

Absorption effects in the elastic scattering of electrons by the CF₄ molecule at intermediate energies

S P Khare, Deo Raj and Piyush Sinha

Physics Department, Meerut University, Meerut-250004, India

Received 15 November 1993, in final form 2 February 1994

Abstract. The independent-atom model (IAM) together with partial waves has been used to study the effect of the absorption potential on the elastic scattering of electrons by the carbon tetrafluoride molecule in the incident energy range 100–700 eV. The atom is represented by an optical potential which is complex, spherically symmetric and energy dependent. The differential, integral elastic and momentum transfer cross sections have been obtained. The present results are in good agreement with the available experimental data.

1. Introduction

Recently Raj (1991a) employed the independent-atom model (IAM) with partial waves to study the \bar{e} -CF₄ elastic scattering at energies ranging from 100–700 eV and obtained the differential, integrated elastic and momentum transfer cross sections. The results were found to be encouraging when compared with the experimental elastic cross sections including the contributions of the rotational and vibrational excitations of Sakae *et al* (1989) on \bar{e} -CF₄ available over a wide range of energies (75–700 eV) and scattering angles (5–135°). However, in general the theory overestimated the differential cross sections. Earlier, Khare and co-workers also used the same approach to study the elastic scattering of electrons by various molecules, namely O₂, CO, CO₂, H₂O and CH₄ in the intermediate energy range (Khare and Raj 1979, 1982, 1991, Raj 1990, 1991b) and obtained quite satisfactory agreement with the available experimental data. However, in all the above investigations only the direct static and the dynamic polarization potentials of the atoms were taken into account. We note that IAM together with partial waves has yielded reasonable results for $E \geq 200$ eV in the case of O₂, CO, CO₂, H₂O and CH₄ molecules while in the case of CF₄ such a situation occurs only at incident energies $E \geq 500$ eV. Since the CF₄ molecule is much heavier in comparison to O₂, CO, CO₂, H₂O and CH₄ it has a number of open inelastic channels at any intermediate energy. Thus the absorption effects may be significant for this molecule. Hence in the present investigation the optical potential is taken to be complex which is a sum of the direct static, dynamic polarization, local exchange and absorption potentials. With such a potential IAM together with the partial wave approach has been employed to obtain the differential, integral elastic and momentum transfer cross sections for electrons elastically scattered by CF₄ over a wide incident energy range (100–700 eV). The present results are compared with the experimental data of Sakae *et al* (1989) and the previous theoretical results of Raj (1991a).

2. Theory

The differential cross section (DCS) averaged over all orientations of the molecular axis in the IAM is given by (Massey *et al* 1969)

$$I_{\text{mol}}(\theta) = \sum_{j=1}^N I_j(\theta) + \sum_{l \neq j=1}^N f_l^*(\theta) f_j(\theta) \sin Kr_{jl}/Kr_{jl} \quad (1)$$

where $I_j(\theta)$ and $f_j(\theta)$ are the atomic DCS and the scattering amplitude, respectively, appropriate to the j th atom. K is the magnitude of the momentum transfer in the collisions. r_{jl} is the separation between the j th and the l th atoms. N represents the total number of atoms present in the molecule. It should be noted that equation (1) considers only one electronic and vibrational state but takes all the rotational states of the molecule into account in an adiabatic manner. However, IAM neglects the multiple scattering, the likely effect of which is to reduce the cross section (Hayashi and Kuchitsu 1976, 1977) and assumes that each atom scatters as if it were free. The valence bond distortion is also neglected which is also known to cause a decrease in the cross section (Bonham and Iijima 1963). For the CF_4 molecule equation (1) reduces to

$$I_{\text{CF}_4}(\theta) = I_{\text{C}}(\theta) + 4I_{\text{F}}(\theta)(1 + 3 \sin Kr_{\text{FF}}/Kr_{\text{FF}}) + 8(\text{FCR} \cdot \text{FFR} + \text{FCI} \cdot \text{FFI}) \frac{\sin Kr_{\text{CF}}}{Kr_{\text{CF}}} \quad (2)$$

where the suffixes C and F stand for carbon and fluorine atoms, respectively. r_{FF} is the separation between the two fluorine atoms in the molecule which has been calculated by using the values of r_{CF} (the bond length = $2.61 a_0$) and the bond angle ($109^\circ 28'$). FCR, FFR and FCI, FFI are the real and imaginary parts of the scattering amplitude for the carbon and fluorine atoms, respectively.

The atomic scattering amplitude $f(\theta)$ in partial waves is given by

$$f(\theta) = \frac{1}{k} \sum_{l=0}^{L_{\text{max}}} (2l+1)(e^{i\delta_l} \sin \delta_l - \delta_l^{\text{B}}) P_l(\cos \theta) + f_{\text{dp}}^{\text{B}}(\theta). \quad (3)$$

To obtain δ_l , the phaseshift for the l th partial wave, the following radial equation is solved numerically under the proper boundary conditions:

$$\left(\frac{d^2}{dr^2} + k^2 - V_{\text{op}}(r) - \frac{l(l+1)}{r^2} \right) U_l(r) = 0 \quad (4)$$

where k^2 is the energy of the incident electron (we employ atomic units in which the length is expressed in a_0 and the energy in Rydberg). $V_{\text{op}}(r)$ is the optical potential. It is complex, spherically symmetric and energy dependent and is given by

$$V_{\text{op}}(r) = V_{\text{R}}(r) + iV_{\text{I}}(r). \quad (5)$$

The real part $V_{\text{R}}(r)$ is given by

$$V_{\text{R}}(r) = V_{\text{ds}}(r) + V_{\text{dp}}(r) + V_{\text{ex}}(r). \quad (6)$$

$V_{\text{ds}}(r)$, $V_{\text{dp}}(r)$ and $V_{\text{ex}}(r)$ are the direct static, dynamic polarization and exchange potential, respectively for \bar{e} -atom interactions. The polarization effects are included by taking spherically symmetric and energy dependent potential as suggested by Jhanwar and

Khare (1976):

$$V_{dp}(r) = -\frac{\alpha_d r^2}{(r^2 + d^2)^3} - \frac{\alpha_q r^4}{(r^2 + d^2)^5} \quad (7)$$

with $d = 0.75 k/\Delta$.

Here α_d and α_q are, respectively, the dipole and quadrupole polarizabilities of the atom and Δ represents the mean excitation energy of the atom. We have taken α_d as 14.2 and 4.05 (Dalgarno and Parkinson 1959), α_q as 55.2 and 10.3 (Gupta *et al* 1975) and Δ as 0.96 and 2.68 (Dehmer *et al* 1975) for carbon and fluorine atoms, respectively.

For the direct static potential $V_{ds}(r)$ and the electron density function $\rho(r)$, we have used the analytical expressions of Salvat *et al* (1987), obtained by a fitting procedure to the Dirac-Hartree-Fock-Slater (DHFS) self-consistent data, and it is given by

$$V_{ds}(r) = -\frac{2Z}{r} \sum_{i=1}^3 A_i e^{-\alpha_i r} \quad (8)$$

and

$$\rho(r) = \frac{Z}{4\pi r} \sum_{i=1}^3 A_i \alpha_i^2 e^{-\alpha_i r}. \quad (9)$$

The parameters A_i and α_i are tabulated in Salvat *et al* (1987). Z is the atomic number of the atom. $V_{ex}(r)$ is the asymptotically adjusted free-electron gas exchange potential of Riley and Truhlar (1976) and is given by

$$V_{ex}(r) = -\frac{4}{\pi} k_F \left(\frac{1}{2} + \frac{1-n^2}{4n} \ln \left| \frac{1+n}{1-n} \right| \right) \quad (10)$$

where

$$k_F = [3\pi^2 \rho(r)]^{1/3} \quad n = S/k_F$$

and

$$S^2 = k^2 + k_F^2.$$

For the imaginary part $V_1(r)$ of the optical potential which is also known as absorption potential we have employed the non-empirical model derived from a quasi-free scattering model by Staszewska *et al* (1983) and it is given by

$$V_1(r) = -\rho(r) T_{loc}^{1/2} \frac{8\pi}{5k^2 k_F^3} H(x) [A_1 + A_2 + A_3] \quad (11)$$

with

$$\begin{aligned} A_1 &= 5k_F^3/\Delta & A_2 &= -k_F^3(5k^2 - 3k_F^2)/(k^2 - k_F^2)^2 \\ A_3 &= 2H(y)y^{5/2}/(k^2 - k_F^2)^2 \end{aligned}$$

where

$$x = k^2 - k_F^2 - \Delta \quad \text{and} \quad y = 2k_F^2 + \Delta - k^2.$$

T_{loc} is the local kinetic energy of the incident electron and $H(x)$ is the Heaviside unit step function. In equation (3) $f_{dp}^B(\theta)$ and δ_l^B are the first Born scattering amplitude and the phaseshifts, respectively, for the dynamic polarization potential $V_{dp}(r)$. We have

used δ_l^S , the semiclassical phaseshifts instead of δ_l^B as the evaluation of the latter is time consuming for the higher partial waves. It may be noted that δ_l^S are found within 3% of δ_l^B and need negligible time for their evaluation (Raj 1981). In the present calculation the first L_{\max} partial wave phaseshifts are taken exactly and the contribution of the remaining $L_{\max} + 1$ to ∞ partial waves is included through the first Born approximation. The value of L_{\max} depends on energy and is chosen such that at $l = L_{\max}$ the difference of δ_l and δ_l^B is less than or equal to 2%. At higher energies if this condition is not satisfied up to $l \leq 30$, L_{\max} is taken to be 30. It may be noted that the higher partial waves contribute to the low scattering angles only. Hence replacement of δ_l by δ_l^B for $l > 30$ is not expected to cause appreciable error in the middle and higher angular regions. Furthermore V_{ds} , V_{ex} and V_I are the short range potentials hence at high l their contribution to δ_l^B is not expected to be appreciable. Finally we calculated $I(\theta)$ from equation (2) and used these values to obtain the integral elastic (Q_1) and the momentum transfer (Q_m) cross sections. The present results of DCS are displayed in figures 1 to 3 together with the experimental data and other theoretical results. The values of the integrated elastic and momentum transfer cross sections are given in table 1.

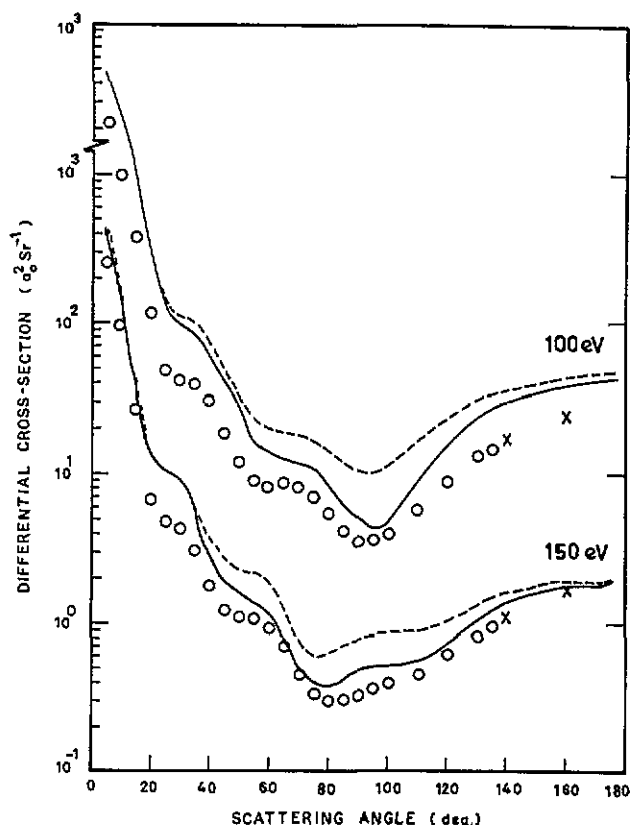


Figure 1. Angular dependence of the differential cross section for \bar{e} -CF₄ elastic scattering at 100 and 150 eV impact energies. Theory: full curve, present results; broken curve, Raj (1991a). Experiment: open circles, Sakae *et al* (1989); crosses, extrapolated data.

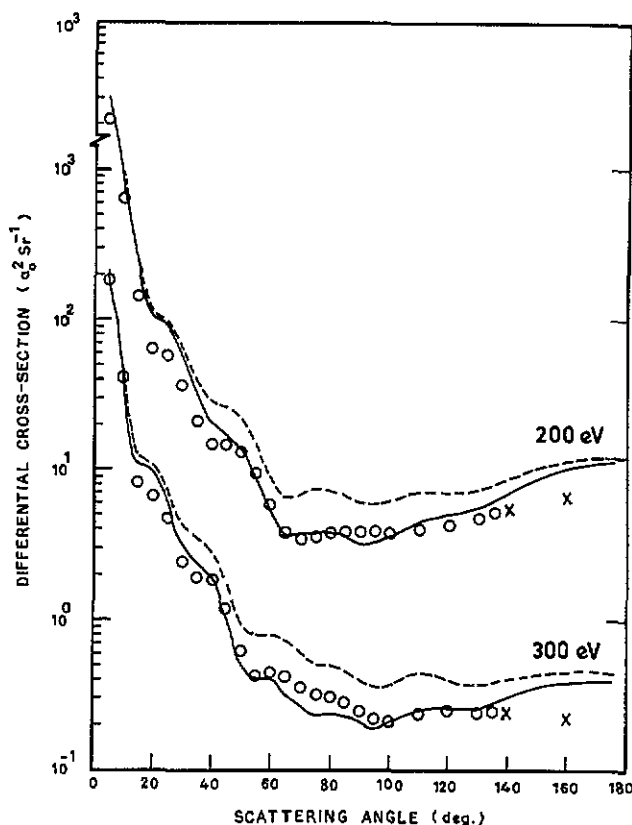


Figure 2. Same as figure 1 except for impact energies of 200 and 300 eV.

3. Results and discussion

In figure 1 the present results (full curve) of DCS at incident energies 100 and 150 eV have been plotted along with the experimental data of Sakae *et al* (1989). The results of the previous calculation of Raj (1991a) (broken curve), in which exchange and absorption effects were neglected, are also included for comparison. It is evident from figure 1 that although the qualitative natures of the two curves are almost the same there has been a significant improvement in the values of DCS when exchange and absorption effects are taken into account particularly at the middle and higher angular ranges of scattering angle. Furthermore the two curves merge with one another for low scattering angles ($\theta \leq 20^\circ$).

At the higher incident energies i.e. 200 and 300 eV (figure 2) the agreement further improves and the present values come closer to the experimental data. The effect of the exchange and absorption is noticeable even below 20° at these incident energies. At 500 and 700 eV (figure 3), although the agreement between the present values and the data of Sakae *et al* (1989) is still satisfactory, the theory now slightly underestimates the cross sections for $\theta > 30^\circ$. In this regard it may be noted that the present imaginary part of the optical potential $V_1(r)$ is known to overestimate the flux loss to the excited electronic states for large scattering angles particularly at high incident energies (Staszewska *et al* 1983) and hence the underestimation of the DCS is according to our

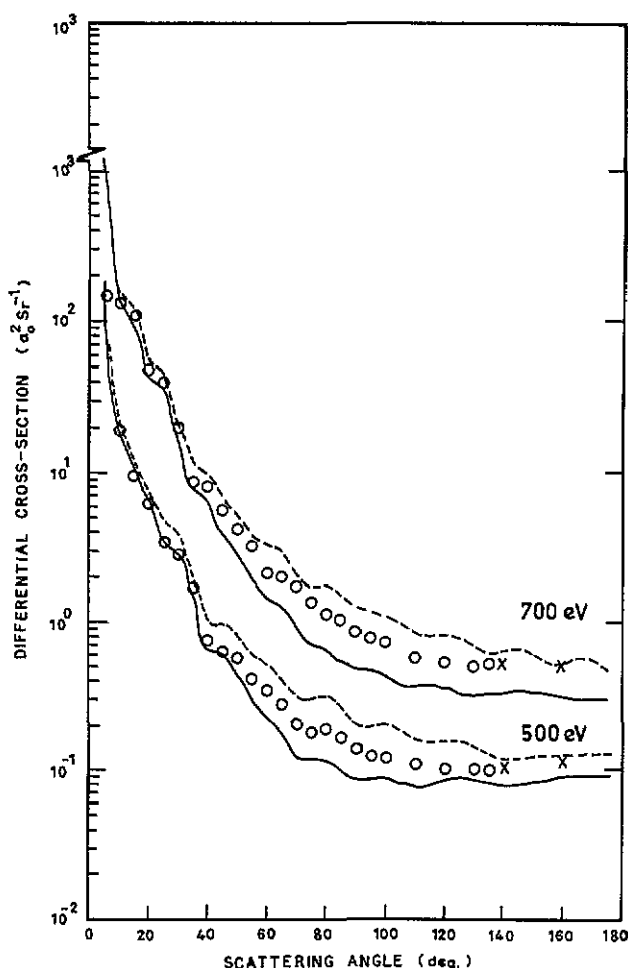


Figure 3. Same as figure 1 except for impact energies of 500 and 700 eV.

Table 1. Integrated elastic (Q_1) and momentum transfer (Q_m) cross sections for \bar{e} -CF₄ scattering at various impact energies in units of a_0^2 . The experimental results (Expt) are from Sakae *et al* (1989).

E (eV)	Q_1			Q_m		
	Raj (1991a)	Present	Expt	Raj (1991a)	Present	Expt
100	103.00	93.04	43.57	33.97	25.75	14.86
150	69.92	62.19	38.57	17.38	13.62	10.68
200	47.51	43.15	30.57	11.65	8.43	6.86
300	31.80	27.32	23.07	6.78	4.43	4.04
500	21.40	15.12	16.71	3.25	1.79	2.26
700	16.29	12.01	13.93	1.97	1.03	1.49

expectation. On the other hand the theoretical values of Raj (1991a) which do not include the exchange and absorption effects overestimate the cross sections.

It is evident from table 1 that the values of the integral elastic cross sections (Q_1) obtained by Raj (1991a) taking only the direct static and the dynamic polarization

effects into account are higher than the experimental cross sections at all the incident energies investigated here. On the other hand the inclusion of the exchange and absorption brings Q_T closer to the experimental data and the agreement improves with energy up to 300 eV. The underestimation of Q_T at 500 and 700 eV is again probably due to too much of the flux loss to the excited electronic states as mentioned above. The present values of the momentum transfer cross section (Q_m) are also in better agreement with the experimental data of Sakae *et al* in comparison with the values obtained by Raj (1991a).

Thus we conclude that the inclusion of the absorption and exchange effects in the present investigation has yielded a better agreement with the experimental data. Since CF_4 is a heavier molecule, the absorption effects are expected to be quite significant and this has been noted in the present investigation. To examine the effect of exchange and absorption potentials separately we have calculated three more sets of DCS—one with $V_{ds} + V_{dp}$, the second with $V_{ds} + V_{dp} + V_{ex}$ and the third with $V_{ds} + V_{dp} + V_I$ at 100 eV (the lowest energy of our calculation). In comparison with the DCS obtained with the first set of potentials, larger DCS were obtained with the second set of potentials while the third set of potentials gave smaller DCS. This shows that the effect of exchange is to increase the DCS and in contrast the absorption potential decreases the cross section. However, in the middle angular region the decrease due to V_I is more than the increase due to exchange. The net effect being the decrease of DCS in comparison with those obtained with $V_{ds} + V_{dp}$ and hence a better agreement with the experimental data. However, we have neglected the multiple scattering and the valence bond distortion effects. CF_4 being a heavy molecule the above effects may have appreciable effect on the cross sections. Hence further investigations including these effects should be carried out. Nevertheless the IAM along with partial waves simplifies the problem and computationally it is easier. Hence its further development to investigate more complex problems like electron-surface scattering is of interest.

Acknowledgment

Financial assistance from the Council of Scientific and Industrial Research, New Delhi is gratefully acknowledged.

References

- Bonham R A and Iijima T 1963 *J. Phys. Chem.* **67** 2266
- Dalgarno A and Parkinson D 1959 *Proc. R. Soc. A* **250** 422
- Dehmer J L, Inokuti M and Saxon R P 1975 *Phys. Rev. A* **12** 102
- Gupta A, Roy H P and Mukherjee P K 1975 *Int. J. Quantum Chem.* **9** 1
- Hayashi S and Kuchitsu K 1976 *Chem. Phys. Lett.* **41** 575
- 1977 *J. Phys. Soc. Japan* **42** 1319
- Jhanwar B L and Khare S P 1976 *J. Phys. B: At. Mol. Phys.* **9** L527
- Khare S P and Raj D 1979 *J. Phys. B: At. Mol. Phys.* **12** L351
- 1982 *Ind. J. Pure Appl. Phys.* **20** 538
- 1991 *J. Phys. B: At. Mol. Opt. Phys.* **24** 3045
- Massey H S W, Burhop E H S and Gilbody H B 1969 *Electronic and Ionic Impact Phenomena* vol 2 (Oxford: Clarendon)
- Raj D 1981 *PhD Thesis* Meerut University
- 1990 *Ind. J. Phys. B* **64** 249
- 1991a *J. Phys. B: At. Mol. Opt. Phys.* **24** L431
- 1991b *Ind. J. Phys. B* **65** 319

Riley M E and Truhlar D G 1976 *J. Chem. Phys.* **65** 792

Sakae T, Sumiyoshi S, Murakami E, Matsumoto Y, Ishibashi K and Katase A 1989 *J. Phys. B: At. Mol. Opt. Phys.* **22** 1385

Salvat F, Martinez J D, Mayol R and Parellada J 1987 *Phys. Rev. A* **36** 467

Staszewska G, Schwenke D W, Thirumalai D and Truhlar D G 1983 *Phys. Rev. A* **28** 2740