LETTER TO THE EDITOR

Cross sections for e^-–CF_4 elastic scattering at intermediate energies

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Abstract. Differential, integral and momentum transfer cross sections have been obtained, using an independent-atom model along with partial waves, for the elastic scattering of electrons by the carbon tetrafluoride molecule over an incident energy range 100–700 eV. The present method yields more structure in DCS at large angles and energies than obtained experimentally.

Recently Sakae *et al* (1989) have measured the differential cross section (DCS) for e^-–CF_4 elastic scattering over a wide range of angles (5°–135°) and incident energies 75–700 eV. They have also integrated their experimental DCS to obtain the values of integral and momentum transfer cross sections (MTCS). They extrapolated their DCS for $\theta < 5°$ and $>135°$. However, at present no theoretical calculation or any other experimental data for e^-–CF_4 elastic scattering seem to be available in the intermediate energy range covered by Sakae *et al* (1989). Hence, a theoretical investigation for e^-–CF_4 elastic scattering in this energy range is needed.

In the recent past we employed an independent-atom model (IAM) along with partial waves to study the elastic scattering of electrons by a number of molecules; namely CO, CO_2, O_2 and H_2O in the intermediate energy range (Khare and Raj 1979, 1982, 1991, Raj 1990). In the above investigations the direct and the polarization potentials of the atoms were taken into account. The model yielded results in satisfactory agreement with the available experimental data for all the molecules, particularly for incident energies $E \geq 200$ eV. Hence, it will be a worthwhile attempt to apply this approach for e^-–CF_4 scattering also to obtain its elastic cross sections which may find their applications in the electron transport properties. In this letter we report the values of DCS, integral and momentum transfer cross sections for the elastic scattering of electrons by the CF_4 molecule over an incident energy range 100–700 eV.

Taking into account all the possible orientations of the internuclear axis in space, the DCS for CF_4 in IAM is given by (Massey *et al* 1969)

$$I_{CF_4}(\theta) = I_C(\theta) + 4I_F(\theta)(3 \sin Kr_{FF}/Kr_{FF} + 1)$$

$$+ 8(\text{FCR} \cdot \text{FFR} + \text{FCI} \cdot \text{FFI}) \sin Kr_{CF}/Kr_{CF} \tag{1}$$

where suffixes C and F stand for carbon and fluorine respectively, $I(\theta)$ is the differential cross section (DCS) and K is the magnitude of momentum transfer. r_{FF}, the separation between the two fluorine atoms in the molecule, may be calculated from the values of r_{CF}, the bond length ($2.608\,a_0$) and the bond angle (109° 28′). FCR, FFR and FCI,

FFl are the real and imaginary parts of the scattering amplitude for the carbon and the fluorine atoms, respectively. Equation (1) neglects the possibility of multiple scattering within the molecule.

To obtain the atomic scattering amplitude in partial waves, we solve the following radial equation numerically under proper boundary conditions for phaseshifts, δ_l

$$\left(\frac{d^2}{dr^2} + k^2 - V_{00}(r) - V_{dp}(r) - \frac{l(l+1)}{r^2}\right) u_l(r) = 0 \tag{2}$$

where k^2 is the energy of the incident electron (atomic units have been used where length is expressed in a_0 and energy in Ryd). $V_{00}(r)$ is the static field of the atom and $V_{dp}(r)$ is the dynamic polarization potential. We have used the approximate HF analytical expressions for $V_{00}(r)$ as obtained by Strand and Bonham (1964) for both the atoms. The polarization effects are included by taking the spherically symmetric and energy-dependent potential as suggested by Jhanwar and Khare (1976). $V_{dp}(r)$ uses the values of α_d, α_q and Δ, dipole and quadrupole polarizabilities and mean excitation energies, respectively, of the atoms. 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 0.961 and 2.68 (Dehmer *et al* 1975) for carbon and fluorine atoms, respectively. The exchange and absorption effects are supposed to be small at the incident energies considered in the present investigation and hence are neglected.

The partial phaseshifts δ_l are then used to calculate the scattering amplitude $f(\theta)$ from the expression

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

$f_{dp}^B(\theta)$ and δ_l^B are the Born scattering amplitude and the phaseshifts, respectively, due to dynamic polarization potential $V_{dp}(r)$. We have used δ_l^S, the semiclassical phaseshift, in place of δ_l^B as the evaluation of δ_l^B is time consuming for the higher partial waves. It may be noted that δ_l^S are within 3% of δ_l^B and need negligible time for their evaluation (Raj 1981). We take the first N partial waves exactly and the contribution of the remaining ones is included through the Born approximation. The value of N depends on the energy. Finally, we calculate $I(\theta)$ from (1) and use these values to obtain the integral, Q_I, and the momentum transfer cross sections (MTCS), Q_M. The present results are displayed in figures 1 to 3 and table 1 along with the experimental results of Sakae *et al* (1989).

It is evident from figure 1 that the present results of DCS at the incident energies 100 and 150 eV reproduce the qualitative behaviour of the experimental data of Sakae *et al* (1989). However, the magnitude of DCS is much higher than the data. At these incident energies the de Broglie wavelength associated with the incident particle is comparable with the bond length r_{CF} of the CF_4 molecule. Hence the multiple scattering will be significant, which is expected to reduce the DCS (Hayashi and Kuchitsu 1976). However, as is evident from figure 2 at 200 and 300 eV the agreement between the theory and the experiment improves with increasing incident energy. Fairly good agreement between the present results and the data is obtained for $E \geq 500$ eV. It may be noted that our present results at higher incident energies show more structure in the large scattering angular region than given by the experiment of Sakae *et al* (1989) (figure 3). However, the variation of the cross section in this region from the smooth curves is less than the experimental accuracy ($\pm 10\%$), and hence, could be missed in
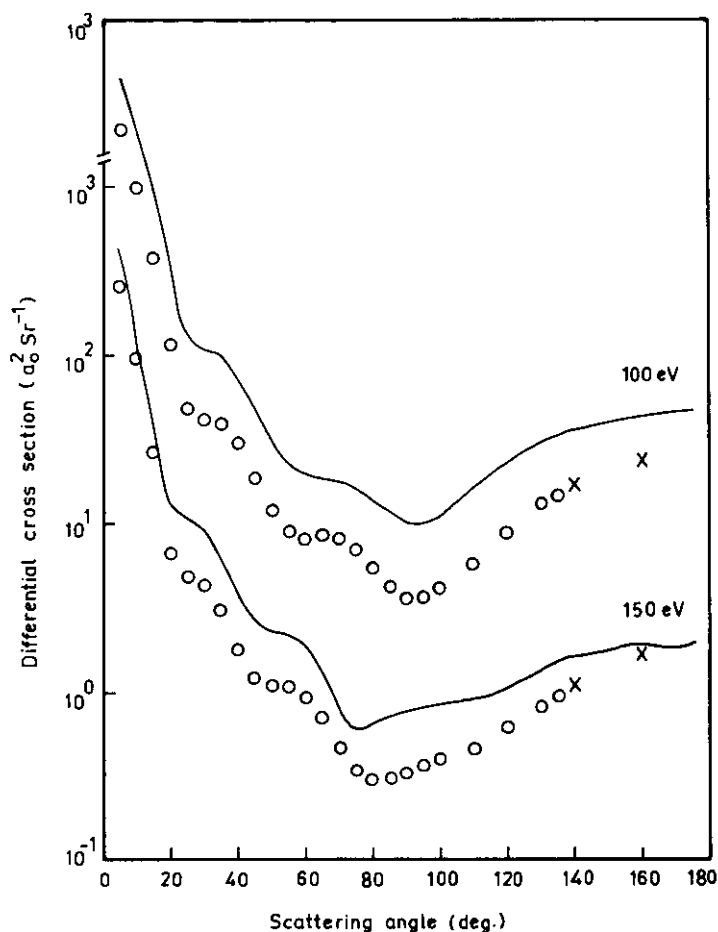
Figure 1. Differential cross section for $e^- - CF_4$ elastic scattering at incident energies 100 and 150 eV. ——, present results; $\bigcirc$, experimental data of Sakae *et al* (1989); $\times$, extrapolated data.

the experiment at 500 and 700 eV (figure 3) within the angular range over which the data are given. However, outside the range of the data ($\theta > 135°$) the difference is up to about 15%. At large incident energies the $\sin Kr_{FF}$ and $\sin Kr_{CF}$ terms oscillate rapidly resulting in more structure in molecular DCS.

In table 1 we have listed our values of the integral and the momentum transfer cross sections for the elastic scattering of electrons by the CF_4 molecule along with the experimental data of Sakae *et al* (1989). Agreement between the theory and the experiment is similar to that obtained for DCS. Here again we get satisfactory agreement between the theory and the experiment for $E \geqslant 500$ eV.

Finally, we conclude that IAM along with the partial waves has yielded satisfactory results for CO, CO_2, O_2 and H_2O molecules for the incident energies $E \geqslant 200$ eV. However, for CF_4 satisfactory results are obtained at a higher energy, i.e. 500 eV. It is well known that in general at low incident energies the values of DCS calculated within the framework of IAM are larger than the measured values because (i) orbital overlap in molecules should decrease the atomic contributions compared with those in the free
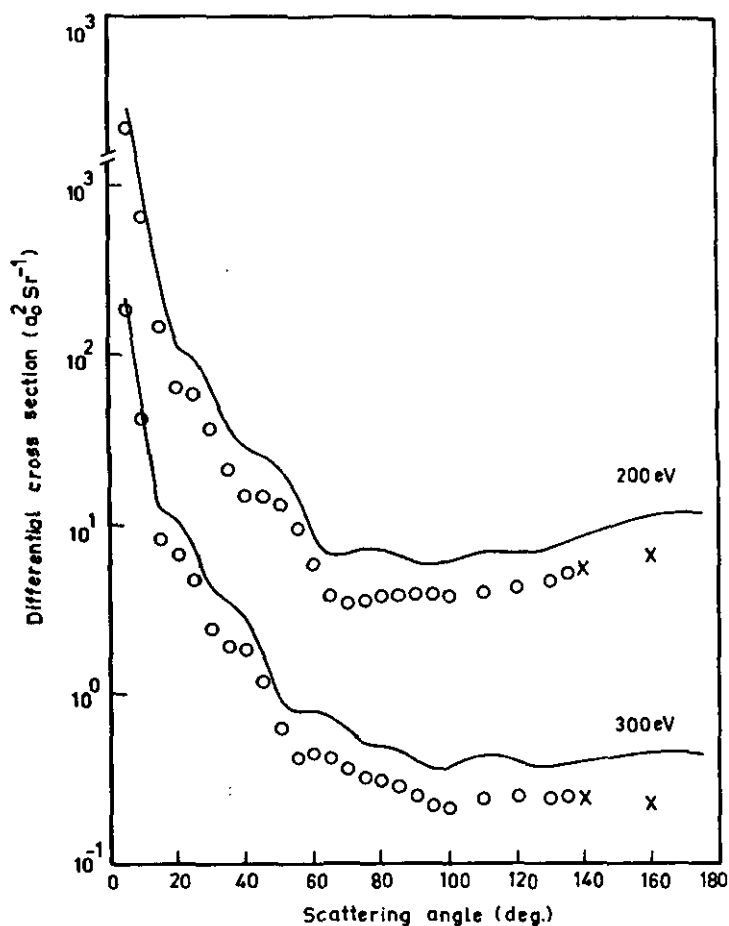
Figure 2. Same as in figure 1 but for 200 and 300 eV.

Table 1. Elastic integral and momentum transfer cross sections for $e^- - CF_4$ scattering in units of a_0^2.

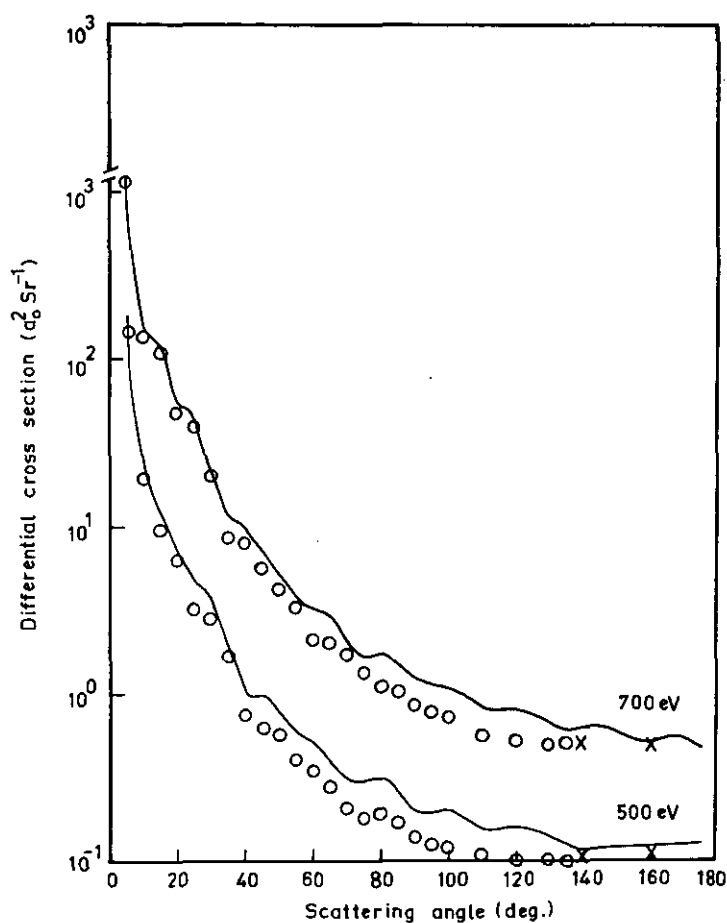| Energy (eV)	Q_I		Q_M	
	Present	Sakae *et al*	Present	Sakae *et al*
100	103.0	43.57	33.97	14.86
150	69.92	38.57	17.38	10.68
200	47.51	30.57	11.65	6.86
300	31.80	23.07	6.78	4.04
500	21.40	16.71	3.25	2.26
700	16.29	13.93	1.97	1.49

Figure 3. Same as in figure 1 but for 500 and 700 eV.

atomic state and (ii) other structural effects (bonding environment, steric crowding, etc) similarly affect the contribution of a given atom. It seems that the above effects are more important for fluorinated molecules, as also noted by Deutsch *et al* (1986) in their e$^-$ impact ionization cross section studies. Although the two processes, i.e. the elastic scattering and the ionization, are quite different the observations in the case of the fluorinated molecules are similar. At present the reason for such behaviour of the fluorinated molecules is not very clear. For a better understanding of the above behaviour of the fluorinated molecules it is desirable to carry out more theoretical and experimental investigations.

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