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A modification potential method for electron scattering total cross section calculations on several molecules at 30–5000eV*

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A complex optical model potential modified by incorporating the concept of bonded atom which takes into consideration the overlapping effect of electron clouds between two atoms in a molecule is employed to calculate the total cross sections for electron scattering in such molecules as N_2, NO, NO_2, CH_4, CF_4, CF_3H, C_2H_2 and C_2H_4 at 30–5000eV using the additivity rule model at Hartree–Fock level. The quantitative total cross sections are compared with those obtained in experiments and other theories, wherever available, and good agreement is obtained at 30–5000eV. It is shown that the modified calculation results are much closer to the available experimental data than the unmodified ones at lower energies, especially below 500eV. Therefore, considering the overlapping effect of electron clouds in the complex optical model potential could be helpful for better calculation results about electron scattering total cross sections from molecules.

Keywords: total cross section, additivity rule, atomic and molecular collision
PACC: 3480, 3440

1. Introduction

In recent years, more and more experimental and theoretical research interest has focused on the total cross sections (TCSs) for electron scattering by molecules in the intermediate- and high-energy range, especially above 2000eV. The reason is that TCSs for electron–molecule scattering have important applications in plasma-assisted material processing, laser, atmospheric science, chemical physics, industrial production, semiconductor devices and military fields etc. However, it is well known that electron–molecule scattering presents a more complex problem than the corresponding electron–atom scattering due to the multi-centre nature, the lack of a centre of symmetry and its nuclear motion. Hence, for electron–molecule scattering, many approaches have been proposed and developed.[1] Here, we are interested in the intermediate- and high-energy range, where almost all inelastic channels are opened.[2] In this energy range, a conventional close-coupling theory for electron–molecule scattering is almost impossible to establish. It is therefore not surprising that many previous TCS calculations for electron–molecule scattering were restricted to low energies.

Recently, a fairly simple approach, namely the additivity rule (AR) model, wherein a molecular TCS is an incoherent sum of the TCSs of the constituent atoms, was employed successfully by Raj[3] to obtain the elastic cross section at 100–500eV. Lately, the AR model has been widely used to calculate total, elastic, inelastic and differential cross sections.[4–6] However, large differences are observed between the theoretical results and experimental data at lower energies, especially below 500eV. At the same time, it has been seldom used to calculate TCSs for electron–molecule scattering above 2000eV, especially above 3000eV. So, in order to acquire accurate calculated results over a wide energy range, many authors gave various modification methods.[6–8] Considering the molecular geometrical properties, Jiang *et al*[7] presented an energy-independent geometry AR(EGAR), but compared with the experimental data, the results are still

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not very good at lower energies. Zecca *et al*[8] took into account the geometrical screening of the component atoms and presented a geometrical approach to the AR, however its accuracy depends on the experimental errors.

In this paper, the complex optical model potential modified by incorporating the concept of bonded atom, which takes into consideration the overlapping effect of electron clouds between two atoms in a molecule, is employed to calculate the TCSs for electron scattering from such molecules as N_2, NO, NO_2, CH_4, CF_4, CF_3H, C_2H_2 and C_2H_4 at 30–5000eV by using AR model at Hartree–Fock level. In Section 2, we describe in detail the complex optical model potential modified by incorporating the concept of bonded atom, and the AR model. In Section 3, we present the TCS calculations and discussion for the target molecules at 30–5000eV and compare them with the available results in experiments and other theories. Final remarks are made in Section 4. Atomic units are employed throughout this paper.

2. Theory and method

The TCS of the AR model for a molecule containing N atoms is given by

$$\begin{aligned} Q_{\mathrm{T}}(E) =& \frac{4\pi}{k}\mathrm{Im}F_m(\theta) \\ \approx& \frac{4\pi}{k}\mathrm{Im}\sum_{j=1}^{N} f_j(\theta=0) = \sum_{j=1}^{N} q_{\mathrm{T}}^j(E), \end{aligned} \quad (1)$$

where $q_{\mathrm{T}}^j(E)$ and f_j are the TCS due to the jth atom of the molecule and the complex scattering amplitude for constituent atoms of the molecule, respectively. Here it is obvious that no molecular geometry is involved in the AR model. So, the electron–molecule scattering problem is reduced to the electron–atom scattering problem which is easier to tackle.

In the present study, the complex optical model potential of a constituent atom in the molecule can be expressed as follows:

$$V_{\mathrm{opt}}(r) = V_{\mathrm{s}}(r) + V_{\mathrm{p}}(r) + V_{\mathrm{e}}(r) + \mathrm{i}V_{\mathrm{a}}(r). \quad (2)$$

Thus V_{opt} incorporates all the important physical effects. In detail, the static potential $V_{\mathrm{s}}(r)$ for an electron–atom scattering system is calculated by using the atomic charge density, determined from the well-known Hartree–Fock atomic wavefunctions.[9] Exchange potential $V_{\mathrm{e}}(r)$ provides a semiclassical energy-dependent form of Riley and Truhlar.[10] Polarization potential $V_{\mathrm{p}}(r)$ was given by our group.[11] And the absorption potential $V_{\mathrm{a}}(r)$[12] represents the combined effect of all the inelastic channels. It is a function of atomic charge density $\rho(r)$, incident energy E of electron, and the mean excitation energy Δ of the target.

In the previous studies,[7] the AR model did not consider the formation of the chemical bond and the overlapping effect of electron clouds between two atoms in a molecule. Thus, calculation errors are great at lower energies. Here, we introduce the concept of bonded atom and consider the overlapping effect of electron clouds between two atoms. That is to say, the atom in a molecule is different from the free one due to the overlapping effect of electron clouds. So, electron charge density $\rho(r)$ may be modified as follows:

$$\rho'(r) = f\rho(r), \quad (3)$$

$$f = 1 - \frac{r}{R} \times \frac{Z}{N}. \quad (4)$$

Here, f is a structural factor; r and R are the bond length and the sum of the radius of the two atoms, respectively. Z and N are the number of electron in the outmost shell and the total number of electron in the atom, respectively. So, Eq.(2) can be modified as

$$V_{\mathrm{opt}}(r) = V_{\mathrm{s}}(r) + V_{\mathrm{p}}(r) + V_{\mathrm{e}}(r) + \mathrm{i}fV_{\mathrm{a}}(r). \quad (5)$$

The q_{T}^j in Eq.(1) is obtained by the method of partial waves from the following radial equation:

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2} + k^2 - V_{\mathrm{opt}} - \frac{l(l+1)}{r^2}\right)u_l(r) = 0; \quad (6)$$

and under the boundary condition $r \to \infty$, we obtain the solution of Eq.(6)

$$u_l(r) \sim kr[j_l(kr) - \mathrm{i}n_l(kr)] + S_l kr[j_l(kr) + \mathrm{i}n_l(kr)], \quad (7)$$

where j_l and n_l are spherical Bessel and Neumann functions, respectively. The limit l_{MAX} is taken, which is large enough to generate the higher partial-wave contributions until a convergence of less than 0.5% is again achieved in the TCS.

Values of the parameter R in target molecules are achieved by using the atomic charge density, determined from the well-known Hartree–Fock atomic wavefunctions.[9]

The structural factor f, derived from Eq.(4), reflects the overlapping effect of electron clouds between two atoms in a molecule. It is very simple, but taking it into consideration, we find that the modified calculations are much closer to the available experiments

than the unmodified ones and the SCOP (Spherical Complex Optical Potential) results obtained by Jain and Baluja,[13,14] at lower energies.

3. Calculations and discussion

Employing the AR model together with the complex optical model potential modified by incorporating the concept of bonded atom, we have calculated the TCSs for electron scattering from a number of molecules (N_2, NO, NO_2, CH_4, CF_4, CF_3H, C_2H_2 and C_2H_4) at 30–5000eV. The modified and unmodified TCS results together with the available experimental and theoretical data are given in Figs.1–8.

Figure 1 shows TCSs for e–N_2 scattering together with the theoretical results obtained by Jain and Baluja[14] at 30–5000eV, and the available experimental data obtained by Blauuw *et al*[15] at 100-750eV, Dalba *et al*[16] at 100–1600eV, Hoffman *et al*[17] at 30–750eV and Garcia *et al*[18] at 600–5000eV. From Fig.1, we can see that the modified calculations are in excellent accord with all the available results in experiments and other theories above 100eV. The differences between the modified calculations and the experimental data of Blauuw *et al*[15] are about 24.2% at 100eV and 23.1% at 225eV. But that between the modified calculation and the data of Dalba *et al*[16] is only about 12.6% at 121eV. And that between the modified calculation and the data of Hoffman *et al*[17] is only about 12.0% at 150eV, too. The modified calculations are higher than all the experimental data, but much closer to them than the SCOP data of Jain and Baluja[14] at lower energies.

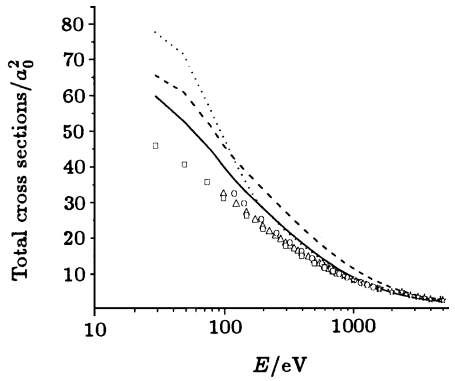


Fig.1. Total cross sections for e–N_2 scattering. Theoretical results: solid line, present modified dashed line, present unmodified line; dotted line, Jain and Baluja[14]; Experimental results: triangle, Blauuw *et al*[15]; circle, Dabla *et al*[16], square, Hoffman *et al*[17], star, Garcia *et al*[18].

The modified calculations are in good accord with the experimental results of Garcia *et al*[18] at 600–5000eV, too. At 600eV, the difference between them is only 15.07%.

The discrepancies between the modified calculations and the data given by Hoffman *et al*[17] are 31.4% at 30eV, and 29.9% at 50eV. Thus, there is also good agreement between them below 100eV.

From Fig.1, we can easily see that, at higher energies, the modified calculations are much closer to the SCOP results of Jain and Baluja.[14] But the unmodified calculations are much higher than the modified ones, all the experimental data, and the SCOP results of Jain and Baluja[14] over a wide energy range. Thus, we can say that using the AR model together with the complex optical model potential which takes into account the overlapping effect of electron clouds can give better TCS calculations.

So far as the TCSs of the e–NO scattering are concerned, experimental data of Dalba *et al*[16] at 121–1440eV, and of Szmytkowski and Maciag[19] at 30–160eV, and theoretical results of Joshipura and Patel[5] at 100–1000eV are shown in Fig.2. From the comparison between theoretical results and experimental data, we find that the results are in excellent agreement with one another at and above 100eV. The modified calculations are slightly higher than the experiments of Dalba *et al*[16] by at most 10.2%, but only larger than the theories of Joshipura and Patel[5] by at most 4.0% in the lower energy range.

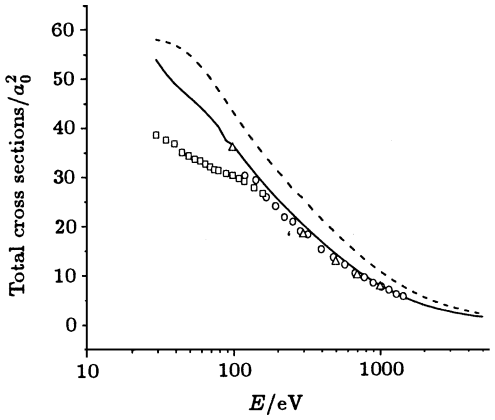


Fig.2. Total cross sections for e–NO scattering. Theoretical results: solid line, present modified results; dashed line, present unmodified results; triangle, Joshipura and Patel[5]; Experimental results; circle, Dabla *et al*[16], square, Szmytkowski and Maciag.[19]

Compared with our calculations and the other experimental data, even though the data obtained by Szmytkowski and Maciag[19] are much smaller, the largest discrepancy between the modified calculations

and the experimental data is only 20.68% at and above 100eV. This is encouraging.

At energies above 1440eV, no experimental data could be found; however, according to the excellent agreement between the modified calculations and the data available at 100–1440eV, we can conclude that the modified calculations are reliable.

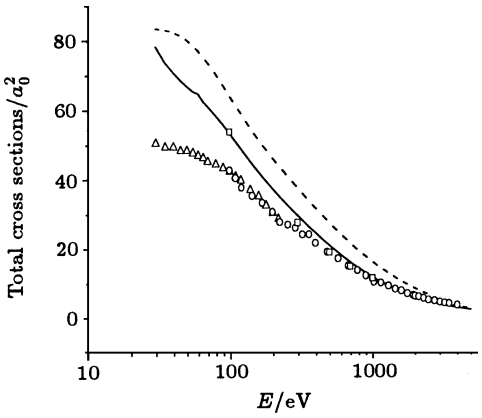


Fig.3. Total cross sections for e–NO_2 scattering. Theoretical results: solid line, present modified results; dashed line, present unmodified results; square, Joshipura and Patel[5]; experimental results; circle, Zecca *et al*[20], triangle, Szmytkowski *et al*[21].

The discrepancies between the modified calculations and the experimental results given by Szmytkowski and Maciag[19] are 36.2% at 35eV, 36.5% at 45eV, 33.4% at 60eV and 22.1% at 90eV. They are in slightly poor agreement at and below 100eV.

Two groups of experimental data of Zecca *et al*[20] at 100–4000eV, and of Szmytkowski *et al*[21] at 30–220eV, and one group of theoretical results of Joshipura and Patel[5] at 100–1000eV together with our modified and unmodified calculations for e–NO_2 are shown in Fig.3. From the comparison among these results, we find that they are also in excellent agreement with one another above 100eV. Figure 3 shows at most 29.0% overestimation of the modified calculations from the measurements of Zecca *et al*,[20] or those of Szmytkowski *et al*[21] at 100–5000eV. But when the energy lies within the range 300–3000eV, the discrepancies between them are at most 15%. Even if the energy is high up to 4000eV, the deviation between the modified calculation and the measurement of Zecca *et al*[20] is only 21.7%.

We also notice that the discrepancies between the modified calculations and the measured results of Szmytkowski *et al*[21] are 49.4% at 35.0eV, 38.0% at 60eV, and 31.4% at 80.0eV. Thus, there is poor agreement between them below 100eV.

Especially, as Zecca *et al*[20] already pointed out, their experimental errors are 5.5%, 3.5% and 5.5% at 100, 110 and 121eV, respectively. And at 144–200eV, the relative experimental errors are at least 2.2%. If we consider this factor within the combined uncertainties, even at 100–220eV, the discrepancies beyond a few energy points may also be below 20%. The same analysis can also be made for the experimental data of Szmytkowski *et al.*[21] So, the AR model together with the complex optical model potential modified by incorporating the concept of bonded atom can be considered to be successful at and above 100eV for e–NO_2.

For e–CH_4 scattering, Zecca *et al*[22] at 30–4000eV, Dababneh *et al*[23] at 30–500eV, Ariyasinghe and Powers[24] at 200–1400eV, and Garcia and Manero[25] at 400–5000eV have given their experimental data of the TCSs recently, as shown in Fig.4. Jain and Baluja[14] also give the calculated results at 30–5000eV. From Fig.4, we find that there is excellent agreement among the modified calculations and the experimental[22–24] or theoretical[25] results in the corresponding energy ranges. Though the deviations between the modified calculation and the data of Zecca *et al*[22], and between the modified calculation and the data of Dababneh *et al*[23] are 25.2% and 32.2% at 100eV, respectively, the difference goes sharply down as the energy goes up. At 300eV, the deviation between the modified calculation and the data of Zecca *et al*[22] is 15.5%, and at the same energy, the difference between our calculation and the data of Dababneh *et al*[23] is 19.5%, whereas at 500eV, the differences are 9.3% and 13.4%, respectively. At 300eV, the deviation between our calculation and the experimental data of Ariyasinghe and Powers[24] is 20.8%. At 500eV, the value is reduced to 13.4%. Unfortunately, at higher energies, especially above 3000eV, the data given by Garcia and Manero[25] are higher than the modified calculations. But, as shown in Fig.4, the discrepancies between them are not large. The situation is similar to the other target molecules in this paper.

In the lower energy range, especially below 1000eV, the theoretical results of Jain and Baluja[14] are obviously smaller than the data obtained by Zecca *et al*[22] and much smaller than the modified calculations. And above 2000eV, the theoretical results of Jain and Baluja[14] are higher than the modified calculations.

In Fig.4, we also give the unmodified calculations. The deviations between the unmodified calculation and the experimental values of Dababneh *et al*[23] at

29.3eV, and between the unmodified calculation and the data of Zecca *et al*[22] at 30eV are 60.0% and 61.4%, respectively. Even at 500eV, the deviations are also 65.3% and 61.2%, respectively. So, the unmodified calculations are obviously higher than the experimental data[22,23] at lower energies, especially at below 800eV.

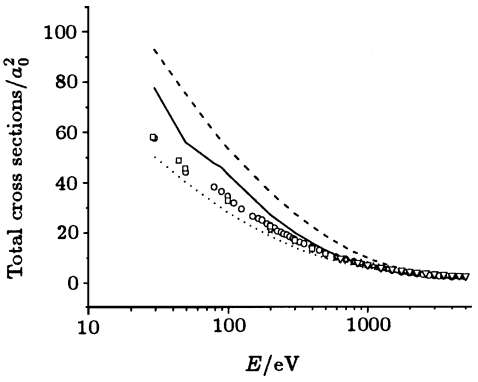


Fig.4. Total cross sections for e–CH_4 scattering. Theoretical results: solid line, present modified results; dashed line, present unmodified calculations; dotted line, Jain and Baluja[14]. Experimental results; circle, Zecca *et al*[22], square Dababneh *et al.*[21], star, Ariyasinghe and Powers[24]; Triangle, Garcia and Manero[25].

For CF_4, one of the fluoromethanes, we also report the comparison between the modified calculations and the available experimental data in Fig.5, from which we notice that there is also an excellent agreement between the modified calculations and the data of Zecca *et al*[26] at 75–4000eV, of Manero *et al*[27] at 300–5000eV, of Sueoka *et al*[28] at 100–400eV, of Szmytkowski *et al*[29] at 100–200eV, and of Ariyasinghe[30] at 100–1500eV. It is shown that the present approach is completely suitable for the calculation of e–CF_4 scattering at above 75eV. Even at 75eV, the deviation between the modified calculation and the experimental values of Zecca *et al*[26] is only 22.5%. Though at 100eV, the deviation between the modified calculation and the data of Sueoka *et al*[28] is 39.9%, at the same energy, the deviations between the modified calculation and the data of Zecca *et al*[26], and between the modified calculation and the data of Szmytkowski *et al*[29] are 19.2% and 22.6%, respectively.

Figure 5 also shows the experimental results of Jones[31] at 30–50eV and the unmodified calculations at 30–5000eV. Obviously, there are large differences between the modified calculations and the experimental results obtained by Jones.[31] At the same time, there are also large differences between the unmodified calculations and all the available data, too. Even at 1000eV, the deviation between the unmodified calculation and the data of Zecca *et al*[26] is up to 30.2%, whereas it is only 7.6% between the modified calculation and the latter.

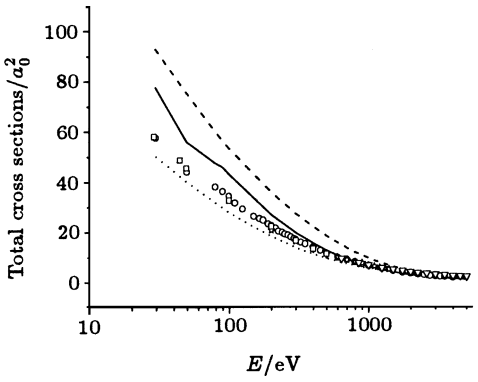


Fig.5. Total cross sections for e–CF_4 scattering. Theoretical results: solid line, present modified results; dashed line, present unmodified results. Experimental results; circle, Zecca *et al*[26]; triangle Manero *et al.*[27]; solid star, Sueoka *et al.*[28]; solid square, Szmytkowski *et al.*[29] square, Ariyasinghe [30]; empty star, Jones[31].

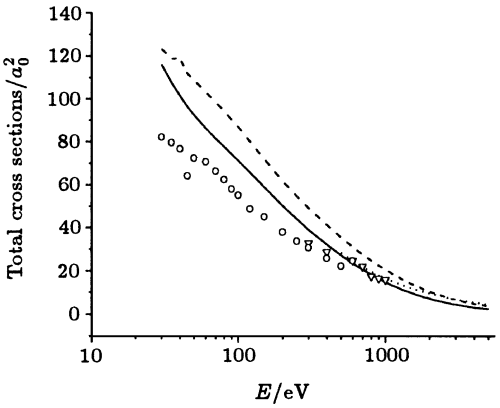


Fig.6. Total cross sections for e–CF_3H scattering. Theoretical results: solid line, present modified calculations; dashed line, present unmodified calculations; dotted line, Manero *et al*[27]. Experimental results; circle, Sueoka *et al*[32], triangle, Iga *et al*[33].

CF_3H is another fluoromethanes. Unfortunately, there are few experiments about e–CF_3H scattering. We only find two groups, which are the experimental data of Sueoka *et al*[32] at 30–600eV, and of Iga *et al*[33] at 300–1000eV. The two groups of experimental data are shown in Fig.6 together with the modified and unmodified calculations, and also the values derived from the empirical formula of Manero *et al*[27] at 500–5000eV. From Fig.6, we can easily see that the modified calculations are still in excellent accord with the two groups of data at above 100eV. The deviation

between the modified calculations and the experimental results of Iga *et al*[33] is at most 18.6%. Even though the difference between the modified calculation and the data of Sueoka *et al*[32] reaches 28.9% at 100eV, this deviation decreases quickly as the energy of incident electron increases.

There is an excellent agreement between the values derived from the empirical formula of Manero *et al*[27] and the modified calculations at below 1500eV, whereas the unmodified calculations are much higher than the modified calculations, the empirical values and the experimental data.

At above 1500eV, no experimental data could be found, but according to the excellent agreement between the above results at 100–1500eV, we guess the modified calculations may be reliable.

Only one group of experimental data[32] could be found at 30–100eV. The discrepancies between them are 35.1% at 35eV, 32.05% at 40eV, and 27.6% at 50eV, 22.0% at 60eV and 24.3% at 80eV. So, there is slightly poor agreement in this energy range.

As shown in Fig.7, the modified calculations are also in excellent accord with the measurements obtained by Xing *et al*[34] at 400–2600eV, Ariyasinghe and Powers[24] at higher energies, and with the theoretical results obtained by Jain and Baluja[14] at 30–5000eV, but in poor accord with the measurements obtained by Sueoka and Mori[35] at 30–400eV, and Ariyasinghe and Powers[24] at lower energies. At below 2000eV, the modified calculations almost overlap with the theoretical results of Jain and Baluja[14] At above 2500eV, the theoretical results of Jain and Baluja[14] are slightly higher than the modified calculations. The difference between the modified calculation and the experimental data of Xing *et al*[34] is about 12.9% at 400eV, whereas it is 0.63% at 1000eV. At 300eV, the deviations between the modified calculation and the experimental values of Ariyasinghe and Powers[24] and between the modified calculation and the data of Sueoka and Mori[35] are about 49.3% and 54.4%, respectively. But this discrepancy quickly goes down as the energy goes up.

At 100–400eV, there are very few experimental data except those of Sueoka and Mori[35] and Ariyasinghe and Powers.[24] We notice that the experimental results of Sueoka and Mori[35] is lower than that of Xing *et al*[34] by about 18.4%. Thus, we guess that large deviations between the modified calculations and the experimental data of Sueoka and Mori[35] are caused in part by the fact that the data of Sueoka and Mori[35] are smaller than the real TCS values. At above 2600eV, no experimental data could be found in the literature, but according to the excellent agreement of the modified calculations with the measurements of Xing *et al*[34] at 100–2600eV, also with the theoretical values of Jain and Baluja[14] at 100–5000eV, we can say that the modified calculations are also reliable.

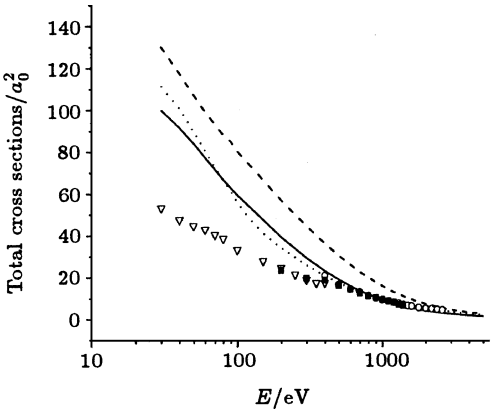


Fig.7. Total cross sections for e–C_2H_2 scattering. Theoretical results: solid line, present modified calculation; dashed line, present unmodified calculations; dotted line, Jain and Baluja[14]. Experimental results; circle, Xing *et al*[34]; triangle, Sueoka and Mori[35]; solid square, Ariyasinghe and Powers[24].

Figure 8 shows the modified and unmodified TCS calculations together with the experimental data of Szmytkowski *et al*[36] at 30–370eV, of Nishimura and Tawara[37] at 100–500eV, of Sueoka and Mori[38] at 30–400eV, and of Ariyasinghe and Powers[24] at 200–1400eV. From Fig.8, we see the excellent agreement between the modified calculations and all the measurements at above 100eV, whereas the unmodified ones are in good accord with the experimental data only at above 1000eV. The discrepancies between the modified calculations and the data of Szmytkowski *et al*[36] are 37.0% at 30eV, 34.7% at 50eV, and 27.4% at 80eV, but rapidly go down to 17.1% at 100eV and 16.8% at 120eV. Thus, the modified calculations are still in good accord with the data given by Szmytkowski *et al*[36] at above 30eV, especially at above 100eV. The deviation between the modified calculations and the data of Ariyasinghe and Powers[24] is at most 20.9%, and the largest deviation lies at 200eV. Though a large deviation between the modified calculation and the data of Nishimura and Tawara[37] is 28.1% at 100eV, it sharply goes down as the energy goes up, and the difference is only about 17.7% at 200eV.

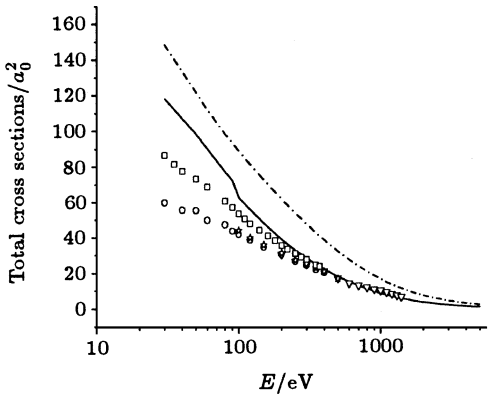


Fig.8. Total cross sections for e–C_2H_4 scattering. Theoretical results: solid line, present modified calculations; dashed line, present unmodified calculations. Experimental results: square, Szmytkowski *et al*[36]; star, Nishimura and Tawara[37]; circle, Sueoka and Mori[38]; triangle, Ariyasinghe and Powers[24].

At above 1400eV, we could not find any previous experimental data. But according to the good accord between the modified calculations and the available measurements at 100–1400eV, and there is only 15.4% of deviation between the modified calculation and the data obtained by Ariyasinghe and Powers[24] at 1400eV, we can almost conclude that the calculations at 1400–5000eV must be reliable, too. But obviously, when the energy is at below 100eV, the modified calculations are in rather poor accord with the data of Sueoka and Mori.[38]

Obviously, the unmodified calculations are largely higher than the four groups of experimental data and the modified calculations.

As seen from Figs.1–8, the modified calculations are obviously better than the unmodified ones over a wide energy range, especially at lower energies. The reason is that the modified model potential takes into consideration the overlapping effect between two atoms in a molecule but the unmodified model potential does not. That is to say, for diatomic and polyatomic molecules, the shielded or overlapped clouds in a molecule are used to calculate an atomic TCS, but in fact they have no contributions to molecular TCS. Thus, the calculations using unmodified model potential give worse results.

At low energies, especially below 100eV, as evidenced from Figs.1–8, the present modified calculations give values that substantially exceed the experimental data because we have ignored the multicentre scattering and the valence-bond effect in the AR model. In addition, a close-packed molecule is not fully transparent for low-energy electrons, and the "inner" atoms are shielded by the "outer" atoms and do not contribute to the molecular TCS.[39] For diatomic and triatomic molecules, because atomic binding and shielding contribute less, we can present better calculated values than those of polyatomic molecules using the same modified model potential. It is obvious that the target molecule is more complex (or contains more electrons) and the TCS calculations produce worse results because the valence-bond effect and shielding effect of the complex molecules have more contributions on the TCS of electron–molecule scattering than those of the simple molecules. For molecules such as N_2, NO_2, CF_4 and C_2H_2, which have only one group of experimental data over the energy range 30–100eV, the modified calculations are about 29.9% higher than the data of Hoffman *et al*,[17] 38.4% higher than the data of Szmytkowski *et al*,[21] 44.1% higher than the data of Jones,[31] and 88.3% higher than the data of Sueoka and Mori[35] at 50eV.

With the increase of the incident energy, the wavelength of the incident electron becomes smaller and smaller compared with the bond length of the molecules, thus the valence-bond effect and shielding effect contribute less and less. Therefore, at 100–300eV, the modified calculations become better and better. And at above 300eV, the contribution of molecular structure and shielding effect on the TCS may be neglected. So, the AR model and the complex optical model potential modified by incorporating the concept of bonded atom can obtain excellent calculated results within the experimental errors, as verified in Figs.1–8. Generally, the modified potential method gives good results compared with available data at above 100eV in Figs.1–8.

4. Conclusion

The AR model refuses molecular geometry and its nuclear motion, so the molecular scattering is reduced to the atomic scattering problem which is easier to tackle. The modified calculations are in excellent agreement with all the available measurements, even though we ignore the molecular multi-centre nature. It is shown that the modified complex optical model potential can successfully be used to calculate the TCSs of electron–molecule scattering at above 100eV, whereas the unmodified one gives larger discrepancies. Since the contributions from the interference occurring between the scattering amplitudes originating from the different constituent atoms of the molecule and molecular shielding effect are not included in the AR

model, even considering the overlapping effect of electron clouds in the modified model potential, the calculated results of TCS using the AR model can show large discrepancies which reach 30.0% and even more.

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