Differential Cross Sections for Elastic Scattering of Low-Energy Electrons by O_2 *

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Differential cross sections for the elastic scattering of electrons by oxygen molecule are calculated for selected impact energies 7 eV and 9 eV. The results are compared with other theoretical results and experimental data. The present results are obtained by the momentum space optical potential method. This method take the polarization of target states into account, which is very important for the scattering problem, particularly at low energies.

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The elastic scattering of low-energy electrons by O_2 plays an important role in various physical processes including the physics of planetary atmosphere, gaseous discharge and both astrophysical and laboratory plasmas. Great experimental efforts have been made to determine the elastic differential cross sections (DCS) for low-energy electrons by oxygen molecule. These works include the early measurements of Trajmar *et al.*,[1] Linder and Schmidt,[2] Dehmel *et al.*,[3] and Shyn and Sharp,[4] and the recent experimental measurements of Refs. [5–8]. Compared to the experimental works, only a few theoretical calculations in this energy region can be found. Recently, the DCS of O_2 by electrons impact has been calculated by Wöste *et al.* using R-matrix method in the energy range from 5 eV to 20 eV and in the scattering angular range from 0° to 160°.[8] Although there has been a quite considerable experimental effort over many years, there is still considerable disagreement among the theoretical and experimental results. Therefore, it is very necessary to calculate the elastic DCS of O_2 to give a consistent data set for the low-energy region. In this Letter, we use an *ab initio* momentum-space optical potential method to calculate the elastic DCS of electrons by O_2 at the incident energies 7 eV and 9 eV, the calculation results are compared with the other theoretical results and experimental data. In this method, the polarization potential describing the effect of higher reaction channels on electron-molecule elastic scattering is approximated by an *ab initio* equivalent-local potential, it is added to the exact static-exchange potential for a momentum-space calculation of electron-molecule scattering. A detailed description of the momentum-space optical potential method to study electron-molecule scattering process can be found by Rossi *et al.*[9] This method has been successfully applied to study the scattering electrons by molecular hydrogen.[10] Here we briefly review the essential features of this method.

The T-matrix element for scattering from the molecular ground state $|0\rangle$ to a state $|i\rangle$ is

$$\langle K'i|T|0K\rangle = \langle K'i|V|0K\rangle + \sum_j \int d^3q \langle K'i|V|jq\rangle \cdot \frac{1}{E^{(+)} - \varepsilon_j - \frac{1}{2}q^2}\langle Kj|T|0K\rangle, \quad (1)$$

where K and K' are the initial and final momentums of the project electron, respectively; i and j represent the ground state of the target for the elastic scattering. Target states are expressed in the independent-particle model. We use the self-consistent field orbitals that are a linear combination of primitive Gaussian centred at the atomic sites. We also use closure over the vibrational and rotational states. The nuclei are assumed to be fixed at their equilibrium sites. Here we make partial wave expansion for Eq. (1).

$$\langle K'L'M'\|T\|KLM\rangle = \langle K'L'M'\|V\|KLM\rangle + \sum_{L''M''}\int dq q^2 \langle k'L'M'\|V\|qL''M''\rangle \cdot \frac{1}{E_0^{(+)} - \frac{1}{2}q^2}\langle qL''M''\|T\|kLM\rangle \quad (2)$$

with

$$V = V_D + V_E + V_O, \quad (3)$$

where V_D is the direct potential,[10] V_E is the exchange potential,[10] and V_O is the optical potential defined by[10]

$$V_O(K,P) = \Big[\int d^3q \frac{\Gamma(k,P,q) - \Gamma(k,P,k_c)}{\frac{1}{2}(k_c^2 - q^2)}\Big] - i\pi k_c \int d\hat{q}\Gamma(k,P,k_c), \quad (4)$$

where

$$K = |k-q|, \quad \hat{k}_c = \hat{q},$$
$$\Gamma(k,P,q) = \frac{\ln(K^2+P^2+2KP) - \ln(K^2+P^2-2KP)}{16\pi^4 K^3 P} \cdot \Big[\Xi(P) - \frac{1}{4\pi}\Xi(K)\int d\hat{P}\Xi(|K+P|)\Big], \quad (5)$$

$$\Xi(P) = 4\pi \sum_{\substack{ijk\\ lml'm'\\ \sigma\xi\rho\varsigma}} (-)^{\rho+\sigma} \cdot \frac{\sqrt{(2l'+1)(2\rho+1)(2\sigma+1)(2l+1)}}{2s+1}$$

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$$\cdot\, c_{kj}c_{ij}\gamma_{kl'm'}\gamma_{ilm}Y^*_{\rho\varsigma}(\hat{R}_i)Y^*_{\sigma\xi}(\hat{R}_k)$$
$$\cdot\, C^{\varsigma m't}_{\rho l's}C^{000}_{\rho l's}C^{\xi mt}_{\sigma ls}C^{000}_{\sigma ls}$$
$$\cdot \int_0^\infty dr\frac{r^{l+l'+1}\sin(Pr)}{P}e^{-\alpha_k(r^2+R_k^2)}$$
$$\cdot\, e^{-\alpha_i(r^2+R_i^2)}i_\sigma(2\alpha_k rR_k)i_\rho(2\alpha_i rR_i). \quad (6)$$

The total reduced V-matrix element reads[10]

$$\langle K'L'M'\|V\|KLM\rangle = \langle k'L'M'\|V_D\|kLM\rangle - \frac{1}{2}\langle K'L'M'\|V_E\|KLM\rangle + \langle k'L'M'\|V_O\|kLM\rangle\delta_{MM'}\delta_{LL'}. \quad (7)$$

The differential cross section for the exit channel i reads

$$\left(\frac{d\sigma_{i0}}{d\Omega}\right) = 4\pi^3 \sum_{L_1M_1L_1'M_1'\mu_1'} \sum_{L_2M_2L_2'M_2'\mu_2'} \cdot \Big\{\sqrt{(2L_1+1)(2L_2+1)}T_{L_1M_1L_1'M_1'} \cdot T^*_{L_2M_2L_2'M_2'}\delta_{\mu_1'\mu_2'}\delta_{M_1+M_2'M_1'+M_2}\sum_J\frac{1}{2J+1} \cdot C^{M_1M_2'M_1+M_2'}_{L_1L_2'J}C^{M_1'M_2M_1'+M_2}_{L_1'L_2J}C^{M_1'M_2M_1'+M_2}_{L_1'L_2J} \cdot C^{0\mu_2'\mu_2'}_{L_1L_2'J}C^{\mu_1'0\mu_1'}_{L_1'L_2J}Y^*_{L_1'\mu_1'}(\hat{P}_i)Y^*_{L_2'\mu_2'}(\hat{P}_i)\Big\}. \quad (8)$$

Here $\hat{P}_i$ is the exit channel momentum in the fixed-space (laboratory) frame.

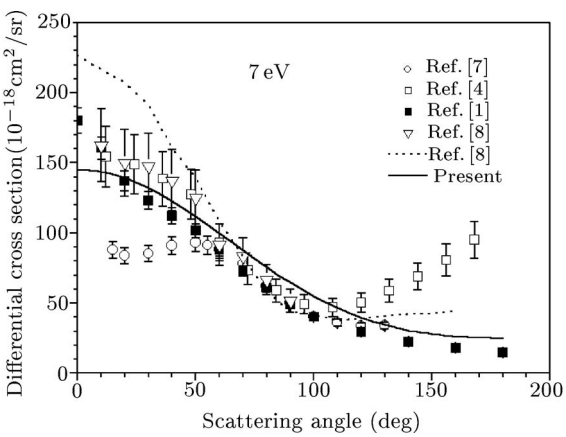


Fig. 1. O_2 elastic differential cross section at incident energies 7 eV.

Figure 1 shows the DCS for elastic scattering from oxygen molecule at 7 eV along with the experimental results of Refs. [1,4,7,8], and the R-matrix calculation result of Wöste *et al.*[8] The present calculation result of 7 eV is in excellent agreement with the experimental data of Trajmar *et al.*[1] and Wöste *et al.*,[8] and also is in good agreement with the experimental data of Shyn *et al.*[4] except slightly lower than the experimental data at large angles ($> 100°$). The present result is much better than the R-matrix calculation result of Wöste *et al.*,[8] their result is slightly higher than the experimental data at small angles ($< 40°$). There appears to be strong evidence that the polarization potential is very important for the scattering problem, particularly at low energies. The present calculation result of 9 eV and the experimental data of Sullivan *et al.*[7] and Wöste *et al.*,[8] and the R-matrix calculation result of Wöste *et al.*[8] is displayed in Fig. 2. There is good agreement between the present result and the experimental data of Wöste *et al.*[8] in the shape and magnitude. There have large discrepancies between the present calculation result, R-matrix calculation result of Wöste *et al.*[8] and the experimental result of Sullivan *et al.*[7] at small scatting angles ($< 60°$). At small scattering angles ($< 60°$), the present result is much better than the R-matrix calculation result of Wöste *et al.*[8] The present results agree well with the experimental data because of taking the polarization of target states into account via the optical potential. The R-matrix calculation result of Wöste *et al.*[8] is more close to experimental data than the present result at large scattering angles ($> 60°$). Probably, this is due to the incomplete description of the polarization effects in the present theoretical model, with the development of a complete theory taking all the reaction channels into account, agreements of the present calculation at the large scattering angles should be improved.

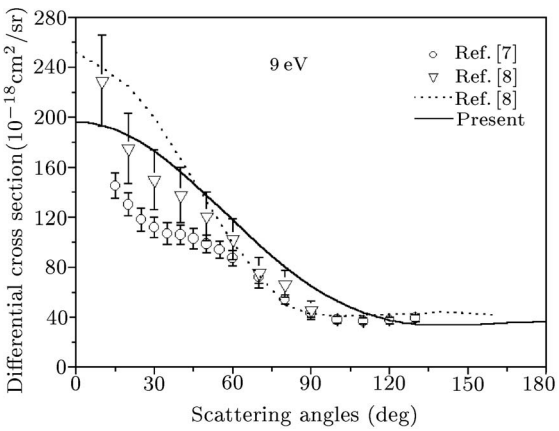


Fig. 2. O_2 elastic differential cross section at incident energies 9 eV.

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