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Absolute differential, elastic integrated and moment transfer cross sections for electron–OCS collisions at intermediate and high energies*

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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 atoms in a molecule, is firstly employed to calculate the absolute differential, elastic integrated and moment transfer cross sections for electron scattering by OCS over the incident energy range from 200 to 1000 eV using the additivity rule model at Hartree–Fock level. The calculated results are compared with those obtained by experiment and other theories wherever available, and good agreement is obtained over a wide energy range. It is shown that the additivity rule model together with the modified potential is completely suitable for calculating the absolute differential, elastic integrated and moment transfer cross sections of electron scattering by molecules such as OCS.

Keywords: electron scattering, additivity rule, differential cross section, elastic integrated cross section
PACC: 3480

1. Introduction

The total cross sections (TCSs), differential cross sections (DCSs), elastic integrated cross sections (ICSs) and moment transfer cross sections (MTCSs) for electron scattering by molecules have important applications in plasma-assisted material processing, gaseous laser, atmospheric science, semiconductor devices and military fields. Thus in recent years in order to calculate the accurate values of TCSs, DCSs, ICSs and MTCSs for electron–molecule scattering, a number of approximate methods have been proposed and developed, such as the Schwinger variational iterative method,[1] the distorted-wave approximation method,[2,3] the Schwinger multichannel method,[4] the complex Kohn variational method,[5,6] the Schwinger variational iterative method combined the distorted-wave approximation method,[7] the Born-closure Schwinger variational method,[8] the R-matrix method,[9,10] the *ab initio* method,[11] the close-coupling method,[12,13] and the Glauber approximation method,[14] etc. As can be seen, these methods operate well at low energies.[1−14] However, at intermediate and high energies, since almost all inelastic channels (rotational, vibrational, electronic excitation and ionization processes, etc) are open, few of the above-mentioned methods can give accurate results. It is, therefore, not surprising that many previous calculations on TCSs, DCSs, ICSs and MTCSs for electron scattering by molecules have been restricted to low energies.

In order to obtain accurate values of TCSs, DCSs, ICSs and MTCSs for electron–molecule scattering at higher energies, recently a simple approach, namely the additivity rule (AR) model, wherein a molecular cross section is taken to be the incoherent sum of the cross sections of the constituent atoms, was employed successfully by Raj[15] to calculate the TCSs, MTCSs and ICSs at 100–500 eV. Lately, the AR model has been widely used to calculate TCSs, DCSs, ICSs and MTCSs.[16,17] However, there are large discrepancies between calculated results and experimental data for relatively large or complex molecules at lower energies, especially below 500 eV. In order to per-

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form accurate calculations using the AR model over a wide energy range, researchers have proposed various modifications[18−22] in the complex optical model potential. Taking into consideration that the presently widely-used absorption potential[23] overestimates the TCS values at lower energies, Raj and Kumar [18] have presented a modification factor $m = 1/k$, but they only calculated the DCSs of electron scattering by O_2. Baluja *et al*[19] have presented a modification factor $m = 1/k^{1/2}r$ and replaced the Δ value (which is the energy gap between the target ground state and the lowest excited state)[23] in the absorption potential with the positronium formation energy, but great TCS differences between theories and experiments are still seen at lower energies for relatively large molecules. Taking into account the polarization of target molecules, Jain[20] has employed the polarized electron density in the absorption potential. Meanwhile, Jain,[20] Raizada *et al*[21] and Joshipura *et al*[22] have replaced the Δ value with the ionization potential of the corresponding atom. However, TCS or DCS calculations on only a few molecules[18−22] can hardly represent the general behaviour.

In this paper, the complex optical model potential is modified by the concept of bonded atom (modified potential), which takes into account the overlapping effect of electron clouds between two atoms in a molecule, is firstly employed to calculate the DCSs, ICSs and MTCSs for electron scattering by OCS molecule using the AR model at intermediate and high energies. OCS is selected as target molecule because it has been detected as a constituent of interstellar clouds.[24] Electron impact DCSs, ICSs and MTCSs are needed in modelling the energy decomposition processes in astrophysical environment and in the optimization of electric-discharge-based devices for the removal of pollutants from industrial fumes. But to our knowledge, investigations[25−31] involving DCSs, ICSs or MTCSs for electron scattering by this molecule are very scarce, whether theoretical or experimental. In these studies, only one group[27] in experiments[25−27] and two groups[27,28] in theories[27−31] are concerned with energies above 100 eV of incident electron energies.

The organization of this paper is as follows: In Section 2, the modified potential and the AR model are briefly described. In Section 3, the calculated results of the DCSs, ICSs and MTCSs for electron–OCS scattering are presented. The comparison between present calculated results with the available measurements and other theories are performed. Finally, in Section 4 concluding remarks are made. Atomic units are used throughout this paper unless otherwise specified.

2. Theory and method

In the AR model, we assume that each atom in a molecule scatters independently. As a result, the theory of scattering by a molecule can be derived from that for the separate atoms. Thus, DCS, ICS and MTCS for a molecule containing N atoms averaged over all the orientations of the rotating molecule are given by

$$I(\theta) = \sum_{j=1}^{N} |f_j(\theta)|^2, \tag{1}$$

$$Q_{\rm I}(E) = 2\pi \int_0^{\pi} I(\theta) \sin\theta {\rm d}\theta, \tag{2}$$

$$Q_{\rm M}(E) = 2\pi \int_0^{\pi} I(\theta)(1-\cos\theta) \sin\theta {\rm d}\theta, \tag{3}$$

where $I(\theta)$ is the DCS for the given molecule; θ is the scattering angle; $f_j(\theta)$ is the scattering amplitude of the jth atom constituting the molecule, $Q_{\rm I}(E)$ and $Q_{\rm M}(E)$ are ICS and MTCS of the molecule, respectively. From Eq.(1), we easily see that the atomic scattering amplitudes referred to a single centre are added incoherently. Thus no molecular geometry is involved. So, a molecular scattering problem is reduced to an atomic one that is easier to handle.

The scattering amplitude of the jth atom in terms of partial waves is given by

$$f_j(\theta) = \frac{1}{2{\rm i}k} \cdot \sum_l (2l+1)(S_l^j - 1) P_l(\cos\theta), \tag{4}$$

where S_l^j is the lth complex scattering matrix of the jth atom and can be obtained by solving the following radial equation,

$$\left(\frac{{\rm d}^2}{{\rm d}r^2} + k^2 - V_{\rm opt} - \frac{l(l+1)}{r^2} \right) u_l(r) = 0, \tag{5}$$

under the boundary condition ($r \sim \infty$)

$$u_l(kr) \sim \; kr[j_l(kr) - {\rm i}n_l(kr)] + S_l kr[j_l(kr) + {\rm i}n_l(kr)]. \tag{6}$$

Here j_l and n_l are spherical Bessel and Neumann functions, respectively. The upper limit of l is taken large enough to take account of the higher partial-wave contributions until a convergence less than 0.5%

is achieved in the DCS. $V_{\rm opt}$ is the appropriate complex optical model potential which includes all the important physical effects. In the present study, the $V_{\rm opt}$ of an atom in a molecule is given by

$$V_{\rm opt}(r) = V_{\rm s}(r) + V_{\rm p}(r) + V_{\rm e}(r) + {\rm i}V_{\rm a}(r). \qquad (7)$$

The static potential $V_{\rm s}(r)$ for e-atom scattering is calculated by using the atomic charge density determined from the well-known Hartree–Fock atomic wavefunction.[32] The exchange potential $V_{\rm e}(r)$ provides a semiclassical energy-dependent form presented by Riley and Truhlar.[33] The polarization potential $V_{\rm p}(r)$ is given by our group.[34] The absorption potential $V_{\rm a}(r)$ represents the combined effect of all the inelastic channels and is given by Staszewska *et al.*[23]

In Eqs.(1)–(3), the DCS, ICS and MTCS of electron–molecule scattering is simply determined from the sum of the DCS, ICS and MTCS of electron scattering by each constituent atom. Thus Eqs.(1)–(3) ignore the formation of the chemical bond and overlapping effect of electron clouds between atoms in a molecule. To reduce the discrepancies between theories and experiments at lower energies, we introduce the concept of bonded atom and consider the overlapping effect of electron clouds between two bonded atoms. Briefly, the atom in a molecule is different from the one in a free state since the overlapping effect may cause the distortion of electron clouds. Thus the modified charge density $\rho'(r)$ of a bonded atom in a molecule must be rewritten in the following form:

$$\rho'(r) = f \cdot \rho(r), \qquad (8)$$

where

$$f = 1 - \frac{\rm d}{R} \cdot \frac{Z}{N}. \qquad (9)$$

Here f is a structural factor; $\rho(r)$ is the charge density of an atom in the free state; d is the bond length, which is presented in Ref.[35]. R is the sum of the radii of the two bonded atoms, which is achieved also by using the aforementioned atomic charge density determined from the Hartree-Fork atomic wavefunction. Z and N are the electron number of the outmost shell and the total electron number of the atom, respectively. So, Eq.(7) can be rewritten as

$$V_{\rm opt}(r) = f \cdot V_{\rm s}(r) + V_{\rm p}(r) + V_{\rm e}(r) + {\rm i}f \cdot V_{\rm a}(r). \qquad (10)$$

According to the concept of bonded atom mentioned above, the DCSs, ICSs and MTCSs for the same atom in different molecules may be different, because the overlapping effect of the electron clouds for the same atom in different molecules may be different.

Employing the modified potential (10), we have calculated the TCSs of electron scattering by numerous molecules such as NH_3, H_2O, CH_4, C_2H_2, C_2H_4, C_2H_6, C_2F_6, CF_3H, CF_4, $CFCl_3$, CF_2Cl_2, CF_3Cl, CCl_4, CO, N_2, NO, NO_2, N_2O, O_2, H_2, HCN, O_3, CO_2 and HF.[36–38] Compared with the unmodified calculations, the modified ones are much closer to the experiments above 100 eV. It is proved that the f factor given in Eq.(9) is reasonable. Now in this paper, we employ this modified potential to calculate the DCSs, ICSs and MTCSs of electron scattering by the relatively complex molecule OCS at intermediate and high energies.

3. Results and discussion

Employing the AR model along with the modified potential, we have calculated the DCSs at 200, 400, 600 and 1000 eV, and the ICSs and MTCSs at 200, 300, 400, 500, 600 and 1000 eV of electron scattering by OCS. Present calculated results together with that of the available measurements[27] and other calculations[27,28] are shown in Figs.1–4 and Table 1, respectively.

Table 1. ICSs and MTCSs for electron–OCS scattering.

	energy/eV					
source	200	300	400	500	600	1000
ICS						
This paper	20.12	14.26	11.71	9.35	7.92	4.29
Exp.[27]	17.90	13.01	10.83	8.82	7.57	—
Theory[28]	29.2	19.8	15.4	12.7	—	6.90
MTCS						
This paper	1.98	1.07	0.66	0.45	0.36	0.18
Theory[28]	3.0	1.5	0.9	0.6	—	0.23

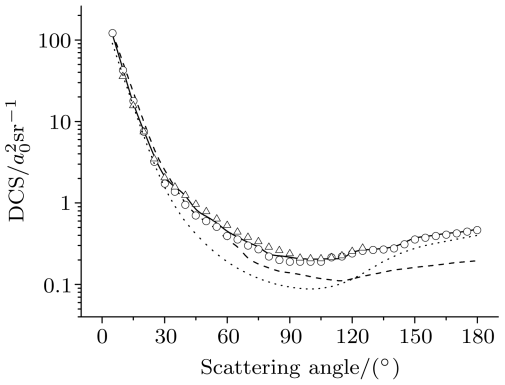


Fig.1. DCSs for e–OCS scattering at 200 eV. The theoretical results: solid line presents modified results; dashed line presents unmodified results; dotted line presents Raj and Tomar's[28] calculations; circles present Michelin *et al*'s[27] calculations. Experimental results: triangles present Michelin *et al*'s[27] measurements.

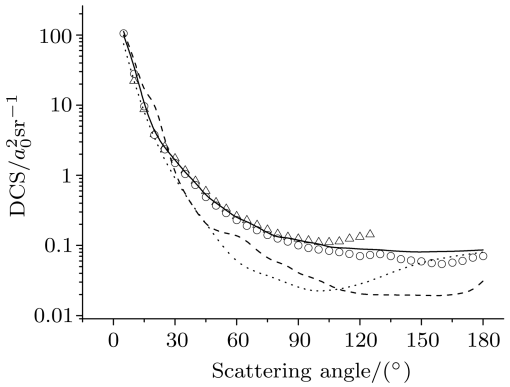


Fig.2. DCSs for e–OCS scattering at 400 eV. The theoretical results: solid line presents modified results; dashed line presents unmodified results; dotted line presents Raj and Tomar's[28] calculations; circle presents Michelin*et al*'s[27] calculations.experimental results: triangle presents Michelin *et al*'s[27] measurements.

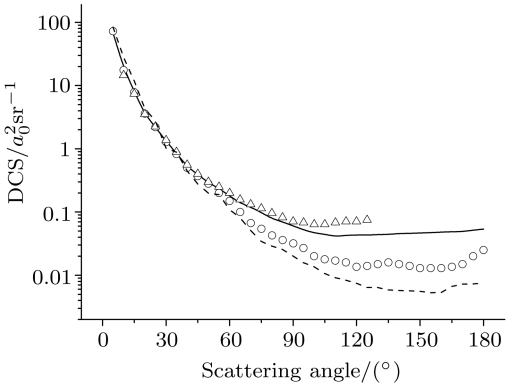


Fig.3. DCSs for e–OCS scattering at 600 eV. The theoretical results: solid line presents modified results; dashed line presents unmodified results; circles present Michelin *et al*'s[27] calculations. Experimental results: triangles present Michelin*et al*'s[27] calculations.

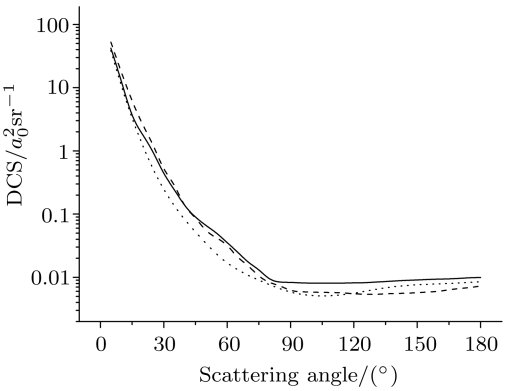


Fig.4. DCSs for e–OCS scattering at 1000 eV. The theoretical results: solid line presents modified results; dashed line presents unmodified results; dotted line presents Raj and Tomar's[28] calculations.

As seen in Figs.1–3, present modified DCS calculations are in good agreement with the only one group of measurements given by Michelin *et al*[27] except at scattering angles from 115° to 125° at 400 eV and from 100° to 125° at 600 eV. Whereas the unmodified DCS results are in poor accordance with this group of measurements[27] almost at all scattering angles. Present modified DCS results are equivalent to the calculations attained by Michelin *et al*[27] in accuracy at small scattering angles, but closer to the measurements[27] than those[27] at larger scattering ones. This shows that the AR model together with the modified potential is suitable for the DCS calculations of electron scattering by the relatively large molecule OCS. Thus our modification is proved successful.

Figure 4 shows the present modified and the unmodified calculations together with the only available group of theories given by Raj and Tomar.[28] From Figs.1–2 we can see that present modified calculations are much closer to the measurements[27] than those obtained by Raj and Tomar [28] at almost all scattering angles. And from Figs.1–3 we can also see that the present modified calculations are in good agreement with the measurements.[27] Thus, accordingly, we conclude that the present modified calculations should be more reliable than the theoretical ones given by Raj and Tomar [28] at 1000 eV, though there are no experimental results and other theoretical values available in the literature to compare with.

Table 1 shows that the present modified ICS calculated values are slightly higher than the measurements of Michelin *et al*[27] at 200–600 eV and coincide with the measurements as the incident electron energy increases. At the same time we also

see that the present modified ICS results are much closer to the measurements[27] than those of Raj and Tomar [28] According to these and the DCS agreement at 200,400 and 600 eV, we believe that the present modified MTCS calculations are more reliable than those of Raj and Tomar [28] though there are no MTCS measurements to compare with in the literature.

From the above calculations, we may consider this modified potential method as a successful attempt at using the AR model to convert a molecular scattering DCS, ICS and MTCS problem into an atomic one that is easier to handle, in particular at intermediate and high energies. Though this approach cannot provide very accurate calculations, the present results are comparable with the available measurements and calculations by and large. They can predict the outcome of experimental research, particularly for these molecules of which the wavefunctions are not available at present. We hope that the modified potential together with the AR model can encourage more experimental work and theoretical calculations of DCSs, ICSs and MTCSs at the intermediate and high energies in the near future.

4. Conclusions

The AR model ignores molecular geometry, thus a molecular scattering problem is reduced to an atomic one that is easier to handle. In this paper, we have employed the AR model and the modified potential to obtain quite encouraging results for the DCSs, ICSs and MTCSs of electron–OCS scattering. In future research, we will employ the AR model and the modified potential to calculate more DCSs, ICSs and MTCSs for electron scattering by more complex molecules, so that we can check to what extent the calculation and measurement agree with each other.

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