

## Elastic and absorption cross sections for electron–nitric oxide collisions

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**Abstract.** In this paper, we report a theoretical study on electron scattering by an open-shell molecule in the low and intermediate energy range. More specifically, calculated elastic differential, integral and momentum transfer cross sections as well as absorption (excitation + ionization) cross sections in the 5–500 eV range are reported for  $e^-$ –NO collisions. In our calculation, a complex optical potential consisting of static, exchange, correlation–polarization plus absorption contributions, derived from a fully molecular wavefunction, is used to describe the electron–molecule interaction. The Schwinger variational iterative method combined with the distorted-wave approximation is applied to calculate scattering amplitudes. Comparison between calculated results and existing experimental and theoretical data is encouraging.

### 1. Introduction

Low-energy electron scattering by small molecules remains a considerable challenge to theorists. For instance, electron elastic scattering on several diatomic molecules at incident energies below 10 eV has shown some unusual small-angle behaviour. A local maximum located at around  $50^\circ$ – $60^\circ$  is seen in the measured differential cross sections (DCS) of  $N_2$  (Sun *et al* 1995),  $O_2$  (Sullivan *et al* 1995), CO (Tanaka *et al* 1978) and NO (Kubo *et al* 1981, Mojarrabi *et al* 1995). Such angular behaviour cannot be reproduced by calculations using approximations at the static-exchange level which may indicate an important role played by polarization–correlation effects on the collisional dynamics in this energy range. Specifically for open-shell molecules such as NO and  $O_2$ , these effects are particularly important due to the presence of low-lying electronically excited states (Tennyson and Noble 1986). In these cases, an investigation on the small-angle scattering behaviour would be very interesting. As the elastic electron– $O_2$  scattering study has been recently reported (Machado *et al* 1999), in this paper, we focus our interest on electron–NO interaction in the low and intermediate energy range.

Despite the important role played by NO in the catalytic destruction of ozone in the atmosphere (Mason and Newell 1989, Kirby 1993), electron scattering by NO has attracted relatively less attention during past decades. The various experimental investigations on electron scattering by NO were reviewed by Mojarrabi *et al* (1995). In particular, absolute elastic electron DCS for this molecule have only been reported by Kubo *et al* (1981) and more recently by Mojarrabi *et al* (1995) for incident energies up to 40 eV. Above this energy, no experimental DCS are reported in the literature. On the theoretical side, the literature is equally scarce. To our knowledge, only the Born-closure Schwinger variational method

(BCSVM) (Lee *et al* 1992), the optical model approach (OMA) of Jain *et al* (1995) and the Schwinger multichannel method (SMC) of da Paixão *et al* (1996) are reported in the literature. The calculations of BCSVM and SMC were performed at the static-exchange level of approximation. Although the OMA has included polarization and absorption contributions in the interaction potential, only the spherical part ( $l = 0$ ) of these contributions was accounted for in their calculation. None of the calculations cited above were capable of reproducing the small angular behaviour in the 3–10 eV energy range.

Recently, Machado *et al* (1999) reported a theoretical investigation on elastic electron scattering by  $O_2$  in the 5–300 eV energy range. In that study, a complex optical potential including the static-exchange-polarization plus absorption contributions was applied in the calculations of DCS and integral cross sections (ICS). In general, the calculated results in that study are in good agreement when compared with available experimental data. Moreover, the authors have shown that the low-energy angular behaviour of the DCS can be well described by the introduction of a polarization–correlation potential.

In this paper, a complex optical potential is applied to study electron scattering by NO. More specifically, calculated elastic DCS, ICS, momentum transfer cross sections (MTCS) and absorption cross sections (ACS) for electron–NO collision in the 5–500 eV energy range are reported. A combination of the Schwinger variational iterative method (SVIM) (Lucchese *et al* 1982) and the distorted-wave approximation (DWA) (Fliflet and McKoy 1980, Lee and McKoy 1983) is used to solve the scattering equations. We expect that the comparison between the calculated and experimental results would reveal interesting insights on the collisional dynamics, particularly for the interaction of low-energy electrons with open-shell molecules.

The organization of this paper is the following: in section 2, we describe briefly the theory used and also some details of the calculation. In section 3 we compare our calculated results with the experimental and theoretical data available in the literature.

## 2. Theory and calculation

Since the details of the SVIM (Lucchese *et al* 1982) and the DWA (Fliflet and McKoy 1980, Lee and McKoy 1983, Lee *et al* 1993) have already been presented in previous papers, here we only outline briefly the theory used. Within the fixed-nuclear framework, the electron–molecule scattering dynamics is represented by a complex optical potential, given by

$$V_{\text{opt}}(\vec{r}) = V^{\text{SEP}}(\vec{r}) + iV_{\text{ab}}(\vec{r}) \quad (1)$$

where  $V^{\text{SEP}}$  is the real part of the interaction potential formed by the static, the exchange and the correlation–polarization contributions, whereas  $V_{\text{ab}}$  is the absorption potential. In our calculation,  $V_{\text{st}}$  and  $V_{\text{ex}}$  are derived exactly from an unrestricted Hartree–Fock SCF target wavefunction. A parameter-free model potential introduced by Padial and Norcross (1984) is used to account for the correlation–polarization contributions. In this model, a short-range correlation potential between the scattering and target electrons is defined in an inner interaction region and a long-range polarization potential in an outer region. The correlation potential is calculated by a free-electron-gas (FEG) model derived using the target electronic density according to equation (9) of Padial and Norcross (1984). In addition, an asymptotic form of the polarization potential is used for the long-range electron–target interactions. The dipole polarizabilities  $\alpha_0 = 11.74$  and  $\alpha_2 = 3.78$  au (Hirschfelder *et al* 1954) were used to calculate the asymptotic form of  $V_{\text{cp}}$ . The first crossing of the correlation and polarization potential curves defines the inner and outer regions. No cut-off or other adjusted parameters are needed in the calculation of  $V_{\text{cp}}$ .

Although the main features of the absorption effects are known, taking these effects into account in an *ab initio* treatment of electron-molecule scattering is very difficult. For instance, close-coupling calculations would require all discrete and continuum open channels to be included in the open-channel  $P$ -space, which is computationally unfeasible. In view of the difficulties, the use of the model absorption potential seems to be presently the only practical manner to account for absorption effects into electron-molecule scattering calculations. In this paper, a modified version of the quasifree scattering model version 3 of Staszewska *et al* (1984) is used to represent the absorption effects. The absorption potential  $V_{\text{ab}}$  in equation (1) is given by

$$V_{\text{ab}}(\vec{r}) = -\rho(\vec{r})(T_L/2)^{1/2}(8\pi/5k^2k_F^3)H(\alpha + \beta - k_F^2)(A + B + C), \quad (2)$$

where

$$T_L = k^2 - V^{\text{SEP}}, \quad (3)$$

$$A = 5k_F^3/(\alpha - k_F^2), \quad (4)$$

$$B = -k_F^3(5(k^2 - \beta) + 2k_F^2)/(k^2 - \beta)^2, \quad (5)$$

and

$$C = 2H(\alpha + \beta - k^2) \frac{(\alpha + \beta - k^2)^{5/2}}{(k^2 - \beta)^2}. \quad (6)$$

In equations (2)–(6),  $k^2$  is the energy (in Ryd) of the incident electron,  $k_F$  the Fermi momentum and  $\rho(\vec{r})$  the local electronic density of the target.  $H(x)$  is a Heaviside function defined by  $H(x) = 1$  for  $x \geq 0$  and  $H(x) = 0$  for  $x < 0$ . According to the quasifree-scattering model version 3 of Staszewska *et al* (1984),

$$\alpha(\vec{r}, E) = k_F^2 + 2(2\Delta - I) - V^{\text{SEP}}, \quad (7)$$

and

$$\beta(\vec{r}, E) = k_F^2 + 2(I - \Delta) - V^{\text{SEP}}, \quad (8)$$

where  $\Delta$  is the average excitation energy and  $I$  is the ionization potential. The calculation of both the model potentials  $V_{\text{cp}}$  and  $V_{\text{ab}}$  depends only on the target electronic density and some molecular properties such as ionization potential, dipole polarizability, etc. Thus, even for an open-shell molecule such as NO, these potentials are spin independent.

Further, the Lippmann-Schwinger scattering equation for the elastic electron-NO collision is solved using the SVIM with the real part of the optical potential. In the SVIM calculations, the continuum wavefunctions are single-centre expanded as

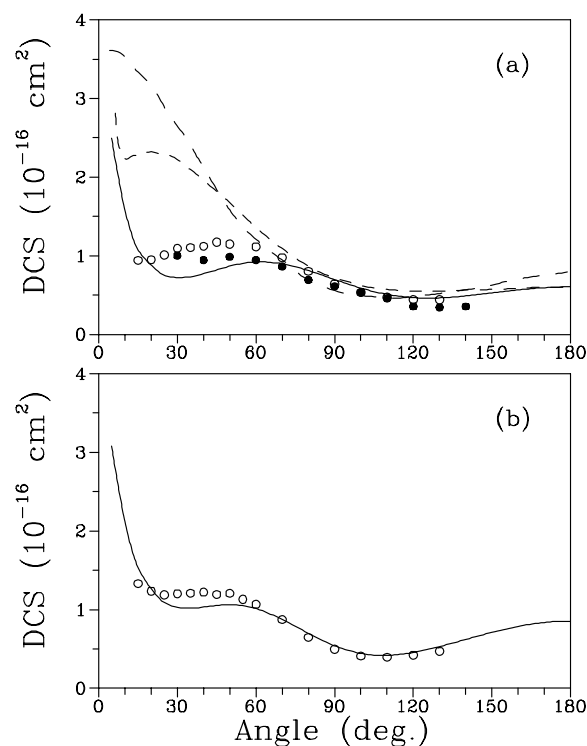
$$\chi_{\vec{k}}^{\pm}(\vec{r}) = (2/\pi)^{1/2} \sum_{lm} \frac{(i)^l}{k} \chi_{klm}^{\pm}(\vec{r}) Y_{lm}(\hat{k}), \quad (9)$$

where the superscripts (+) and (−) denote the incoming- and outgoing-wave boundary conditions, respectively, and  $Y_{lm}(\hat{k})$  are the usual spherical harmonics. The absorption part of the  $T$  matrix is calculated via the DWA as

$$T_{\text{abs}} = i\langle \chi_f^- | V_{\text{ab}} | \chi_i^+ \rangle. \quad (10)$$

Since NO is an open-shell molecule with the ground-state configuration  $X^2\Pi^-$ , two spin-specific scattering channels, the singlet and triplet couplings between the scattering electron and the isolated  $2\pi$  electron of the target are considered in this paper. Therefore the statistical average of the elastic scattering DCS is written as

$$\frac{d\sigma}{d\Omega} = \frac{1}{4} \left[ 3 \left( \frac{d\sigma}{d\Omega} \right)^1 + \left( \frac{d\sigma}{d\Omega} \right)^0 \right] \quad (11)$$

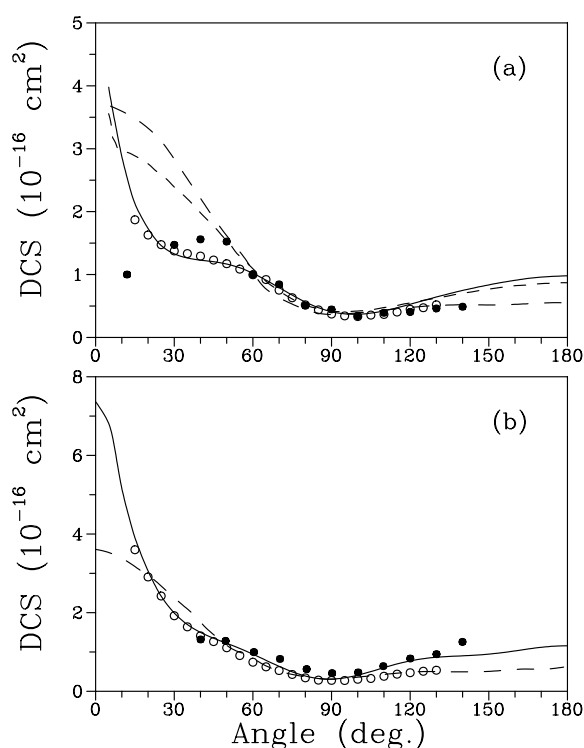


**Figure 1.** DCS for elastic electron-NO scattering at (a) 5 eV, (b) 7.5 eV. Solid curve, present calculated results; dashed curve, the calculated results of Lee *et al* (1992) using the static-exchange approximation; long-dashed curve, calculated results of da Paixão *et al* (1996); open circles, experimental data of Mojarrabi *et al* (1995); full circles, measured data of Kubo *et al* (1981).

where  $(d\sigma/d\Omega)^1$  and  $(d\sigma/d\Omega)^0$  are the multiplet-specific DCS averaged over molecular orientations for the total ( $e^- + \text{NO}$ ) spin  $S = 1$  (triplet) and 0 (singlet) couplings, respectively.

In this paper, a standard [9s5p/3s2p] basis set (Dunning and Hay 1977) augmented by three s ( $\alpha = 0.028, 0.012$  and  $0.005$ ), two p ( $\alpha = 0.027$  and  $0.008$ ), and one d ( $\alpha = 0.8$ ) uncontracted functions for the nitrogen atom and three s ( $\alpha = 0.032, 0.015$  and  $0.007$ ), two p ( $\alpha = 0.032$  and  $0.01$ ), and one d ( $\alpha = 0.85$ ) for the oxygen atom is used for the calculation of the SCF wavefunction of the target. With this basis set, the calculated UHF SCF energy and dipole moment, at the experimental equilibrium geometry of the NO ground-state of 2.1747 au, are  $-129.15017$  and  $0.0745$  au, respectively, compared with the near-Hartree-Fock values of  $-129.2953$  and  $0.260$  au (Green 1972) and with the experimental dipole moment of  $0.066$  au (Huber and Herzberg 1979).

In this paper, we have limited the partial-wave expansion for the continuum wavefunctions as well as for the  $T$ -matrix elements up to  $l_{\text{max}} = 30$  and  $m_{\text{max}} = 17$  for incident energies up to 150 eV. Above that energy,  $l_{\text{max}} = 35$  and  $m_{\text{max}} = 30$  were used. Considering the small dipole moment of NO, no further corrections were carried out to account for higher partial-wave contributions. In addition, it is well known that a fixed-nuclei (FN) treatment of electron scattering by polar molecules would lead to divergent DCS in the forward direction if all the partial-wave contributions are included. Consequently, the calculated ICS would also diverge at all incident energies. Nevertheless, as pointed out by Winstead and McKoy (1998), this

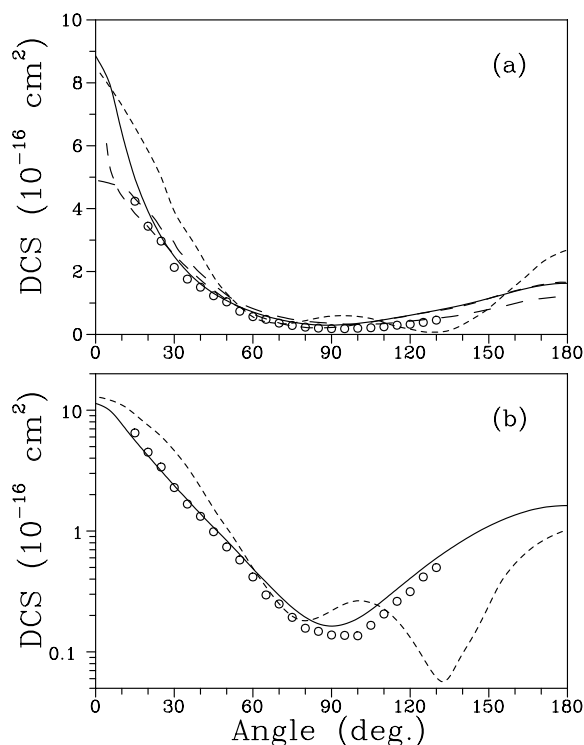


**Figure 2.** DCS for elastic electron-NO scattering at (a) 10 eV (b) 15 eV. Solid curve, present calculated results; dashed curve, the calculated results of Lee *et al* (1992) using the static-exchange approximation; long-dashed curve, calculated results of da Paixão *et al* (1996); open circles, experimental data of Mojarrabi *et al* (1995); full circles, measured data of Kubo *et al* (1981).

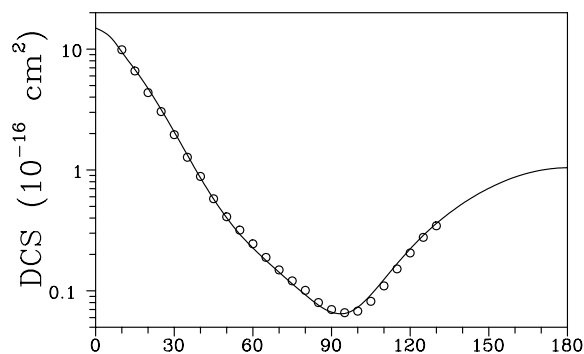
divergent behaviour of ICS is unphysical since the rotation of the molecule during the collision weakens the effective interaction field. Thus, although this divergence can be removed by the introduction of the nuclear motion in the Hamiltonian, the use of a FN approximation with sufficient partial waves can still provide accurate DCS away from the forward direction. The truncation parameters used in this paper have ensured the convergence of DCS from  $5^\circ$  to be better than 2%. The ICS and MTCS obtained directly via appropriate integration over scattering angles are also meaningful. Such approximations have also been applied for low-energy electron scattering by other polar molecules (Winstead and McKoy 1998, Sarpal *et al* 1996, Morgan *et al* 1997). Finally, the total cross sections (TCS) for electron-molecule scattering are obtained with the truncated  $T$ -matrix elements using the optical theorem. The ACS are calculated by the difference between the TCS and elastic ICS.

### 3. Results and discussion

In figures 1–4 we show our calculated DCS for elastic electron-NO scattering in the 5–40 eV energy range along with the available experimental data of Kubo *et al* (1981) and Mojarrabi *et al* (1995). The previous calculated BCSVM DCS using the static-exchange potential (Lee *et al* 1992) along with the calculated results of da Paixão *et al* (1996) and of Jain *et al* (1995) are also shown for comparison. At incident energies below 10 eV, our calculation reproduces successfully the local maximum at scattering angles around  $50^\circ$ – $60^\circ$ . Since this feature was



**Figure 3.** DCS for elastic electron–NO scattering at (a) 20 eV (b) 30 eV. Solid curve, present calculated results; dashed curve, the calculated results of Lee *et al* (1992) using the static-exchange approximation; short-dashed curve, calculated results of Jain *et al* (1995); open circles, experimental data of Mojarabi *et al* (1995).



**Figure 4.** DCS for elastic electron–NO scattering at 40 eV. Solid curve, present calculated results; open circles, experimental data of Mojarabi *et al* (1995).

not seen in the previous calculated DCS using the static-exchange approximation (Lee *et al* 1992, da Paixão *et al* 1996), we conclude that a combination of accurate short- and long-range interaction potentials is essential to describe the low-energy electron–NO collisional dynamics. On the other hand, the calculated DCS of Jain *et al* (1995) show a double-minimum feature, in disagreement with all calculated and experimental data. Quantitatively, the agreement between

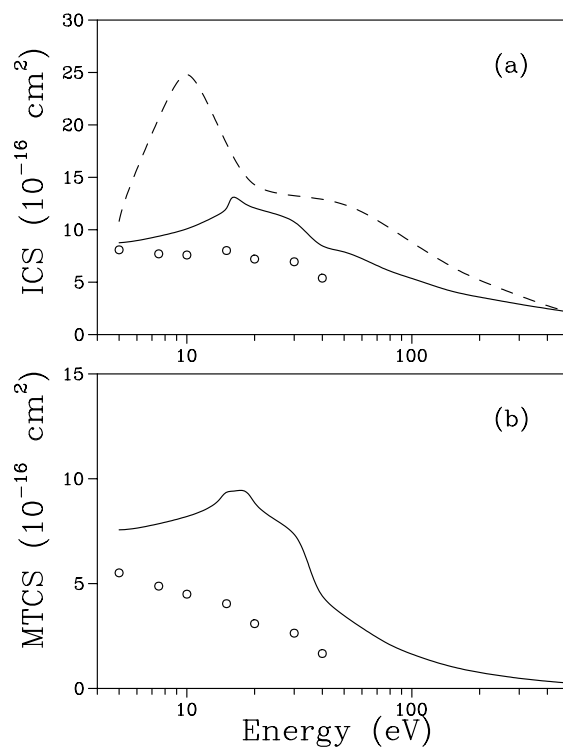
**Table 1.** Calculated DCS, ICS and MTCS (in  $10^{-16}$  cm<sup>2</sup>) for  $e^-$ -NO scattering.

Angle (deg)	Energy (eV)					
	50	75	100	150	300	500
0	0.171(2) <sup>a</sup>	0.192(2)	0.205(2)	0.213(2)	0.246(2)	0.264(2)
5	0.145(2)	0.157(2)	0.162(2)	0.160(2)	0.159(2)	0.146(2)
10	0.103(2)	0.104(2)	0.102(2)	0.895(1)	0.679(1)	0.484(1)
15	0.726(1)	0.671(1)	0.614(1)	0.474(1)	0.276(1)	0.160(1)
20	0.486(1)	0.402(1)	0.338(1)	0.227(1)	0.107(1)	0.679(0)
25	0.310(1)	0.226(1)	0.172(1)	0.105(1)	0.518(0)	0.415(0)
30	0.191(1)	0.122(1)	0.855(0)	0.501(0)	0.322(0)	0.277(0)
35	0.115(1)	0.655(0)	0.440(0)	0.278(0)	0.226(0)	0.184(0)
40	0.694(0)	0.365(0)	0.249(0)	0.176(0)	0.169(0)	0.119(0)
45	0.439(0)	0.228(0)	0.166(0)	0.130(0)	0.129(0)	0.791(−1)
50	0.293(0)	0.157(0)	0.123(0)	0.103(0)	0.967(−1)	0.597(−1)
60	0.164(0)	0.963(−1)	0.847(−1)	0.804(−1)	0.569(−1)	0.447(−1)
70	0.110(0)	0.723(−1)	0.740(−1)	0.662(−1)	0.438(−1)	0.304(−1)
80	0.784(−1)	0.628(−1)	0.704(−1)	0.524(−1)	0.399(−1)	0.204(−1)
90	0.609(−1)	0.605(−1)	0.657(−1)	0.457(−1)	0.346(−1)	0.168(−1)
100	0.685(−1)	0.688(−1)	0.638(−1)	0.476(−1)	0.288(−1)	0.145(−1)
110	0.113(0)	0.939(−1)	0.713(−1)	0.560(−1)	0.257(−1)	0.119(−1)
120	0.192(0)	0.136(0)	0.911(−1)	0.682(−1)	0.252(−1)	0.101(−1)
130	0.296(0)	0.186(0)	0.121(0)	0.812(−1)	0.256(−1)	0.947(−2)
140	0.409(0)	0.240(0)	0.158(0)	0.920(−1)	0.257(−1)	0.917(−2)
150	0.520(0)	0.295(0)	0.199(0)	0.998(−1)	0.253(−1)	0.892(−2)
160	0.619(0)	0.348(0)	0.240(0)	0.106(0)	0.247(−1)	0.858(−2)
170	0.691(0)	0.388(0)	0.273(0)	0.113(0)	0.251(−1)	0.853(−2)
180	0.719(0)	0.403(0)	0.288(0)	0.117(0)	0.258(−1)	0.861(−2)
ICS	0.788(1)	0.615(1)	0.536(1)	0.414(1)	0.290(1)	0.216(1)
MTCS	0.347(1)	0.213(1)	0.163(1)	0.103(1)	0.485(0)	0.258(0)

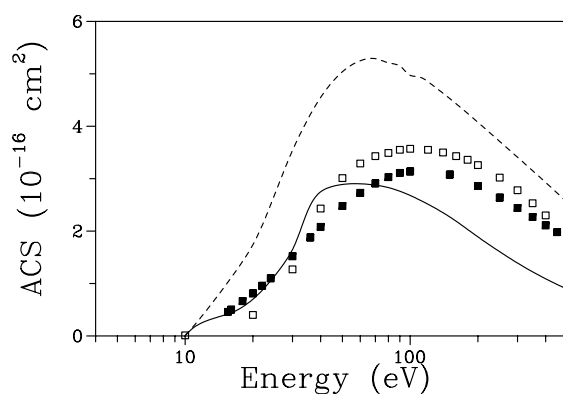
<sup>a</sup> (*n*) means  $\times 10^n$ .

our calculated results and experimental data is also good. In the 10–40 eV range, our calculated results are in excellent agreement with the measured data, particularly with those of Mojarrabi *et al* (1995), both qualitatively and quantitatively. On the other hand, the calculated results of Lee *et al* (1992) and da Paixão *et al* (1996) strongly overestimate the DCS for scattering angles below 60° at 5 and 10 eV. These discrepancies reflect the importance of the correlation–polarization effects at low incident energies, not accounted for in those calculations. At 20 eV, the agreement between the present results and those of static-exchange-level calculations is good. Unfortunately, there is no experimental DCS reported in the literature for incident energies above 40 eV for comparison. Therefore, our calculated DCS in the 50–500 eV range are also not shown in the figures. However, they are presented in table 1, along with the calculated ICS and MTCS. We expect these results to be useful for further theoretical and experimental investigations on electron–NO scattering in the intermediate energy range.

In figure 5 we compare our calculated ICS and MTCS in the 5–500 eV range with the experimental data of Mojarrabi *et al* (1995) and the calculated ICS of Jain *et al* (1995) using the OMA. Considering the excellent agreement between the calculated and measured DCS seen in figures 1–4, it is quite surprising that the experimental ICS and MTCS of Mojarrabi *et al* lie well below our calculated data. We suspect that the discrepancies are probably due to the extrapolation procedure adopted by these authors. In order to understand these differences, we performed numerical integrations using their published DCS in the 5–40 eV energy range



**Figure 5.** (a) ICS and (b) MTCS for elastic electron-NO collisions. Solid curve, present calculated results; dashed curve, the OMA results of Jain *et al* (1995); open circles, experimental data of Mojarrabi *et al* (1995).



**Figure 6.** ACS for electron-NO collisions. Solid curve, present calculated results; dashed curve, the OMA results of Jain *et al* (1995); open squares, measured data of Iga *et al* (1996); full squares, measured data of Rapp and Englander-Golden (1965).

to estimate ICS and MTCS. These integrals were carried out only over the angular range covered in their experiments and no extrapolation in the forward and backward directions was performed. The ICS and MTCS obtained through this procedure agree with their published data to within 2%. So, although the authors have stated the use of the extrapolation procedure



in their work, the published ICS and MTCS were in fact obtained without the contributions of the DCS beyond the scattering angles covered in their measurement. On the other hand, the calculated ICS of Jain *et al* (1995) lie systematically above our results. At the lower incident energies, their calculation overestimates strongly the cross sections which indicates clearly that the use of a spherical potential is inadequate for electron-NO collisions. The agreement between the calculated results improves with increasing incident energies.

Figure 6 shows our calculated ACS in the 5–500 eV energy range along with some available measured data on the electron-impact ionization cross section (Rapp and Englander-Golden 1965, Iga *et al* 1996) and with the calculated ACS of Jain *et al* (1995). Our calculated ACS are in good agreement with the measured data (Rapp and Englander-Golden 1965, Iga *et al* 1996) for incident energies below 100 eV. At higher energies our calculation underestimates the ACS. Again, the calculated ACS of Jain *et al* (1995) lie systematically and substantially above our results.

In summary, we have presented a theoretical study on electron scattering by NO molecules in the low and intermediate energy range. A complex optical potential has been used to represent the collisional dynamics. The calculated results are very encouraging considering the simplicity of the model potential used in this paper. Our calculated DCS are in general good agreement with the experimental results available in the literature. In particular, our study clearly shows that an appropriate combination of short- and long-range potentials is responsible for the local maximum seen in the DCS at around  $50^\circ$ – $60^\circ$  for incident energies below 10 eV. In addition, although our calculation underestimates the ACS at higher incident energies, the agreement with experiments is good below 100 eV. The successful application of a complex optical model potential to electron scattering by an open-shell molecule is particularly meaningful because it opens the possibility for estimation of reliable cross sections for electron-radical scattering. These cross sections are important in many fields of application but difficult to measure experimentally. Efforts in this direction are underway.

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## References

- da Paixão F J, Lima M A P and McKoy V 1996 *Phys. Rev. A* **53** 1400
- Dunning T H Jr and Hay J P 1977 *Modern Theoretical Chemistry* vol 3 (New York: Plenum) p 1
- Fliflet A W and McKoy V 1980 *Phys. Rev. A* **21** 1863
- Green S 1972 *Chem. Phys. Lett.* **13** 552
- Hirschfelder J O, Curtis C F and Bird R B 1954 *Molecular Theory of Gases and Liquids* (New York: Wiley)
- Huber K and Herzberg G 1979 *Constants of Diatomic Molecules* (New York: Van Nostrand-Reinhold)
- Iga I, Rao M V V S and Srivastava S K 1996 *J. Geophys. Res. (Planets)* **101** 9261
- Jain A K, Kumar P and Tripathi A N 1995 *PRAMANA J. Phys.* **44** 555
- Kirby K P 1993 *The Physics of Electronic and Atomic Collisions* (New York: AIP) pp 48–58
- Kubo M, Matsunaga D, Suzuki T and Tanaka H 1981 *At. Coll. Res. Japan* **7** 4
- Lee M-T, Fujimoto M M, Michelin S E, Machado L E and Bescansin L M 1992 *J. Phys. B: At. Mol. Opt. Phys.* **25** L505
- Lee M-T and McKoy V 1983 *Phys. Rev. A* **28** 697
- Lee M-T, Michelin S E, Machado L E and Bescansin L M 1993 *J. Phys. B: At. Mol. Opt. Phys.* **23** 4331
- Lucchese R R, Raseev G and McKoy V 1982 *Phys. Rev. A* **25** 2572
- Machado L E, Ribeiro E M S, Lee M-T, Fujimoto M M and Bescansin L M 1999 *Phys. Rev. A* **60** 1199
- Mason N J and Newell W R 1989 *J. Phys. B: At. Mol. Opt. Phys.* **22** 2297

- Mojarrabi B, Gulley R J, Middleton A G, Cartwright D C, Teubner P J O, Buckman S J and Brunger M J 1995 *J. Phys. B: At. Mol. Opt. Phys.* **28** 487
- Morgan L A, Gillan C J, Tennyson J and Chen X 1997 *J. Phys. B: At. Mol. Opt. Phys.* **30** 4087
- Padial N T and Norcross D W 1984 *Phys. Rev. A* **29** 1742
- Rapp D and Englander-Golden D 1965 *J. Chem. Phys.* **43** 1480
- Sarpal B K, Pfingst K, Nestmann B M and Peyerimhoff S D 1996 *J. Phys. B: At. Mol. Opt. Phys.* **29** 857
- Staszewska G, Schwenke D W and Truhlar D G 1984 *Phys. Rev. A* **29** 3078
- Sullivan J P, Gibson J G, Gulley R J and Buckman S J 1995 *J. Phys. B: At. Mol. Opt. Phys.* **28** 4319
- Sun W G, Morrison M A, Isaacs W A, Trail W K, Alle D T, Gulley R J, Brennan M J and Buckman S J 1995 *Phys. Rev. A* **52** 1229
- Tanaka H, Srivastava S K and Chutjian A 1978 *J. Chem. Phys.* **69** 5329
- Tennyson J and Noble C J 1986 *J. Phys. B: At. Mol. Phys.* **19** 4025
- Winstead C and McKoy V 1998 *Phys. Rev. A* **57** 3589