Momentum-space calculation of electron–CO elastic collision

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We report a momentum-space study on low-energy electron-CO collisions. Elastic differential cross sections (DCS) are obtained using a static-exchange-optical (SEO) model for the incident energies of 2, 3, 5, and 10 eV. Polarization effect of higher reaction channels, including the ionization continuum, on the elastic collision is represented by an *ab initio* equivalent-local optical potential. The cross sections are compared with experimental measurements and other theoretical results.

Keywords: electron scattering, carbon monoxide, differential cross section

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1. Introduction

The study of electron collision with CO plays an important role in several applied sciences such as laser, gas discharges, plasmas,[1] and magnetohydrodynamic (MHD) power generation.[2] The CO molecule is also a significant constituent of the atmosphere and the interstellar medium. In addition, it offers a relatively simple method of investigating a reasonably small and closed shell molecule which is weakly polar.

Elastic scattering is a dominant process in electron–molecule collisions. The elastic cross sections of e–CO collisions have been measured by Tanaka *et al.*,[3] Jung *et al.*,[4] Nickel *et al.*,[5] Middleton *et al.*,[6] Gote and Ehrhardt,[7] Gibson *et al.*,[8] and more recently by Allan.[9] Compared with the experimentally measured data,[3–9] results obtained by theoretical calculation[10–15] are less. Jain and Norcross[10] have used an exact static-exchange plus a parameter-free correlation-polarization model (ESEP) to calculate rotationally elastic and inelastic differential cross sections (DCS) for incident energy up to 10 eV. Calculations based on *R*-matrix (RM) approach were reported by Morgan,[11] Morgan and Tennyson,[12] Salvini *et al.*,[13] and latest by Gibson *et al.*[8] All the above mentioned calculations were performed at incident energies below 10 eV. More recently, Lee *et al.*[14] reported the elastic DCS by using the Schwinger variational iterative method (SVIM) combined with the distorted-wave approximation in the low and intermediate energy range.

The momentum space static-exchange-optical model has been applied to calculating the electron scattering from nonpolar diatomic molecules: H_2, N_2, and O_2,[15–19] which has shown good agreement with the experimental data. The present work is a test of electron scattering from a polar molecule system. This method is attractive from two points of view. First, differential cross sections are expressed in terms of the initial and final electron momenta so that the amplitudes involved in the calculation are directly based on experiment. Second, the electron–molecule system has a single center in the momentum space, whereas a tractable coordinate-space representation is multi-centered.[20]

In this work, we report the electronically elastic differential scattering cross sections of electron scattering from CO at 2, 3, 5, and 10 eV by using the momentum space static-exchange-optical model.

2. Model and method

A detailed description of the momentum space static-exchange-optical model for electron–molecule scattering has been given by Rossi and McCarthy.[16] Here, we briefly review the essential features of the static-exchange-optical model. The electronically elastic cross section is calculated by solving the momentum space Lippmann–Schwinger equation as

$$\langle \boldsymbol{k}'0|T|0\boldsymbol{k}\rangle = \langle \boldsymbol{k}'0|V|0\boldsymbol{k}\rangle + \sum_j \int \mathrm{d}^3q \langle \boldsymbol{k}'0|V|j\boldsymbol{q}\rangle \times \frac{1}{E^{(+)} - \varepsilon_j - q^2/2} \langle \boldsymbol{q}j|T|0\boldsymbol{k}\rangle, \quad (1)$$

where $\boldsymbol{k}$ and $\boldsymbol{k}'$ are the initial and final momenta of project electron, respectively.

We use the projection operators P and Q for the sets of states. In the present derivation only the elastic channel is incorporated.

$$P = |\phi_0\rangle\langle\phi_0|. \quad (2)$$

The remaining channels including the continuum are projected by the complementary operator Q,

$$P + Q = 1. \quad (3)$$

The bound state energy eigenvalues of ε_j include only the ground state ε_0. Then $E^{(+)} - \varepsilon_j = E_0^{(+)} = k_j^2/2$, where k_j is

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the incident electron momentum. The electronic ground state of the CO molecule is given in terms of the electronic Hamiltonian $H_{\rm T}$ as

$$(\varepsilon_0 - H_{\rm T})|0\rangle = 0. \tag{4}$$

The electron–molecule potential is V. The total energy of the electron–molecule system is E. The potential consists of direct potential $V_{\rm D}$, exchange potential $V_{\rm E}$, and optical potential W

$$V = V_{\rm D} + V_{\rm E} + W. \tag{5}$$

The coordinate-space representations of direct and exchange potentials are

$$V_{\rm D}(\boldsymbol{r}_0) = \sum_{j=1}^{N} \int {\rm d}^3 r_1 \langle \phi_j | \boldsymbol{r}_1 \rangle \frac{1}{|\boldsymbol{r}_0 - \boldsymbol{r}_1|} \langle \boldsymbol{r}_1 | \phi_j \rangle - \sum_{n=1}^{M} \frac{Z_n}{|\boldsymbol{r}_0 - \boldsymbol{R}_n|}, \tag{6}$$

and

$$V_{\rm E}(\boldsymbol{r}_0, \boldsymbol{r}_1) = -\sum_{j=1}^{N/2} \langle \phi_j | \boldsymbol{r}_1 \rangle [E_0 - \varepsilon_j - \frac{1}{|\boldsymbol{r}_0 - \boldsymbol{r}_1|}] \langle \boldsymbol{r}_0 | \phi_j \rangle. \tag{7}$$

Here E_0 is the energy of the incident electron. The Hartree–Fock orbital and the corresponding energies are ϕ_j and ε_j, respectively. The coordinate of the i-th N-electron is $\boldsymbol{r}_i$. The coordinate of the n-th M nuclei is $\boldsymbol{R}_i$ and the corresponding charge is Z_n. The sum in Eq. (4) is taken over the $N/2$ electron with the same spin projection.

To implement the calculation of the polarization matrix elements $\langle \boldsymbol{k}'0|W|0\boldsymbol{k}\rangle$, we first make the approximation of weak coupling of channels for which the target state is in the Q-space. The time-reversed state vector for scattering from entrance channel n is $|\Psi_n^{(-)}\rangle$. Here, n is a discrete notation for a one- or two-body continuum. The projection operator Q in this notation is

$$Q = \sum_n |\Psi_n^{(-)}\rangle \langle \Psi_n^{(-)}|, \tag{8}$$

and the approximation gives as

$$\langle \boldsymbol{k}'0|W|0\boldsymbol{k}\rangle = \sum_{n\in Q} \langle \boldsymbol{k}'0|V|\Psi_n^{(-)}\rangle \frac{1}{E^{(+)} - E_n} \langle \Psi_n^{(-)}|V|0\boldsymbol{k}\rangle. \tag{9}$$

Note that equation (9) contains exact amplitudes for the excitation of channel n from the entrance channel. We proceed by making the Born approximation for these amplitudes. This high-energy approximation has been proved to be excellent for optical-potential matrix elements in electron–atom scattering.[21]

The localized and spherically averaged optical potential is

$$W(k,P) = \Big[\int {\rm d}^3 q \frac{\Gamma(k,P,q) - \Gamma(k,P,k_{\rm C})}{(k_{\rm C}^2 - q^2)/2}\Big] - {\rm i}\pi k_{\rm C} \int {\rm d}\hat{q} \Gamma(k,P,k_{\rm C}), \tag{10}$$

where

$$\Gamma(k,P,q) = \frac{\ln(K^2+P^2+2KP) - \ln(K^2+P^2-2KP)}{16\pi^4 K^3 P} \times \Big[\bar{\Xi}(P) - (4\pi)^{-1} \bar{\Xi}(K) \int {\rm d}\hat{P} \bar{\Xi}(|K-P|)\Big]. \tag{11}$$

Details of the expansion of the optical potential have been given by Rossi and McCarthy.[16]

For target molecules in the gas phase, we assume random initial orientations and treat rotational excitation as an adiabatic process. This is equivalent to averaging the DCS over molecular orientations. Following the work of Gallup,[22] we transform our entrance and exit channel momenta $\boldsymbol{k}_0$ and $\boldsymbol{k}_i$, which are expressed in the body-fixed frame, into momenta $\boldsymbol{p}_0$ and $\boldsymbol{p}_i$ in the space-fixed (laboratory) frame. The transformation is affected by the rotation matrices,

$$\langle \boldsymbol{p}_i 0|V|0\boldsymbol{p}_0\rangle = \sum_{LML'M'\mu\mu'} \langle k_I L'M' \| T \| k_0 LM\rangle D^L_{M\mu} D^{L'*}_{M'\mu'} Y_{L\mu}(\hat{\boldsymbol{p}}_0) Y^*_{L'\mu'}(\hat{\boldsymbol{p}}_i). \tag{12}$$

We choose the positive $\hat{z}$ axis to be $\hat{\boldsymbol{p}}_0$.

The DCS is

$$\frac{{\rm d}\sigma_{i0}}{{\rm d}\Omega} = 4\pi^3 \sum_{L_1M_1L'_1M'_1\mu'_1} \sum_{L_2M_2L'_2M'_2\mu'_2} \Big\{ \sqrt{(2L_1+1)(2L_2+1)} T_{L_1M_1L'_1M'_1} T_{L_2M_2L'_2M'_2} \delta_{\mu'_1\mu'_2} \delta_{M_1+M'_2M'_1+M_2} \times \sum_J \frac{1}{2J+1} C^{M_1M'_2M_1+M'_2}_{L_1L'_2J} C^{M'_1M_2M'_1+M_2}_{L'_1L_2J} C^{0\mu'_2\mu'_2}_{L_1L'_2J} C^{\mu'_1 0\mu'_1}_{L'_1L_2J} Y^*_{L'_1\mu'_1}(\hat{\boldsymbol{p}}_i) Y_{L'_2\mu'_2}(\hat{\boldsymbol{p}}_0) \Big\}. \tag{13}$$

The integrated cross section for exit channel i is obtained by integrating the expression over $\hat{\boldsymbol{p}}_i$,

$$\sigma_{i0} = 4\pi^3 \sum_{L_1M_1L_2M_2M'_1M'_2L} \Big\{ T_{L_1M_1LM'_1} T_{L_2M_2LM'_2} \sum_{\mu J} \frac{1}{2J+1} C^{M_1M'_2M_1+M'_2}_{L_1LJ} C^{M'_1M_2M'_1+M_2}_{LL_2J} C^{0\mu\mu}_{LL_2J} C^{\mu 0\mu}_{LL_2J} \Big\}. \tag{14}$$

3. Results and discussion

Coupling between partial waves is observed to become negligible beyond $L = 10$ for a carbon monoxide molecule. Selection rules are responsible for the fact that off-diagonal V-matrix elements with odd partial-wave quantum number L or L' and M or $M' \neq 0$ are zero. On-diagonal matrix elements are included up to $L = 20$. The real part of the optical potential is found to display the asymptotic behavior typical of an induced

dipole potential, namely

$$V(r) = -\frac{\alpha_0}{2r^4}. \quad (15)$$

where α_0 is the dipole polarizability for the CO molecule.

The DCS for elastic scattering from CO at 2, 3, 5, and 10 eV are presented in Figs. 1–4 along with the measured values of Tanaka *et al.*,[3] Gibson *et al.*[8] and Allan,[9] as well as the theoretical results of Jain and Norcross[10] using an ESEP model, Gibson *et al.*[8] using RM method and Lee *et al.*[14] using SVIM combined with the distorted-wave approximation method.

We compare the present results of DCS at 2 eV with measurements and other theoretical results in Fig. 1. Exceptionally good agreement with experimental data can be find. Our SEO curve lies almost consistently within the error bars of the measurements of Gibson *et al.*[8] (at an energy of 1.91 eV). Agreement within the experimental error of Allan[9]'s data is comprehensive over the full angular range. We see disagreement among these curves obtained with different theoretical models. The results of RM[8] (at 1.91 eV) are slightly higher than the experimental data at forward scattering angles, and the results of ESEP [10] (at 2.1 eV) are higher than the measurements at both forward and backward angles. We attribute the discrepancies among these theoretical results to the different descriptions of the target polarization.

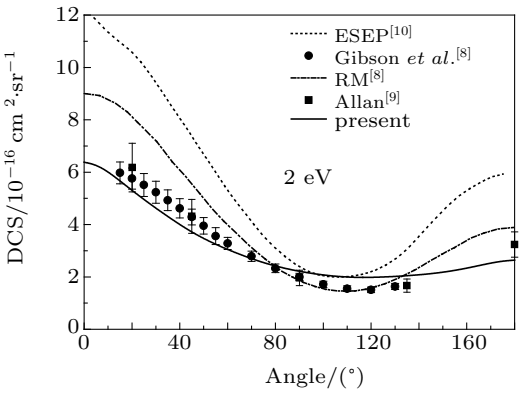


Fig. 1. CO elastic DCS at the incident energy of 2 eV. Theoretical work: full curve, SEO; dot, ESEP;[10] dash dot, RM.[8] Experimental: bullet, Gibson *et al.*; [8] black square, Allan.[9]

Disagreement among these curves obtained with different theoretical models at incident energy of 3 eV can be seen in Fig. 2. At forward scattering angles, the experimental and theoretical results do not all agree with each other. Our curve underestimates the experimental data of Gibson *et al.*[8] as much as 30% at forward angles. For intermediate angles, the RM[8] curve lies within the error bars of Tanaka *et al.*,[3] while ESEP [10] agrees with the experimental data of Gibson *et al.*[8] For backward scattering, agreement between the theoretical results is qualitatively good. The angular isotropy of our curve is probably due to the lack of anisotropic polarization effects.

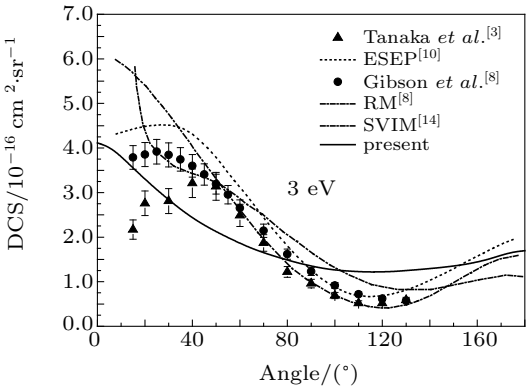


Fig. 2. CO elastic DCS at the incident energy of 3 eV. Theoretical work: full curve, SEO; dot, ESEP;[10] dash dot, RM;[8] dash dot dot, SVIM.[14] Experimental: black triangle, Tanaka *et al.*;[3] bullet, Gibson *et al.*.[8]

Comparison of our DCS with other experimental and theoretical results for 5 eV is presented in Fig. 3. Discrepancy exists among these results at forward angles. For forward scattering, ESEP [10] and SVIM[14] overestimate the experimental data, while RM[8] agrees well with the measurements. Note that our curve lies below all the other results for angles from 30° to 70°, which is probably due to omitting the rotational excitation. The agreement is excellent for backward scattering within the error bars of Tanaka *et al.*[3] and Allan,[8] and other theoretical results.

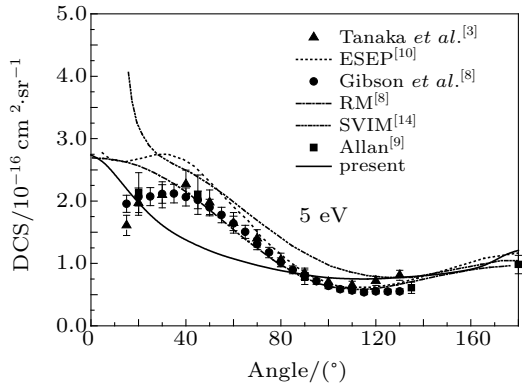


Fig. 3. CO elastic DCS at the incident energy 5 eV. Theoretical work: full curve, SEO; dot, ESEP;[10] dash dot, RM;[8] dash dot dot, SVIM.[14] Experimental: black triangle, Tanaka *et al.*;[3] bullet, Gibson *et al.*;[8] black square, Allan.[9]

At an energy of 10 eV (Fig. 4) all the calculated and measured data agree quite well with each other. Our curve underestimates the experimental error of Tanaka *et al.*[3] and Gibson *et al.*[8] (at 9.9 eV) for angles from 40° to 50°. At backward scattering angles, agreement with the results of Gibson *et al.*[8] and Allan[9] is excellent. At this incident energy, the present result and ESEP [10] result present larger cross sections than experimental data in the forward direction. At this incident energy 7 electronic state channels are open, the RM[8] approach produces different results (at 9.9 eV), because the absorption effect of excitation target states is considered, which is neglected in the ESEP [10] and present calculation results.

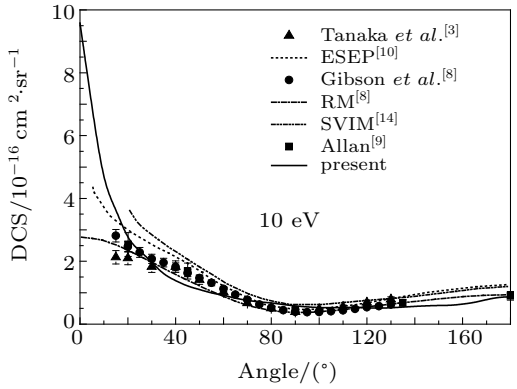


Fig. 4. CO elastic DCS at the incident energy of 10 eV. Theoretical work: full curve, SEO; dot, ESEP;[10] dash dot, RM;[8] dash dot dot, SVIM.[14] Experimental: black triangle, Tanaka *et al.*;[3] bullet, Gibson *et al.*;[8] black square, Allan.[9]

In general, we produced a more angularly isotropic curve than rotationally summed DCS. At backward scattering angles, the present results are in good agreement with experimental and other theoretical results. For forward scattering, our results underestimate the experimental values and other theoretical calculations, probably due to omitting the rotational excitation in the polar molecule system. For the polar molecule, the rotational-excitation cross sections are enhanced and tend to dominate all forward scattering at low energies.[23] In future work rotational excitation will be incorporated to calculate the DCS.

4. Conclusions

In summary, we reported a theoretical investigation on the electron scattering by CO in the low energy range. The momentum space static-exchange-optical model is used to solve the scattering equations, while an *ab initio* optical potential is used to represent the interaction dynamics. The present results are similar in shape and magnitude to results of experimental and other theoretical work. Some discrepancies exist and this may be due to omitting rotational excitation. Our intention is to further develop this method taking into account rotational excitation and anisotropic polarization potential. We expect this will lead to a better agreement with experimental results.

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