Elastic cross sections for $e^- - CH_4$ collisions at intermediate energies

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A joint theoretical and experimental investigation on $e^- - CH_4$ elastic scattering in the intermediate energy range is reported. More specifically, calculated cross sections in the (1–500)-eV incident energy range, as well as measured absolute cross sections from 100 to 500 eV, are presented. A complex optical potential consisting of static, exchange, correlation-polarization, plus absorption contributions is used to describe the electron-molecule interaction. The Schwinger variational iterative method combined with the distorted-wave approximation is applied to calculate the scattering amplitudes. The experimental absolute elastic differential cross sections are determined using the relative flow technique. In general, our calculated results are in very good agreement with our experimental data and with other experimental and theoretical results available in the literature. Our study has shown the significant role played by the absorption effects on the calculated cross sections for incident energies of 50 eV and above. The importance of the nonspherical components of the $e^- - CH_4$ interaction potential has also been verified in our calculations.

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I. INTRODUCTION

Methane is an interesting system from both pure and applied research points of view. It has been identified as a source of infrared absorption in the atmospheres of Jupiter and Saturn, and is a primary constituent of the atmospheres of outer planets such as Uranus and Neptune [1]. Also, methane is an important molecule in plasma processing [2] and plays a role in edge plasmas of fusion devices [3]. On more basic grounds, electron collision with methane is a very well studied problem, both experimentally and theoretically, mostly in the low incident-energy range. For instance, recent experimental data on differential cross sections (DCS’s) were reported in a number of works: Curry, Newell, and Smith [4]; Tanaka et al. [5]; Vuskovic and Trajmar [6]; Sohn et al. [7]; Shyn and Cravens [8]; Boesten and Tanaka [9]; Kanik, Trajmar, and Nickel [10]; and Mapstone and Newell [11], just to cite a few.

On the theoretical side, the literature for low-energy electron-CH$_4$ scattering is equally rich. DCS’s, momentum transfer cross sections (MTCS’s), and integral cross sections (ICS’s) for elastic $e^- - CH_4$ scattering have been calculated in the past fifteen years at different levels of approximation. Model potentials at static-exchange (SE) and at static-exchange-polarization (SEP) levels were used by several authors [12–15]. The Schwinger multichannel method using pseudopotentials was applied by Bettega et al. [16] to study elastic scattering of electrons by XH$_4$ molecules ($X = C, Si, Ge, Pb$). An exact SE calculation for elastic $e^- - CH_4$ scattering was reported by Lima et al. [17]. Beyond the exact SE level, the correlation-polarization contributions to the interaction potential has been taken into account either via an approximated local function [18–20] or via a multichannel treatment of the scattering equations [21,22].

Comparatively speaking, far fewer studies, both experimental and theoretical, have been carried out for intermediate-to-high energies ($E_0 \approx 50$ eV). The literature for experimental investigations is strongly concentrated in grand total (elastic plus inelastic) cross section measurements [23–26]. Some of these works also report the partitioning of the total cross sections into elastic plus inelastic (ionization and neutral dissociation) cross sections [24,26]. The only two sets of absolute measurements of DCS’s, ICS’s, and MTCS’s for elastic $e^- - CH_4$ scattering have been reported by Vuskovic and Trajmar [6] at 20, 30, and 200 eV and by Sakae et al. [27] in the (75–750)-eV energy range. Theoretically, elastic $e^- - CH_4$ cross sections were reported by Dhal, Srivastava, and Shingal [28] for incident energies from 205 to 820 eV. Very simple theoretical models were used in their calculations. Recently, elastic $e^- - CH_4$ DCS’s for incident energies up to 500 eV were calculated by Jain [12] using a spherical SEP plus local absorption model potentials. This study showed the important influences of absorption effects for $E_0 \approx 50$ eV. Nevertheless, his calculated DCS’s are in strong disagreement with the measured data [6,9,27] for $E_0 \approx 100$ eV. Recently, we applied the Schwinger variational iterative method (SVIM, Ref. [29]) combined with the distorted-wave approximation (DWA, Ref. [30]) to study the elastic electron scattering by N$_2$ [31] and O$_2$ [32] in a wide energy range. A complex optical potential, derived from a fully molecular near-Hartree-Fock self-consistent-field (SCF) wave function, is used to describe the electron-molecule interaction. For these two systems, the comparison between the calculated DCS’s and experimental results available in the literature was very encouraging. In view of the important role played by absorption effects on
electron-molecule scattering in the intermediate energy range, the application of this method to the study of electron collisions with polyatomic targets is clearly of interest.

In the present investigation, we report a theoretical study on electron scattering by CH$_4$ in the intermediate energy range. More specifically, calculated elastic DCS’s in the (20–500)-eV energy range as well as ICS’s and MTCS’s in the (1–500)-eV range are presented. Considering the scarcity of absolute experimental cross sections for elastic e$^-$.CH$_4$ collisions above 100 eV, we have also measured DCS’s, ICS’s, and MTCS’s in the (100–500)-eV energy range. These quantities are also reported here.

This paper is organized as follows. In Sec. II, we describe briefly the theory used and also give some details of the calculation. In Sec. III we present briefly some experimental details. Finally, in Sec. IV we compare our calculated results with our and the existing experimental data and with other theoretical data available in the literature.

II. THEORY AND CALCULATION

Since the details of the SVIM and the DWA have already been presented in previous works [29,30], here we will only outline briefly the theory used. After carrying out the average over the molecular orientations, the laboratory-frame DCS’s for elastic electron-CH$_4$ scattering is given by

$$\frac{d\sigma}{d\Omega} = \sum_{L} A_L(k) P_L(\cos \theta),$$  

where $\theta$ is the scattering angle. The coefficients $A_L(k)$ in Eq. (1) are given by the formula

$$A_L(k) = \frac{1}{2L+1} \sum_{p \mu \lambda} \frac{(1-\mu')^{m'-m}}{p_1 \mu_1 j_{1}^{l_1} l_{1}^{m_1} l_{1}^{p_1} \mu_1^{l_1} m_1^{l_1} m_1} \times \sqrt{(2l+1)(2l_1+1)} b^{p_1 \mu_1} l_{1}^{p_1} m_1^{p_1} m_1^{p_1} \times b^{p \mu} l_{1}^{p} m_1^{p} m_1^{p} \times (1+\mu') \times (1+\mu) \times \frac{1}{2l'} \times L(1,0,0|L) \times (1-\mu) \times \frac{1}{2l'} \times L(1,-1,0|L),$$

where $(j_1 m_1 j_2 m_2 | j_3 m_3)$ are the usual Clebsch-Gordan coefficients and the auxiliary amplitudes $d^{p \mu}_{l_{1}^{h}, l_{1}^{h}}(k)$ are defined as

$$d^{p \mu}_{l_{1}^{h}, l_{1}^{h}}(k) = -\frac{\sqrt{\pi}}{k} i^{l_{1}^{l_{1}^{l_{1}}} - 1} \times \left( 2l' + 1 \right)^{l_{1}^{l_{1}^{l_{1}}} - 1} \times \frac{1}{2l'} \times T^{p \mu}_{l_{1}^{h}, l_{1}^{h}, l_{1}^{h}}.$$  

In Eqs. (1)–(3), $p$ is an irreducible representation (IR) of the molecular point group, $\mu$ is a component of this representation and $h$ distinguishes between different bases of the same IR corresponding to the same value of $l$, and $T^{p \mu}_{l_{1}^{h}, l_{1}^{h}, l_{1}^{h}}$ is a partial-wave component of the elastic transition $T$ matrix defined as

$$T = \langle \Phi_{i} | V_{opt} | \psi_{f} \rangle.$$  

The coefficients $b^{p \mu}_{l_{1}^{m_{1}}} \mu_{1}$ satisfy important orthogonality conditions and are tabulated for the $C_{2v}$ and $O_{h}$ groups by Burke, Chandra, and Gianturco [33].

The dynamics of the electron-CH$_4$ interaction is described by a complex optical potential, given as

$$V_{opt} = V^{SEP} + iV_{ab},$$

where $V^{SEP}$ is the real part of the interaction potential composed of the static, the exchange, and the correlation-polarization contributions as

$$V^{SEP} = V_{st} + V_{ex} + V_{cp},$$

and $V_{ab}$ is the absorption potential. In our calculation, $V_{st}$ and $V_{ex}$ are treated exactly, while $V_{cp}$ is obtained in the framework of the free-electron-gas model derived from a parameter-free local density, as prescribed by Padial and Norcross [34].

Concerning the absorption potential, several models of both empirical [35–37] and nonempirical [38,39] natures have been proposed for more than 20 years. Among these model potentials, the quasifree scattering model (QFSM) proposed by Staszewska et al. [39] is particularly interesting. The QFSM is derived nonempirically to reproduce the absorption probability per unit time for an electron passing through a free-electron gas. Recently, Blanco and García [40] pointed out an error (a factor of 2) in the derivation of this model potential. On the other hand, the original QFSM [39] was modified empirically by Staszewska et al. [41] in order to introduce some target properties, such as ionization potentials and mean excitation energies, into the collisional dynamics. Two modified versions, namely, versions 2 and 3 of the QFSM, are the most successful. Unlike other empirical models [35–37], these semiempirical QFSM versions do not require any parameters to be adjusted for a given target and for a given incident energy. Therefore, they are easy to use, and can provide cross sections for predictive purposes. For instance, the elastic DCS calculated by Staszewska et al. [41] using the QFSM version 3 for rare gases He, Ne, and Ar in a wide energy range are in very good agreement when compared with experimental data. In our calculation, the absorption potential $V_{ab}$ appearing in Eq. (5) is that of the QFSM version 3 of Staszewska et al. [41].

In the two-potential formalism, the interaction potential is split as

$$V_{opt} = U_{1} + U_{2},$$

where $U_{1}$ is taken as the real part of the complex optical potential, whereas $U_{2}$ is the imaginary absorption potential. The corresponding distorted-wave functions satisfy the following scattering equation:

$$(H_{0} + U_{1} - E) \chi = 0,$$

which is solved using the SVIM (Ref. [29]). Furthermore, the absorption part of the $T$ matrix is calculated via DWA as...
where the superscripts ± denote the incoming-wave and outgoing-wave boundary conditions.

In order to take advantage of the symmetry of the target, in the SVIM calculations the scattering-wave functions can be partial-wave expanded as

$$X_{k}^{(\pm)}(\hat{r}) = \left(\frac{2}{\pi}\right)^{1/2} \frac{1}{k} \sum_{\mu \nu \lambda} i^{\lambda} X_{k,\nu}^{\mu}(\hat{r}) X_{\nu}^{\mu}(k),$$

(10)

where $X_{\nu}^{\mu}(\hat{r})$ are generalized spherical harmonics, related to the usual spherical harmonics $Y_{l m}$ by

$$X_{\nu}^{\mu}(\hat{r}) = \sum_{m} b_{\nu,m} Y_{l m}(\hat{r}).$$

(11)

Despite its $T_d$ symmetry, CH$_4$ is considered to belong to the $C_{2v}$ point group in the present calculation.

The initial scattering-wave functions can be expanded into a set $R_0$ of $L^2$ basis functions $\alpha_i(\hat{r}) = \langle \hat{r} | \alpha_i \rangle$:

$$X_{k,\nu}^{(\pm)}(\hat{r}) = \sum_{i=1}^{N} a_{\nu,i}^{(\pm)} \langle \hat{r} | \alpha_i \rangle.$$

(12)

Variational $T_{\pm}^{(\pm)\mu \nu}$ matrix elements can be derived as

$$T_{k,\nu'}^{(\pm)\mu\nu} = \sum_{i,j=1}^{N} \langle \Phi_{k,\nu}^{(\pm)\mu} | U_1 | \alpha_i \rangle \langle D^{(\pm)^{-1}} \rangle_{ij} \langle \alpha_j | U_1 | \Phi_{k,\nu'}^{(\pm)\mu} \rangle,$$

(13)

where

$$D^{(\pm)^{-1}} = \langle \alpha_i | U_1 - U_1 G^{(\pm)} U_1 | \alpha_j \rangle^{-1}.$$

(14)

and the corresponding approximate scattering solution with outgoing-wave boundary condition becomes (from now on the superscript + will be omitted)

$$X_{k,\nu}^{(S)}(\hat{r}) = \Phi_{k,\nu}^{(\pm)}(\hat{r}) + \sum_{i,j=1}^{M} \langle \Phi_{k,\nu}^{(\pm)} | U_1 | \Phi_{k,\nu'}^{(\pm)} \rangle \langle D^{-1} \rangle_{ij} \langle \alpha_j | U_1 | \alpha_i \rangle.$$

(15)

Converged outgoing solutions of Eq. (8) can be obtained via an iterative procedure. The method consists in augmenting the basis set $R_0$ by the set $S_0 = \{X_{k,\nu}^{(S)}(\hat{r}) | X_{k,\nu}^{(S)}(\hat{r}) \ldots X_{k,\nu}^{(S)}(\hat{r}) \ldots \}$

(16)

where $l_c$ is the maximum value of $l$ for which the expansion of the scattering solution of Eq. (10) is truncated. A new set of partial-wave scattering solutions can now be obtained from

$$\begin{array}{lll}
\text{TABLE I. Cartesian Gaussian functions used in the SCF calculations. Cartesian Gaussian basis functions are defined as } \\
\Psi_{\alpha}^{\mu,m,n}(r) = N(x - A_i)^{\mu}(y - A_j)^{m}(z - A_k)^{n} \exp(-\alpha|x - A|^2), \text{ with } N \text{ a normalization constant.} \\
\hline
\text{Atom} & s & p & d \\
\text{Expt.} & \text{Coeff.} & \text{Expt.} & \text{Coeff.} & \text{Expt.} & \text{Coeff.} \\
\hline
\text{C} & 14.1892 & 0.791751 & 1.926600 & 0.321870 & 5.147700 & 1.000000 & 0.359400 & 1.000000 & 1.500 & 1.000000 \\
& & & & & & & & & 0.496200 & 1.000000 & 0.114600 & 1.000000 & 0.750 & 1.000000 \\
& & & & & & & & & 0.153300 & 1.000000 & 0.04584 & 1.000000 & 0.300 & 1.000000 \\
& & & & & & & & & 0.06132 & 1.000000 & 0.02000 & 1.000000 & & & & & & \\
\text{H} & 33.6444 & 1.000000 & 0.10000 & 1.000000 & 5.057960 & 1.000000 & 0.500000 & 1.000000 & & & & & & & & & & & \\
\end{array}
\end{array}$$

In our study, $U_1$ is derived from the ground-state wave function of methane. This one-determinant near-Hartree-Fock wave function is composed of linear-combination-of-atomic-orbitals molecular spin orbitals that are calculated using the contracted cartesian Gaussian basis set shown in Table I. At the equilibrium C—H bond distance ($R_{C-H} = 1.0503a_0$) this basis set gives an SCF energy of $-40.1987$ a.u., which can be compared with the $-40.2155$ a.u. value of Nishimura and Itikawa [15]. The correlation-polarization (CP) potential is constructed using
the electronic density given by the SCF wave function. The asymptotic form of this polarization potential is given for $T_d$ molecules by

$$V_{p}(r) = -\frac{1}{2} \frac{\alpha_0}{r^2},$$  \hspace{1cm} (19)

where $\alpha_0$ is the spherical part of the molecular dipole polarizability. In our calculations the experimental value $\alpha_0 = 17.5$ a.u. was used [43]. All parameters used to generate the absorption potential were taken from Jain and Baluja [44].

Additional terms that account for the contributions of angular momenta higher than $l_c$ are included in the scattering amplitude calculation as follows:

$$f(k',k_0) = \sum_{l,h,l',h'} f_{l,h,l',h'}(2l+1)e^{2i\delta_l}P_l(\cos \theta) + f^{\text{(higher)}},$$  \hspace{1cm} (20)

where

$$f^{\text{(higher)}} = \frac{1}{2i\kappa} \sum_{l=0}^{l_{\text{max}}} (2l+1)(e^{2i\delta_l} - 1)P_l(\cos \theta)$$  \hspace{1cm} (21)

and $\delta_l$ is the partial-wave phase shift, given by a closed formula,

$$\tan \delta_l = -\frac{\pi k^2 \alpha_0}{(2l-1)(2l+1)(2l+3)}.$$  \hspace{1cm} (22)

In the present calculation, the cutoff parameter used in the expansions of the target bound orbitals and of the static-plus-CP potential is $l_c = 18$. All possible values of $h = l$ are retained. With this cutoff, the normalization of all bound orbitals is better than 0.999. In SVIM calculations, we have also limited the partial-wave expansions to $l_c = 18$. In addition, for incident energies $E_0 \geq 20$ eV angular momentum phase shifts up to $l_{\text{max}} = 200$ were used in Eq. (21).

III. EXPERIMENT

Details of our experimental procedure will be presented elsewhere [45] and thus will only be briefly presented here. Our experimental setup, a crossed-beam apparatus, is built inside a vacuum chamber pumped by a 6-in. diffusion pump. The typical background pressure (no gas load) in the vacuum chamber is about $1 \times 10^{-7}$ Torr. Three pairs of Helmholtz coils around the chamber reduce the magnetic field in the collision region to less than 15 mG.

The electron gun used is composed of a hairpin tungsten filament, a triode extraction, a set of einzel lenses, and two sets of electrostatic deflectors in perpendicular directions. The electron beam is generated without prior energy selection. In the (100–1000)-eV range, the typical beam has a diameter of 1 mm and its current is around 1 $\mu$A. Its energy resolution is about 0.5 eV. A molecular beam flows into the vacuum chamber perpendicularly to the electron beam via a capillary array. This array has an external diameter of 1 mm with individual capillaries of diameter $D = 0.05$ mm and length $L = 5$ mm (aspect ratio $\gamma = D/L = 0.01$). Scattered electrons are collected in the angular range covered by $5^\circ$–$135^\circ$ and $-5^\circ$–$-60^\circ$. A pair of apertures with diameters of 1 mm in the detector/analyzer system limits the viewcone of the detector, and the resulting angular resolution is about $0.2^\circ$. The scattered electrons are energy-filtered by a retarding-field energy selector (RFES). The resolution of the RFES is about 1.5 eV for an incident energy of 500 eV. This resolution is sufficient to distinguish inelastically scattered electrons resulting from electronic excitation for most small molecules, but it is unable to resolve vibrational excitation processes. After being energy-analyzed, the elastically scattered electrons are detected by a channeltron.

During the measurement, the working pressure in the vacuum chamber is around $5 \times 10^{-7}$ Torr with the gas beam turned on. For each scattering angle and each incident energy, records of the scattering intensities are taken at least three times. The counting time is monitored to ensure that the statistical deviations of the counts are less than 3%. In order to discount the background scattering contributions, the gas beam is deviated to a side leak far from the collision region and the scattering intensities are recorded. These contributions are subtracted from the measured scattering intensities for each angle.

It is well known that electron-molecule collisions in the intermediate energy range may result in a variety of charged and neutral molecular fragments. Ultraviolet (uv) photons can also be generated via radiative decay processes from excited molecules. Although the potentials applied at RFES and at the channeltron coincide during the measurements prevent both positively and negatively charged molecular fragments from reaching the detector, they have no effect on uv photons or neutral fragments. In order to measure the contributions of these species, polarities of the potentials applied at the RFES and at the channeltron are inverted. This procedure prevents any charged species (ions and electrons) from reaching the detector. Thus, the contributions due to the uv photons and/or neutral fragments can be measured. Nevertheless, in our experiment it is found that the contribution of these neutral species is negligible.

The recorded scattering intensities are converted into absolute elastic DCS’s using the relative flow technique (RFT). The RFT has been widely used [46–53] in measurements of electron-atom (molecule) collisional cross sections. This technique bypasses the determination of many experimental parameters required for an absolute measurement of the cross sections. Basically, it relates the scattering intensities of the gas under study (x) with those of a reference gas (std) of known DCS’s, under identical experimental conditions, via the expression

$$\left< \frac{d\sigma}{d\Omega} \right>_x = \left< \frac{d\sigma}{d\Omega} \right>_{\text{std}} \frac{I_x}{n_x} \frac{n_{\text{std}}}{M_x} \frac{M_{\text{std}}}{M_x}^{1/2},$$  \hspace{1cm} (23)

where $I$ is the scattered electron intensity, $n$ is the flow rate, and $M$ is the molecular weight. The above equation is valid if the beam profiles (density distribution) of both gases, $x$ and std, are closely the same. According to Olander and Kruger
this requirement is fulfilled under two conditions: the mean free paths ($\lambda$) of both gases behind the capillaries must be equal and the Knudsen number $K_L$ defined as ($\lambda/L$) of the beam flow must satisfy $\gamma \approx K_L \lesssim 10$.

Recently, the applicability of RFT for absolute cross section determinations has been extensively discussed [52,53,55,56]. Some studies [53,55] have shown that even at beam flow regimes where the $K_L$’s are significantly lower than $\gamma$, the density distribution of most gases measured in their works can still be very similar to each other. In particular, a systematic study of the influences of the secondary standards as well as on the range of working pressure was recently carried out by our group [45]. It was shown that at flow conditions where $0.002 \approx K_L \approx 10$, reliable DCS’s for elastic $e^- - \text{N}_2$ scattering in the (300–500)-eV range are obtained using CH$_4$, Ne, Ar, and Kr as secondary standards. In some manner, our findings agree with the study carried out by Buckman et al. [55]. In that work, the authors have reported that the profile full width at half maximum of the gaseous beam of several gases heavier than He are about the same even at flow conditions where $K_L$ is significantly lower than $\gamma$.

In the present study, Ne is used as the reference gas. The collisional diameters of Ne and CH$_4$ are 2.38 [57] and 3.24 Å [58], respectively, and thus the theoretical pressure

FIG. 3. DCS’s for elastic $e^- - \text{CH}_4$ collision at 20 eV. Solid line, present calculated results; short-dashed line, theoretical results of Jain [12]; long-dashed line, theoretical results of Nishimura and Itikawa [15]; full circles, present experimental results; open circles, experimental data of Sohn et al. [7]; open triangles, experimental data of Vuskovic and Trajmar [6]; full squares, experimental data of Boesten and Tanaka [9]; open squares, experimental data of Sakae et al. [27]; asterisks, experimental data of Shyn and Cravens [8].

FIG. 4. Same as Fig. 3, but for 50 eV.
ratio for equal $K_L$ would be 1.9:1. We used 9.8 Torr for the pressure of Ne and 5.0 Torr for that of CH$_4$. This corresponds to the mean free path of 13.2 $\mu$m and $K_L = 0.0026$ for both gases. In addition, the absolute cross sections of Jansen et al. [59] for Ne is used for normalization of our data. Besides the uncertainties due to the normalization procedure, errors of a random nature such as fluctuations on primary electron beam currents, pressure fluctuations, etc., contribute to the overall experimental error of the measured data. In our experiments, the uncertainty due to pressure fluctuations is less than 0.2%, the accuracy of the measurements of the electron beam current is better than 1%, errors due to the uncertainties of scattering-angle readings are estimated to be 1%, and the error due to background scattering is less than 1%. These contributions combined with the estimated statistical error of 3% give an overall error of 4% in the relative DCS’s for each gas. Moreover, the quoted error in the absolute DCS’s of Jansen et al. [59] is 6.5%. In addition, the experimental uncertainty associated with the normalization procedure is estimated to be 5.7%. Therefore, the overall experimental uncertainty in our absolute DCS’s is about 10.3%. In order to obtain the ICS’s and MTCS’s, the values of the DCS’s obtained in a limited angular range must be extrapolated to both low and high scattering angles. A manual extrapolation procedure was adopted, following the trends of the extrapolated DCS’s of Sakae et al. [27]. The uncertainties of this procedure are estimated to be 10% at small angles and 20% at large angles, which leads to overall errors of 18% in the ICS’s and 20% in the MTCS’s.

IV. RESULTS AND DISCUSSION

In Figs. 1 and 2 we present our calculated ICS’s and MTCS’s, respectively, for elastic $e^-\text{-CH}_4$ scattering, in the (1–500)-eV energy range. Our measured ICS’s and MTCS’s at 100 eV and above are also presented. Some selected ex-
perimental [6–9,27] and theoretical [12,15,18] results are also shown for comparison. In general, there is a good agreement among the calculated and measured data. Our calculation has predicted a shape resonance in ICS’s at around 10 eV, in good agreement with the theoretical results of Jain [12] and McNaugthen et al. [18]. It is interesting to note that although the measured ICS’s of Shyn and Cravens [8] and those of Boesten and Tanaka [9] agree fairly well with each other, there is a significant difference between their measured MTCS’s, particularly in the region of the maximum. This discrepancy may reflect differences in the extrapolation procedures used by the authors for large scattering angles.

Figures 3 and 4 show our calculated DCS’s for elastic e–CH₄ scattering at 20 and 50 eV, respectively, along with some available experimental [4,6,8,9] and theoretical [12,15] results. In general, our calculated DCS’s agree very well with the measured data, both qualitatively and quantitatively. Our results also agree fairly well with the calculated results of Jain [12] and Nishimura and Itikawa et al. [15]. Particularly at 50 eV, although the theoretical DCS’s of Nishimura and Itikawa [15] agree qualitatively well with our calculated results, they are overestimated at scattering angles above 30°. This disagreement is probably due to the neglect of absorption effects in their study.

In Figs. 5–9 we present our calculated and measured DCS’s for elastic e–CH₄ scattering in the (100–500)-eV range, along with other available experimental [6,9,27] and theoretical [12,28] results. Good agreement is seen between our measured DCS’s and other available experimental data. In general, our calculated DCS’s agree qualitatively very well with the present and other measured data in the above noted energy range. Quantitatively, this agreement is also good for incident energies $E_0 \approx 300$ eV. The calculated results of Jain [12] disagree significantly with the present calculated data. This discrepancy can probably be attributed to the neglect of nonspherical components of the interaction potential in his calculation.

In order to illustrate the importance of the role played by the absorption effects on the cross sections, in Fig. 5 we also show the DCS’s at 100 eV calculated without the inclusion of the absorption potential. Our measured DCS’s lie between the two sets of calculated results, slightly closer to that without absorption. Nevertheless our calculated DCS’s with absorption are in better agreement with the measured data of Boesten and Tanaka [9].

For the sake of completeness, in Table II we present our measured DCS’s, ICS’s, and MTCS’s for energies ranging from 100 to 500 eV.

In summary, we report calculated cross sections for elastic e–CH₄ scattering in the (1–500)-eV incident energy range and measured absolute cross sections from 100 to 500 eV. In general, our calculated results are in good agreement with our experimental data and with other experimental and theoretical results available in the literature. Our study has shown the significant role played by the absorption effects on the calculated cross sections for incident energies of 50 eV and above. In addition, the importance of the nonspherical components of the e–CH₄ interaction potential has also been verified in our calculations. Application of this method to other molecular systems is under way.

**TABLE II.** Experimental DCS’s, ICS’s, and MTCS’s (in $10^{-16}$ cm²) for elastic e–CH₄ scattering.

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<th>Angle (deg)</th>
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<th>200</th>
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<th>400</th>
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**ACKNOWLEDGMENTS**

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[57] A. Roth, Vacuum Technology (North-Holland, Amsterdam, 1982).

[58] Value calculated using the Van der Waals constant reported in Handbook of Chemistry and Physics, edited by R. Lide (CRC Press, Boca Raton, 1992).