

Electron-scattering cross sections of fluoromethanes in the energy range from 0.1 to 10 keVF. Manero,¹ F. Blanco,² and G. García¹¹*Centro de Investigaciones Energéticas Medioambientales y Tecnológicas (CIEMAT), Departamento de Fusión y Física de Partículas Elementales, Avenida Complutense 22, 28040 Madrid, Spain*²*Universidad Complutense de Madrid, Facultad de Física, Departamento de Física Atómica Molecular y Nuclear, Avenida Complutense s/n, 28040 Madrid, Spain*

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Total electron-scattering cross section for CF₄ has been measured in the energy range from 300 to 5000 eV. Semiempirical values for the total cross sections of CF₄, CF₃H, CF₂H₂, and CFH₃ between 0.5 and 10 keV are also given, obtained by means of a formula that depends only on the total number of electrons and the polarizability of the molecule, and which was previously deduced by the authors. Experimental and semiempirical values have been compared with previously published experimental data. Differential and integral elastic cross sections are given at several incident electron energies in the range from 100 to 10 keV, calculated by means of a scattering potential method, assuming that the independent-atom model is valid, and the results compared with other published data. Integral inelastic cross-section values are also given as the difference between the total cross section and the integral elastic cross-section data. Finally, in order to facilitate the use of the present results in computation work, our integral elastic and inelastic cross sections have been fitted to expressions based on Born-Bethe formulas, which allows one to obtain these cross sections at any energy within the energy range considered.

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I. INTRODUCTION

Relations between cross sections for electron scattering and the physical-chemical parameters of groups of molecules have been searched for since the earliest systematic measurements of cross sections. Such relationships may indicate the role of some microscopic target properties in the scattering process, and semiempirical formulas describing these correlations can help to estimate cross sections of targets where there is a lack of experimental data or calculations. In this context, an increased interest has recently been shown in the halogenated hydrocarbons. These are artificial gases of wide technological interest. In particular, carbontetrafluoride has been used as a refrigerant and in the semiconductor industry as a plasma etching gas [1,2]. Moreover, halocarbons play an important role in atmospheric chemistry [3]. Free Cl radicals formed by ultraviolet induced dissociation act as catalysts in the chain reactions leading to the destruction of the atmospheric ozone [4]. Also, the high potential of these gases for greenhouse warming is recognized [5].

Hence, cross-section data for electron scattering from partially fluorinated hydrocarbons are urgently needed in plasma processing, material and earth sciences, since these molecules, which have a shorter lifetime than CF₄ in the atmosphere, are considered to be environmentally acceptable plasma processing gases [6]. Therefore, studies on electron-scattering cross sections have increasingly been carried out for halogenated hydrocarbons in recent years. Nevertheless, for some molecules, mainly fluoromethanes, experimental data or calculations are scarce or lacking at intermediate and high energies.

Zecca and co-workers [7] have measured the total cross section of CF₄ in the 75–4000 eV energy range, using a modified Ramsauer setup. Szmytkowski *et al.* [8] have reported absolute total cross sections for e^- -CF₄ scattering,

using the linear transmission technique, for energies ranging from 0.5 to 200 eV. Normalized total cross sections for CF₄ have been published by Sueoka, Mori, and Hamada [9] for electron-impact energies from 1.0 to 400 eV. Absolute total cross-section values for CH₃F have been obtained in a transmission experiment by Krzysztofowicz and Szmytkowski [10] in the energy range between 0.3 and 250 eV, and total cross sections for CHF₃ have been measured by Sueoka and co-workers [11] for energies from 0.1 to 600 eV and by Iga, Pinto, and Homem [12] from 300 to 1000 eV. In addition, differential elastic cross sections have been measured by Sakae and co-workers [13] for CF₄ in the energy range from 75 to 700 eV, and integral- and momentum-transfer cross sections obtained. Differential elastic cross sections have been measured by Boesten *et al.* [14] for CF₄ below 100 eV. Differential and integral elastic cross sections have been reported by Iga, Pinto, and Homem [12,15] for CHF₃ for energies from 300 to 1000 eV. Fluorination effects in the elastic differential cross sections have been reported by Tanaka *et al.* [16] and Natalense and co-workers [17] below 100 eV for CH₃F, CH₂F₂, CHF₃ and CF₄.

The electron-impact total ionization cross section of CF₄ has been measured as a function of the incident electron energy from threshold to 3 keV by Nishimura *et al.* [18] and the values obtained compared with theoretical cross sections calculated from the binary-encounter-Bethe (BEB) method developed by Kim and co-workers [19,20]. Absolute partial and total electron-impact ionization cross sections have also been measured by Ma, Bruce, and Bonham [21–23] for CF₄ from threshold to 500 eV and by Stephan, Deutsch, and Mark [24] from threshold up to 180 eV. Finally, the total dissociation cross sections have been measured by Winters and Inokuti [25] for CF₄ and CF₃H for electron-impact energies between the threshold and 600 eV and by Motlagh and

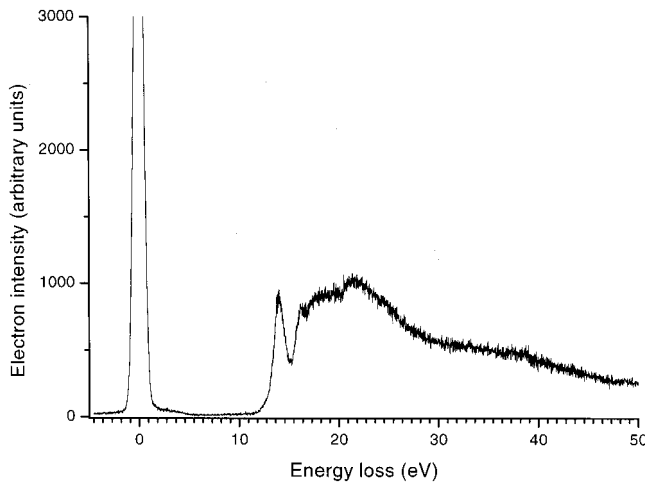


FIG. 1. Energy spectrum of electrons scattered by CF₄ at 0° for 2000 eV incident energy.

Moore [26] for CF₄, CF₃H, and CFH₃ between 10 and 500 eV.

Calculations of the total (elastic plus inelastic) cross sections for electron scattering from CF₄ have been made by Baluja *et al.* [27] in the energy range of 10–5000 eV by using a parameter-free spherical complex optical potential approach. Jiang, Sun, and Wan [28] have used an atom independent model to calculate the total cross section of CF₄ between 10 and 1000 eV. Finally, an extensive review of electron-scattering integral cross sections for hydrocarbons and halides can be found in Karwasz, Brusa, and Zecca [29].

However, in spite of the scientific and technological interest of fluoromethanes, there are very few cross-section data for these molecules, except for CF₄, and in this case only for energies up to 4–5 keV. This fact has prompted the present work. Experimental values are given for the total cross section of CF₄ in the energy range from 0.3 to 5.0 keV, as well as calculated total cross sections for the four fluoromethanes up to 10 keV, obtained by means of a semiempirical formula previously derived by the authors [30]. Differential and integral elastic cross sections for fluoromethanes are also calculated at several incident electron energies up to 10 keV. The suitability of the semiempirical formula for fluorocarbons above 1 keV has been confirmed by comparing our total cross-section values with those obtained by adding our integral elastic cross-section data to the ionization values of Kim and Rudd [31].

II. TOTAL CROSS SECTIONS

A. Experimental values

Absolute total cross sections for electron scattering by CF₄ have been measured in a transmission beam system for electron energies from 300 to 5000 eV. The experimental setup has been previously described [32–34] and will be only briefly referred to here. The primary electron beam, produced by an emitting filament, was collimated into a 1-mm-diameter beam and deflected by a combination of electrostatic plates and a transverse magnetic field. Typical

TABLE I. Total cross sections for electron scattering by CF₄ (in units of a_0^2)

| Energy (keV) | Present work | Eq. (1) | Zecca [7] | Szmytkowski [8] | Sueoka [9] | Jiang [28] |
|--------------|--------------|---------|-----------|-----------------|------------|------------|
| 0.100 | | | 66.07 | 64.28 | 56.36 | 75.83 |
| 0.110 | | | 65.00 | | | |
| 0.120 | | | | 61.78 | 53.68 | |
| 0.125 | | | 60.71 | | | |
| 0.140 | | | | 59.99 | | |
| 0.150 | | | 58.21 | | 49.46 | |
| 0.160 | | | | 56.07 | | |
| 0.175 | | | 55.36 | | | |
| 0.180 | | | | 54.99 | | |
| 0.200 | | | 51.43 | 52.12 | 44.71 | 53.47 |
| 0.225 | | | 47.14 | | | |
| 0.250 | | | 45.36 | | 40.11 | |
| 0.275 | | | 43.21 | | | |
| 0.300 | 39.7 | | 41.43 | | 36.03 | 41.50 |
| 0.350 | | | 38.57 | | | 33.50 |
| 0.400 | 32.4 | | 35.71 | | 30.32 | 34.68 |
| 0.450 | | | 33.46 | | | |
| 0.500 | 28.2 | 34.50 | 29.89 | | | 29.78 |
| 0.600 | | 29.92 | 26.71 | | | 26.04 |
| 0.700 | 23.3 | 26.53 | 24.07 | | | 23.28 |
| 0.800 | | 23.91 | 22.21 | | | 20.89 |
| 0.850 | 21.0 | 22.80 | | | | |
| 0.900 | | 21.81 | 20.39 | | | 19.06 |
| 1.000 | 18.7 | 20.09 | 18.78 | | | 17.65 |
| 1.200 | 16.1 | 17.43 | | | | |
| 1.250 | | 16.88 | 15.61 | | | |
| 1.500 | 14.0 | 14.64 | 13.61 | | | |
| 1.750 | | 12.98 | 11.46 | | | |
| 2.000 | 10.8 | 11.70 | 10.50 | | | |
| 2.250 | | 10.67 | 9.43 | | | |
| 2.500 | 9.11 | 9.83 | 8.54 | | | |
| 2.750 | | 9.13 | 7.89 | | | |
| 3.000 | 8.19 | 8.53 | 7.25 | | | |
| 3.250 | | 8.01 | 6.71 | | | |
| 3.500 | 7.14 | 7.56 | 6.32 | | | |
| 4.000 | 6.43 | 6.81 | 5.39 | | | |
| 5.000 | 5.43 | 5.72 | | | | |
| 5.500 | | 5.31 | | | | |
| 6.000 | | 4.97 | | | | |
| 6.500 | | 4.67 | | | | |
| 7.000 | | 4.40 | | | | |
| 7.500 | | 4.17 | | | | |
| 8.000 | | 3.97 | | | | |
| 8.500 | | 3.78 | | | | |
| 9.000 | | 3.62 | | | | |
| 9.500 | | 3.47 | | | | |
| 10.000 | | 3.33 | | | | |

operating currents were between 10^{-9} and 10^{-10} A when recording energy-loss spectra and between 10^{-13} and 10^{-14} A when performing attenuation measurements. The

TABLE II. Fluoromethane polarizabilities (in units of a_0^3).

| | CF ₄ | CF ₃ H | CF ₂ H ₂ | CFH ₃ |
|-----------------------------|-----------------|-------------------|--------------------------------|------------------|
| Polarizability (α) | 25.900 | 24.092 | 22.037 | 20.043 |

typical electron-energy resolution under these conditions was 500 meV. The collision chamber was defined by two apertures each of 1 mm in diameter, separated by 100 mm. The transmitted electrons were analyzed in energy by an electrostatic hemispherical spectrometer combined with a retarding field. Under these conditions a constant energy resolution of about 0.8 eV was obtained over the whole energy range considered. The acceptance angle of the analyzer was of the

order of 10^{-5} sr. Electrons were detected at the exit of the energy analyzer by a two-stage microchannel plate operating in pulse counting mode. The gas pressure in the chamber was measured with an absolute capacitance manometer (MKS Baratron 127 A), and the ultimate pressure in the region of the energy analyzer and electron detector was of the order of 10^{-7} Torr. Figure 1 shows a typical energy-loss spectrum of the electrons transmitted through the gas cell, and the excellent discrimination against the inelastic component of the transmitted electrons.

Statistical uncertainties in the measured data were less than 2%, other error sources have been previously discussed in [32–34]. By quadratic combination of all possible sources of error a total uncertainty of about 3% was obtained for the

TABLE III. Total cross sections for electron scattering by CF₃H, CF₂H₂, and CFH₃ (in units of a_0^2).

| Energy (keV) | CF ₃ H | | | CF ₂ H ₂ | | CFH ₃ | | | |
|--------------|-------------------|-------------|----------|--------------------------------|---------|------------------|---------|---------------------|---------------|
| | Eq. (1) | Sueoka [11] | Iga [12] | Addition rule | Eq. (1) | Addition rule | Eq. (1) | Krzysztofowicz [10] | Addition rule |
| 0.100 | | 55.36 | | 67.07 | | 58.30 | | 42.14 | 49.59 |
| 0.110 | | | | | | | | 40.71 | |
| 0.120 | | 48.93 | | | | | | 40.00 | |
| 0.140 | | | | | | | | 36.43 | |
| 0.150 | | 45.36 | | | | | | | |
| 0.160 | | | | | | | | 32.89 | |
| 0.180 | | | | | | | | 31.03 | |
| 0.200 | | 38.21 | | 46.29 | | 39.11 | | 28.82 | 31.94 |
| 0.220 | | | | | | | | | |
| 0.250 | | 33.93 | | | | | | 23.82 | |
| 0.300 | | 31.07 | 33.14 | 35.62 | | 29.73 | | | 23.84 |
| 0.400 | | 26.07 | 29.00 | 29.52 | | 24.38 | | | 19.23 |
| 0.500 | 28.69 | 22.14 | | 25.17 | 22.84 | 20.61 | 17.01 | | 16.05 |
| 0.600 | 24.89 | 20.00 | 25.07 | 21.96 | 19.82 | 17.87 | 14.75 | | 13.77 |
| 0.700 | 22.07 | | 22.18 | 19.54 | 17.57 | 15.81 | 13.08 | | 12.07 |
| 0.800 | 19.89 | | 17.75 | 17.50 | 15.83 | 14.10 | 11.79 | | 10.70 |
| 0.900 | 18.14 | | 16.71 | 15.97 | 14.44 | 12.89 | 10.75 | | 9.81 |
| 1.000 | 16.71 | | 16.14 | 14.84 | 13.30 | 11.99 | 9.90 | | 9.15 |
| 1.250 | 14.04 | | | | 11.18 | | 8.32 | | |
| 1.500 | 12.18 | | | | 9.70 | | 7.22 | | |
| 1.750 | 10.80 | | | | 8.60 | | 6.40 | | |
| 2.000 | 9.73 | | | | 7.75 | | 5.77 | | |
| 2.500 | 8.18 | | | | 6.51 | | 4.85 | | |
| 3.000 | 7.09 | | | | 5.65 | | 4.20 | | |
| 3.500 | 6.29 | | | | 5.01 | | 3.73 | | |
| 4.000 | 5.67 | | | | 4.51 | | 3.36 | | |
| 4.500 | 5.17 | | | | 4.12 | | 3.06 | | |
| 5.000 | 4.76 | | | | 3.79 | | 2.82 | | |
| 5.500 | 4.42 | | | | 3.52 | | 2.62 | | |
| 6.000 | 4.13 | | | | 3.29 | | 2.45 | | |
| 6.500 | 3.88 | | | | 3.09 | | 2.30 | | |
| 7.000 | 3.66 | | | | 2.92 | | 2.17 | | |
| 8.000 | 3.30 | | | | 2.63 | | 1.96 | | |
| 9.000 | 3.01 | | | | 2.40 | | 1.78 | | |
| 10.000 | 2.77 | | | | 2.21 | | 1.64 | | |

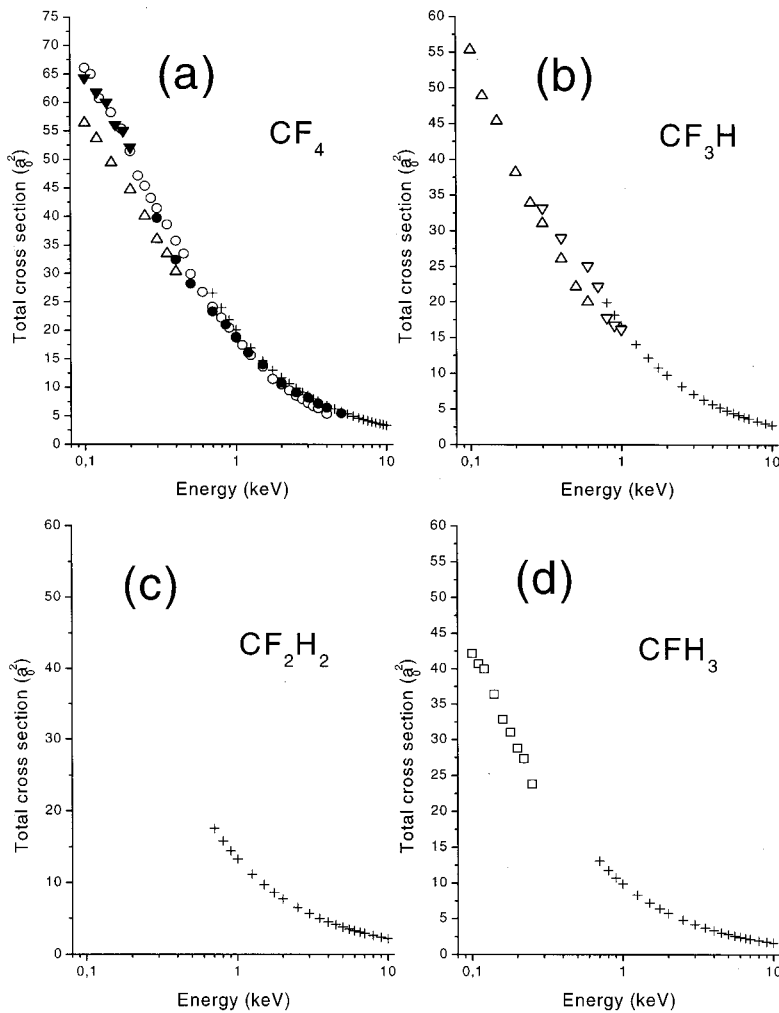


FIG. 2. Total cross section for fluoromethanes vs incident electron energy E . (a) CF_4 total cross section: ●, present experimental values; +, semiempirical values of Eq. (1); ○, experimental data by Zecca, Karwasz, and Brusa [7]; ▼, experimental data by Szmytkowski *et al.* [8]; △, data by Sueoka, Mori, and Hamada [9]. (b) CF_3H total cross section: +, semiempirical values of Eq. (1); △; data by Sueoka *et al.* [11]; ▽, experimental data by Iga, Pinto, and Homem [12]. (c) CF_2H_2 total cross section: +, semiempirical values of Eq. (1). (d) CFH_3 total cross section: +, semiempirical values of Eq. (1); □, experimental data by Krzysztofowicz and Szmytkowski [10].

measured values of the total cross section of CF_4 from 300 to 5000 eV. The values obtained are listed in Table I together with the experimental values of Zecca, Karwasz, and Brusa [7], Szmytkowski *et al.* [8], and Sueoka, Mori, Hamada [9] and the calculated values of Jiang, Sun, and Wan [28], as well as the result of our semiempirical calculations, explained below. Figure 1(a) shows a plot of all the experimental data for CF_4 and our empirical calculations for this molecule.

B. Empirical values

As mentioned in the Introduction, there are no experimental data for the total cross section of CF_4 at energies about 4.0 keV, and there are only data for CF_3H at energies below 1.00 keV, for CFH_3 at energies between 0.3 and 250 eV, and no data at all for CF_2H_2 .

In a recent paper García and Manero [30] proposed an empirical expression to calculate total cross sections for electron scattering by molecules, which was based on their measurements performed in a linear transmission beam configuration. This expression depends only on two parameters; the molecular polarizabilities (α) and the number of target electrons (Z), as follows:

$$\sigma_T(E) = (0.4Z + 0.1\alpha + 0.7)E^{-0.78}, \quad (1)$$

where $\sigma_T(E)$ and α are given in atomic units (a_0^2 and a_0^3 , respectively) and E in keV. This formula can be used for energies ranging from ≈ 1 to 10 keV. The total error associated with the values obtained using Eq. (1) was estimated to be better than 10%, as shown in [30] from the comparison with the experimental and theoretical data of other molecules.

By using Eq. (1) and the polarizability values given in Table II, taken from [35], (for CF_2H_2 , polarizability was obtained from a linear regression fit of the other three values), total cross-sections values have been deduced for the fluoromethanes for energies from 500 eV to 10 keV. As already mentioned, Table I lists the values obtained for CF_4 . In Table III are listed our empirically calculated values for the total cross sections of CF_3H , CF_2H_2 , and CFH_3 in the energy range from 0.5 to 10 keV, together with the experimental values of Sueoka *et al.* [11] and Iga, Pinto, and Homem [12] for CF_3H and those of Krzysztofowicz and Szmytkowski [10] for CFH_3 , as well as calculated values obtained by applying the addition rule to the atomic cross-section values of Jiang, Sun, and Wan [28] for H, C, and F. Figures 2(b)–2(d) shows plots of the data for CF, H, CF_2H_2 ,

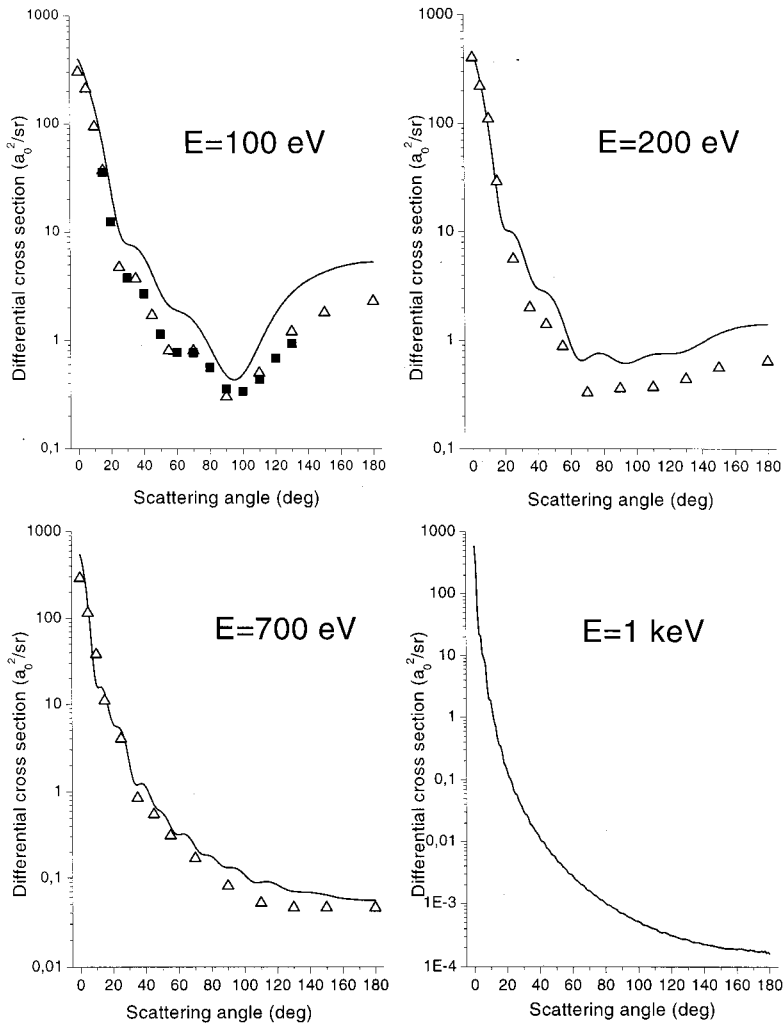


FIG. 3. Differential elastic cross section for CF_4 at 100, 200, 700 eV, and 1 keV incident electron energy: —, present calculations, Δ , data by Sakae *et al.* [13]; \blacksquare , data by Tanaka *et al.* [16].

and CFH_3 , respectively.

As shown in Fig. 2(a) and Table I, the values obtained using Eq. (1) for CF_4 are in excellent agreement with our experimental ones, the discrepancy being less than 8% for energies above 900 eV, and also in good agreement with other experimental data. As shown in Table III and Figs. 2(b)–2(d) there is also good agreement between the values obtained using Eq. (1) and other experimental or calculated data.

III. ELECTRON ELASTIC-SCATTERING CROSS SECTIONS

A. Differential cross sections

As shown recently [36], accurate differential and integral cross-section data for electron scattering by atoms in the energy range from 0.5 to 10 keV can be calculated by means of a scattering potential method. A similar procedure can be applied to molecular targets [37,38] by assuming that the incident electron energy is high enough to validate the independent atom model [39]. In these conditions, the differential cross section averaged over all orientations of the molecular axis is given by

$$\sigma_M(\theta) = \sum_{i,j=1}^N f_j(\theta) f_j^*(\theta) \sin(qr_{ij}/qr_{ij}), \quad (2)$$

where N represents the number of atoms in the molecule, (here, $N=5$), $f_j(\theta)$ is the scattering amplitude due to the j th atom of the molecule, $q [=2k \sin(\theta)/2]$ is the magnitude of the momentum (k) transferred in the collision, and r_{ij} is the distance between the i th and the j th atom. The atomic scattering amplitudes $f_j(\theta)$ for fluorine, carbon, and hydrogen were obtained in a partial-wave expansion, given by

$$f_j(\theta) = \frac{1}{2ik} \sum_l (2l+1)(e^{2i\delta_{lj}} - 1) P_l(\cos \theta), \quad (3)$$

where $P_l(\cos \theta)$ are the Legendre polynomials and δ_{lj} the l th partial-wave phase shift for the j th atom of the molecule. To obtain δ_{lj} , the appropriate scattering equation was solved numerically with proper boundary conditions [36]. The constituent atoms were replaced by a local spherically symmetric potential V_{so} which, as shown in [36], can be described for elastic processes as

$$V_{sc} = V_s(r) + V_e(r) + V_p(r), \quad (4)$$

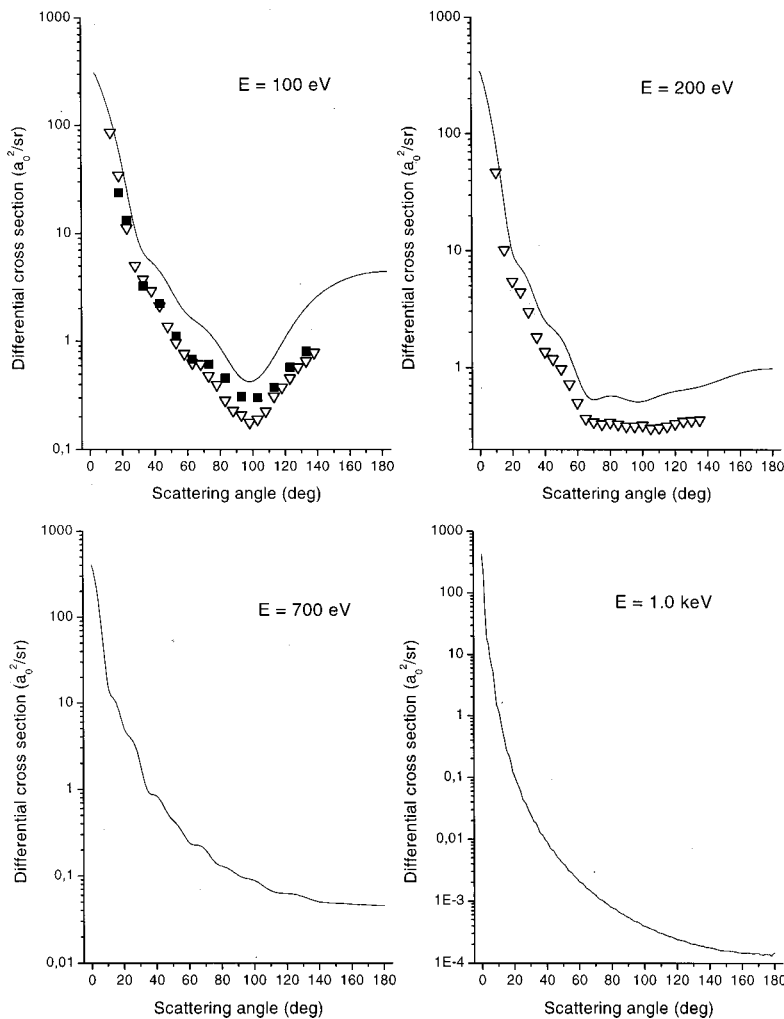


FIG. 4. Differential elastic cross section for CF_3H at 100, 200, 700 eV, and 1 keV incident electron energy: —, present calculations; ∇ , data by Homem and Iga [15]; \blacksquare , data by Tanaka *et al.* [16].

where $V_s(r)$ is the static potential for the electron-atom system, which has been calculated by using the atomic charge density deduced from Hartee-Fock wave functions [40], and $V_e(r)$ and $V_p(r)$ represent the exchange and target polarization contributions, respectively, as described in [36].

As an example of the results obtained, in Fig. 3 are plotted the differential elastic cross sections for electron scattering by CF_4 at several incident energies, together with the experimental data of Sakae *et al.* [13] and Tanaka *et al.* [16], and in Fig. 4 we plot the differential elastic cross sections for electron scattering by CF_3H at the same energies, together with the experimental data of Homem and Iga [15] and Tanaka *et al.* [16]. Similar results have also been obtained for CF_2H_2 and CFH_3 .

As can be seen in Figs. 3 and 4, our differential elastic cross-section data are in good qualitative agreement over the whole angular range with previous experimental data and in good quantitative agreement also at small angles, where the contribution to the total elastic cross section is more important. At large angles our values are higher than the experimental ones, probably due to the fact that the independent atom model oversimplifies the electron molecule scattering process and other contributions should be included. In the case of the data of Homem and Iga [15] for CF_3H , it should be pointed out that they reported that their data were a factor

of 2 lower than those obtained from an independent atom model calculation.

B. Integral cross sections

By integrating over all the scattering angles, integral elastic cross sections have been obtained from the differential ones for CF_4 , CF_3H , CF_2H_2 , and CFH_3 . The results obtained by this procedure are plotted in Fig. 5 and listed in Table IV, together with the data of Sakae *et al.* [13], the data of Raj [41] obtained by means of the addition rule for CF_4 and the data of Iga and co-workers [12] for CF_3H .

It can be seen from Table IV and Fig. 4 that there is very good qualitative and quantitative agreement for all the CF_4 data, but that the data of Iga, Pinto, and Homem [12] for CF_3H are about 50% lower than ours, showing a similar trend as their differential cross-section data.

In accordance with Refs. [42,43] the total elastic ($\sigma_{\text{el}}^{\text{BB}}$) and the total inelastic ($\sigma_{\text{inel}}^{\text{BB}}$) cross sections for electron scattering by atoms, in a combined Born-Bethe approximation, can be written as

$$\frac{\sigma_{\text{el}}^{\text{BB}}}{a_0^2} = \pi \left[A_{\text{el}} \left(\frac{R}{E_0} \right) + B_{\text{el}} \left(\frac{R}{E_0} \right)^2 + C_{\text{el}} \left(\frac{R}{E_0} \right)^3 + \dots \right] \quad (5)$$

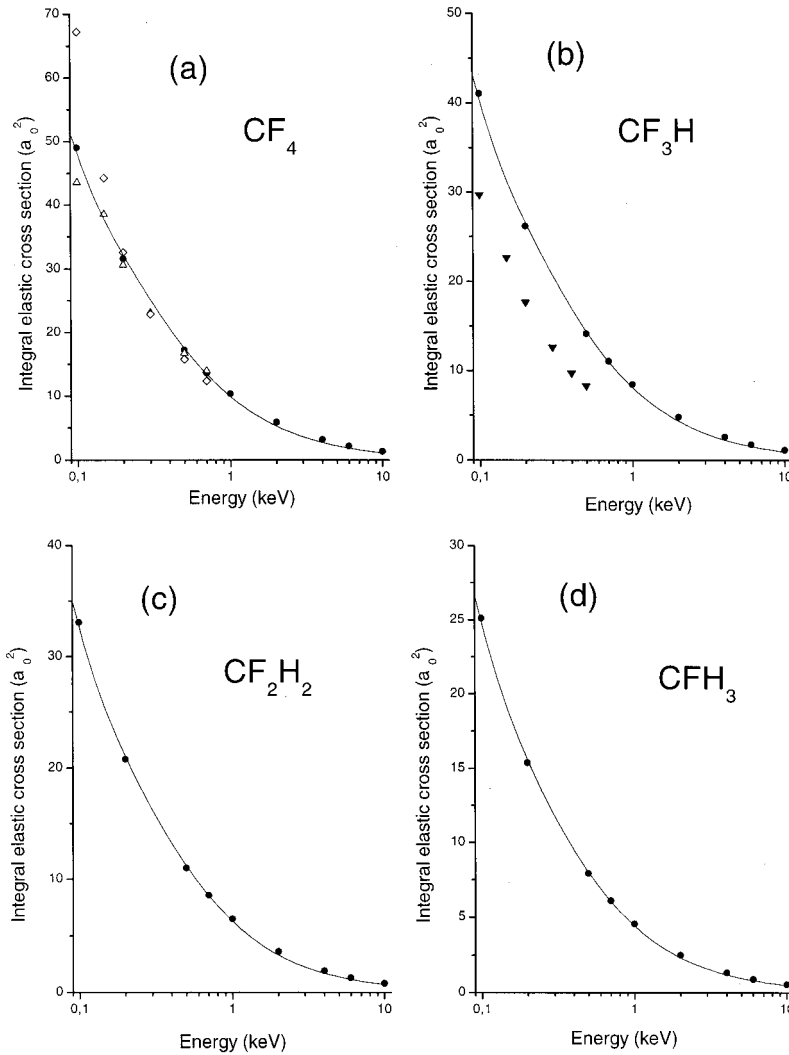


FIG. 5. Integral elastic cross section for fluoromethanes vs incident electron energy. (a) CF_4 integral cross section: \bullet , present calculations; Δ , data by Sakae *et al.* [13]; \diamond , data by Raj [41]; \circ , result of the nonlinear least-squares fit. (b) CF_3H integral cross section: \bullet , present calculations; \blacktriangledown , data by Iga, Pinto, and Homem [12]; --- , result of the nonlinear least-squares fit. (c) CF_2H_2 integral cross section: \bullet , present calculations; --- , result of the nonlinear least squares fit. (d) CFH_3 integral cross section: \bullet , present calculations; --- , result of the nonlinear least-squares fit.

and

$$\frac{\sigma_{\text{inel}}^{\text{BB}}}{a_0^2} = 4\pi \left[M_{\text{inel}}^2 \left(\frac{R}{E_0} \right) \ln \left(4c_{\text{inel}} \frac{E_0}{R} \right) + \gamma_{\text{inel}} \left(\frac{R}{E_0} \right)^2 + \dots \right], \quad (6)$$

respectively, where E_0/R is the incident energy in Rydberg units ($1 \text{ Ry} = 13.605 \text{ eV}$) and a_0 is the Bohr radius.

Accordingly, and in order to facilitate calculations, we have carried out a nonlinear least-squares fit of the integral elastic cross-section data to several expressions similar to Born-Bethe formulas. The best fit was obtained using the expression

$$\sigma_{\text{el}}(E) = \frac{1}{E} \left(A_1 + \frac{A_2}{E} + \frac{A_3}{E^2} + \frac{A_4}{E^3} \right), \quad (7)$$

where the cross sections are given in units of a_0^2 and the energy in keV. Table V lists the values of the parameters obtained for the four fluoromethanes. Therefore Eq. (7), with the coefficients of Table V, allows one to calculate the total elastic cross sections for fluoromethanes in the energy range from 0.1 to 10.0 keV.

We have checked for CF_4 , the coherence between the total cross-section values given by Eq. (1) and the integral cross section values obtained as mentioned above, by comparing the values of Eq. (1) with those obtained by adding to our integral cross-section values the total ionization values of Kim and Rudd [31], calculated through a BEB method. The result of this comparison is plotted in Fig. 6, which shows that there is a good agreement between the total cross-section values and the added ones, the latter being about 10% lower in the energy range from 1.0 to 10.0 keV, where Eq. (1) applies. This is expected, because the sum of integral cross sections and ionization does not include the contribution of other channels, such as electronic excitations, which are open at these impact energies.

IV. INELASTIC SCATTERING CROSS SECTIONS

There are neither experimental data nor calculated values for the electron inelastic-scattering cross sections of fluoromethanes, due to the large number of channels open in inelastic collisions at these energies. We have deduced inelastic cross-section values for CF_4 , CF_3H , CF_2H_2 , and CFH_3 as the difference between the total cross-section val-

TABLE IV. Integral elastic cross sections for electron scattering by fluoromethanes (in units of a_0^2).

| Energy (keV) | CF ₄ | | | CF ₃ H | | CF ₂ H ₂ | CFH ₃ |
|--------------|-----------------|------------|----------|-------------------|----------|--------------------------------|------------------|
| | Present work | Sakae [13] | Raj [41] | Present work | Iga [12] | Present work | Present work |
| 0.100 | 49.010 | 43.57 | 67.17 | 41.030 | 29.696 | 33.060 | 25.080 |
| 0.150 | | 38.57 | 44.26 | | 22.671 | | |
| 0.200 | 31.580 | 30.57 | 32.56 | 26.180 | 17.654 | 20.780 | 15.370 |
| 0.250 | | | | | | | |
| 0.300 | | 23.07 | 22.88 | | 12.639 | | |
| 0.350 | | | | | | | |
| 0.400 | | | | | 9.728 | | |
| 0.450 | | | | | | | |
| 0.500 | 17.200 | 16.71 | 15.75 | 14.100 | 8.261 | 11.000 | 7.907 |
| 0.600 | | | | | | | |
| 0.700 | 13.540 | 13.93 | 12.35 | 11.060 | | 8.579 | 6.097 |
| 1.000 | 10.350 | | | 8.428 | | 6.499 | 4.569 |
| 2.000 | 5.881 | | | 4.759 | | 3.637 | 2.515 |
| 4.000 | 3.172 | | | 2.558 | | 1.944 | 1.331 |
| 6.000 | 2.172 | | | 1.750 | | 1.327 | 0.905 |
| 10.000 | 1.333 | | | 1.073 | | 0.813 | 0.552 |

ues, given by Eq. (1), and the integral elastic cross-section data obtained from the least-squares fit [Eq. (7)]. Table VI lists the integral inelastic cross-section values obtained in this way for the four fluoromethanes.

As in the case of the elastic cross sections, a least-squares fit to several expressions similar to Born-Bethe formulas was carried out. The best fit was obtained for the expression

$$\sigma_{inel}(E) = \frac{1}{E} \left[B_1 + B_2 \ln(E) + \frac{B_3}{E} \right], \quad (8)$$

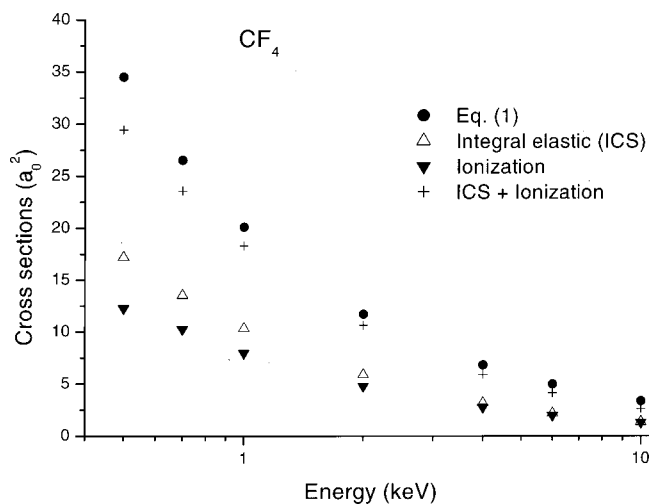


FIG. 6. Comparison of the total cross section values of Eq. (1) with the sum of the integral elastic and the ionization cross-section values for CF₄. ●, values of Eq. (1); △, integral cross-section values; ▼, ionization cross section values; +, sum of integral and ionization cross-section values.

where the cross sections are given in units of a_0^2 and the energy in keV. Table VII lists the values of the coefficients of Eq. (8) for the four fluoromethanes and Fig. 7 shows the excellent agreement obtained between the fitted curves and the inelastic cross section values in all cases.

V. CONCLUSIONS

Total electron-scattering cross sections for CF₄ were measured from 300 to 5000 eV, which show good agreement with other previously published experimental data. Total cross-section values for electron scattering by the fluoromethanes are given for the energy range from 0.5 to 10.0 keV. These are obtained by means of an empirical formula that depends on only two parameters—the total number of electrons and the polarizability of the molecule. The values obtained using this formula have been compared with the present and previous experimental and evaluated data, and are in good agreement, to within 8%, in the energy range considered.

Differential and integral elastic cross sections are also given at several incident electron energies up to 10 keV, calculated by means of a scattering potential method, in which it was assumed that the independent atom model is valid.

TABLE V. Coefficients of formula (7) for the fluoromethanes.

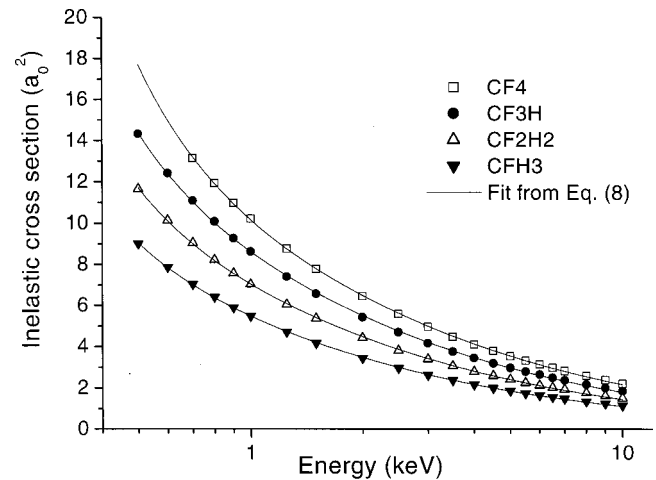
| | A1 | A2 | A3 | A4 |
|--------------------------------|---------|---------|--------|---------|
| CF ₄ | 11.2225 | -1.4517 | 0.1160 | -0.0035 |
| CF ₃ H | 9.1782 | -1.1758 | 0.0948 | -0.0029 |
| CF ₂ H ₂ | 7.0788 | -0.8741 | 0.0704 | -0.0021 |
| CFH ₃ | 4.9317 | -0.5466 | 0.0429 | -0.0013 |

TABLE VI. Inelastic cross sections for electron scattering by fluoromethanes (in units of a_0^2).

| Energy (keV) | CF ₄ | CF ₃ H | CF ₂ H ₂ | CFH ₃ |
|--------------|-----------------|-------------------|--------------------------------|------------------|
| 0.50 | | 14.32 | 11.65 | 9.01 |
| 0.60 | | 12.41 | 10.14 | 7.86 |
| 0.70 | 13.14 | 11.09 | 9.05 | 7.03 |
| 0.80 | 11.93 | 10.08 | 8.22 | 6.40 |
| 0.90 | 10.98 | 9.27 | 7.56 | 5.89 |
| 1.00 | 10.21 | 8.62 | 7.03 | 5.47 |
| 1.25 | 8.76 | 7.40 | 6.04 | 4.70 |
| 1.50 | 7.77 | 6.56 | 5.35 | 4.16 |
| 1.75 | 7.02 | 5.92 | 4.83 | 3.75 |
| 2.00 | 6.44 | 5.42 | 4.42 | 3.44 |
| 2.50 | 5.57 | 4.69 | 3.81 | 2.96 |
| 3.00 | 4.95 | 4.16 | 3.39 | 2.62 |
| 3.50 | 4.47 | 3.76 | 3.06 | 2.37 |
| 4.00 | 4.09 | 3.45 | 2.79 | 2.16 |
| 4.50 | 3.79 | 3.19 | 2.59 | 1.99 |
| 5.00 | 3.53 | 2.97 | 2.41 | 1.86 |
| 5.50 | 3.32 | 2.79 | 2.25 | 1.74 |
| 6.00 | 3.14 | 2.65 | 2.13 | 1.64 |
| 6.50 | 2.98 | 2.50 | 2.02 | 1.55 |
| 7.00 | 2.82 | 2.37 | 1.93 | 1.48 |
| 8.00 | 2.59 | 2.17 | 1.76 | 1.35 |
| 9.00 | 2.39 | 2.00 | 1.62 | 1.24 |
| 10.00 | 2.22 | 1.86 | 1.51 | 1.15 |

TABLE VII. Coefficients of formula (8) for the fluoromethanes.

| | B1 | B2 | B3 |
|--------------------------------|--------|--------|--------|
| CF ₄ | 7.2020 | 6.1571 | 2.9604 |
| CF ₃ H | 6.7223 | 4.7895 | 1.8933 |
| CF ₂ H ₂ | 5.5635 | 3.8206 | 1.4688 |
| CFH ₃ | 4.4441 | 2.8623 | 1.0318 |

FIG. 7. Integral inelastic cross sections for the fluoromethanes: ■, CF₄ cross section; ●, CF₃H cross section; ▼, CF₂H₂ cross section; ▲, CFH₃ cross section; —, results of the nonlinear least-squares fit.

The results obtained are, in general, in good agreement with other published data.

Integral inelastic cross section values have been deduced as the difference between total cross-section and integral elastic cross-section values. Nonlinear least-squares fits were made to the integral elastic and inelastic data, and formulas were given which allow one to calculate these cross sections at any energy within the energy range considered.

Finally, the coherence for CF₄ of the present cross-section values has been checked by comparing our total cross-section values with those obtained by adding to our integral elastic cross-section values the total ionization data of Kim and Rudd [31]. This comparison showed a good agreement between both sets of data.

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