Improved collision strengths and line ratios for forbidden [O III] far-infrared and optical lines

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ABSTRACT

Far-infrared and optical [O III] lines are useful temperature-density diagnostics of nebulae as well as dust obscured astrophysical sources. Fine structure transitions among the ground state levels 1s²2s²2p³ 3P₀,1,2 give rise to the 52 and 88 µm lines, whereas transitions among the 3P₀,1,2, 1D₂, 1S₀ levels yield the well-known optical lines λλ 4363, 4959 and 5007 Â. These lines are excited primarily by electron impact excitation. But despite their importance in nebula diagnostics collision strengths for the associated fine structure transitions have not been computed taking full account of relativistic effects. We present Breit-Pauli R-matrix calculations for the collision strengths with highly resolved resonance structures. We find significant differences of up to 20% in the Maxwellian averaged rate coefficients from previous works. We also tabulate these to lower temperatures down to 100 K to enable determination of physical conditions in cold dusty environments such photo-dissociation regions and ultra-luminous infrared galaxies observed with the Herschel space observatory. We also examine the effect of improved collision strengths on temperature and density sensitive line ratios.

Key words: Gaseous Nebulae – Optical Spectra: H II Regions – Line Ratios: Atomic Processes – Atomic Data

1 INTRODUCTION

Ω3 optical lines have long been standard nebular temperature diagnostics with wavelengths almost in the middle of the optical spectrum at λλ 4363, 4959, 5007 (viz. Aller 1956, Dopita and Sutherland 2003, Pradhan and Nahar 2011). In recent years, owing to the advent of far-infrared (FIR) space observatories and instruments such as the Infrared Space Observatory - Long Wavelength Spectrograph (ISO-LWS), the Spitzer Infrared Spectrograph, and the Herschel Photodetector Array Camera and Spectrometer (PACS) the Ω3 FIR lines have proven to have great potential in providing diagnostics of physical conditions in a variety of astrophysical objects that are generally obscured by dust extinction at optical or shorter wavelengths. These range from Galactic H II regions (Martin-Hernandez et al. 2002, Morisset et al. 2002) to star-forming galaxies at intermediate redshift (Liu et al. 2008) and ultra-luminous infrared galaxies (ULIRGs). For example, the Ω3 FIR lines at λλ 88 and 52 µm are observed from dusty ULIRGs, which are copious IR emitters and become more prominent with increasing redshift (Nagao et al. 2011). They may be valuable indicators of the metallicity evolution from otherwise inaccessible star-forming regions buried deep within the galaxies (Houck et al. 2004, 2005).

The forbidden FIR lines arise from very low-energy excitations within the fine structure levels of the ground state of atomic ions, such as the Ω3 ³P₂ →³P₁ transition at 88.36 µm and the ³P₁ →³P₂ transition at 51.81 µm. As such they can be excited by electron impact at low temperatures, even T<sub>e</sub> ~ 1000 K or less. That also accounts for their utility since the FIR lines can be formed in (and therefore probe) not only H II regions but also photo-dissociation regions (PDRs) where the temperaure-density gradients are large (Nagao et al. 2011).

However, excitation of levels lying very close to each other implies that the associated cross sections need to be computed with great accuracy at very low energies in order to yield reliable rate coefficients. The Maxwellian electron distribution at low temperatures samples only the near-threshold energies above the small excitation energy of the fine structure transition. Relativistic fine structure separations therefore assume special importance even for low-Z atomic ions in determining not only the energy separation but also the interaction of the incident electron with the target levels. Owing to its prominence in astrophysical spectra, a large number of previous studies have been carried out on electron impact excitation of O III (viz. compilation of evaluated data by Pradhan and Zhang 2001). Among the recent ones, whose collision strengths are employed in astrophysical models, are Burke et al. (1989) and Aggarwal and
Keenan (1999). But these calculations are basically in LS coupling (Burke et al. 1989), or with intermediate coupling effects introduced perturbatively via an algebraic transformation from the LS to LSJ scheme (Aggarwal and Keenan 1999). Although the earlier calculations employed the coupled channel R-matrix method which takes account of the extensive resonance structures, the fine structure separations are not considered. In this report we take account of both the resonances and fine structure in an ab initio manner.

Another recent development in relativistic R-matrix codes is the inclusion of the two-body fine structure Breit interaction terms in the Breit-Pauli hamiltonian (Eissner and Chen 2012, Nahar et al. 2011). A relativistic calculation of collision strengths can therefore be carried out, including fine structure explicitly and more accurately than in previous works. Relativistic effects are likely to be insignificant for optical transitions compared to the FIR transitions since the former involve relatively larger energy separations and relativistic corrections are small. Nevertheless, we consider all 10 forbidden transitions among the levels dominated by the ground configuration of OIII.

2 THEORY AND COMPUTATIONS

A brief theoretical description of the calculations is given. In particular, we describe relativistic effects and the representation of the (e + ion) system.

2.1 Relativistic fine structure

The relativistic Hamiltonian (Ryderh units) in the Breit-Pauli R-matrix (BPRM) approximation is given by

\[ H_{\text{BP}}^{r} = \sum_{i=1}^{N+1} \left\{-\nabla_{i}^{2} - \frac{2Z}{r_{i}} + \sum_{j>i}^{N+1} \frac{2}{r_{ij}}\right\} + H_{\text{mass}}^{r} + H_{\text{Dar}}^{r} + H_{\text{so}}^{r}, \]

where the last three terms are relativistic corrections, respectively:

- the mass correction term, \( H_{\text{mass}}^{r} = -\frac{\alpha^{2}}{4\pi} \sum_{i} p_{i}^{4} \),
- the Darwin term, \( H_{\text{Dar}}^{r} = \frac{Z\alpha^{2}}{2\pi} \sum_{i} \frac{3}{r_{i}} \sum_{j} \frac{1}{r_{ij}} \),
- the spin – orbit interaction term, \( H_{\text{so}}^{r} = Z\alpha^{2} \sum_{i} \frac{1}{r_{i}} l_{i}s_{i} \).

Equ. (2) represents the one-body terms of the Breit interaction. In addition, another version of BPRM codes including the two-body terms of the Breit-interaction (Nahar et al. 2011; W. Eissner and G. X. Chen, in preparation) has been developed, and is employed in the present work.

2.2 Effective collision strengths

Cross sections or collision strengths at very low energies may be inordinately influenced by near-threshold resonances. Those, in turn, affect the effective collision strengths or rate coefficients computed by convolving the collision strengths over a Maxwellian function at a given temperature T as

\[ \Upsilon_{ij}(T_{c}) = \int_{0}^{\infty} \Omega_{ij}(\epsilon) \exp(-\epsilon/kT_{e}) d(\epsilon/kT_{e}), \]

where \( \epsilon_{ij} \) is the energy difference and \( \Omega_{ij} \) is the collision strength for the transition \( i \to j \). The exponentially decaying Maxwellian factor implies that at low temperatures only the very low energy \( \Omega_{ij}(\epsilon) \) would determine the \( \Upsilon(T) \).

2.3 Wavefunction representation and calculations

Based on the coupled channel approximation, the R-matrix method (Burke et al. 1971) entails a wavefunction expansion of the (e + ion) system in terms of the eigenfunctions for the target ion. In the present case we are interested in low-lying O/FIR transitions of the ground configuration 2\( s^{2}p^{2} \). Therefore we confine ourselves to an accurate wavefunction representation for the first 19 levels dominated by the spectroscopic configurations [1s\(^{2}\)]2s\(^{2}\)2p\(^{2}\), 2s\(^{2}\)2p\(^{2}\)p, 2s\(^{2}\)2p\(^{3}\)d, 2s\(^{2}\)2p\(^{4}\)s, 2s\(^{2}\)2p\(^{4}\)p, 2s\(^{2}\)2p\(^{5}\)s, 2s\(^{2}\)2p\(^{5}\)p, 2s\(^{2}\)2p\(^{6}\)3d, 2s\(^{2}\)3s\(^{2}\), 2s\(^{2}\)3p\(^{2}\), 2s\(^{2}\)3d\(^{2}\), 2s\(^{2}\)4s\(^{2}\), 2s\(^{2}\)4p\(^{2}\). We note here
that the crucial fine structure separations between the ground state \(^3P_{0,1,2}\) levels reproduced theoretically agree with experimentally measured values to \(\sim 3\%\) (Nahar et al. 2011, see Pradhan and Nahar (2011) for a general description of atomic processes and calculations). The observed energies were substituted for theoretical ones in order to reproduce the threshold energies more accurately. This is of particular importance for excitation at low temperatures dominated by near-threshold resonances. Even though the observed and experimental values are close, a small difference in resonance positions relative to threshold can introduce a significant uncertainty in the effective collision strengths.

The collision strengths were computed employing the extended Breit-Pauli R-matrix (BPRM) codes (Eissner and Chen 2012). Particular care is taken to test and ensure convergence of collision strengths with respect to partial waves and energy resolution. Total (e + ion) symmetries up to \((LS)J\pi\) with \(J \leq 19.5\) were included in the calculations, though it was found that the collision strengths for all forbidden transition transitions converged for \(J \leq 9.5\). An energy mesh of \(\Delta E < 10^{-4}\) Rydbergs was used to resolve the near-threshold resonances. The resonances were delineated in detail prior to averaging over the Maxwellian distribution.

\section{RESULTS AND DISCUSSION}

We describe the two main sets of results for the FIR and the optical transitions, as well as diagnostics line ratios.

\subsection{Far-infrared transitions}

The BPRM collision strengths for the two FIR fine structure transitions \(\lambda\lambda\, 52, 52 \mu m\) are shown in Fig. 1a,b. Although the resonance structures look similar the magnitude and energy variations are not the same. The Maxwellian averaged effective collision strengths \(Y(T)\) are quite different, as shown in Fig. 2. While \(Y(T;^3P_{1/2}^0 - ^3P_{1/2}^1)\) for the 88 \(\mu m\) transition is relatively constant over three orders of magnitude in temperature, the \(Y(T;^3P_{1/2}^1 - ^3P_{1/2}^3)\) for the 52 \(\mu m\) transition varies by about a factor of 1.5 from the low-temperature limit of 100 K to temperatures \(T > 10,000\) K. A comparison with the earlier work by Aggarwal and Keenan (1999) is shown as dashed lines, which range down to their lowest tabulated temperature 2500K. It can be noted that if the Aggarwal and Keenan values are extrapolated linearly to lower temperatures then one would obtain fairly constant effective collision strengths. But the present results show marked difference owing to resonance structures as in Fig. 1.

Such temperature sensitivity of the otherwise density sensitive 52/88 line ratio is illustrated in Fig. 3a,b. In Fig. 3a the solid lines are ratios with the present collision strengths, and the dashed lines are using previous results (Aggarwal and Keenan 1999). We find very good agreement, implying that at all temperatures down to 2500K the differences in line ratios would be negligible. Fig. 3b shows the 52/88 ratio at various temperatures between 100K and 10,000K. Whereas the ratio is relatively constant with density at 100K, its dependence on density varies significantly with increasing temperature. The density-temperature diagnostic value of the 52/88 ratio is apparent from these curves.

Therefore, care must be exercised to establish a temperature regime for the emitting region. Fig. 3a shows line ratios computed at 2500 K and 10,000K, and with variations with electron density. It is also found that the values of line ratios at 2500K and 1000K are very close together, implying coverage for \(T \sim 1000K\). Fig. 3b clearly demonstrates that the line ratio decreases rapidly for \(T < 1000K\) to almost flat at 100K. The low-temperature regime 100-1000K is therefore indicated by the curves shown in Fig. 3b, as well as the limit where the 52/88 ratio is temperature invariant. So the 52/88 ratio is excellent density diagnostics in the typical density range \(\log N_e \sim 3-4\) for \(T > 1000K\) without much dependence on temperature (Fig. 3a). However, at lower temperatures the ratio may differ by up to a factor of ten (Fig. 3b). Whereas the primary variations are owing to the exponential factors in \(Y(T)\), (Eq. 3), we emphasize the role of relativistic fine structure splitting between the \(^3P_{0,1,2}\) levels and near-threshold resonances lying in between.

\subsection{Forbidden optical transitions}

Fig. 4 shows the collision strengths for the optical transitions \(^3P_{1/2}^1 - ^3D_{2/2}, \, ^3P_{1/2}^1 - ^3D_{2,3}^1, \, ^1S_0^1 - ^1D_2\) at \(\lambda\lambda 4959, 5007, 4363\) respectively. The effective collision strengths for the \(\delta\beta\) optical lines are shown in Fig. 5. These also differ significantly from previously available ones, by up to 15%. The new results are also obtained down to 100K; their limiting values at low temperatures tend to 0.4-0.6:1.0. Since \(\lambda\lambda 4959, 5007\) are often blended, it is common to plot the blended line ratio (4959+5007)/4363 shown in Fig. 6. This ratio varies over orders of magnitude since the upper-most \(^1S_0\) level is far less excited at low energies than the \(^1D_2\), and therefore the level populations and line intensities depend drastically on temperature. A comparison is made with fine structure collision strengths derived from the LS term values of Aggarwal and Keenan (1999) divided according to statistical weights, again shown as dashed lines in Figs. 5 and 6. However, similar to Fig. 3a), the differences in effective collision strengths do not translate into any significant differences in line ratios even at \(\log T = 4.5\) (\(\approx 30000K\)) where the values differ most.
3.3 Maxwellian averaged collision strengths

In Table 1 we present the effective collision strengths (Eq. 3) for the 10 transitions among the ground configuration levels and their wavelengths. The tabulation is carried out at a range of temperatures typical of nebular environments, including the low temperature range $T \leq 1000K$ not heretofore considered.

3.4 Conclusion

Improved collision strengths including fine structure with relativistic effects are computed. Owing to the diagnostic importance of the $\Omega 3$ forbidden FIR and optical lines, the relatively small but significant differences of up to 20% should provide more accurate line ratios. Particular attention is paid to the resolution of resonances in the very small energy region above threshold(s), enabling the study of low temperature behavior.

The line emissivities and ratios computed in this work demonstrate the temperature-density behaviour at low temperatures and at typical nebular temperatures. However, depending on the astrophysical sources a complete model of line emissivities may also need to take into consideration the Bowen fluorescence mechanism: the radiative excitation of $2p^3 P_2 - 2p3d^3 P'_2$ by He II Ly$\alpha$ at 304Å and cascades into the upper levels of the forbidden transitions considered herein (viz. Saraph and Seaton 1980, Pradhan and Nahar 2011). In addition, for higher temperatures $T > 20,000$K proton impact excitation of the ground state fine structure levels $^3P_{0,1,2}$ needs to be taken into account; at lower temperatures the excitation rate coefficient due to electrons far exceeds that due to protons (Ryans et al. 1999). Finally, there may be some contribution from $(e +$ ion) recombination from O IV to $\Omega 3$, since recombination rate coefficients increase sharply towards lower temperatures while collisional excitation rates decrease (level-specific and total recombination rate coefficients may be obtained from S. N. Nahar’s database NORAD at: www.astronomy.ohio-state.edu/$\sim$sinnahar). Recombination contribution depends on the O IV/$\Omega 3$ ionization fraction, which at low temperatures would be small.

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REFERENCES

Aggarwal, K. M. and Keenan, F. P., 1999, Astrophys. J. Supp. Ser., 123, 311
Aller, L. H. 1956, Gaseous Nebulae, Wiley, New York
Berrington K. A., Eissner W. & Norrington P. H., 1995, Comput. Phys. Commun. 92, 290
Burke, V. M., Lennon, D. J., and Seaton, M. J., 1989, Mon. Not. R. astr. Soc., 236, 353
Table 1. Effective Maxwellian averaged collision strengths

| Transition | λ   | Υ(100) | Υ(500) | Υ(1000) | Υ(5000) | Υ(10000) | Υ(20000) | Υ(30000) |
|------------|-----|---------|---------|----------|----------|----------|----------|----------|
| $^3P_0 - ^3P_3$ | 88 μm | 5.814(-1) | 5.005(-1) | 4.866(-1) | 5.240(-1) | 5.648(-1) | 6.007(-1) | 6.116(-1) |
| $^3P_2 - ^3P_0$ | 33 μm | 2.142(-1) | 2.153(-1) | 2.234(-1) | 2.469(-1) | 2.766(-1) | 3.106(-1) | 3.264(-1) |
| $^3P_2 - ^3P_1$ | 33 μm | 1.036(0) | 1.032(0) | 1.072(0) | 1.210(0) | 1.330(0) | 1.451(0) | 1.499(0) |
| $^1D_2 - ^3P_0$ | 4933 Å | 1.959(-1) | 2.088(-1) | 2.154(-1) | 2.347(-1) | 2.693(-1) | 3.106(-1) | 3.264(-1) |
| $^1D_2 - ^3P_1$ | 4959 Å | 5.903(-1) | 6.285(-1) | 6.483(-1) | 7.067(-1) | 8.108(-1) | 9.313(-1) | 9.802(-1) |
| $^1D_2 - ^3P_2$ | 5007 Å | 9.934(-1) | 1.056(0) | 1.089(0) | 1.188(0) | 1.363(0) | 1.564(0) | 1.645(0) |
| $^1S_0 - ^1D_2$ | 4363 Å | 3.900(-1) | 3.899(-1) | 3.899(-1) | 4.544(-1) | 5.661(-1) | 6.230(-1) | 6.219(-1) |
| $^1S_0 - ^3P_1$ | 2321 Å | 1.765(-1) | 1.590(-1) | 1.477(-1) | 1.228(-1) | 1.223(-1) | 1.294(-1) | 1.332(-1) |
| $^1S_0 - ^3P_2$ | 2332 Å | 2.850(-1) | 2.587(-1) | 2.421(-1) | 2.045(-1) | 2.046(-1) | 2.170(-1) | 2.235(-1) |
| $^1S_0 - ^3P_0$ | 2317 Å | 5.965(-2) | 5.354(-2) | 4.959(-2) | 4.994(-2) | 4.096(-2) | 4.299(-2) | 4.424(-2) |

Crawford, F. J., Keenan, F. P., Aggarwal, K. M., Wickstead, A. W., Aller, L. H. and Feibelman, W. A., 2000, 362, 730
Dopita M. A. & Sutherland R. S., 2003, Astrophysics of the Diffuse Universe, Springer-Verlag
Eissner W. & Seaton M. J., 1972, J. Phys. B 5, 2187
Houck, J. R. et al., 2004, Astrophys. J. Supp. Ser., 154, 18
Houck, J. R. et al., 2005, Astrophys. J. Lett., 622, L105
Liu, X., Shapley, A. E., Coil, A. L., Benchmann, J. and Ma C-P., 2008, Astrophys. J., 678, 758
Martin-Hernandez et al., 2002, Astron. Astrophys., 381, 606
Morisset, C., Schaerer, D., Martin-Hernandez, N. L., Peeters, E., Damour, F., Baluteau, J.-P., Cox, P., and Roelofsema, P., 2002, Astron. Astrophys., 386, 558
Nahar, S. N., Eissner, W., Chen, G.-X., Pradhan, A. K., 2003, 408, 789
Nahar, S. N., Pradhan, A. K., Montenegro, M., Eissner, W., 2011, Phys. Rev. A, 83, 053417
Nagao, T., Maiolino, R., Marconi, A., and Matsuhara, H. 2011, Astron. Astrophys., 526, A149
Pradhan, A. K. and Nahar, S. N., 2011, Atomic Astrophysics and Spectroscopy, Cambridge University Press
Pradhan, A. K. and Zhang, H. L., Landolt-Börnstein Volume 17 Photon and Electron Interactions with Atoms, Molecules, Ions, Springer-Verlag, 2001, (Ed: Y. Itikawa), I.17.B, 1
Ryans, R. S. I., Foster-Woods, V. J., Reid, R. H. G., Keenan, F. P., 1999, Astron. Astrophys., 345, 663
Saraph, H. E. & Seaton, M. J., 1980, Mon. Not. R. astr. Soc., 193, 617