Electron collision strengths for the far-infrared lines of O III

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Dedication. It is a great pleasure for the authors to dedicate this paper to Professor M. J. Seaton, FRS on the occasion of his sixtieth birthday.

Summary. New collision strengths for electron impact excitation of the ${}^3P_{\rm J} \rightarrow {}^3P_{\rm J'}$ fine structure transitions within the ground configuration of O⁺⁺ are presented. These were obtained by using a suitable transformation of LS-coupling reactance matrix elements computed with the well-known R-matrix method. The results exhibit a complex pattern of resonances and are given graphically for electron energies below 7.36 eV. The thermally averaged collision strengths (from which rate coefficients can readily be determined) have been evaluated and are tabulated as functions of the electron temperature in the range $0 \le T_{\rm e} \le 2 \times 10^4 \, {\rm K}$.

1 Introduction

The radiative magnetic dipole transitions ${}^3P_{2\rightarrow1}$ and ${}^3P_{1\rightarrow0}$ within the ground configuration of O III give rise to the fine structure lines at 51.82 and 88.35 μ m. These far infrared (IR) lines are likely to be emitted by H II regions where O⁺⁺ is an abundant form of oxygen. If the electron density of a thermal plasma at 10^4 K is sufficiently low ($N_e \leq 10^3$) then a comparable amount of energy will be radiated in the IR and nebular lines ($\lambda\lambda$ 5007, 4959). The importance of infrared line emission for diagnosing the ionized gas that lies in the plane of the Galaxy has been remarked upon by many authors (see, for example, Gould 1963; Delmer, Gould & Ramsay 1967; Osterbrock 1969; Pottasch 1969).

The first successful measurement of galactic O III infrared emission was made by Ward et al. (1975) from an aeroplane flying at an altitude of about $14 \,\mathrm{km}$. They detected the $88.35 \,\mu$ line in the IR spectrum of M17 (Omega Nebula in Saggitarius). An earlier attempt by Ward (1975) to observe this emission line in the spectrum of M42 (Orion Nebula) proved unsuccessful.

Airborne spectrometers with greater resolution have since been used to study a variety of sources (cf. Baluteau et al. 1976, 1981; Dain et al. 1978; Melnick et al. 1978, 1979; Moorwood et al. 1978, 1980a, b; Storey et al. 1979; Watson, Storey & Townes 1980). Note that balloons, which have the advantage of being able to ascend much higher in the atmosphere than aircraft, have so far only been used by Moorwood et al. (1980b). Their observations were made from altitudes of 30.8 and 36.9 km. Some of the more recent papers quoted here report detection of the 51.82μ emission line as well as 88.35μ . The observed intensities of these two lines can be used to obtain information about the emitting plasma, for example the electron temperature, density and ionic abundance (cf. Petrosian 1970; Simpson 1975). They also enable one to estimate the effective temperature of the ionizing radiation field (cf. Watson et al. 1980).

When interpreting the observational data it is necessary to solve the statistical equilibrium equations that determine the instantaneous populations of the ${}^3P_{0,1,2}$ levels, for departures from a Boltzmann distribution are likely to occur in low density astrophysical plasmas ($N_e \leq 10^4 \, \mathrm{cm}^{-3}$). In gaseous nebulae, where kinetic temperatures are of the order of $10^4 \, \mathrm{K}$ and the diffuse radiation field is very dilute, the upper fine structure levels will be mainly populated directly from the ground state by thermal electron collisions (see, for example, Lequeux 1979; Smeding & Pottasch 1979). It is therefore desirable to have accurate rate coefficients for electron induced transitions between the $2p^2$ 3P_1 levels.

In this paper we present the results of new calculations based on a variant of the close coupling approximation known as the R-matrix method (cf. Burke, Hibbert & Robb 1971). Our collision strengths are rapidly varying functions of the electron energy owing to the presence of resonances. They are shown graphically for energies up to 7.36 eV and have been thermally averaged in order to give rate coefficients.

We give a brief historical survey in Section 4, comparing the results of past and present calculations and discussing in some detail the recent atomic data of Bhatia, Doschek & Feldman (1979). In Section 5 we solve the statistical equilibrium equations for the three fine structure levels and compare the relative populations obtained using the best atomic data with those corresponding to the use of older estimates of collision strengths and transition probabilities.

2 Collision strengths

We made use of the LS-coupling reactance matrix elements which Baluja, Burke & Kingston (1980, 1981) computed using the R-matrix form of the close coupling approximation (Burke et al. 1971). We extended their results by running the RMATRX code of Berrington et al. (1978) for partial waves with $4 \le L \le 9$. Note that the target is represented by a 12-state model ion comprising those LS terms which arise in the configurations $2s^2 2p^2$, $2s 2p^3$ and $2p^4$. Each LS state is approximated by a configuration interaction wavefunction obtained by means of Hibbert's (1975) program CIV3. In Table 1 we list the mixing

Table 1. OIII mixing coefficients from the configuration interaction program CIV3. Details of the configurations to which these coefficients refer are given in the paper by Baluja et al. (1980).

State			Coefficients			Energy (AU)
$2p^4 3P^e$	-0.127360	0.991576	0.013993	0.016877	0.003955	-71.764964
	0.003995	-0.006623				
$2p^{4} D^{e}$	-0.126923	0.991644	0.020729	0.005108	-0.002200	-71.661224
	0.005446	-0.006526				
$2p^{4} {}^{1}S^{e}$	0.247418	0.954239	-0.014392	-0.010019	-0.008859	-71. 496014
	0.166211	0.014161				

coefficients which are used to describe the three highest states: $2p^4(^3P, ^1D, ^1S)$. Coefficients for the remaining nine states, as well as details of the radial functions, are given in the paper by Baluja *et al.* (1980).

The reactance matrix elements, which are stored in a data bank that is being developed at The Queen's University of Belfast, were unitarily transformed to pair coupling by Saraph's (1972, 1978) program JAJOM. We assumed relativistic effects to be negligible and did not allow for intermediate coupling of the target ion, i.e. we used equation (5) in Saraph (1972). The transformed matrix elements were processed by JAJOM in order to give partial collision strengths for transitions between the three fine structure levels. These were summed to yield the total collision strengths $\Omega(^3P_0-^3P_1)$, $\Omega(^3P_0-^3P_2)$ and $\Omega(^3P_1-^3P_2)$ shown in Figs 1, 2 and 3, respectively. We ran JAJOM at 436 energy points in order to be able to draw the complex resonance patterns which occur between 0.0 and 0.541 Ryd. Note that the highest energy we considered lies just below the $2s2p^3$ $^5S_2^0$ threshold at 0.5583 Ryd (cf. Baluja et al. 1980).

Until now, all previous calculations have ignored the resonance contributions to these collision strengths, and therefore have only provided estimates of the background scattering. Our results show that there are numerous resonances, both broad and narrow, in the energy range of importance at astrophysical temperatures (i.e. $T_e \lesssim 20\,000\,\mathrm{K}$).

3 Rate coefficients

For most astrophysical applications the free electrons are thermalized at a temperature T_e and have a Maxwellian distribution. In this case the de-excitation rate coefficient $q(j \rightarrow i)$ is given by

$$q(j \to i) = \frac{8.6287 \times 10^{-6}}{\omega_i T_a^{1/2}} \Upsilon(i-j) \text{ cm}^3 \text{ s}^{-1}$$
 (1)

where $\Upsilon(i-j)$ is the thermally averaged (or effective) collision strength:

$$\Upsilon(i-j) = \int_0^\infty \Omega(i-j) \exp(-E_j/kT_e) d(E_j/kT_e). \tag{2}$$

 E_j is the colliding electron's energy after it has produced the inelastic transition $i \rightarrow j$. The excitation rate coefficient $q(i \rightarrow j)$ is given by

$$q(i \to j) = \frac{\omega_j}{\omega_i} q(j \to i) \exp(-E_{ij}/kT_e)$$
(3)

where ω_i and ω_j are the statistical weights of the lower and upper levels, respectively, and E_{ij} is the transition energy. It is convenient to recall here that if energies are given in Rydberg units then $k = 6.3335 \times 10^{-6}$.

We assumed Ω to vary linearly between adjacent tabulation points and so were able to evaluate Υ by summing the analytically derived contributions from each energy interval. The intervals used were quite small (0.001 and 0.002 Ryd) and 436 steps were required to span the energy range $0.00 \le E_j \le 0.541$ Ryd. The high energy contribution to Υ was estimated by assuming Ω to be constant for $E_j \ge 0.541$ Ryd. This was deemed a satisfactory approximation to make since the contribution is very small (less than 2 per cent of Υ) when $T_e \le 2 \times 10^4$ K.

Table 2. Thermally averaged collision strengths $\Upsilon(J-J')$ for the electron induced fine structure transitions $O^{++}({}^3P_J \rightarrow {}^3P_{J'})$.

$T_{\rm e}/10^{4}$	$\Upsilon(0-1)$	Y (0−2)	Υ(1-2)
0.00	0.518	0.247	1.204
0.25	0.504	0.250	1.193
0.50	0.517	0.257	1.224
0.75	0.531	0.265	1.259
1.00	0.542	0.271	1.288
1.25	0.549	0.277	1.309
1.50	0.553	0.281	1.324
1.75	0.555	0.284	1.335
2.00	0.556	0.288	1.342
∞	0.000	0.169	0.379

Our results for $\Upsilon(J-J')$ are given in Table 2 as functions of the electron temperature in the range from 0 to 20000 K. Note that

$$\Upsilon \sim \Omega(E_j = 0); \qquad \Upsilon \sim \Omega(E_j = \infty)$$

$$T_{e \to \infty} \Omega(E_j = \infty)$$
(4)

and in Table 2 we show our estimates of the threshold collision strengths as well as the high energy limits obtained using the Born approximation in a way similar to that described by Tully & Baluja (1981). At very low temperatures, which are of no astrophysical significance, the thermally averaged collision strengths all pass through minima. This just reflects the fact

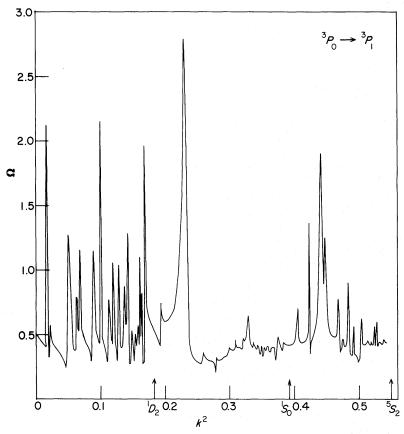


Figure 1. Collision strength for the transition ${}^3P_0 \rightarrow {}^3P_1$ in O III as a function of electron energy in Ryd using the R-matrix method.

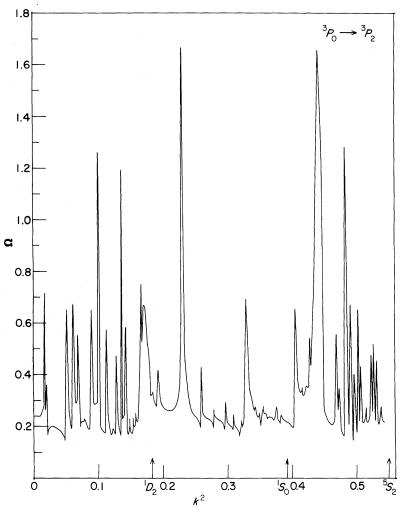


Figure 2. Collision strength for the transition ${}^3P_0 \rightarrow {}^3P_2$ in O III as a function of electron energy in Ryd using the R-matrix method.

that the collision strengths are decreasing functions of energy for $E_j \gtrsim 0.0$, as can be seen from Fig. 1, 2 and 3. It is clear from Table 2 that the temperature dependence of Υ is slight when $T_e \leq 2 \times 10^4$ K. However, with increasing temperature the Υ functions will eventually begin to decrease and descend towards the high temperature limits given in the table.

4 Historical survey

In this section we consider the evolution of theoretical estimates for the O III fine structure collision strengths during the past 40 years. Hebb & Menzel (1940) carried out the first quantal calculation that allowed for distortion of the colliding electron's motion by the net charge on the ion. To do so they used the product of post and prior Coulomb—Born—Oppenheimer (CBO) scattering amplitudes, and rightly concluded that the CBO collision strengths would be non-zero at threshold and roughly independent of the electron velocity. They therefore performed calculations for zero velocity incident electrons which correspond to threshold energy. Note that in a fully non-relativistic treatment of the collision, $E_{ij} = 0$ for the fine structure transitions. Although only a limited number of partial waves were considered, their 'total' collision strengths for the three transitions we are interested in are nevertheless too large. This was first suspected by Bates *et al.* (1950), who showed from flux conservation arguments that the CBO approximation sometimes overestimates cross-sections

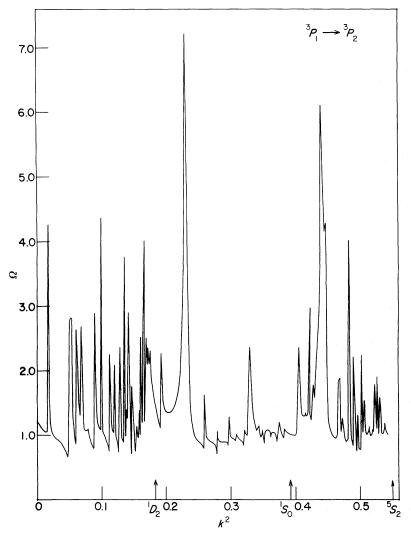


Figure 3. Collision strength for the transition ${}^3P_1 \rightarrow {}^3P_2$ in O III as a function of electron energy in Ryd using the R-matrix method.

at low energies. Quantitative confirmation was later provided by Seaton (1953, 1955) who used a more reliable exchange approximation than CBO. Seaton's (1955) results are smaller than Hebb & Menzel's by factors ranging from 6 to 16 (see Table 3, where the various theoretical results are compared).

The transitions ${}^3P_0 - {}^3P_2$ and ${}^3P_1 - {}^3P_2$ have electric quadrupole moments (cf. Seaton 1955) and finite collision strengths are predicted by non-exchange weak coupling approxi-

Table 3. Fine structure collision strengths $\Omega(J-J')$ at zero impact energy.

Source	0-1	0-2	1-2
Hebb & Menzel (1940)	1.72	4.06	11.2
Seaton (1955)	0.31	0.25	0.96
Blaha (1968)	0.0	0.298	0.671
Blaha (1969)	0.389	0.232	1.009
Saraph et al. (1969)	0.376	0.213	0.948
Bhatia et al. (1979)	0.627*	0.243*	1.332*
Present work	0.518	0.247	1.204

^{*}Obtained by linear extrapolation of Bhatia et al.'s results at 0.5 and 0.8 Ryd.

mations. Blaha (1968), for example, used the Coulomb-Born (CB) approximation at zero energy. He also used a simple distorted wave exchange approximation (Blaha 1969), which, in the light of later work, provides remarkably good estimates of the collision strengths at threshold.

The exact resonance and distorted wave approximations which Seaton (1953, 1955) introduced, were further developed and improved upon by Seaton and his co-workers, and eventually led to the publication by Saraph, Seaton & Shemming (1969) of fine structure collision strengths at three energies close to threshold including zero energy. Osterbrock (1974) used Saraph *et al.*'s results to obtain $\Upsilon(J-J')$ at $T_e = 10^4$ K, and these effective collision strengths have been widely used by astrophysicists and are also reproduced by Spitzer (1978) in his book on the interstellar medium.

Bhatia et al. (1979) have recently calculated collision strengths at several fairly high energies for many transitions in OIII using the distorted wave method of Eissner & Seaton (1972). Their published results for the ground term fine structure transitions were obtained allowing for intermediate coupling (i.e. they used the appropriate transformation in Saraph's 1972 JAJOM program). However, they also verified that relativistic effects are small for the ${}^{3}P_{J} - {}^{3}P_{J'}$ transitions in OIII (Bhatia 1981, private communication), thus justifying in retrospect our use of the algebraic transformation from LS to ij coupling.

In Table 3 we list the collision strengths at threshold (i.e. zero) energy obtained by the authors referred to above, while in Table 4 we give the effective collision strengths at 10000 K from Osterbrock (1974), Bhatia et al. (1979) and the present method. By comparison it can be seen that our results are significantly larger (30 to 40 per cent) than those which have been extensively used until now. Finally, we see that the results of Bhatia et al. (1979) are in very good agreement with our effective collision strengths. This must of course be considered as largely fortuitous since they did not allow for the contribution from resonances.

5 Level populations and line emissivities

In some of the most recent astrophysical papers on OIII infrared emission (e.g. Storey, Watson & Townes 1979) the fine structure collision strengths and transition probabilities quoted by Osterbrock (1974) and Spitzer (1978) have been used to determine the distribution of doubly ionized oxygen amongst the $2p^2 \, ^3P_J$ levels as a function of N_e and T_e . It is interesting to note that use of the present results (Table 2) together with the A-values computed by Baluja & Doyle (1981) leads to sizeable changes (20 to 40 per cent) in the populations compared with the results of Storey et al. (1979) and Moorwood et al. (1980a, b). The excited levels are both enhanced relative to the ground state and the important ratio $N(^3P_2)/N(^3P_1)$ is increased by about 20 per cent in the region where it is most sensitive to

Table 4. Thermally averaged collision strengths $\Upsilon(J-J')$ for $T_e = 10^4 \, \text{K}$.

Source	0-1	0-2	1 - 2
Osterbrock (1974) Bhatia et al. (1979)	0.39 * 0.619†	0.21 * 0.242†	0.95 * 1.320†
Present work	0.542	0.271	1.288

^{*}Calculated by Osterbrock using the collision strengths of Saraph et al. (1969).

[†] Calculated by the present authors using linear interpolation and extrapolation of Bhatia et al.'s collision strengths.

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Table 5. Population ratio $N(^3P_2)/N(^3P_1)$ of the fine structure levels in O⁺⁺. $T_e = 10^4$ K. Statistical equilibrium equations solved using (a) old atomic data (Osterbrock 1974) and (b) new atomic data (present work; Baluja et al. 1981; Baluja & Doyle 1981).

	3-level ion		5-level ion	
$\log N_{ m e}$	old	new	old	new
0.0	0.09119	0.08968	0.09388	0.09154
2.0	0.1199	0.1324	0.1236	0.1352
2.5	0.1786	0.2171	0.1843	0.2218
3.0	0.3371	0.4312	0.3479	0.4401
3.5	0.6683	0.8183	0.6878	0.8331
4.0	1.096	1.225	1.123	1.244
4.5	1.404	1.469	1.434	1.488
5.0	1.545	1.569	1.573	1.588
∞	1.621	1.621	1.621	1.621

density (i.e. $N_{\rm e} \sim 10^{2.5}-10^{3.5}\,{\rm cm}^{-3}$). Some results for this ratio at $T_{\rm e}=10^4\,{\rm K}$ are given in Table 5 for the purpose of comparison. It can be seen that the 1D_2 and 1S_0 levels have quite a small effect on the ratio in question since they increase it by only about 2 per cent. In all of our calculations we used the following energies (in Rydberg units): $E_{12}=1.031\times 10^{-4}$, $E_{13}=2.79\times 10^{-4}$, $E_{14}=0.1848$, $E_{15}=0.3936$. It is useful to note here that 1 Ryd = $2.1793\times 10^{-11}\,{\rm erg}$. We used the proton excitation rate coefficients computed by Faucher, Masnou-Seeuws & Prudhomme (1980) in order to verify that protons have a negligible effect at the temperatures we are interested in. For example, at $T_{\rm e}=2\times 10^4$ they add about 1 or 2 per cent to the electron rate coefficients.

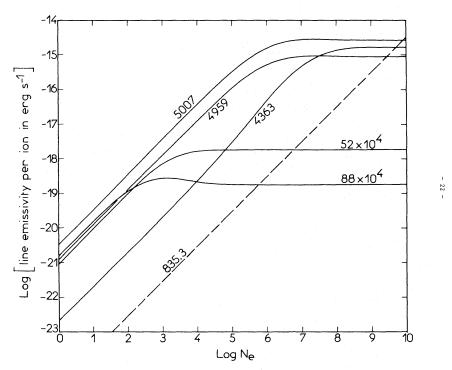


Figure 4. The forbidden line power radiated by a single O⁺⁺ ion in a transparent, homogeneous plasma at 10^4 K. The resonance line 835.292 Å $(2s2p^3 ^3D_3 \rightarrow 2s^22p^2 ^3P_2)$ is shown for comparison. It is seen to have a negligible emissivity at nebular temperatures $(T_e \sim 10^4$ K) and densities $(N_e \sim 10^3$ cm⁻³).

As mentioned in the introduction the temperature and density of HII regions are such that collisionally excited O^{++} ions emit most of their energy in two pairs of lines: the IR (88.35 μ m, 51.82 μ m) and nebular (5007 and 4959 Å) lines. This is illustrated in Fig. 4 where the power (in erg s⁻¹) radiated in the forbidden IR, nebular and auroral lines by a single O^{++} ion from 10^4 K transparent, time independent, homogeneous plasma is plotted as a function of the electron density N_e . The power or emissivity per ion for the line associated with the transition $j \rightarrow i$ is given by the product $(N_j/N) A_{ji} E_{ij}$, where N_j/N is the fraction of O^{++} ions in the level j. The fine structure levels begin to saturate when $N_e \sim 10^3$ cm⁻³ but for electron densities lower than this the power radiated in the IR and nebular lines is of comparable magnitude. We have also indicated the emissivity of the 835.3 Å UV line which belongs to the first resonance multiplet. In order to compute this quantity we used the collision strengths of Bhatia *et al.* (1979). As is well known, the power in this and other UV lines is quite insignificant at nebular densities and temperatures; this is clearly seen from the kind of plot given in Fig. 4.

6 A remark concerning stimulated emission

In the introduction we stressed the importance of our results for interpreting O III infrared emission from hot galactic nebulae. The background radiation in these regions is generally very weak, being composed of the big-bang remnant (2.7 K blackbody spectrum) together with the photon flux from imbedded stars. The latter corresponds roughly to a 4×10^4 K blackbody distribution with a dilution factor W between 10^{-12} and 10^{-13} .

Bhatia et al. (1979) have calculated $e + O^{++}$ collision strengths for application to the Sun's transition zone. They solved the statistical equilibrium equations for a 20-level model ion under conditions appropriate to the solar atmosphere. Their calculations were therefore carried out with $T_e = 6 \times 10^4 \, \text{K}$, and they took account of the photospheric radiation field by assuming the oxygen ions to be irradiated by a dilute (W = 1/2) blackbody spectrum at a temperature of $6 \times 10^3 \, \text{K}$. Stimulated emission was omitted (Bhatia 1981, private communication). While this has a negligible effect on visible and UV lines, it becomes increasingly important as one moves towards IR wavelengths and is quite significant at 52 and 88 μ m. A population inversion, i.e.

$$N_j/N_i > \omega_j/\omega_i, \tag{5}$$

which Bhatia et al. (1979, fig. 1) found to exist for the ground term levels in the low density limit $(N_e \to 0)$, does not occur if one allows for stimulated emission. When $N_e = 0$ one has

$$\frac{N_j}{N_i} = \frac{\omega_j}{\omega_i} \frac{W}{\left[\exp(E_{ij}/kT) - 1 + W\right]} \le \frac{\omega_j}{\omega_i} \exp(-E_{ij}/kT). \tag{6}$$

Note that the population ratio in (6) never exceeds that given by the Boltzmann distribution (i.e. when W = 1). If stimulated emission is neglected then equation (6) becomes

$$\frac{N_j}{N_i} = \frac{\omega_j}{\omega_i} \frac{W}{\left[\exp(E_{ij}/kT) - 1\right]} \ge \frac{\omega_j}{\omega_i} \exp(-E_{ij}/kT) \tag{7}$$

which, for W = 1/2 and T = 6000 K, predicts $N(^{3}P_{1})/N(^{3}P_{0})$ to be 54.4 instead of 2.84.

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