

Electron scattering by O₂ at intermediate and high energies

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A complex optical model potential correlated by the concept of bonded atoms, which considers the overlapping effect of electron clouds between two atoms in a molecule, is firstly employed to calculate the absolute differential cross sections, the integrated and momentum transfer cross sections for electrons scattered by O₂ at intermediate and high energies by using additivity rule model at Hartree-Fock level. In the study, the complex optical model potential is composed of static, exchange, correlation polarization plus absorption contributions. The quantitative absolute differential cross sections, the integrated and momentum transfer cross sections are obtained. Compared with available experimental data, this approach presents good results. It is shown that the additivity rule model together with the complex optical model potential correlated by the concept of bonded atoms is completely suitable for the calculations of the absolute differential cross sections, the integrated and momentum transfer cross sections.

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In recent years, there has been a renewed interest in the calculations of absolute differential cross sections (DCSs), integrated cross sections (ICSs), and momentum transfer cross sections (MCSs) for electrons scattered by gas molecules such as O₂, N₂, CO, and CO₂^[1-5]. The reason is that, firstly, the availability of new absolute DCS, ICS, and MCS measurements (especially at higher incident energies) allows a fairly detailed comparison between theories and measurements, and secondly, the need for absolute DCSs, ICSs, and MCSs becomes apparent, since these theories over wide energy range can be used for a variety of plasma-assisted material processing, laser, atmospheric science, and aeronautical 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 multicenter nature, the lack of a center of symmetry (in the case of polyatomic and hetero-nuclear molecules) and its nuclear motion. Hence, for electron-molecule scattering, many different approaches have been proposed^[6,7]. At the intermediate and high energies, since acquiring molecular wave functions is very difficult, where almost all inelastic channels (rotational, vibrational, electronic excitation, and ionization process, etc.) are open, a conventional close-coupling theory for electron-molecule scattering is almost impossible to establish. It is therefore unsurprising that many previous calculations on the absolute DCSs, ICSs, and MCSs for electron-molecule scattering have been restricted to low-energy region.

Very recently, a fairly simple approach, namely, the additivity rule (AR) model, was employed successfully to obtain the total cross sections (TCSs) for electrons scattered by a sample of molecules (N₂, O₂, NO, NO₂, and N₂O) at intermediate and high energies^[8], but we never use it to calculate the DCSs, ICSs, and MCSs of any atom and any molecule. In the AR model, we assume

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

$$I(\theta) = \sum_{i=1}^N |f_i(\theta)|^2, \quad (1)$$

$$Q_I(E) = 2\pi \int_0^\pi I(\theta) \sin \theta d\theta, \quad (2)$$

$$Q_M(E) = 2\pi \int_0^\pi I(\theta)(1 - \cos \theta) \sin \theta d\theta, \quad (3)$$

where $I(\theta)$ is the DCS for the relevant molecule, $f_i(\theta)$ is the scattering amplitude proper to the i th atom constituting the molecule, $Q_I(E)$ and $Q_M(E)$ are ICS and MCS of the molecule, respectively. From Eq. (1), we can easily see that the atomic scattering amplitudes referred to a single center are added incoherently. So, no molecular geometry is involved in the AR model of the DCS.

The scattering amplitude of the i th atom in term of partial waves is given by

$$f_i(\theta) = \frac{1}{2ik} \cdot \sum_l (2l+1)(S_l - 1)P_l(\cos \theta), \quad (4)$$

where S_l is the complex scattering matrix and can be obtained by solving the radial equation of

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

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

$$u_l(kr) \sim kr[j_l(kr) - in_l(kr)] + S_l kr[j_l(kr) + in_l(kr)], \quad (6)$$

where j_l and n_l are spherical Bessel and Neumann functions, respectively, k is energetic energy of incident electron. The limit l is taken to be large enough to generate the higher partial-wave contributions until again a convergence of less than 0.5% is achieved in the DCS. V_{opt} is the appropriate complex optical model potential which incorporates all the important physical effects and is given by

$$V_{\text{opt}}(r) = f \cdot V_s(r) + V_p(r) + V_e(r) + if \cdot V_a(r). \quad (7)$$

In detail, the static potential $V_s(r)$ for e-atom scattering is calculated by using the atomic charge density, determined from the well-known Hartree-Fock atomic wavefunctions^[9]. The exchange potential $V_e(r)$ provides a semiclassical energy-dependent form^[10]. $V_p(r)$ is the polarization potential^[11]. The absorption potential $V_a(r)$ represents the combined effect of all the inelastic channels^[12]. f is a structure factor given in Ref. [8].

Using the AR model and $V_p(r)$ given by Eq. (7), we have calculated the TCSs of more than twenty molecules and got excellent results^[8,13–15], which showed that the AR model together with the polarization potential is completely successful in the TCS calculations.

In this letter, employing the AR model along with the complex optical model potential correlated by the concept of bonded atoms, we firstly calculate the DCS, ICS, and MCS of electrons scattered by O_2 at 300, 400, 500, 700, 800, and 1000 eV. An effective range formula

$$\tan \delta_l = \frac{\pi \alpha k^2}{(2l+1)(2l+3)(2l-1)} \quad (8)$$

is used to generate the higher partial-wave contributions until again a convergence of less than 0.5% is achieved in the DCS, ICS, and MCS. To the best of our knowledge, there is no other theoretical calculations at these energies. Our results together with the available measurements at 300, 400, 500, 700, 800, and 1000 eV are shown in Figs. 1–5 and Table 1. Atomic units are employed throughout this letter unless specified.

From Fig. 1 to Fig. 4, we can easily see that the DCS calculation results are in fairly excellent agreement with the available measurements of Iga *et al.*^[16] and Bromberg^[17]. It is obvious that the higher the incident energy is, the better the agreement between the theories and the measurements is. The discrepancies are about 15%–20% at lower energies for small angles. These prove that the complex optical model potential correlated by

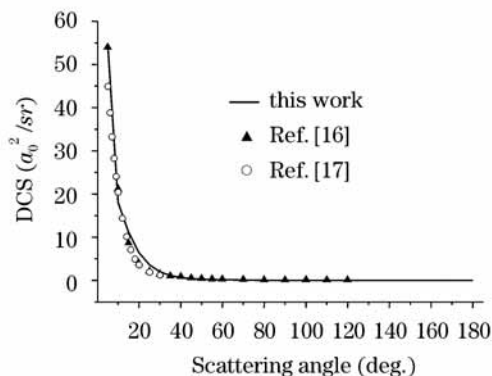


Fig. 1. DCSs for e- O_2 scattering at 300 eV.

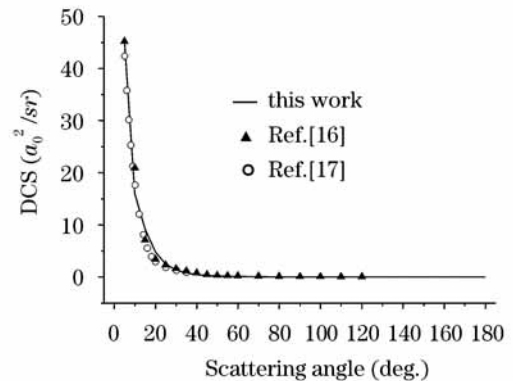


Fig. 2. DCSs for e- O_2 scattering at 400 eV.

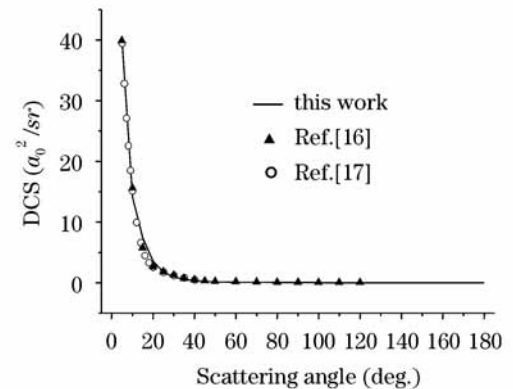


Fig. 3. DCSs for e- O_2 scattering at 500 eV.

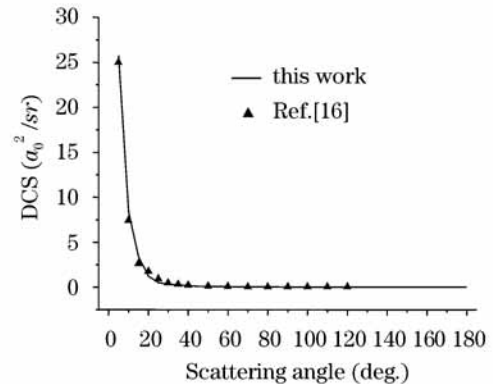
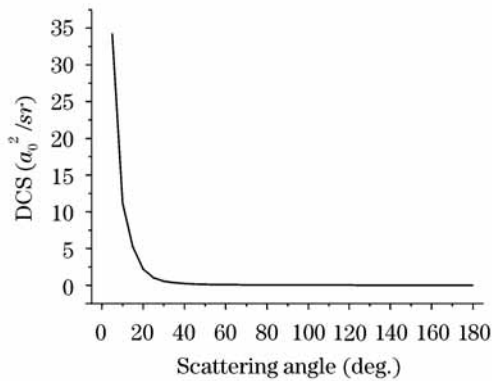
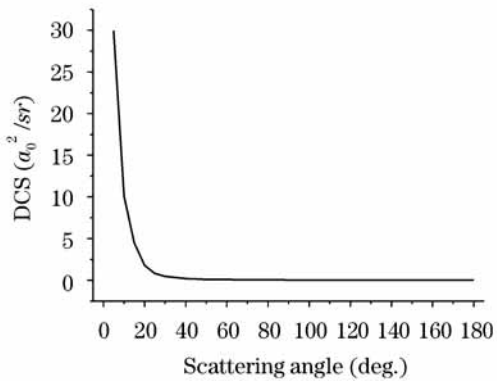


Fig. 4. DCSs for e- O_2 scattering at 1000 eV.

the concept of bonded atoms is completely suitable for the calculations of the absolute differential cross sections.

It may be noted that the present DCS results are higher than the measurements at lower energies for small angles from 15° to 30° . The reason might be the multiple scattering and the valence distortion which have been neglected in the study. At lower incident energies, the de Broglie wavelength associated with the incident particle becomes comparable to the internuclear distance which increases the possibility of multiple scattering. It is expected that the inclusion of multiple scattering effects at lower energies reduce the DCS values by a significant amount^[18]. The likely effect of the valence bond distortion is also to reduce the DCS values at lower energies^[19]. The further work to investigate the quantitative results of multiple scattering effects on DCS is proceeding.

Fig. 5. DCSs for e-O₂ scattering at 700 eV.Fig. 6. DCSs for e-O₂ scattering at 800 eV.Table 1. ICSs and MCSs for e-O₂ Scattering

Energy (eV)	300	400	500	700	800	1000
ICS						
This Work	12.44	10.46	7.73	5.52	4.72	3.75
Ref. [16]	10.3	9.08	7.15	—	—	3.74
MCS						
This Work	1.83	1.48	1.01	0.691	0.492	0.354
Ref. [16]	1.60	1.31	0.921	—	—	0.353

Figures 5 and 6 show the DCS results at 700 and 800 eV derived from the AR model and the complex optical model potential correlated by the concept of bonded atoms. There are no experimental data at these energies, but according to the excellent agreement between calculations and measurements at 300, 400, 500, and 1000 eV, we may conclude the calculation results must be reliable.

Table 1 shows that the present ICS results are slightly higher than the measurements of Iga *et al.*^[16] over the energy range of 300–1000 eV and merge well with the experimental data as the incident electron energy increases. For example, at 300 and 400 eV, our ICS results are about 20.8% and 15.2% higher, as compared with the data of Iga *et al.*^[16], respectively. For MCS, the differences between our calculations and the experimental data^[16] are within 15.0%, they are in good agreement in the whole energy range of 300–1000 eV. Though there are no measurements about ICS and MCS at 700 and 800 eV, according to the excellent agreement between theories and measurements at 300, 400, 500, and 1000 eV, our results

at 700 and 800 eV must be reliable, too.

Employing the AR model and the complex optical model potential correlated by the concept of bonded atoms, we also calculate the DCS, ICS, and MCS for electron scattering from N₂, CO, and CO₂. Our results are in good agreement with the measurements^[1–3,17]. Thus, the calculations of DCS, ICS, and MCS for e-O₂ scattering employing the AR model and local optical model potential are encouraging.

Obviously, the present results show a good agreement over the energy range of 300–1000 eV. From the above, we may consider this approach as a successful attempt using the AR model to transform the molecular scattering problem into an atomic scattering problem which is easier to handle, in particular at higher energies. Though this method cannot lead to very exact calculations, the present results are proved qualitatively well. They can be used to predict the outcome of experimental research, particularly for the molecules which wave functions are not available at present. We also hope that the AR model can lead to more work for DCS, ICS, and MCS in the intermediate and high energy ranges in the near future.

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