Mon. Not. R. Astron. Soc. **312**, 813–816 (2000)

Theoretical values for the [O III] 5007/4959 line-intensity ratio and homologous cases

P. J. Storey[1]★ and C. J. Zeippen[2]★
[1]*University College London, Department of Physics and Astronomy, Gower Street, London WC1E 6BT*
[2]*UMR 8631 (associée au CNRS et à l'Université Paris 7) et DAEC, Observatoire de Paris, F-92195 Meudon, France*

Accepted 1999 October 15. Received 1999 October 11; in original form 1999 July 23

ABSTRACT

The magnetic-dipole probabilities for the $^1D_2$–$^3P_2$ and $^1D_2$–$^3P_1$ transitions in carbon-like and oxygen-like ions are calculated up to atomic number $Z = 12$, including relativistic corrections to the magnetic dipole operator. The ratio of the probabilities for these two transitions is found to change by up to 5 per cent compared with previous theoretical work, none of which included these relativistic corrections, with the effect being largest for the near neutral ions. The transition probability ratio for the [O III] 5007 and 4959 Å lines is found to be 3.01, implying an intensity ratio of 2.98, in significantly better agreement with the observed ratio than the earlier theoretical work.

Key words: atomic data – line: formation – techniques: spectroscopic – H II regions – planetary nebulae: general.

1 INTRODUCTION

Several authors have commented on the apparent discrepancy between the intensity ratio of the [O III] 5007, 4959 Å lines predicted from the best atomic theory and that observed in high signal-to-noise astronomical spectra. In the 1980s, observations of this ratio and other apparently theoretically well-determined intensity ratios were used to probe the non-linearity of photon counting systems (e.g. Peimbert & Torres-Peimbert 1987). After allowing for such non-linearity, Rosa (1985) suggested that the correct value for the 5007/4959 intensity ratio was 3.03 ± 0.03, significantly different to the best theoretical value at the time of 2.88 (Nussbaumer & Storey 1981). The most recent and elaborate theoretical work on the carbon isoelectronic sequence still predicts an intensity ratio of 2.89 (Galavís, Mendoza & Zeippen 1997). The advent of charge-coupled device (CCD) detectors has confirmed that the measured value is significantly higher with Iye, Ulrich & Peimbert (1987) quoting a value of 3.17 ± 0.04 while Leisy & Dennefeld (1996) give 3.00 ± 0.08. The difference between theory and observation is small, lying between 4 and 9 per cent, but must be considered well-established because the 5007 Å and 4959 Å lines can be observed with very high signal-to-noise ratio in the spectra of gaseous nebulae and the theoretical ratio has not changed significantly with the increasing complexity of the atomic computations.

In this paper we will show that the probabilities for the 5007 Å and 4959 Å transitions, and the equivalent transitions in other carbon-like and oxygen-like ions, are affected by small relativistic corrections to the magnetic dipole operator. These corrections to the operator were first considered for a multi-electron ion by Eissner & Zeippen (1981) in the context of a line-intensity ratio in [O II], where a much larger discrepancy was resolved. The N-like sequence was subsequently treated (Butler & Zeippen 1984; Zeippen 1987; Becker, Butler & Zeippen 1989 and references therein). The case of [S II], together with the P-like sequence, was considered by Mendoza & Zeippen (1982). The effect is important in [O II] and [S II] because the spin–orbit interaction vanishes to first order between the terms of the $2p^3$ and $3p^3$ ground electron configurations of these ions. Such effects were expected to be small for ions, such as those of the carbon and oxygen sequences, where the spin–orbit interaction does not vanish, but are not small enough to be neglected when differences of a few per cent are at issue.

2 METHOD

2.1 The atomic structure calculation

A comprehensive calculation of radiative forbidden transition probabilities for members of the carbon and oxygen isoelectronic sequences has been made by Galavís et al. (1997). They give results for atomic numbers $Z \leqslant 28$ and consider that their results are accurate to 10 per cent or better, with the exception of weak electric quadrupole transitions in ions with $Z \leqslant 11$. We will work in the same configuration interaction model as Galavís et al. (1997), using the computer code SUPERSTRUCTURE (Eissner, Jones & Nussbaumer 1974; Nussbaumer and Storey, 1978). The ions of the carbon isoelectronic sequence are described by a basis of 18 electron configurations, created from the 1s, 2s, 2p, $\bar{3}$s, $\bar{3}$p, $\bar{3}$d and $\bar{4}$f electron radial wave functions. The 1s, 2s and 2p wave functions are calculated in scaled Thomas–Fermi–Dirac model potentials, while the remainder are calculated in a scaled Coulomb

---

★ E-mail: pjs@star.ucl.ac.uk (PJS); zeippen@obspm.fr (CJZ) potential (Nussbaumer & Storey 1978). The ions of the oxygen sequence are described in a 12 configuration basis using the 1s, 2s, 2p, $\bar{3}$s, $\bar{3}$p, $\bar{3}$d, $\bar{4}$p and $\bar{4}$f orbitals. The lists of configurations in these basis sets have been given by Galavís et al. (1997) as have the scaling parameters of the potentials for the radial wave functions. The Hamiltonian matrix incorporates the Coulomb interactions between the electrons and the Breit–Pauli relativistic corrections described by Eissner et al. (1974). These include all the one-body and two-body magnetic fine-structure interactions, spin–orbit, spin–spin etc. Galavís et al. (1997) also use the so-called term energy corrections (TEC) introduced into SUPERSTRUCTURE by Zeippen, Seaton & Morton (1977), in which the Hamiltonian matrix is empirically adjusted to give the best agreement between experimental energies and the final calculated term energies including the relativistic effects. Galavís et al. (1997) also use experimental energies to compute the final transition probabilities from the calculated line strengths for each transition, thereby eliminating any error resulting from differences of the calculated level energies from the experimental values.

2.2 The intensity ratio for the magnetic dipole transitions

We are concerned here only with the $^1D_2$–$^3P_2$ and $^1D_2$–$^3P_1$ transitions in the carbon and oxygen-like ions. These two transitions occur primarily by magnetic dipole radiation, but there is also a small contribution from electric quadrupole radiation. We take these electric quadrupole probabilities directly from the work of Galavís et al. (1997) as deposited in the Centre de Données astronomiques de Strasbourg (CDS). These values are given in Tables 1 and 2, and they contribute less than 0.6 per cent to the total probability in all cases. The usual form for the magnetic dipole operator **M1** is

$$\mathbf{M1} = \mathbf{L} + \mathbf{2S}, \tag{1}$$

in atomic units, where **L** and **S** are the operators for the total orbital and spin angular momentum of the ion. This operator has the property that its matrix elements are only non-zero for transitions within the same term *SL*. With this operator it can be shown that the ratio of the line strengths *S* for the $^1D_2$–$^3P_2$ and $^1D_2$–$^3P_1$ transitions, in the limit of *LS*-coupling when all magnetic interactions become negligible, is

$$\frac{S(^1D_2\text{–}^3P_2)}{S(^1D_2\text{–}^3P_1)} = 3. \tag{2}$$

Using the configuration bases referred to in Section 2.1, we find that the line-strength ratio differs from 3 by no more than 0.1 per cent for any O-like or C-like ion with $Z \leqslant 12$, with the largest difference being for the largest *Z*. The ratio of the transition probabilities *A* is then

$$\frac{A(^1D_2\text{–}^3P_2)}{A(^1D_2\text{–}^3P_1)} = 3\,\frac{E(^1D_2\text{–}^3P_2)^3}{E(^1D_2\text{–}^3P_1)^3}, \tag{3}$$

where *E* are the energy differences. The difference in energy between the $^1D_2$–$^3P_2$ and $^1D_2$–$^3P_1$ transitions arises from the fine-structure splitting of the levels of the ^3P term and it is therefore the magnitude of these magnetic interactions that determines the transition probability and intensity ratio for low-*Z* members of both the O-like and C-like sequences. For [O III] for example, these are $E(^1D_2\text{–}^3P_2) = 19\,967\,\mathrm{cm^{-1}}$ and $20\,160\,\mathrm{cm^{-1}}$, respectively (Edlén 1983, 1985), giving a transition probability ratio of 2.915 in close agreement with the value of 2.918 derived from the probabilities given by Galavís et al. (1997), which include the small electric quadrupole contribution. The intensity ratio corresponding to the Galavís et al. transition probabilities is then 2.890. Because the ratio of the magnetic dipole line strengths does not depend upon the configuration expansion used, and the electric quadrupole contribution is very small, it is clear that as long as the standard formulation for the magnetic dipole operator is used, this value is definitive.

Table 1. *A*-values ($\mathrm{s^{-1}}$) for the $^1D_2$–$^3P_1$ and $^1D_2$–$^3P_2$ transitions in the carbon sequence. E2: electric quadrupole, M1: standard magnetic dipole, RM1: magnetic dipole including relativistic corrections to the operator. The E2 and M1 values are from Galavís et al. (1997). $a \pm b$ denotes $a \times 10^{\pm b}$.

Ion		$^1D_2$–$^3P_1$			$^1D_2$–$^3P_2$	
	E2	M1	RM1	E2	M1	RM1
C I	1.813−7	7.449−5	7.136−5	1.249−6	2.217−4	2.228−4
N II	1.198−6	1.015−3	9.807−4	7.937−6	2.997−3	3.007−3
O III	5.508−6	6.989−3	6.785−3	3.583−5	2.037−2	2.042−2
F IV	1.942−5	3.396−2	3.308−2	1.230−4	9.719−2	9.736−2
Ne V	5.589−5	1.251−1	1.221−1	3.450−4	3.496−1	3.501−1
Na VI	1.452−4	4.130−1	4.041−1	8.516−4	1.118 0	1.119 0
Mg VII	3.416−4	1.192 0	1.169 0	1.878−3	3.105 0	3.105 0

Table 2. *A*-values ($\mathrm{s^{-1}}$) for the $^1D_2$–$^3P_1$ and $^1D_2$–$^3P_2$ transitions in the oxygen sequence. E2: electric quadrupole, M1: standard magnetic dipole, RM1: magnetic dipole including relativistic corrections to the operator. The E2 and M1 values are from Galavís et al. (1997). $a \pm b$ denotes $a \times 10^{\pm b}$.

Ion		$^1D_2$–$^3P_1$			$^1D_2$–$^3P_2$	
	E2	M1	RM1	E2	M1	RM1
O I	3.754−6	2.107−3	2.147−3	2.218−5	6.513−3	6.424−3
F II	1.256−5	1.248−2	1.268−2	8.270−5	3.933−2	3.885−2
Ne III	3.605−5	5.340−2	5.413−2	2.578−4	1.727−1	1.708−1
Na IV	9.021−5	1.836−1	1.859−1	6.957−4	6.142−1	6.079−1
Mg V	1.999−4	5.346−1	5.404−1	1.676−3	1.866 0	1.848 0

2.3 The corrections to the magnetic dipole operator

Following the work of Drake (1971) on two-electron systems, Eissner & Zeippen (1981) introduced relativistic corrections to the magnetic dipole operator in the code SUPERSTRUCTURE for a general *N*-electron system. The corrected operator is

$$\mathbf{M1}' = \sum_{j=1}^{N}\mathbf{M}(j) + \sum_{i=1}^{N}\sum_{j<i}\mathbf{M}(ij), \tag{4}$$

where $\mathbf{M}(j)$ contains one-body operators including the first-order magnetic dipole operator of equation (1), plus corrections of order α^2, while $\mathbf{M}(ij)$ contains two-body operators also of order α^2, where α is the fine-structure constant. Technical details of the operators and their evaluation were given by Eissner & Zeippen (1981) and will not be repeated here.

3 RESULTS AND DISCUSSION

We calculate the relativistically corrected magnetic-dipole-transition probabilities $A(\mathbf{RM1})$ from

$$A(\mathbf{RM1}) = \mathrm{A}(\mathbf{M1})\frac{\mathrm{S}(\mathbf{M1}')}{\mathrm{S}(\mathbf{M1})}, \tag{5}$$

where the values of $A(\mathbf{M1})$ are obtained form the work of Galavís et al. (1997), as deposited in the CDS, while the line strengths $S(\mathbf{M1}')$ and $S(\mathbf{M1})$ are obtained using the operators described in Sections 2.2 and 2.3 above. We note that the $A(\mathbf{M1})$ have therefore been calculated in a model that incorporates term energy corrections and uses experimental level energies.

Tables 1 and 2 contain *A*-values for the $^1D_2$–$^3P_1$ and $^1D_2$–$^3P_2$ transitions in the carbon and oxygen sequences, respectively, for ions with $Z \leqslant 12$. The data from Galavís et al. (1997) are given together with the relativistically corrected *A*-values (RM1) for the magnetic dipole transitions. Table 1 shows that, for the C-sequence, only the $^1D_2$–$^3P_1$ transition shows significant sensitivity to relativistic corrections in the M1 operator, with an increase of the corresponding *A*-value of 4 per cent ($Z = 6$) to 2 per cent ($Z = 12$). The situation is similar for the O-sequence in Table 2, but here the *A*-values decrease by 2 per cent ($Z = 8$) to 1 per cent ($Z = 12$). The magnitude of the relativistic corrections is therefore consistent with the 10 per cent uncertainty estimated by Galavís et al. (1997) for their results for these transitions.

Tables 3 and 4 present the total *A*-values for the $^1D_2$–$^3P_1$ and $^1D_2$–$^3P_2$ transitions, including the relativistic corrections to the **M1** operator. They also give the *A*-value ratios calculated without and with **M1** relativistic corrections. As expected from the results in Tables 1 and 2, the ratios are affected by the use of the more elaborate formalism: a 5 per cent to 2 per cent increase is found in the C-sequence and a 3 per cent to 2 per cent decrease is seen in the O-sequence, with the larger differences being for the elements of smaller *Z*.

In [O III], the new *A*-value ratio is 3.01, implying a line-intensity ratio of 2.98, compared with the previous value of 2.89 from the data of Galavís et al. (1997). This new value for the ratio differs by 2 per cent or less from the values deduced by Rosa (1985) and Leisy & Dennefeld (1996) from astronomical spectra, while the discrepancy with the value of Iye et al. (1987) has been reduced to 6 per cent.

4 CONCLUSIONS

We have shown that the incorporation of relativistic corrections to the magnetic dipole operator causes observable changes in the magnetic dipole transition probabilities for the $^1D_2$–$^3P_2$ and $^1D_2$–$^3P_1$ transitions in C-sequence and O-sequence ions. These changes are large relative to those that have arisen from improvements to the wave-function expansions, which have left the transition probability ratios effectively unchanged over the last 20 yr.

In the case of [O III], although there is substantial scatter in the values of the $^1D_2$–$^3P_2$ to $^1D_2$–$^3P_1$ intensity ratio derived from astronomical observations, these values are in significantly better agreement with the new theoretical values given here than with previous theory.

Of the C-sequence and O-sequence lines considered in this paper, the [O III] 5007 Å and 4959 Å lines are the most prominent in the spectra of photoionized nebulae, owing to the relatively high

Table 3. Total *A*-values and ratios for the $^1D_2$–$^3P_1$ and $^1D_2$–$^3P_2$ transitions in the carbon sequence. GMZ refers to Galavís et al. (1997). $a \pm b$ denotes $a \times 10^{\pm b}$.

Ion	$^1D_2$–$^3P_1$ λ_{air}(Å)	A(s^{-1})	$^1D_2$–$^3P_2$ λ_{air}(Å)	A(s^{-1})	$A(^1D_2$–$^3P_2)/A(^1D_2$–$^3P_1)$ GMZ	Present
C I	9824.1	7.154−5	9850.3	2.240−4	2.985	3.131
N II	6548.1	9.819−4	6583.5	3.015−3	2.958	3.071
O III	4958.9	6.791−3	5006.8	2.046−2	2.918	3.013
F IV	3996.9	3.310−2	4059.9	9.748−2	2.864	2.945
Ne V	3345.9	1.222−1	3425.9	3.504−1	2.795	2.867
Na VI	2872.7	4.042−1	2971.9	1.120 0	2.709	2.771
Mg VII	2509.2	1.169 0	2629.1	3.107 0	2.607	2.658

Table 4. Total *A*-values and ratios for the $^1D_2$–$^3P_1$ and $^1D_2$–$^3P_2$ transitions in the oxygen sequence. GMZ refers to Galavís et al. (1997). $a \pm b$ denotes $a \times 10^{\pm b}$.

ion	$^1D_2$–$^3P_1$ λ_{air}(Å)	A(s^{-1})	$^1D_2$–$^3P_2$ λ_{air}(Å)	A(s^{-1})	$A(^1D_2$–$^3P_2)/A(^1D_2$–$^3P_1)$ GMZ	Present
O I	6363.8	2.151−3	6300.3	6.446−3	3.096	2.997
F II	4869.0	1.269−2	4789.4	3.893−2	3.155	3.068
Ne III	3967.5	5.417−2	3868.8	1.711−1	3.237	3.159
Na IV	3362.2	1.860−1	3241.6	6.086−1	3.347	3.272
Mg V	2927.5	5.406−1	2782.2	1.850 0	3.493	3.422

abundance of O^{2+} ions in these objects and the position of the lines in the centre of the visible spectral range. We note, however, that homologous lines of [C I] and [N II] in the C-sequence and [O I] and [Ne III] in the O-sequence are also observed, albeit at much lower intensity (e.g. Liu et al. 2000). A careful analysis of the relative intensities of these lines from high signal-to-noise spectra could provide a further test of the theory employed here.

ACKNOWLEDGMENTS

The present collaboration benefited from visits to Meudon by PJS with support provided by the Observatoire de Paris and the Université Paris 7. The hospitality of the Observatoire de Paris was much appreciated.

REFERENCES

Becker S. R., Butler K., Zeippen C. J., 1989, A&A, 221, 375
Butler K., Zeippen C. J., 1984, A&A, 141, 274
Drake G. W. F., 1971, Phys. Rev. A, 3, 908
Edlén B., 1983, Phys. Scr., 28, 51
Edlén B., 1985, Phys. Scr., 31, 345
Eissner W., Zeippen C. J., 1981, J. Phys. B, 14, 2125
Eissner W., Jones M., Nussbaumer H., 1974, Comput. Phys. Commun., 8, 270
Galavís M. E., Mendoza C., Zeippen C. J., 1997, A&AS, 123, 159
Iye M., Ulrich M. H., Peimbert M., 1987, A&A, 186, 84
Leisy P., Dennefeld M., 1996, A&AS, 116, 95
Liu X.-W., Storey P. J., Barlow M. J., Danziger I. J., Cohen M., Bryce M., 2000, MNRAS, in press
Mendoza C., Zeippen C. J., 1982, MNRAS, 198, 127
Nussbaumer H., Storey P. J., 1978, A&A, 64, 139
Nussbaumer H., Storey P. J., 1981, A&A, 99, 177
Peimbert M., Torres-Peimbert S., 1987, Rev. Mex. Astron. Astrofis., 14, 540
Rosa M., 1985, The Messenger, 39, 15
Zeippen C. J., 1987, A&A, 173, 410
Zeippen C. J., Seaton M. J., Morton D. C., 1977, MNRAS, 181, 527

This paper has been typeset from a TEX/LATEX file prepared by the author.