

Electron-CF₄ elastic scattering in the static-exchange approximation

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We report differential, integral, and momentum-transfer cross sections for the elastic scattering of electrons by CF₄ from 5 to 35 eV. The calculations were carried out at the fixed-nuclei, static-exchange level using the Schwinger variational principle. Analyses of the partial channel amplitudes show four broad shape resonances; two in T_2 , one in A_1 , and one in E symmetries. The positions of these resonances agree with experimental data from total-cross-section measurements, dissociative attachment studies, and low-energy electron excitation spectra, the only exception being the 8.9-eV structure in the total-cross-section data. No experimental measurements on differential cross sections are available, but comparing with the corresponding static-exchange calculations for the e -CH₄ system, the e -CF₄ cross sections generally are less backward peaked.

I. INTRODUCTION

The scattering of low-energy electrons by polyatomic molecules has attracted considerable theoretical interest.¹ So far, most of the theoretical treatments relied on single-center expansion techniques^{1,2} as well as the use of model exchange^{1,3,4} and polarization^{1,4-6} potentials. For a few polyatomic hydrides, true multicenter, *ab initio* studies have also been reported.⁷⁻⁹ The latter calculations are based on a multichannel extension of the Schwinger variational principle¹⁰ (SMC) where the $(N+1)$ -electron wave function is expanded in a set of Gaussian functions at the nuclear centers and any other centers deemed suitable. The proper boundary condition is retrieved from a projected Lippmann-Schwinger equation. The SMC method allows the direct use of target wave functions from bound-state calculations without possible loss of accuracy due to one-center expansions. In addition, the use of an antisymmetrized wave function automatically incorporates nonlocal exchange effects in the calculation. So far, most of the SMC calculations have been carried out at the static-exchange level, but limited polarization calculations have been reported for CH₄.⁹ In all the cases studied so far, the SMC cross sections calculated in the static-exchange approximation are in good agreement with available experimental data at incident energies 10 eV and above, indicating that polarization effects probably are small in this energy region.

Ab initio studies of low-energy e -CF₄ scattering pose additional challenges as it represents the largest molecule studied so far. Both the tight fluorine 1s electrons and the longer bond length makes it a less suitable candidate for single-center techniques. The large basis set required to represent the target molecule also makes this a demanding calculation using the SMC method. On the other hand, these cross sections are needed to unravel the energy deposition pathways of the ionizing radiation in the upper atmosphere and to model the atmospheric chemistry of fluorocarbons. In addition, they are useful in the design of gaseous dielectrics and plasma etchings.

An interesting aspect in the electron scattering of heavy polyatomic molecules is the rich resonance structures observed in elastic scattering, rotational, vibrational, and electronic excitations, as well as dissociative attachment processes. The nature of these resonances can be inferred only indirectly from experiment. Most theoretical studies of resonances in polyatomic molecules are limited to structural calculations on the target states and infer the symmetry and position of the negative-ion states from the low-lying unoccupied orbitals.¹¹ Only in a few cases have the resonances been studied directly by solving the scattering problem. Notable examples include the coupled-channel studies by Morrison and co-workers^{12,13} on the low-energy $^2\Sigma_g^+$ resonance in CO₂ using a model potential and single-center coordinates. Also, the single-center model-potential calculations of Jain and Thompson¹⁴ on the electronically elastic e -H₂S scattering showed a B₂ shape resonance at about 2 eV and a broad resonance around 6–8 eV due to A_1 scattering. Using a similar technique, Gianturco and Scialla¹⁵ reproduced the broad peak in the 7–8 eV region in e -CH₄ elastic scattering due to a shape resonance in the T_2 symmetry. This structure has also been obtained by Jain¹⁶ using a single-centered spherical optical potential. Similarly, the Schwinger, multicenter, static-exchange calculation of Lima *et al.*⁷ showed a broad peak for this system but the position of the peak was shifted to 10–12 eV. No analyses were made in the last two calculations to identify this structure as a resonance. Experimental studies on the e -CF₄ system have led to the assignment of a number of resonances. In his total-cross-section measurements, Jones¹⁷ observed a broad shoulder around 3.6 eV, a peak at 8.9 eV, and a very broad maximum around 25 eV and attributed those features to resonances. Verhaart *et al.*¹⁸ observed sharp structures in the derivative of the transmitted current in the 0–2 eV region. They ascribed these features to the vibrational levels of a resonance state where the attached electron is in a Rydberg orbital. Resonant dissociative attachments in CF₄ have been reported by Verhaart *et al.*,¹⁸ Harland and

Franklin,¹⁹ and MacNeil and Thynne.²⁰ The resonant production of CF_3^- is centered at 6.9 eV and for F^- , between 6.15 and 7.5 eV. In addition, Verhaart *et al.*¹⁸ ascribed two humps in their low-energy electron-impact spectra, located at 12.0 and 13.0 eV and not observable in the corresponding high-energy electron-impact spectra, to core-excited resonances in which the Rydberg orbital in the negative-ion state is doubly occupied. In the present fixed-nuclei, static-exchange study of elastic $e\text{-CF}_4$ scattering between 5 and 35 eV, we found four resonances. This represents the first determination of resonances in a polyatomic molecule using a multicenter, *ab initio* technique. The only previous calculations on this system are by Tossell and Davenport²¹ using the multiple-scattering $X\alpha$ approximation. Their calculations showed a resonance in the T_2 channel centered at 3.2 eV, but both the calculated position and intensity of the resonance are extremely sensitive to the bond distance.

No absolute measurements of the elastic or momentum-transfer cross sections for the $e\text{-CF}_4$ system have been reported in the energy range of interest. In addition to the experiments cited above, measurements in the low-energy regime include the work of Field *et al.*²² who reported a Ramsauer-Townsend minimum for this system at 0.162 eV. Leiter *et al.*²³ measured the ionization cross section from threshold to 180 eV, and Winters and co-workers^{24,25} reported dissociation cross sections. Swarm measurements of drift velocities have been reported by Christophorou *et al.*²⁶ and Naidu and Prasad.²⁷ Values of the ratio of the diffusion coefficient versus mobility have been determined by Naidu and Prasad²⁷ and by Lakshminarashimha *et al.*²⁸ Hayashi²⁹ deduced momentum-transfer, vibrational excitation, and electronic excitation cross sections by fitting available swarm data. His vibrational excitation cross sections for the ν_3 mode are much larger than the corresponding values in CH_4 .

A brief description of the computational procedure is given in Sec. II. Section III presents our results and discussions and Sec. IV concludes the paper.

II. COMPUTATIONAL PROCEDURE

Detailed descriptions of the computational procedure in the SMC method have been presented elsewhere.^{30,31} Briefly, the Hamiltonian for the collision system is

$$H = (H_N + T_{N+1}) + V, \quad (1)$$

with H_N the target Hamiltonian, T_{N+1} the kinetic energy operator of the incident electron, and V the interaction potential. Let $\Psi_n^{(+)}$ be the total $(N+1)$ -electron antisymmetrized wave function with incoming-plane-wave and outgoing-wave boundary conditions for the n th channel. A projected Lippman-Schwinger equation for $\Psi_n^{(+)}$ is

$$P\Psi_n^{(+)} = S_n + G_P^{(+)}V\Psi_n^{(+)}. \quad (2)$$

The projection operator P defines the open-channel space in terms of the target eigenfunctions Φ_m ,

$$P = \sum_{m=1}^M |\Phi_m(1,2,\dots,N)\rangle \langle \Phi_m(1,2,\dots,N)|, \quad (3)$$

with M the total number of energy accessible target states under consideration. In Eq. (2), S_n is the eigenfunction of the unperturbed Hamiltonian $H_N + T_{N+1}$, and is given by

$$S_n = \left[\frac{k_n}{(2\pi)^3} \right]^{1/2} \exp(ik_n \cdot \mathbf{r}_{N+1}) \Phi_n. \quad (4)$$

The projected outgoing-wave Green's function $G_P^{(+)}$, defined in the open-channel space, is given by

$$G_P^{(+)} = -\frac{1}{2\pi} \sum_{m=1}^M \left| \Phi_m \right\rangle \frac{\exp(ik_m |\mathbf{r}_{N+1} - \mathbf{r}'_{N+1}|)}{|\mathbf{r}_{N+1} - \mathbf{r}'_{N+1}|} \left\langle \Phi_m \right|. \quad (5)$$

A complete equation for $\Psi_n^{(+)}$ is obtained by the requirement that it must satisfy the Schrödinger equation as well as the projected Lippmann-Schwinger equation. After some rearrangement, the resulting equation is¹⁰

$$A^{(+)}\Psi_n^{(+)} = VS_n, \quad (6)$$

with

$$A^{(+)} = \frac{1}{2}(PV + VP) - VG_P^{(+)}V + \frac{1}{N+1}\hat{H} - \frac{1}{2}(P\hat{H} + \hat{H}P), \quad (7)$$

where $\hat{H} = E - H$. Based on Eq. (7), a variational expression for the fixed-nuclei scattering amplitude is

$$f_{mn} = -\frac{1}{2\pi} \frac{\langle S_m | V | \Psi_n^{(+)} \rangle \langle \Psi_m^{(-)} | V | S_n \rangle}{\langle \Psi_m^{(-)} | A^{(+)} | \Psi_n^{(+)} \rangle}. \quad (8)$$

The above quantity is calculated in the molecular frame using the fixed-nuclei approximation. Transformation to the laboratory frame is achieved via partial-wave decompositions.³²

In the static-exchange approximation, the quality of the SMC cross section depends entirely on the choice of basis sets.³⁰ Generally, two basis sets are involved: one set to represent the $(N+1)$ -electron wave function and the second set as an insertion basis for $G_P^{(+)}$. All previous SMC calculations on polyatomic hydrides used large, uncontracted Gaussian bases. However, the size of the CF_4 calculation necessitates the use of a contracted basis. Thus, in the representation of $\Psi_0^{(+)}$, we use Dunning's³³ $9s5p/4s2p$ basis for fluorine, augmented by one set of d functions. For carbon we use an uncontracted basis of $10s6p3d$ functions obtained by adding one diffuse s , one diffuse p , and three d functions to Huzinaga's $9s5p$ carbon basis.³⁴ This carbon basis is similar but smaller than the $12s8p4d$ basis used in the CH_4 calculations.⁷ The choice of an uncontracted basis at carbon is motivated by the fact that the continuum electron is most conveniently represented by a basis at the center of mass of the colliding system and a large, uncontracted basis should be used for this purpose. Table I presents the basis set used for $\Psi_0^{(+)}$. The target wave function used is a self-consistent-field (SCF) wave function calculated at the experimental

TABLE I. Gaussian basis set used in the representation of $\Psi_0^{(+)}$.

Atom and type	Exponent
C, 10s	4233.0, 634.9, 146.1, 42.5, 14.19, 5.148, 1.967, 0.4962, 0.1533, 0.02789
C, 6p	18.16, 3.986, 1.143, 0.3594, 0.1146, 0.0361
C, 3d	0.626, 0.15, 0.0375
F, 4s	Dunning ^a 9s/4s set
F, 2p	Dunning ^a 5p/2p set
F, 1d	1.58

^aReference 33.

geometry³⁵ using the same basis set. A C—F bond distance of 2.4944 a.u. is used. The SCF energy is -435.766214 a.u., to be compared with the value of -435.760499 a.u. by Sekino and Bartlett³⁶ using double zeta plus polarization basis.

The second basis set is used as an insertion basis to represent the principal-value part of $G_p^{(+)}$. The procedure for choosing this basis has been discussed previously.³⁰ As in our study of the shape resonance in N₃,³⁰ we found that calculations in the resonance region are particularly sensitive to the insertion basis. Large, judiciously chosen insertion bases are required to obtain converged results. Table II presents the insertion bases used in the present calculation. The insertion bases are grouped in C_{2v} symmetry because the computer code used in the calculation of the target wave function is based on this point group. Note that molecular orbitals in C_{2v} symmetry can be readily regrouped into the T_d point group. For example, the A_1 orbitals in the C_{2v} point group include the A_1 orbitals as well as one component each of the degenerate E and T_2 orbitals in the T_d point group and the subsets do not mix with each other. Thus we determine partial cross sections belonging to a

given irreducible representation of the T_d point group simply by choosing a subset of scattering orbitals of the correct symmetry. Such regrouping was not done for the insertion bases. For this reason, the partial cross sections show small deviations from T_d symmetry.

III. RESULTS AND DISCUSSIONS

Figure 1 presents the elastic integral cross sections of CF₄. For the purpose of comparison, the elastic cross sections of CH₄ calculated in the static-exchange approximation⁷ also are included in the figure. The two sets of cross sections are noticeably different. While the CH₄ data show one broad peak around 11 eV, the CF₄ cross sections have more structures, with one strong peak around 6.5 eV, and two secondary structures at approximately 12 and 26 eV. Also, the magnitude of the CF₄ cross sections are generally below those of CH₄ except at its primary peak.

To understand the nature of the CF₄ cross-section curve, we investigated the possibilities of resonances. From the analyses of the eigenphase sums and the K matrices, four shape resonances are found in the region of

TABLE II. Gaussian basis sets used in the representation of $G_p^{(+)}$.

Insertion basis set	Exponent
A_1 symmetry ^a : Basis set from Table I plus	
C, 8s	19 200, 9600, 2400, 1200, 300, 60, 30, 0.001
C, 8p _y	9600, 3600, 1200, 600, 240, 60, 30, 0.001
C, 6d _{x²−y²}, 6d_{y²−z²}, 6d_{z²−x²}}}}	9600, 3200, 600, 120, 30, 4
B_1 symmetry ^a : Basis set from Table I plus	
C, 16p _x	19 200, 9600, 4800, 2400, 1200, 900, 600, 300
C, 18d _{xy}	120, 60, 30, 8, 0.6, 0.01, 0.001
	39 400, 19 200, 9600, 4800, 2400, 1200, 900, 600
	300, 120, 60, 30, 16, 8, 4, 1.6, 0.01, 0.001
B_2 symmetry ^a : Basis set from Table I plus	
C, 16p _z	19 200, 9600, 4800, 2400, 1200, 900, 600, 300
C, 18d _{yz}	120, 60, 30, 8, 2, 0.6, 0.01, 0.001
	39 400, 19 200, 9600, 4800, 2400, 1200, 900, 600
	300, 120, 60, 30, 16, 8, 4, 1.6, 0.01, 0.001
A_2 symmetry ^a : Basis set from Table I plus	
C, 18d _{xz}	39 400, 19 200, 9600, 4800, 2400, 1200, 900, 600
	300, 120, 60, 30, 16, 8, 4, 1.6, 0.01, 0.001

^aThe insertion bases are grouped according to C_{2v} symmetry. See text for more details.

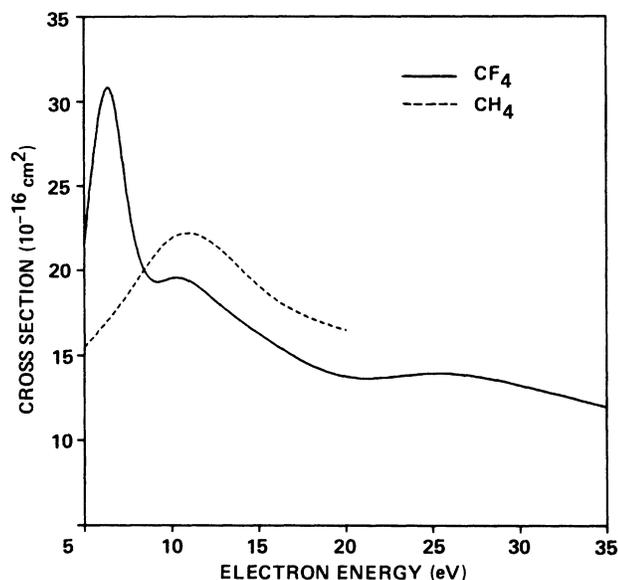


FIG. 1. Elastic integral cross sections in the static-exchange approximation for e -CF₄ and e -CH₄ scattering. The CH₄ data are from the SMC calculations in Ref. 7.

energy under study, two in T_2 , one in A_1 and one in E symmetries. Figure 2 presents the eigenphase sums from these three partial channels and in Fig. 3 the corresponding partial cross sections are presented. The resonance positions and widths, obtained by spline fits of the eigen-

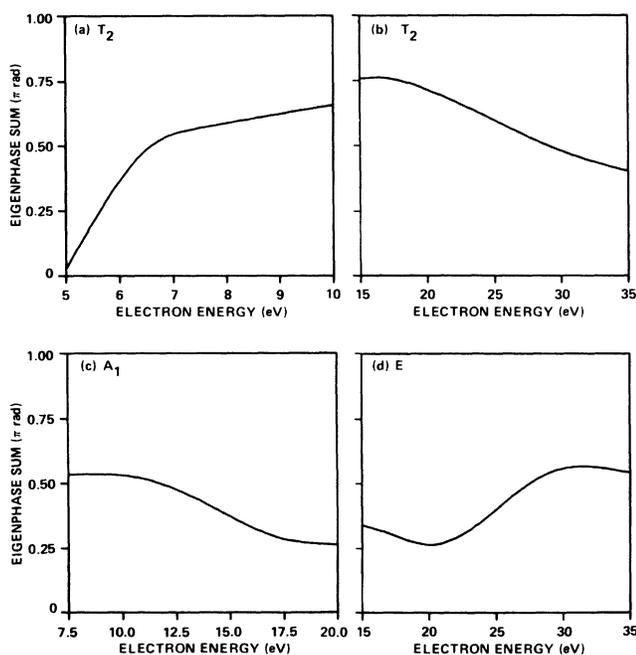


FIG. 2. Eigenphase sums (in π rad) near the resonances in e -CF₄ elastic scattering. (a) First resonance in T_2 symmetry, (b) second resonance in T_2 symmetry, (c) A_1 symmetry, and (d) E symmetry.

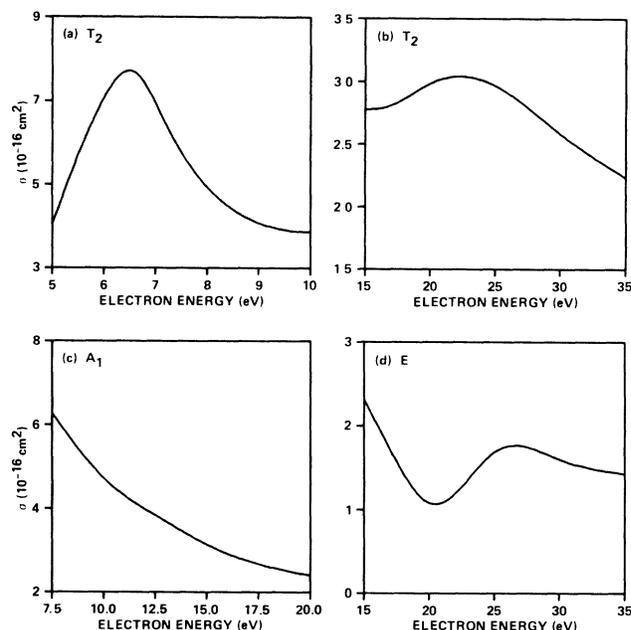


FIG. 3. Partial cross sections near the resonances in e -CF₄ elastic scattering. (a) First resonance in T_2 symmetry, (b) second resonance in T_2 symmetry, (c) A_1 symmetry, and (d) E symmetry.

phase sums, are presented in Table III. Notice that all the resonances are very broad. Thus it is necessary to use both the eigenphase sums and the K matrices to confirm their existence. We note that the resonance positions deduced from the K matrices generally are shifted slightly, indicating that the insertion bases may still be deficient. Also notice that the SMC calculations include both resonant and nonresonant contributions. Since these resonances occur at relatively high energies, the nonresonant contributions are not negligible. For these reasons, the resonance positions and widths in Table III can only be considered approximate. More accurate determinations of these parameters will require larger basis sets, closer energy intervals, as well as more sophisticated data analysis in the SMC calculations. Alternative procedures include the use of the Feshbach projection operator technique,³⁷ or a complex coordinate treatment.³⁸ The strong nonresonant contribution in the A_1 partial channel also reduces the resonant contribution to inflections in the A_1 cross-section curve in Fig. 3, whereas for the other partial channels the resonant structures are much more prominent.

TABLE III. Estimated positions and widths of the resonances in e -CF₄ elastic scattering.

Symmetry	Position (eV)	Width (eV)
T_2	6.6	4.1
	29.1	29.8
A_1	11.7	22.8
E	27.5	18.4

TABLE IV. Integral and momentum-transfer cross sections for e -CF₄ elastic scattering (present SMC calculation) and total scattering cross sections (experiment of Jones, Ref. 17).

Electron energy (eV)	Cross sections (10^{-16} cm ²)		
	Integral elastic ^a	Momentum transfer ^a	Total ^b
5.0	21.50	18.83	13.85
6.5	30.69	15.87	17.21 ^c
7.5	24.09	14.16	20.11
10.0	19.58	13.34	20.89
12.5	18.23	12.90	18.26
15.0	16.31	11.83	17.89
17.0	14.99	10.82	18.17
20.0	13.78	10.31	19.03
25.0	13.97	11.47	20.13
30.0	13.27	10.93	19.94
35.0	11.99	9.52	19.77

^aPresent SMC calculation.

^bExperiment of Jones, Ref. 17.

^cAt an incident energy of 6.6 eV.

Partial-wave analyses show that the first T_2 resonance is dominated by the $l = 1, m = 0, 1$ partial waves and the second resonance comes from the $l = 2, m = 1, 2$ partial waves. The A_1 resonance is an s -wave resonance and the E resonance comes from $l = 2, m = 0, 2$, with a small contribution from $l = 4, m = 0$. Because the widths are large, all the resonances overlap to a certain extent. This is particularly true of the second T_2 resonance and the E resonance. For this reason, the calculated integral cross sections show only three peaks instead of four.

The integral and momentum-transfer cross sections for e -CH₄ elastic scattering are given in Table IV. Also presented there are the total scattering cross sections of Jones.¹⁷ Comparing with Jones's total cross sections, the present elastic calculations reproduce the position of the broad maximum around 25 eV, but neither of the two peaks at 6.6 and 12.5 eV corresponds to the broad peak at 8.9 eV in his experiment. Part of the discrepancy may be due to the fact that elastic and total cross sections do not necessarily exhibit resonances at exactly the same positions. Hayashi's analysis of swarm data²⁹ shows that resonant enhanced vibrational excitation cross sections contribute significantly to the total cross sections, and their contributions may shift and merge the two elastic peaks. The static-exchange approximation may also play a role in the discrepancy. It is well known that the position of the $^2\Pi_g$ resonance in N₂ is shifted from ≈ 2.3 eV in a polarization calculation to ≈ 4.5 eV in the static-exchange approximation.^{30,39,40} Also, the broad maximum between 7 and 8 eV in the experimental cross section⁴¹ of CH₄ is shifted to ≈ 11 eV in the static-exchange approximation.⁷ A similar shift may also apply to CF₄. On the other hand, the position of the 6.6-eV resonance in the present calculation coincides well with the resonances between 6.15 and 7.5 eV from dissociative attachment experiments.¹⁸⁻²⁰ Whether this agreement with experiment will stand in a polarization calculation remains to be seen. The 11.7-eV resonance from our calculation is also close to the 12.0 and 13.0 eV resonances determined

by Verhaart *et al.*¹⁸ from their low-energy electron-impact spectra, but our result does not support their conjecture regarding the nature of this resonance. They attribute the resonances between 12 and 13 eV to core-excited resonances where the incident electron is temporarily attached to a Rydberg state of the target. In the present static-exchange calculation, excited target states are excluded from the representation of $\Psi_0^{(+)}$ and the resonances from such calculation cannot be ascribed to core-excited resonances. On the whole, it appears that, with the exception of the broad peak at 8.9 eV in Jones's

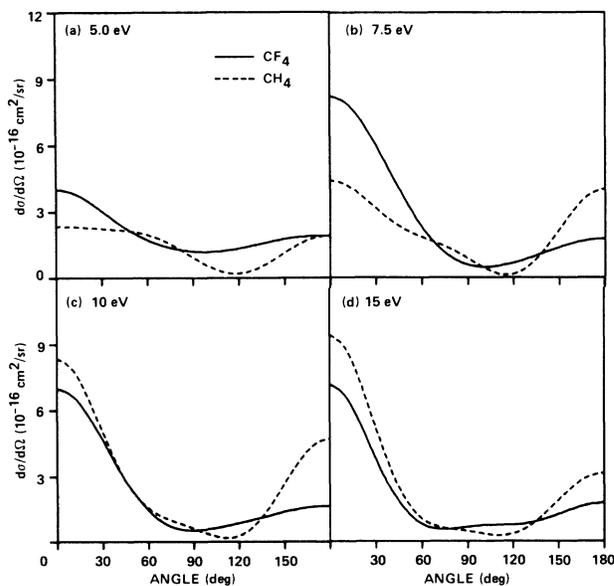


FIG. 4. Elastic differential cross sections for e -CF₄ and e -CH₄ scattering at (a) 5 eV, (b) 7.5 eV, (c) 10 eV, and (d) 15 eV incident energies. The CH₄ data are from the SMC calculations in Ref. 7.

total scattering cross section, the positions of the resonances from the present study relate rather well with available experiment. Theory also provides more information regarding the nature of these resonances. We believe the 8.9-eV structure in the total cross section can be reconciled only with polarization and nuclear dynamics calculations.

The magnitude of the total cross section should provide an upper limit to the elastic integral cross section. We note, however, that in the presence of a resonance, a fixed-nuclei calculation without proper account of nuclear dynamics tends to give a stronger and narrower peak than experiment and may even overshoot the total cross section. A good example is found in the ${}^2\Pi_g$ resonance in N_2 .⁴² In the present case, both the lack of polarization and nuclear dynamics calculations most likely are responsible for the fact that between 5 and 7.5 eV, the elastic cross sections are larger than the corresponding total cross sections (see Table IV). As the incident energy increases to 10 eV and above, the elastic cross section becomes smaller than the total cross section. At 20 eV, it is $\approx 72\%$ of the total cross section and at 35 eV it is 61%. While the elastic cross section at high energies may appear to be too small in comparison with the total cross section, it should be remembered that Hayashi²⁹ deduced a very large vibrational excitation cross section for this molecule. The experimental ionization²³ and dissociation cross sections^{24,25} for this molecule also are large. When these inelastic process are taken into consideration, the difference between the present elastic cross section and the total cross section appears to be reasonable. Future experiments will be required to verify this point.

The differential cross section (DCS's) at 5.0, 7.5, 10, and 15 eV are presented in Fig. 4 where the SMC static-

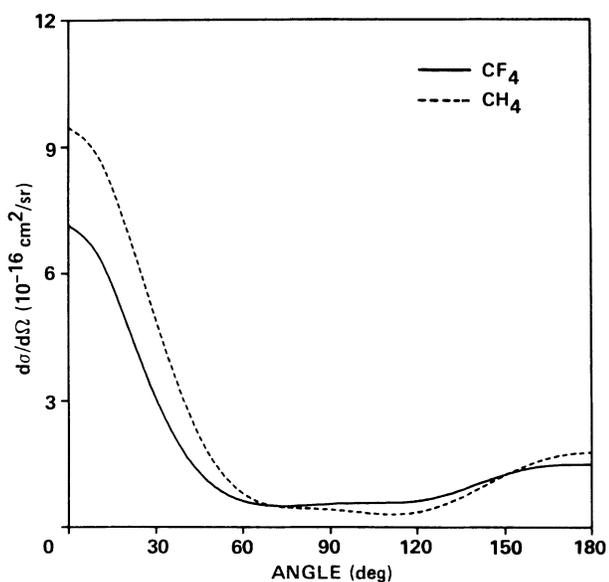


FIG. 5. Elastic differential cross sections for e - CF_4 and e - CH_4 scattering at 20 eV. The CH_4 data are from the SMC calculations in Ref. 7.

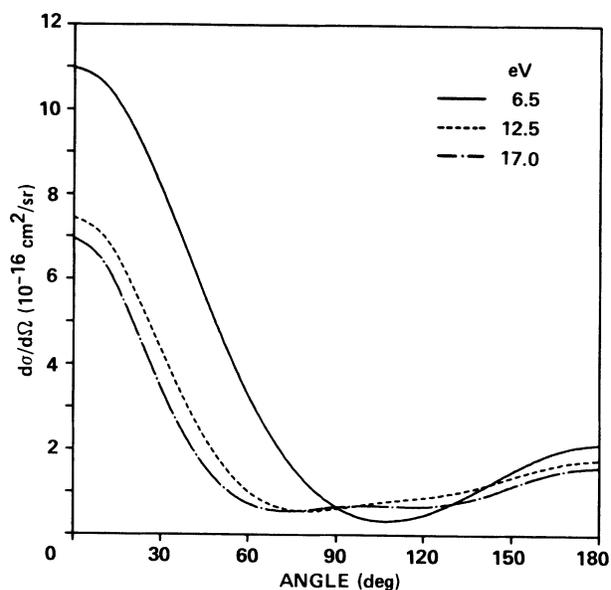


FIG. 6. Elastic differential cross sections for e - CF_4 scattering at 6.5, 12.5, and 17 eV.

exchange results of CH_4 are also presented for comparison. Figure 5 presents the DCS's for these two molecules at 20 eV. The CF_4 DCS's generally show less backward peaking than the CH_4 data. At 5.0 and 7.5 eV, near the first, strong T_2 resonance in CF_4 , the DCS curves for these two molecules are significantly different, but become more similar at higher energies. Figure 6 presents the DCS of CF_4 at 6.5, 12.5, and 17 eV. Comparing the 6.5-eV DCS curve, which is almost on top of the first T_2 resonance, with the DCS curves at 12.5 and 17 eV shows

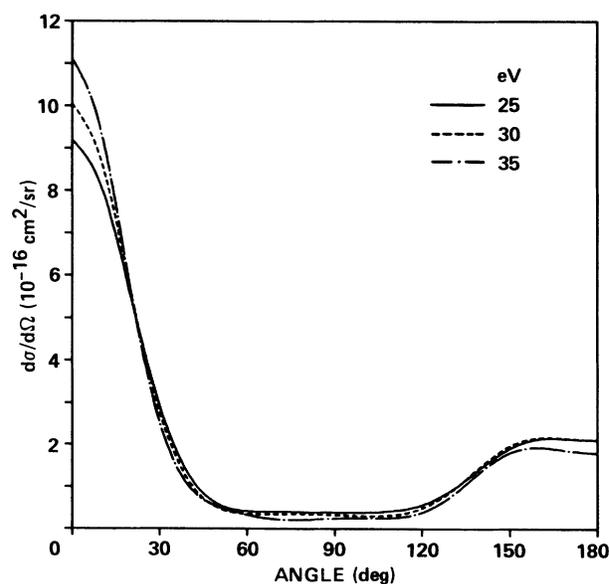


FIG. 7. Elastic differential cross sections for e - CF_4 scattering at 25, 30, and 35 eV.

that the first T_2 resonance affects the forward scattering much more strongly than at large angles. Notice that the DCS's at 12.5 and 17 eV are affected by the broad A_1 resonance at 11.7 eV as well as the T_2 and E resonances near 27 eV. However, those resonances are so broad that their effects on the DCS curves are much weaker. The DCS's at 25, 30, and 35 eV, shown in Fig. 7, are close to each other. The major difference is found at forward scattering, which decreases with increasing energy.

IV. CONCLUSIONS

The results of the present study show that state-of-the-art calculations, using a multicenter, *ab initio* method,

can be used to treat electron-heavy polyatomic molecule scattering successfully. The broad, overlapping shape resonances from different partial channels mean that electron-impact excitation of mixed vibrational modes should be effective in this molecule. Such broad resonances introduce complications in theoretical treatments since most of the theoretical formulations of resonant vibrational excitations assume a single, relatively narrow resonance. Present results also indicate that Hayashi's assumption²⁹ of ν_3 being the only vibrational mode with strong resonant enhancements may be questionable. We hope that this study will stimulate further experimental and theoretical studies on electron scattering of polyatomic molecules.

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