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Differential and integral cross sections for electron collisional excitation of ^3P–^1D and ^3P–^1S transitions in atomic oxygen

S S Tayal†

Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803-4001, USA

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Abstract. Differential and integral cross sections for excitation of the ^3P-^1D and ^3P-^1S transitions by electron impact in atomic oxygen are presented in the energy region from 4 to 30 eV and these are compared, where available, with other calculations and experiments. The R-matrix method is used in the three-state ($2p^4\,^3P$, ^1D and ^1S) and six-state ($2p^4\,^3P$, ^1D, ^1S, $^3\bar{S}^o$, $^3\bar{P}^o$ and $^3\bar{D}^o$) levels of the close-coupling approximation. The present results for the ^3P-^1D transition are in good agreement with the measurement of Shyn and Sharp, but normally discrepancies exist with the experiment of Doering and Gulcicek at low energies ($E \lesssim 20$ eV). The calculated integral cross sections for the ^3P-^1S transition are generally smaller than the available experiments.

1. Introduction

Electron impact excitation of the $2p^4\,^1D$ and ^1S states of atomic oxygen gives rise to emission features at 6300 and 2959 Å in the spectra of the atmospheres of Earth, Mars and Venus. Accurate knowledge of excitation cross sections for the $2p^4\,^3P$-^1D and $2p^4\,^3P$-^1S transitions is needed in the study of Earth's upper atmosphere. Shyn and Sharp (1986) and Shyn *et al* (1986) measured electron impact excitation absolute differential cross sections of atomic oxygen for the ^3P-^1D and ^3P-^1S transitions, respectively, using a crossed-beam technique. Recently, Doering and Gulcicek (1989) also reported low-energy absolute differential and integral electron excitation cross sections for these transitions in atomic oxygen. The theoretical calculations of integral and differential cross sections for these transitions have been carried out by Thomas and Nesbet (1975) in the energy region from 0.14 to 11 eV using a matrix variational method. Henry *et al* (1969) performed a close-coupling calculation in the energy region from threshold to 50 eV and Vo Ky Lan *et al* (1972) used a polarized close-coupling method. Berrington (1988) calculated collision strengths for the fine-structure transitions between the $2p^4\,^3P_2$, $^3P_1$ and $^3P_0$ levels of atomic oxygen using the R-matrix method. He included three pseudostates, $^3\bar{S}^o$, $^3\bar{P}^o$ and $^3\bar{D}^o$ along with the $2p^4\,^3P$, ^1D and ^1S states of atomic oxygen in the close-coupling expansion. He chose the three pseudostates to represent the dipole polarizability of the ground state. Berrington and Burke (1981) reported effective collsion strengths for electron impact excitation of the $2p^4\,^3P$, ^1D and ^1S states of atomic oxygen obtained in a six-state ($2p^4\,^3P$, ^1D, ^1S, $2s2p^5\,^3P^o$,

† Present address: Department of Physics and Centre for Theoretical Studies of Physical Systems, Clark Atlanta University, Atlanta, GA 30314, USA.

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$^1P^o$ and $2p^6\ ^1S$) *R*-matrix calculation. They used the Hartree–Fock representation for the $2p^4\ ^3P$, ^1D, $2s2p^5\ ^3P^o$, $^1P^o$ states and allowed configuration interaction for the $2p^4\ ^1S$ and $2p^6\ ^1S$ states.

Significant discrepancies in the shape and magnitude of the cross sections from the two sets of measurement and also between calculated results and measurements exist. For example, the integral cross sections obtained by Shyn *et al* (1986) for the ^3P–^1S transition are larger than the measurement of Doering and Gulcicek (1989) over the entire energy range by up to a factor of 2.7, while for the ^3P–^1D transition the integral cross sections of Doering and Gulcicek (1989) are larger than the results of Shyn and Sharp (1986) in the low-energy region ($E \leqslant 20$ eV). The calculated results of Henry *et al* (1969) for the ^3P–^1S transiton are smaller than both the measurements in the low energy region ($E \leqslant 20$ eV).

Tayal and Henry (1988, 1990) recently reported theoretical integral and differential cross sections for electron impact excitation of atomic oxygen for the electric dipole-allowed ^3P–$3s\ ^3S^o$ and dipole-forbidden ^3P–$3p\ ^3P$ transitions. Theoretical cross sections are in good agreement with the measured values of Vaughan and Doering (1987) and Gulcicek and Doering (1988) for the resonance ^3P–$3s\ ^3S^o$ transition, but for the forbidden ^3P–$3p\ ^3P$ transition a large discrepancy exists with the measurement of Gulcicek *et al* (1988). Because of the existing significant discrepancy among the various measured and calculated cross sections for excitation of the $2p^4\ ^1D$ and $2p^4\ ^1S$ states of atomic oxygen and also due to the importance of these cross sections in the studies of planetary atmospheres, we performed detailed close-coupling calculations to obtain integral and differential cross sections for ^3P–^1D and ^3P–^1S transitions over the energy region from 4 to 30 eV.

2. Calculation

We performed two independent three- and six-state close-coupling (CC) calculations. The three terms of the ground state configuration ($2p^4\ ^3P$, ^1D, ^1S) are included in the three-state CC calculation, while in the six-state CC calculation, in addition to these three states the $^3\bar{S}^o$, $^3\bar{P}^o$ and $^3\bar{D}^o$ pseudostates are also included. The inclusion of pseudostates gives rise to spurious pseudoresonances. Care has been taken in choosing the pseudostates so that their excitation thresholds lie outside the energy range of interest (4–30 eV) in our calculation (see table 1).

Table 1. The calculated and experimental energies (eV) of the excited $2p^4\ ^1D$ and ^1S states and $^3\bar{S}^o$, $^3\bar{P}^o$ and $^3\bar{D}^o$ pseudostates relative to the ground $2p^4\ ^3P$ state.

	Energy			
State	Present theory	Baluja and Zeippen (1988)	Berrington (1988)	Moore (1971)
$2p^4\ ^3P$	0.0	0.0	0.0	0.0
$2p^4\ ^1D$	2.09	2.08	2.25	1.97
$2p^4\ ^1S$	4.23	4.23	4.97	4.19
$2p^3(^4S^o)3s\ ^3\bar{S}^o$	42.35		18.00	
$2p^3(^2P^o)3s\ ^3\bar{P}^o$	43.65		21.68	
$2p^3(^2D^o)3s\ ^3\bar{D}^o$	41.74		23.79	

These states are represented by extensive configuration-interaction (CI) wavefunctions constructed from the same six orthogonal one-electron orbitals: 1s, 2s, 2p, 3s, 3p and 3d. We start with the 1s, 2s and 2p radial functions of the ^{3}P ground state of O I given by Clementi and Roetti (1974). The radial part of each orbital is expressed in analytic form as a sum of the Slater-type orbitals and the parameters of the 3s, 3p and 3d orbitals are obtained by using the computer code CIV3 (Hibbert 1975). The 3s, 3p and 3d orbitals are optimized on the $2p^4\ ^1$S state. Baluja and Zeippen (1988) used the same procedure to obtain these orbitals in their calculation of excitation energies and oscillator strengths. They have listed the parameters of these orbitals. In order to account for the important correlation effects in target wavefunctions, up to two electron replacements are considered. In our scattering calculation, we used 28, 17 and 14 configurations to describe the ^{3}P, ^{1}D and ^{1}S states, respectively. In the description of the $^3\bar{S}^o$, $^3\bar{P}^o$ and $^3\bar{D}^o$ pseudostates, we used eight, ten and nine configurations, respectively. The calculated excitation thresholds are given in table 1, where these are compared with the calculations of Baluja and Zeippen (1988) and Berrington (1988) and the measurement of Moore (1971). The present calculated and measured values agree within 1% for the $2p^4\ ^1$S state, while for the $2p^4\ ^1$D state the calculated result is larger by about 6%. The calculated results of Berrington (1988) for the $2p^4\ ^1$D and $2p^4\ ^1$S states are larger than the measurement by 14% and 18%, respectively.

The total wavefunction representing the electron–oxygen-atom collision is expanded in terms of the eight-electron target wavefunctions and nine-electron bound-state-type functions ϕ_j by the close-coupling expansion

$$\Psi_k = A\sum_{ij} c_{ijk}\Phi_i(1, 2, \ldots, 8; \hat{r}_9\sigma_9)\bar{r}_9^1 u_{ij}(r_9) + \sum_j d_{jk}\phi_j(1, 2, \ldots, 9) \qquad (1)$$

where A is the antisymmetrization operator, the Φ_i are channel functions formed by coupling the spin and angular functions and u_{ij} are the numerical basis functions describing the radial motion of the scattered electron. The coefficients c_{ijk} and d_{jk} determined by diagonalizing the total Hamiltonian of the nine-electron system in the usual way. The functions ϕ_j are included to compensate for the imposition of orthogonality conditions and to adequately account for the short-range correlation effects. Application of a variation principle leads to a set of coupled integrodifferential equations which are numerically solved by the R-matrix method (Berrington *et al* 1978). Each term in the first summation of equation (1) gives rise to an interaction channel. At each incident electron energy, results are obtained for seven values of angular momenta $L = 0$–6. These partial waves gave converged cross sections for both the ^{3}P–^{1}D and ^{3}P–^{1}S transitions considered in the present work.

3. Results and discussion

3.1. ^3P–^1D transition

Electron-impact excitation differential cross sections (DCS) for the ^{3}P–^{1}D transition in atomic oxygen are displayed in figures 1–6 over incident electron energies from 4 to 30 eV. These are compared with the available measured values of Doering and Gulcicek (1989) and Shyn and Sharp (1986). The theoretical cross sections obtained in the three- and six-state CC approximations are shown by full and broken curves, respectively. The full circles represent the measured values of Doering and Gulcicek (1989), while the results of Shyn and Sharp (1986) are shown by full squares. Shyn and Sharp (1986)

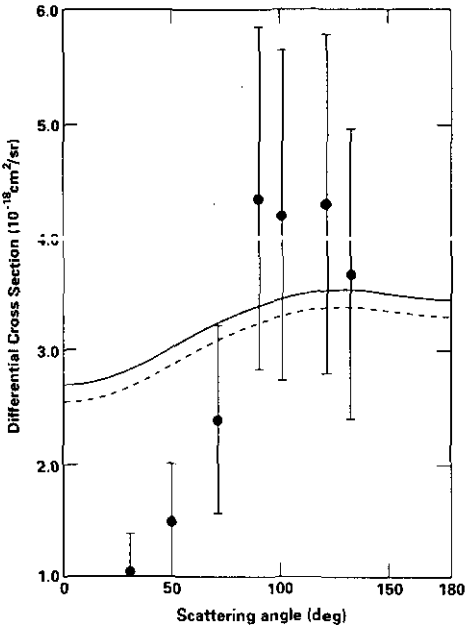

Figure 1. Differential cross sections for electron impact excitation of the ^3P–^1D transition as a function of scattering angle at 4 eV. Full curve, present three-state close-coupling cross sections; broken curve, present six-state close-coupling cross sections; full circles, measured values of Doering and Gulcicek (1989).

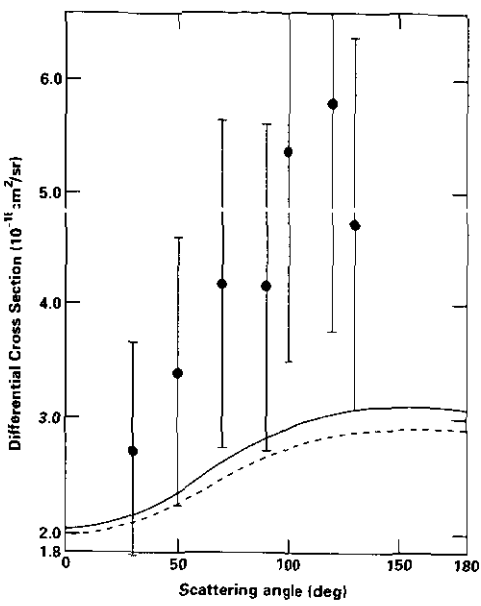

Figure 2. Differential cross sections for electron impact excitation of the ^3P–^1D transition as a function of scattering angle at 5 eV. Notations are as in figure 1.

reported DCS in the energy region from 7 to 30 eV and angular range 30–150°, while Doering and Gulcicek (1989) also measured cross sections close to the threshold region (4 and 5 eV) in the angular range 0–135°. Doering and Gulcicek (1989) put their cross sections on an absolute scale by the use of well established cross sections in atomic oxygen and other species.

The theoretical DCS at all energies are peaked in the backward direction, in agreement with both the experiments. This is the expected behaviour of a spin-changing forbidden transition. The peak in the backward direction becomes stronger as the incident electron energy increases. This trend is in agreement with the calculation of Thomas and Nesbet (1975) and also with measurements. The theoretical DCS obtained in the six-state calculation are lower than those obtained in the three-state approximation at 4 and 5 eV over the entire angular range, while at 7 and 10 eV the six-state results are larger at small scattering angles and become smaller at large scattering angles than the three-state results. In the low-energy region close to the ^1D threshold (figures 1 and 2), there are significant differences in the shape and magnitude of the calculated and measured cross sections. At 7 eV, the present results are lower than the measurement of Doering and Gulcicek (1989) by up to a factor of 1.6, while at 30 eV, the calculated results overestimate compared to the measurement of Doering and Gulcicek (1989), particularly for scattering angles $\leq 100°$. On the other hand, the calculated DCS at 7, 8, 10, 20 and 30 eV (figures 3–6) lie within the error limits of the measured values of Shyn and Sharp (1986) at almost all scattering angles.

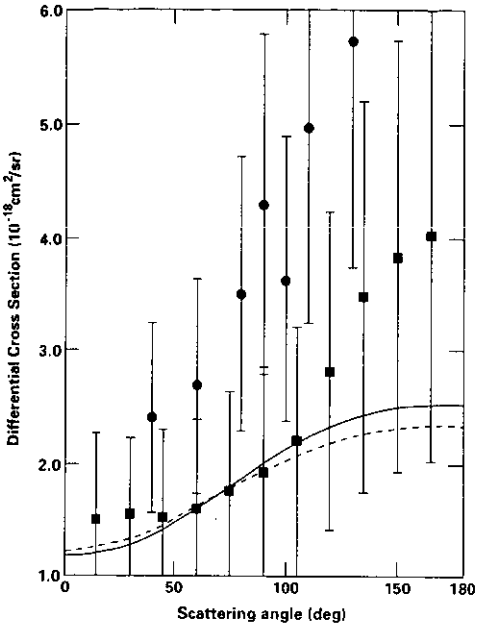

Figure 3. Differential cross sections for electron impact excitation of the ^{3}P–^{1}D transition as a function of scattering angle at 7 eV. Full squares, measured values of Shyn and Sharp (1986) and other notations are as in figure 1.

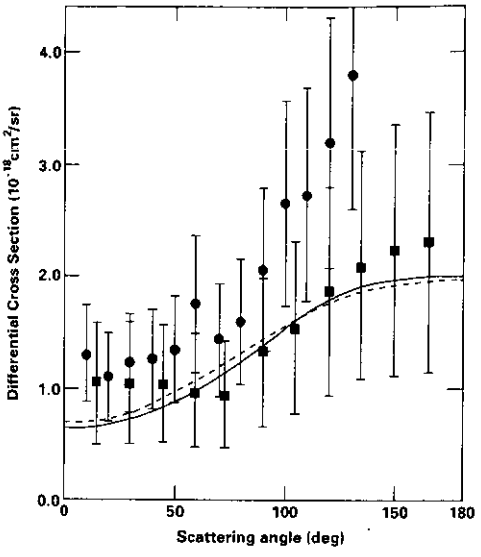

Figure 4. Differential cross sections for electron impact excitation of the ^{3}P–^{1}D transition as a function of scattering angle at 10 eV. Notations are as in figure 3.

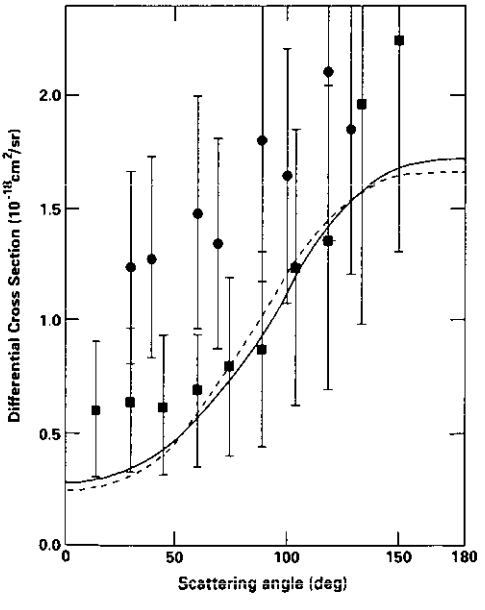

Figure 5. Differential cross sections for electron impact excitation of the ^{3}P–^{1}D transition as a function of scattering angle at 20 eV. Notations are as in figure 3.

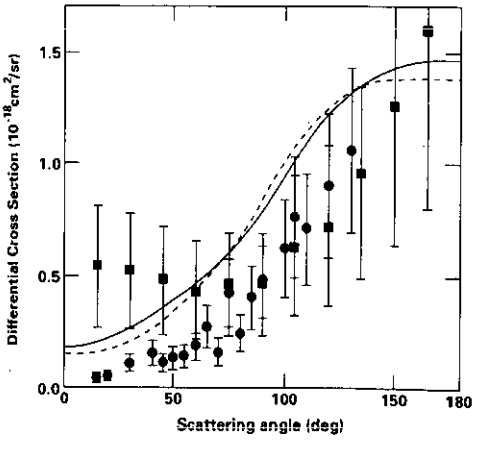

Figure 6. Differential cross sections for electron impact excitation of the ^{3}P–^{1}D transition as a function of scattering angle at 30 eV. Notations are as in figure 3.

The integral excitation cross sections for the ^3P–^1D transition are listed in table 2 and plotted in figure 7, where they are compared with the two sets of measurement (Doering and Gulcicek 1989, Shyn and Sharp 1986). The agreement between the calculated results and the measurement of Shyn and Sharp (1986) is good at all energies, while the present results are smaller than the measurement of Doering and Gulcicek (1989) at 5, 7, 10 and 20 eV. At 30 eV, the present results are larger than the measured values of Doering and Gulcicek (1989). Doering and Gulcicek (1989) predicted a peak in the cross section in the energy region between 5 and 7 eV, while our calculation exhibits this peak at lower energy around 3 eV. Henry *et al* (1969) predicted 17.0×10^{-18} cm^2 integrated cross section at 20 eV which is about 35% larger than the present results. There is very good agreement between the present calculation and the earlier six-state R-matrix results of Berrington and Burke (1981; also see Itikawa and Ichimura 1990) for the excitation cross section of the ^3P–^1D transition.

3.2. ^3P–^1S transition

In figures 8–11, we show the present theoretical DCS for the ^3P–^1S transition in O I at 7, 10, 20 and 30 eV, where these are compared with the measured values (Doering and

Table 2. Integral excitation cross sections (10^{-18} cm^2) for the ^3P–^1D transition in atomic oxygen.

Energy (eV)	Theory		Experiment	
	3-state	6-state	Doering and Gulcicek (1989)	Shyn and Sharp (1986)
2.5	43.90	41.27		
3.0	50.06	46.82		
3.5	46.17	43.64		
4.0	41.32	39.45	39.60	
5.0	34.25	32.27	54.10	
7.0	24.25	23.60	52.40	29.00
10.0	17.18	17.68	31.40	18.00
20.0	12.33	12.65	20.40	15.00
30.0	10.43	10.41	6.97	8.3

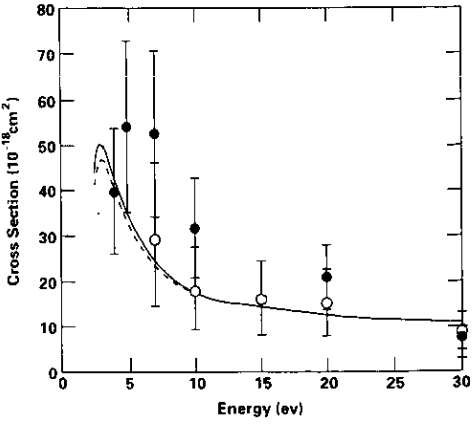

Figure 7. Integral cross sections for electron impact excitation of the ^3P–^1D transition as a function of electron energy. Open circles, measured values of Shyn and Sharp (1986) and other notations are as in figure 1.

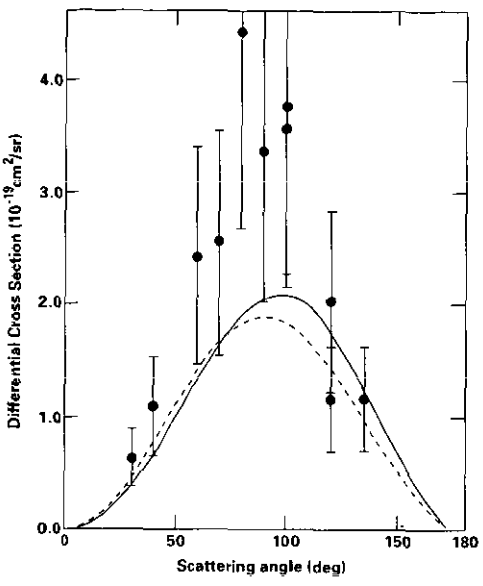

Figure 8. Differential cross sections for electron impact excitation of the ^{3}P-^{1}S transition as a function of scattering angle at 7 eV. Notations are as in figure 1.

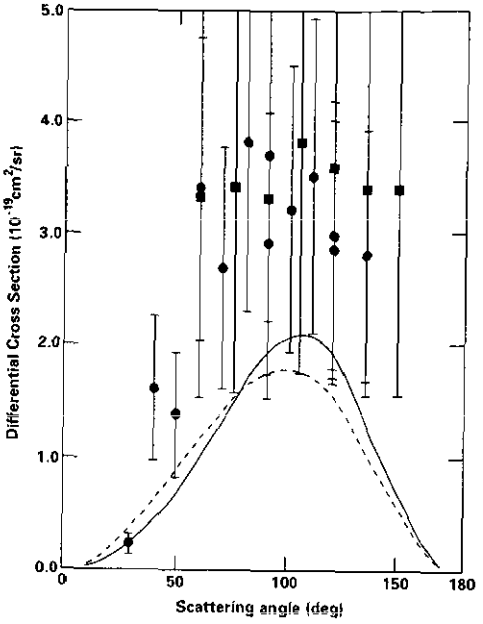

Figure 9. Differential cross sections for electron impact excitation of the ^{3}P-^{1}S transition as a function of scattering angle at 10 eV. Full squares, the measured values of Shyn *et al* (1986) and other notations are as in figure 1.

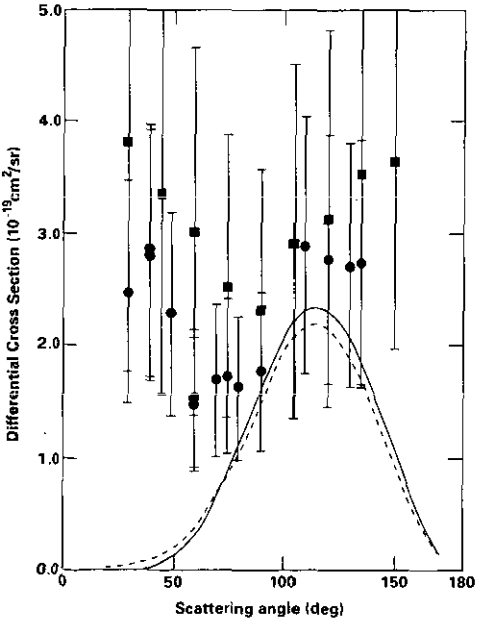

Figure 10. Differential cross sections for electron impact excitation of the ^{3}P-^{1}S transition as a function of scattering angle at 20 eV. Notations are as in figure 9.

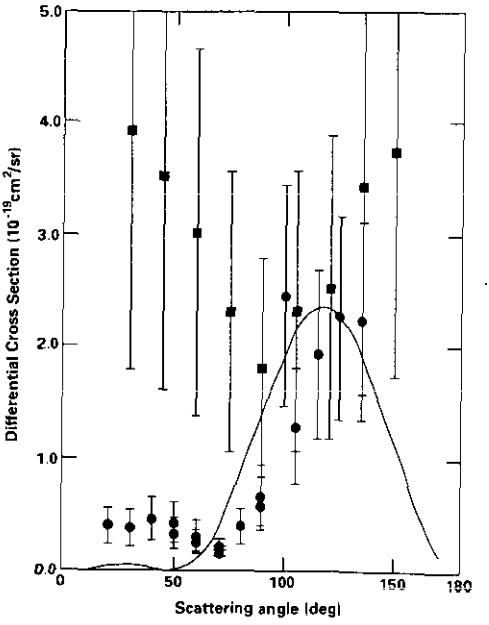

Figure 11. Differential cross sections for electron impact excitation of the ^{3}P-^{1}S transition as a function of scattering angle at 30 eV. Notations are as in figure 9.

Gulcicek 1989, Shyn *et al* 1986). The present theoretical calculations predict the bell shape of the cross sections at all energies considered here, which is in agreement with the prediction of the earleir calculation of Thomas and Nesbet (1975). The theoretical DCS for the ^3P-^1S transition are peaked around the 100-120° angular range. The position of the peak shifts towards the larger scattering angles as the incident energy increases. At 30 eV the two calculations give almost identical results. The measured values of Doering and Gulcicek (1989) are shown by full circles, while the full squares indicate the results of Shyn *et al* (1986). There are substantial differences in the magnitude and shape of the cross sections obtained in the two sets of measurement. Doering and Gulcicek (1989) reported DCS at 7, 10, 20 and 30 eV in the angular range 0-135°. They normalize their cross sections to an absolute scale by the use of measured DCS for the ^3P-^1D transition. On the other hand Shyn *et al* (1986) measured cross sections in the energy range 10-30 eV and angular range 30-150°. At 7 eV the present DCS agree with the measurement of Doering and Gulcicek (1989) at all scattering angles, except in the peak region. The shape of the measured DCS at 7 and 10 eV is in agreement with the calculation. At 20 and 30 eV, both the measurements predict a dip in the cross section in the 70-90° angular region and peaks in the forward and backward directions. The calculated cross sections exhibit only a slight dip around 50° at 30 eV, while the measurement of Doering and Gulcicek (1989) shows the dip at 70°. Except for a shift in the positions of dip and peak, the shape of the calculated and measured values of Doering and Gulcicek appears to be in agreement at 30 eV.

The integral excitation cross section for the ^3P-^1S transition are given in table 3. It is clear from this table that the calculated cross sections are smaller than the measured values of Doering and Gulcicek (1989) at energies $\leq$20 eV and also smaller than the results of Shyn *et al* (1986), typically by a factor of 2.7. Itikawa and Ichimura (1990) reported that the six-state *R*-matrix calculation of Berrington and Burke (1981) is in fairly good agreement with the measurements at 15 and 20 eV for this transition.

Table 3. Integral excitation cross sections (10^{-18} cm^2) for the ^3P-^1S transition in atomic oxygen.

Energy (eV)	Theory		Experiment	
	3-state	6-state	Doering and Gulcicek (1989)	Shyn *et al* (1986)
5	1.19	0.92		
7	1.69	1.57	2.72	
10	1.61	1.50	3.35	4.3
20	1.42	1.38	3.19	3.9
30	1.38	1.32	1.31	3.6

4. Conclusion

We have presented theoretical integral and differential cross sections for electron impact excitation of the ^3P-^1D and ^3P-^1S transitions in atomic oxygen. These transitions give rise to prominent emission features in the aurora and dayglow. The theoretical

cross sections for the ^3P-^1D transition are normally in good agreement with the measurement of Shyn and Sharp and display the characteristic shape of the spin-changing forbidden transition. However, for the forbidden ^3P-^1S transition there are discrepancies between the calculated results and both the measurements. Further theoretical and experimental investigations are required to resolve the discrepancy.

In this work we have used the well tested *R*-matrix approach to numerically solve the coupled integrodifferential equations which should be accurate to well within 5%. To first order the accuracy of the scattering calculation depends directly on the accuracy of the target-state wavefunctions. Theoretical excitation energies differ from the measured values by up to 6%. This difference is caused by the use of approximate wavefunctions and by the neglect of some correlation effects. Further errors are introduced into the scattering calculation by the truncation of the target-state expansion. However, some allowance is made for the higher states by the pseudostates. The calculated results can be further improved by choosing the pseudostates that accurately represent the dipole polarizabilities of initial and final states. In the present calculation we have not considered this aspect of low-energy scattering process which may introduce some errors into our results. The present theoretical results are probably accurate to 20%.

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