data points. We have not shown the IAM results in the Born approximation, which are larger than both the present theory and the experiments even at 1000 eV.

Practically all general comments of e - O_2 results apply also to the e - O_3 system also. From our results on the O_2 molecule, we expect that our results on the O_3 molecules

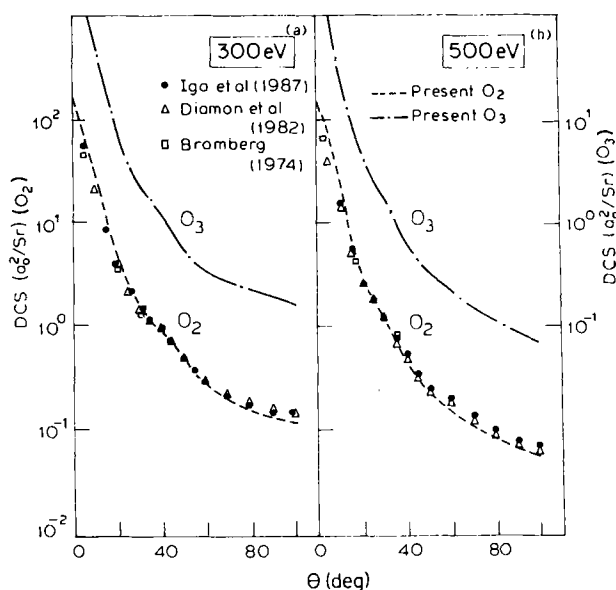


Figure 1. DCS of e - O_2 and e - O_3 scattering.

would also be satisfactory except for an overestimation at small angles. Better results would be obtained by starting directly with the molecular wavefunctions. In conclusion it may be pointed out that the optical potential in the present work does not include absorption effects.

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