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Geometric shielding corrections for total cross section calculations of electron scattering by CH_4, C_2H_6, $C_2H_3F_3$, C_2H_4, C_2F_4, C_2Cl_4 and $C_2Cl_2F_2$ from 30–5000 eV

D.H. Shi[1,a], J.F. Sun[1,2], Z.L. Zhu[1], H. Ma[1], and Y.F. Liu[1]

[1] Department of Physics, Henan Normal University, Xinxiang 453007, P.R. China
[2] Department of Physics, Luoyang Normal University, Luoyang 471022, P.R. China

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Abstract. To quantify the changes in the geometric shielding effect in a molecule as the incident electron energy varies, an empirical fraction, which represents the total cross section contributions of shielded atoms in a molecule at different energies, is presented. Using this empirical fraction, the total cross sections for electron scattering by CH_4, C_2H_6, $C_2H_3F_3$, C_2H_4, C_2F_4, C_2Cl_4 and $C_2Cl_2F_2$ are calculated over a wide energy range from 30 to 5000 eV by the additivity rule model at the Hartree-Fock level. The quantitative total cross sections are compared with those obtained by experiment and other theories where available. Good agreement is attained above 100 eV.

PACS. 34.80.Bm Elastic scattering of electrons by atoms and molecules

1 Introduction

There has been significant progress in the development of computational methods for the calculation of total cross section (TCS) of electron scattering by molecules. In the past several decades, many approaches have been developed, such as the Schwinger iterative variational method [1], the Schwinger multichannel method [2], the complex Kohn variational method [3], the Schwinger iterative variational method combined with the distorted-wave approximation method [4,5], the Born-closure Schwinger variational method [6], the *R*-matrix method [7], the close-coupling method [8] and the Glauber approximation method [9]. However, at intermediate and high energies, since almost all the inelastic channels (rotational, vibrational, electronic excitation and ionization process, etc.) are open, few of the above-mentioned methods can give accurate results. It is therefore not surprising that many previous calculations on the TCS for electron-molecule scattering have been restricted to the low energy range.

In order to obtain accurate TCS's for electron scattering by molecules at higher energies, some new approximation methods have been proposed in the past twenty years. Of these methods, the additivity rule (AR) model [10] is a fairly simple and practical one, particularly for simpler and smaller molecules at high enough energies. However, for complex polyatomic molecules [11,12] or polyatomic molecules [13,14] containing heavier atoms, great discrepancies still exist even at energies of several hundreds of eV.

To extend the AR model validity to lower energies, a number of investigations have been performed in recent years. Bobeldijk et al. [15] have presented two geometric AR methods, and obtained encouraging electron impact ionization cross sections (ICS's) of some molecules at energies of several tens of eV, but they did not investigate the TCS's of electron scattering by molecules. Deutsch et al. [16] have applied a modified AR (with an atomic weight factor) to the molecular ICS's, but they too did not calculate the TCS's of electron scattering by molecules. Joshipura et al. [17] have separated the polarization interaction from the optical potential, and obtained the atomic cross sections from the remainder. Then, they summed the atomic cross sections with the cross section for scattering on the molecular polarization potential. Employing this approach, they have calculated the TCS's for a number of molecules and improved their results in this way. Karwasz et al. [18] have proposed a formation of the AR, where a molecular cross section can be approximated by a Born-like two-parameter formula. Though this method can give satisfactory results over a wide energy range, the applications are still limited since the two adjustable parameter values are different for each target, and require experimental determination. Zecca et al. [19] have presented a new AR formula, which takes into account the geometrical screening of the component atoms. Using this formula, they have calculated the TCS's of electron scattering by linear (NO, N_2O, CO_2), bent triatomic (NO_2) and spherical (CH_4) molecules. Encouraging TCS results are obtained at intermediate and high energies. However,

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[a] e-mail: `scattering@sina.com.cn`

the accuracy of the TCS they obtain depends on the experimental errors present in the starting data of measured molecular cross sections. Recently, Joshipura et al. [20] have also provided a modified AR named the group additivity method, where the cross section arising from each constituent group of a molecule is added together to obtain the molecular TCS. Using this method, Joshipura et al. have computed the TCS's of electron scattering by several molecules such as CF_4, C_2F_4, C_2F_6, C_3F_8 and CF_3I. Good agreement with experiment is obtained over a wide energy range. Jiang et al. [21] have proposed a modified method named the energy-dependent geometric AR (EGAR) approach, and calculated the TCS's for electron scattering by a number of molecules. Since the target molecular dimension is not considered, obvious deviations still exist at lower energies for complex polyatomic molecules or polyatomic molecules containing heavier atoms. To improve the agreement between theory and experiment, in this paper, we will take into consideration the shielding effect of atoms in a molecule and discuss further modifications to the EGAR model [21], which depends on the target molecular dimension and the energy of the incident electrons.

2 Theoretical methodology

In the original AR model [22], the implicit assumption is made that the molecular orbitals can be described by the sum of the valence orbitals of all the atoms in the molecule. Therefore, we can assume that each atom in a molecule can scatter independently. Thus, the molecular TCS containing N atoms can be written as

$$Q_{AR}(E) = \frac{4\pi}{k}\mathrm{Im}F_m(\theta=0) \approx \frac{4\pi}{k}\mathrm{Im}\sum_{j=1}^{N} f_j(\theta=0) = \sum_{j=1}^{N} q_T^j(E) \quad (1)$$

where, $F_m(\theta=0)$ denotes the electron-molecule scattering amplitude for the forward direction; $q_T^j(E)$ and $f_j(\theta=0)$ are the TCS and the complex scattering amplitude for the jth constituent atom, respectively.

In equation (1), one main effect is not considered: a close-packed molecule is not fully transparent for low-energy electrons, and the "inner" atoms are partially shielded by the "outer" atoms and contribute less to the molecular TCS at lower energies than those at higher energies. The shielding effect, which leads to negative contributions to the TCS in the AR model, is dependent on the molecular geometry. Accounting for the shielding effect, Bobeldijk et al. [15] have introduced a geometric additivity rule (GAR) to calculate the molecular ICS. We find that the GAR model, which incorporates the geometrical shielding effect in a molecule, is a good approach to obtain the TCS's for electron scattering by molecules, particularly for complex polyatomic molecules at low energies [21]. When the GAR model is applied to determine the TCS, it can be expressed as

$$Q_{GAR}(E) = \frac{1}{3}Q_{\parallel}(E) + \frac{2}{3}Q_{\perp}(E). \quad (2)$$

Where $Q_{\parallel}(E)$ and $Q_{\perp}(E)$ are the TCS for electrons approaching the molecule parallel ($\theta = 0°$) and perpendicular ($\theta = 90°$) to the Z-axis, respectively. In the case of molecule CH_4, $Q_{\parallel}(E)$ and $Q_{\perp}(E)$ are both equal to Q_{CH_3}. More precisely, Q_{CH_3} is the TCS of electron scattering by CH_3 and is obtained with the AR model (Eq. (1)). In the case of C_2H_6, C_2H_4, C_2F_4 and C_2Cl_4, $Q_{\parallel}(E)$ and $Q_{\perp}(E)$ are equal to Q_{CH_3}, Q_{CH_2}, Q_{CF_2}, Q_{CCl_2} and $Q_{CH_2}+Q_{CH_2}$, $Q_{CH_2}+Q_{CH_2}$, $Q_{CF_2}+Q_{CF_2}$ and $Q_{CCl_2}+Q_{CCl_2}$, respectively. And in the case of $C_2H_3F_3$ and $C_2Cl_2F_2$, $Q_{\parallel}(E)$ and $Q_{\perp}(E)$ are set to $\frac{1}{2}(Q_{CH_3}+Q_{CF_3})$, $\frac{1}{2}(Q_{CCl_2}+Q_{CF_2})$ and $Q_{CH_2}+Q_{CF_2}$, $Q_{CCl_2}+Q_{CF_2}$, respectively (for detailed information, see Ref. [15]). Similarly to Q_{CH_3}, Q_{CH_2}, Q_{CF_2} and Q_{CCl_2} are obtained still by equation (1).

Calculations have shown that the GAR model is valid at lower energies [21] and overestimates the shielding effect in molecules over the high-energy region, resulting in lower TCS results. In comparison, the AR model is accurate at higher energies [11–14] and disregards the shielding effect at lower energies, resulting in higher TCS results compared with experimental findings, especially for complex polyatomic molecules or polyatomic molecules containing heavier atoms. It is well known that a close-packed molecule is not fully transparent for low-energy electrons, but the transparency will increase with the electron energy. That is to say, when the incident electron energy is very low, the "inner" atoms are shielded partially by the "outer" atoms, thus the GAR model can give encouraging results, but the AR model does not. When the energy is high enough, the molecule is fully transparent and each atom in the molecule can scatter independently. Thus the interaction effect between atoms can be neglected at sufficiently high energies. Hence, the AR model is valid, but the GAR model not. Taking into account these factors, we incorporate the GAR and AR, and present a semi-empirical formula,

$$Q_{TCS}(E) = Q_{GAR}(E) + A[Q_{AR}(E) - Q_{GAR}(E)]. \quad (3)$$

Here, A is an empirical fraction, which signifies the TCS contribution of shielded atoms for different molecules at different energies. There are two methods to determine the parameter A: through theoretical calculation or using an empirical approach. The formal calculation of the contribution of a shielded unit to the molecular TCS is highly complicated by the geometry and composition of the molecule as the incident electron energy is varied [16]. Thus, we choose the empirical approach. In determining the parameter A, two factors should be considered. First of all, when the incident electron energy is low enough, since the GAR model is valid, the value of A must satisfy $Q_{TCS}(E) \approx Q_{GAR}(E)$. And when the incident electron energy is high enough, because the AR model is accurate, the A must satisfy $Q_{TCS}(E) \approx Q_{AR}(E)$. It means that the empirical fraction $A \longrightarrow 0$ if $E \longrightarrow 0$, and $A \longrightarrow 1$ if $E \longrightarrow \infty$. That is to say, the higher the energy is, the less effect geometrical shielding will have on the TCS of the molecule. In addition, the empirical fraction A is related to both the incident electron energy E and the total electron number in the molecule m. A should also ensure a reasonable shape for the TCS when compared to experimental data in the wide energy range. Hence, Jiang et al. [21] proposed that

$$A = \frac{E}{mC + E}. \quad (4)$$

Here, E is in units of eV and C is a constant, which is equal to 1 eV. Equation (4) does not take into consideration the molecular specifications, such as molecular geometric dimension or total atomic number in the molecule. Therefore, for relatively larger or more complex molecules, it does not give encouraging TCS results at lower energies. In order to obtain more accurate TCS's, we propose that at least two additional factors should be taken into account in equation (4). Firstly, at a given energy, calculations have shown that the larger the size of a molecule, the greater is the discrepancy between the TCS's calculated by equations (3) and (4) and the experimental values. It implies that the larger the volume of a molecule is, the smaller the empirical fraction A should be. Calculations have also shown that when molecules have the same total number of electrons, the greater the total atomic number in the molecule, the smaller the empirical fraction A should be. Secondly, equation (4) can still not give the correct shape of the TCS curve. This can be clearly seen in log-log curves plotted using the TCS results calculated by equations (3) and (4). The main problem is that these log-log curves are still steeper than those obtained by the corresponding experimental findings. In accordance with the above discussion, we assume the empirical fraction A over the whole energy range behaves as

$$A = \frac{E}{mndC + E}. \quad (5)$$

Here, n is the total atomic number in a molecule, and d is the molecular dimension in atomic units, which can be roughly determined by the bond length and bond angle given in reference [24]. C is a constant to take into account the reasonable dimension relation, which is equal to 1 eV/a_0. According to a proposal by Bobeldijk et al. [16], molecules can be appropriately partitioned into two groups: one group possessing a circular form, which can be approximated by a torus-like shape, and the other having a cylindrical form, which can be approximated by a rod-like shape. For example, the molecule CH_4 has circular pattern and can be approximated by a torus-like shape. The molecules C_2H_6, $C_2H_3F_3$, C_2H_4, C_2F_4, C_2Cl_4 and $C_2Cl_2F_2$ have cylindrical patterns and are therefore approximated by a rod-like shape with a coordinate system attached to the center of the molecule and the Z-axis attached to the axis of the symmetry. Thus, the parameter d in equation (5) can be regarded as the largest length of the molecular size projected to the Z-axis.

The $q_T^j(E)$ in equation (1) can be determined by the method of partial waves given in reference [14]. Here, it is to be noted that Δ in the absorption potential $V_a(r)$ is equal to the ionization potential of the atom, as opposed to the energy gap between the target ground state and the lowest excited electronic state [24].

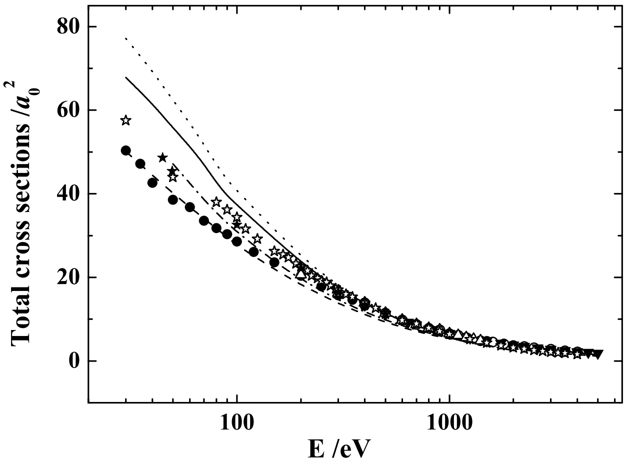

Fig. 1. TCS's for electron-CH_4 scattering. Theoretical calculations: solid line, present modified AR results; dotted line, present unmodified AR results; dashed line, Jain et al. [31]; dash-dotted line, Vinodkumar et al. [32]. Experimental findings: open triangle, Ariyasinghe et al. [25]; full triangle, García et al. [26]; open circle, Ariyasinghe et al. [27]; open star, Zecca et al. [28]; full star, Dababneh et al. [29]; full circle, Sueoka et al. [30].

3 Results and discussion

Using the complex spherical optical potential V_{opt}, we have recently calculated the TCS's for electron scattering by atoms of He, Ne and Ar [14] at 30–5000 eV. Compared with the experimental data, the calculated TCS results are encouraging at the energies studied. It appears that the electron-atom potential used in this paper is satisfactory, at least for the TCS calculations of electron scattering by these atoms over the present energy range.

Employing equations (3) and (5) together with the complex spherical optical potential, we have calculated the TCS's for electron scattering by molecules of CH_4, C_2H_6, $C_2H_3F_3$, C_2H_4, C_2F_4, C_2Cl_4 and $C_2Cl_2F_2$ for energies from 30–5000 eV. The TCS results calculated by equations (3) and (5) (the present modified AR results), the TCS results calculated by equation (1) (the present unmodified AR results) as well as some other available measurements and theories are illustrated in Figures 1–7.

Being a very well-known molecule, CH_4 offers a large amount of experimental as well as theoretical data for comparison. Figure 1 shows the present modified and unmodified AR results together with measurements obtained by Ariyasinghe et al. [25], García et al. [26], Ariyasinghe et al. [27], Zecca et al. [28], Dababneh et al. [29], Sueoka et al. [30] as well as theoretical results obtained by Jain et al. [31] and Vinodkumar et al. [32]. For the sake of clarity, numbers of results, such as the ones obtained by Zecca et al. [19], Joshipura et al. [33]

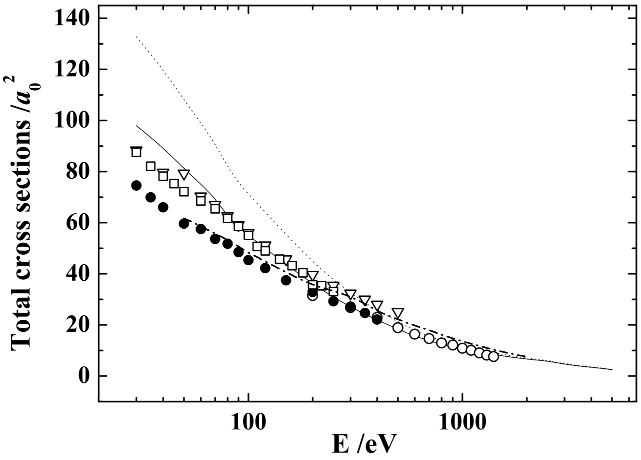

Fig. 2. TCS's for electron-C_2H_6 scattering. Theoretical calculations: solid line, present modified AR results; dotted line, present unmodified AR results; dash-dotted line, Vinodkumar et al. [32]. Experimental findings: open circle, Ariyasinghe et al. [25]; full circle, Sueoka et al. [30]; open triangle, Nishmura et al. [35]; open square, Szmytkowski et al. [36].

and Jain [34], are not included in Figure 1. The present modified AR results are in excellent agreement with the measurements obtained by Ariyasinghe et al. [25], García et al. [26] and Ariyasinghe et al. [27] at all the overlapping energies, and agree well with the experimental results obtained by Zecca et al. [28] above 90 eV, those of Dababneh et al. [29] above 100 eV and those of Sueoka et al. [30] above 200 eV. However, the present unmodified AR results show obvious deviations when they are compared with all the mentioned measurements at intermediate and low energies. Thus, for the proposed formula, good agreement with measurements [25–30] can be obtained when the incident electron energy is above 100 eV or so.

C_2H_6 is another target molecule, for which a large number of experimental and theoretical results are available for comparison. In Figure 2, we depict the present modified and unmodified AR results together with the measurements reported by Ariyasinghe et al. [25], Sueoka et al. [30], Nishimura et al. [35] and Szmytkowski et al. [36] as well as theoretical results obtained by Vinodkumar et al. [32]. Similarly to Figure 1, to avoid congestion, some results, such as the ones obtained by Joshipura et al. [37], are not shown in Figure 2. It should be pointed out that the present modified AR results are in excellent agreement with the experimental findings obtained by Ariyasinghe et al. [25] and Szmytkowski et al. [36] at all of the overlapping energies, and are in good agreement with the ones attained by Sueoka et al. [30] above 200 eV and Nishimura et al. [35] below 300 eV. In comparison, the present unmodified AR results are in poor agreement with all the measurements at intermediate and low energies. For instance, the present modified AR results are higher than the measurements [36] only by 6.1% and 0.3% at 70 and 200 eV, respectively. However, the deviations between the present unmodified AR results and the measurements [36] are 38% and 23% at 70 and 200 eV, respectively.

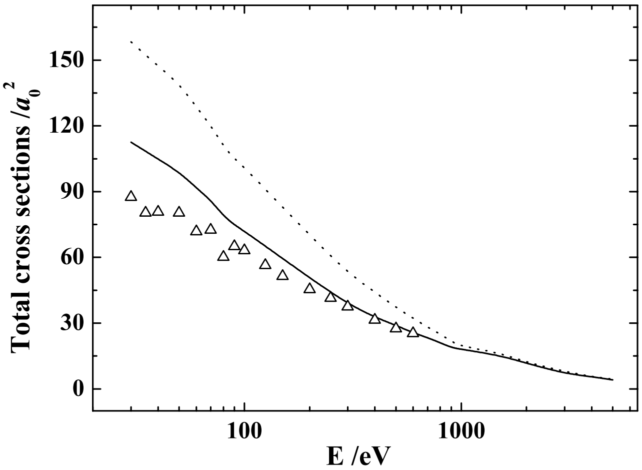

Fig. 3. TCS's for electron-$C_2H_3F_3$ scattering. Theoretical calculations: solid line, present modified AR results; dotted line, present unmodified AR results. Experimental findings: open triangle, Sueoka et al. [38].

From Figures 1 and 2, we notice that the present modified AR results for electron-C_2H_6 scattering are better than those for electron-CH_4 scattering when compared with measurements, and the modified effect for electron-C_2H_6 scattering is more obvious than that for electron-CH_4 scattering. The reason is that in a molecule of CH_4 at low energies, only the contribution of one hydrogen atom to the molecular TCS is shielded; in a molecule of C_2H_6, one-third of the contribution of a carbon atom and two and one-third of the contribution of a hydrogen atom to the molecular TCS are shielded, as per the GAR model [15].

As far as the TCS's of electron scattering by $C_2H_3F_3$ are concerned, to our knowledge only one group of experiments [38] above 30 eV has been performed. The present modified and unmodified AR results together with these measurements are plotted in Figure 3. As shown in Figure 3, the present modified AR calculations compare favorably with the measurements above 100 eV, whereas the present unmodified AR results show great deviations even at intermediate energies.

C_2H_6 and $C_2H_3F_3$ have the same number of atoms, but the molecule $C_2H_3F_3$ contains heavier F. For this reason, the modified effect on electron-$C_2H_3F_3$ scattering is more obvious than that on electron-C_2H_6 scattering. The situation for C_2H_4 and C_2F_4 is the same as for C_2H_6 and $C_2H_3F_3$.

The two molecules, C_2H_6 and $C_2H_3F_3$, are analogous in structure. From their comparison, we can see that the present modified AR results for the two molecules agree well with the afore-mentioned measurements above 100 eV or so.

For C_2H_4, we have made use of the TCS measurements obtained by Ariyasinghe et al. [25], Sueoka et al. [30], Nishimura et al. [35] and Szmytkowski et al. [39], and the theories given by Vinodkumar et al. [32] and Joshipura et al. [37] in the energy range of interest. We depict the present modified and unmodified AR results,

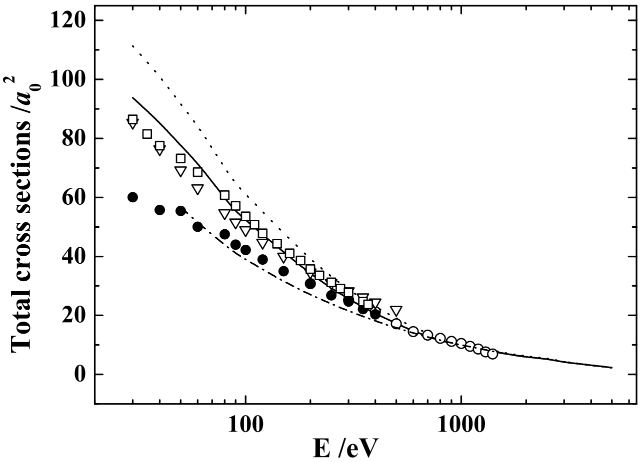

Fig. 4. TCS's for electron-C_2H_4 scattering. Theoretical calculations: solid line, present modified AR results; dotted line, present unmodified AR results; dash-dotted line, Vinodkumar et al. [32]. Experimental findings: open circle, Ariyasinghe et al. [25]; full circle, Sueoka et al. [30]; open triangle, Nishmura et al. [35]; open square, Szmytkowski et al. [39].

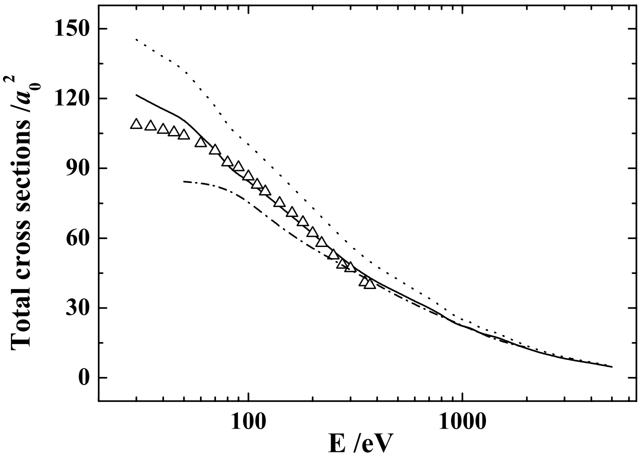

Fig. 5. TCS's for electron-C_2F_4 scattering. Theoretical calculations: solid line, present modified AR results; dotted line, present unmodified AR results; dash-dotted, Antony et al. [40]. Experimental findings: open triangle, Szmytkowski et al. [39].

four groups of measurements, and the theoretical results given by Vinodkumar et al. [32] in Figure 4. The present modified AR results are in slightly better agreement with some of the experimental measurements [25,35,39], but in poorer accord with others [30] when compared with the theoretical results of Vinodkumar et al. [32] at intermediate and low energies. As for experimental results, the present modified AR results are in excellent agreement with all the measurements [25,30,35,39] at all the overlapping energies, except those obtained by Sueoka et al. [30] below 200 eV.

Experimental and theoretical results on electron scattering by C_2F_4 above 30 eV are scarce. The only available experimental results are those reported by Szmytkowski et al. [39]. The only theoretical results are those given by Jiang et al. [21] and Antony et al. [40]. The present modified AR results are smaller than those given by Jiang et al. [21] (not shown in Fig. 5) at lower energies, thus much closer to the measurements [39]. As shown in Figure 5, the present modified AR results agree well with the available measurements above 50 eV.

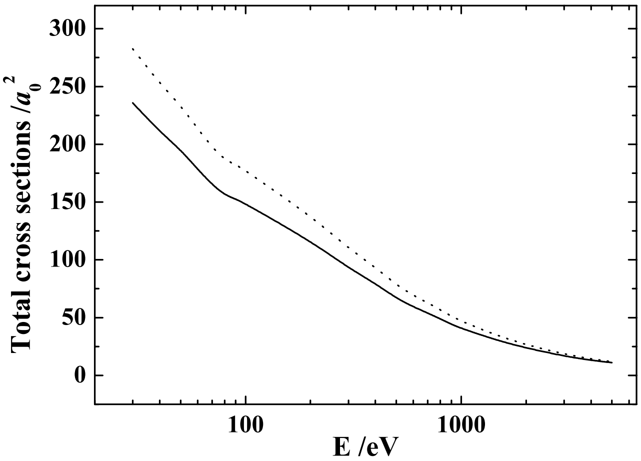

Fig. 6. TCS's for electron-C_2Cl_4 scattering. Theoretical calculations: solid line, present modified AR results; dotted line, present unmodified AR results.

As with molecules C_2H_6 and $C_2H_3F_3$, C_2H_4 and C_2F_4 are analogical in structure, too. From their comparison above 100 eV or so, the present modified AR results for agreement with available experimental measurements. And the higher the energy, the smaller are the discrepancies between the present modified AR results and the measurements.

To the best of our knowledge, neither experimental nor theoretical results exist in the literature for molecules C_2Cl_4 and CCl_2F_2. Thus, we cannot carry out a direct comparison for the present modified AR results (which are presented independently in Figs. 6 and 7). Because the molecules C_2H_4, C_2F_4, C_2Cl_4 and CCl_2F_2 are analogous in structure, and the previous calculations have pointed out that the two groups of analogous molecules in structure (one group being C_2H_6 and $C_2H_3F_3$, the other being C_2H_4 and C_2F_4) have good accord between the present modified AR results and the measurements wherever available above 100 eV, we believe that the present modified AR results for C_2Cl_4 and CCl_2F_2 must also be reliable above 100 eV.

At lower energies, as illustrated in Figures 1–7, the present modified AR results are obviously higher than all the measurements since we do not consider the interference effect originating from each constituent group in a molecule [40]. This effect may be important below 100 eV or so when the de Broglie wavelength (∼0.123 nm) associated with the incident particle will become comparable to the bond length of the molecule. (For instance, the C-H bond lengths in C_2H_6 and C_2H_4 are of 0.111 and 0.108 nm [23], respectively.) This complication may lead to an overestimation of the calculated TCS's [40]. In addition, multiple scattering events and valence-bond

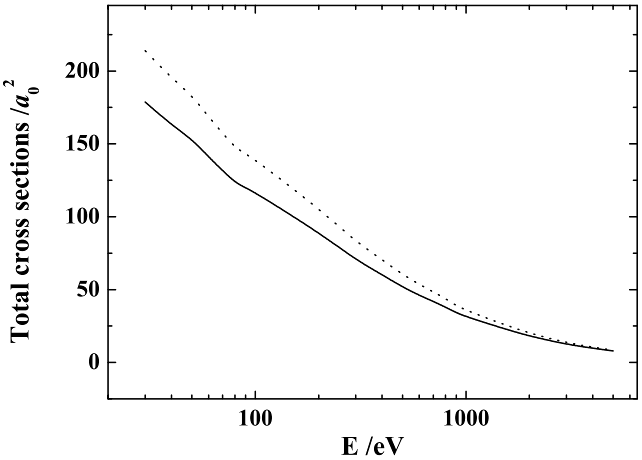

Fig. 7. TCS's for electron-$C_2Cl_2F_2$ scattering. Theoretical calculations: solid line, present modified AR results; dotted line, present unmodified AR results.

distortions [41,42] are also neglected in the present investigations. The possibility of multiple scattering is increased when the de Broglie wavelength of the incident electrons is comparable to the internuclear distance of the molecule at energies of several tens of eV. It is expected that the inclusion of multiple scattering effects at lower energies will reduce the TCS's by a significant amount [41]. The likely effect of any valence-bond distortions is also to reduce the cross section [42]. So, though we have taken into consideration the geometric shielding effect in the molecule, TCS differences still exist between the present modified AR results and the experimental findings at lower energies.

With increasing energy, the de Broglie wavelength of the incident electrons becomes smaller and smaller compared with the bond ength of the molecule, the interactions amongst the atoms in the molecule become weaker and weaker, and thus the above-mentioned effects contribute less and less. Therefore, the higher the energy, the better are the present modified AR results, as already demonstrated in Figures 1–7.

Finally, we briefly state the results for the present modified AR in predicting electron scattering by C_3H_8, C_3F_8, C_4H_{10}, C_4F_{10}, C_6H_6 and C_6F_6. From a comparison between the present modified AR results and available experimental measurements, as a whole, we find good agreement above 100 eV. In similarity with the molecules shown in Figures 1–7, the higher the energy, the smaller are the discrepancies between the present modified AR results and the measurements. The present unmodified AR results, however, show great discrepancies, especially at intermediate and low energies. More detailed results and a comparison with experimental results where available will be published in the near future.

4 Conclusions

Taking into consideration the geometric shielding effect in a molecule, an empirical fraction, which depends on the target's molecular dimension and the energy of the incident electrons, is presented. Employing this fraction, we successfully combine the advantages of the GAR and AR approaches and generate more reliable TCS results for electron scattering by complex polyatomic molecules over a certain energy range. Excellent agreement has been found at lower energies, especially above 100 eV, despite the fact that the interference effect originating from each constituent group [40], the multicenter scattering effect [41] and the valence-bond distortion effect [42] were not taken into account in the present work. In future investigations, we will take these effects into consideration so that we can extend the validity of the AR model to energies of several tens of eV for even more complex molecules.

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