The impact of strong recombination on temperature determination in planetary nebulae

V. Gómez-Llanos, C. Morisset, J. García-Rojas, D. Jones, R. Wesson, R. L. M. Corradi and H. M. J. Boffin

ABSTRACT

The long-standing difference in chemical abundances determined from optical recombination lines and collisionally excited lines raises questions about our understanding of atomic physics, as well as the assumptions made when determining physical conditions and chemical abundances in astrophysical nebulae. Here, we study the recombination contribution of [O III] 4363 and the validity of the line ratio [O III] 4363/[O II] 4959 as a temperature diagnostic in planetary nebulae with a high abundance discrepancy. We derive a fit for the recombination coefficient of [O III] 4363 that takes into account the radiative and dielectronic recombinations, for electron temperatures from 200 to 30 000 K. We estimate the recombination contribution of [O III] 4363 for the planetary nebulae Abell 46 and NGC 6778 by subtracting the collisional contribution from the total observed flux. We find that the spatial distribution for the estimated recombination contribution in [O III] 4363 follows that of the O II 4649 recombination line, both peaking in the central regions of the nebula, especially in the case of Abell 46 that has a much higher abundance discrepancy. The estimated recombination contribution reaches up to 70 and 40 per cent of the total [O III] 4363 observed flux, for Abell 46 and NGC 6778, respectively.

Key words: atomic data – stars: AGB and post-AGB – ISM: abundances – planetary nebulae: individual: Abell 46, NGC 6778.

1 INTRODUCTION

When measuring chemical abundances from faint heavy-element optical recombination lines (ORLs), it is found that they are always greater than those measured from the much brighter collisionally excited lines (CELS). Being known for more than 70 yr, this abundance discrepancy problem is probably the most important challenge to our understanding of the physics of photoionized nebulae (see García-Rojas et al. 2019, and references therein). Several scenarios have been proposed to resolve the issue, the two most popular being (i) the existence of temperature fluctuations within a chemically homogeneous plasma (Peimbert 1967; Torres-Peimbert, Peimbert & Dallabuìt 1980) and (ii) the presence of cold, metal-rich gaseous clumps in the nebula, which are very efficiently cooled by the heavy elements (Liu et al. 2000).

However, neither of these scenarios seems appropriate to universally explain the complete range of abundance discrepancy factors (ADFs, i.e. the ratio between the abundances determined from ORLs and CELs) observed in both H II regions and planetary nebulae (PNe; see Wesson et al. 2018). Moreover, the mechanisms producing, and allowing for the survival of, temperature fluctuations in a photoionized plasma are still under debate (Peimbert, Peimbert & Delgado-Ingla 2017), while the same is true for the physical origin of the metal-rich component (Stasińska et al. 2007; Corradi et al. 2015). Nevertheless, some observational evidence of the existence of two or more gaseous phases in PNe has been found by several authors in recent years (Wesson, Liu & Barlow 2003; Liu et al. 2006; Wesson et al. 2008; Richer et al. 2013, 2017; Peña et al. 2017).

In particular, PNe with ADFs >10 have proven to be very interesting objects, as their extreme ADFs seem to be linked with the evolution of a central close-binary system that has experienced a common envelope phase (Liu et al. 2006; Corradi et al. 2015; García-Rojas et al. 2016; Jones et al. 2016; Wesson et al. 2018), even if the nature of the relationship is still a mystery. Detailed analysis of the physical conditions and chemical abundances of a few objects has led several authors to suggest that the ionized gas comprises two different phases: an H-rich phase, which is dominated by hydrogen and helium recombination lines and CELs from heavy elements (O, N, Ne, Ar, etc.), alongside a much colder, H-poor phase with strong emission in
the ORLs of heavy elements (C, N, O, Ne) and almost no CEL emission (Liu et al. 2000; Wesson, Liu & Barlow 2005; Corradi et al. 2015; Wesson et al. 2018). Under this hypothesis, accurately determining the physical conditions (electron temperature, $T_e$, and electron density, $n_e$) from different CEL and ORL diagnostics is crucial to properly determine the chemical abundances in each phase. However, having two gas-phase components with different chemical contents in an ionized gas complicates the computation of physical conditions and chemical abundances from an observational point of view.

A first estimate of how the presence of multiple gas components could affect the determination of physical conditions and chemical abundances in the main nebular shell was made by Liu et al. (2000), who computed new recombination coefficients for the $T_e$-sensitive [N II] $\lambda$5754 and [O II] $\lambda\lambda$ 7320+30 auroral lines and found that recombination excitation was important in exciting these lines and that ignoring it would lead to an overestimated $T_e$. These authors also proposed a fit to the contribution of radiative recombination (RR) to the widely used [O III] $\lambda$4363 auroral line, valid for $T_e > 8000$ K.

In this letter, we want to explore the classical [O III] $\lambda$4363/4959 $T_e$ diagnostic, which can be strongly contaminated by recombination in extreme ADF PNe and therefore is no longer suitable for the measurement of $T_e$. In this work, we try to determine the contribution of the recombination to the [O III] $\lambda$4363 line, for the PNe NGC 6778 and Abell 46. In Section 2, we briefly describe the observational data used in this paper; in Section 3, we present new calculations to compute the recombination contribution to the [O III] $\lambda$4363 CEL emissivity; in Section 4, we estimate the recombination contribution from an observational point of view; and finally, in Section 5, we discuss our results.

2 OBSERVATIONS

We have used long-slit, intermediate-resolution spectra taken by our group of the extreme ADF PNe NGC 6778 (with FORS2-VLT 8.2 m; see Jones et al. 2016, ADF ∼ 18) and Abell 46 (with ISIS-WHT 4.2 m; see Corradi et al. 2015, ADF ∼ 120), respectively. The FORS2 observations covered the wavelength range of 3600–5000 Å with an average spectral resolution of 1.5 Å. The ISIS observations covered the wavelength range of 3610–5050 Å with a spectral resolution of 0.8 Å. For additional details on the observations and data reduction, we refer the reader to the original references.

For each long-slit, we split the 2D spectrum into several spatial bins along the slit – 2.5 and 0.5 arcsec wide for Abell 46 and NGC 6778, respectively – which provides enough signal to noise for the faintest lines of interest to be measured. The fluxes of the [O III] $\lambda$4363 and $\lambda$4959 CELs and the O II $\lambda\lambda$4649+50 ORL are obtained by automatically fitting Gaussian profiles to each line (for the ORL line, a double Gaussian is used to take into account the two members of the multiplet at 4649.13 and 4650.25 Å; we ignore the contribution of C III $\lambda$4650.25 because other lines of the same multiplet such as C III $\lambda$4647.42 have not been reported in the literature spectra of either object; Corradi et al. 2015; Jones et al. 2016). The uncertainties are determined in each spatial bin through a quadratic mean of the difference between the Gaussian fit and the signal.

In Fig. 1, we show examples of the line fitting process for the two PNe considered in this paper (upper panels for Abell 46 and lower panels for NGC 6778).

3 THE LIMITS IN COMPUTING [O III] $\lambda$4363 INTENSITY

To compute the [O III] $\lambda$4363 emission, we first consider the contribution from the radiative de-excitation of the O $^{3+}$ ion following an excitation of the level $^1$S$_0$ by collision with a free electron of the plasma. This is obtained using PYNEB (Luridiana, Morisset & Shaw 2015) version 1.1.10, based on collision strengths by Storey, Sochi & Badnell (2014) and transition probabilities by Froese Fischer & Tachiev (2004).

We also have to carefully take into account the RR computed by the fit from Pequignot, Petitjean & Boisson (1991) and the dielectronic recombination (DR) from Nussbaumer & Storey (1984). A fit for the total recombination contribution is given by Liu et al. (2000) as

$$\frac{I(4363)}{I(\beta)} = 12.4 \times t^{0.59} \times \frac{O^{3+}}{H^+}, \quad (1)$$

This line ratio [O III] $\lambda$4363/H $\beta$ leads to a recombination coefficient of the single [O III] $\lambda$4363 line close to

$$\alpha_{4363}[cm^3s^{-1}] \simeq 3.3 \times 10^{-13} \times t^{-0.21}, \quad (2)$$

where $t = T_e/10^4$ K and considering $\alpha_{\text{HI}} \simeq 2.94 \times 10^{-14} \times t^{-0.80} cm^3 s^{-1}$. This fit has been obtained when the DR has a considerable effect on the total recombination. This occurs for $T_e$ between 8000 and 20 000 K. For $T_e < 5000$ K, the DR is negligible compared to the RR and the dependence on $T_e$ does not follow the fit by Liu et al. (2000) anymore. We computed a new fit that reproduces the sum RR + DR within 3 per cent from 200 to 30 000 K:

$$\alpha_{4363} \simeq 2.63 \times 10^{-13} \times t^{-0.6} + 1.4 \times 10^{-13} \times e^{-0.89/t}. \quad (3)$$

This fit is used in the multipurpose photoionization code CLOUDY (Ferland et al. 2017) since v17.02. In Fig. 2, we can see the variation of recombination coefficients with $T_e$ for the RR and DR computed from Pequignot et al. (1991) and Nussbaumer & Storey (1984), respectively, as well as the fit by Liu et al. (2000) and our fit from equation (3). Note that the recombination computed in CLOUDY until v17.02 is rather overestimated as it uses Burgess & Seaton (1960) upper limits (purple line in Fig. 2).

It is important to notice here that, in general, no simple fit to the line ratio [O III] $\lambda$4363/H $\beta$ (like the one obtained by Liu et al. 2000; see equation 1) can be obtained, as the regions where the recombination lines [O III] $\lambda$4363 and H $\beta$ are produced can be very different, especially in terms of temperature, densities, and volume. The complete relation is

$$\frac{I(4363)}{I(\beta)} = \int_\nu E_\nu \alpha_{4363}(T_e) n(O^{3+}) n(e) \frac{dV}{d\nu} = \int_\nu E_\nu \beta(T_e) n(H^+) n(e) \frac{dV}{d\nu}. \quad (4)$$

where $E_\nu$ is the energy of the corresponding emission line and $n(X)$ is the density (by number) of the ion X responsible for the line emission (namely O $^{3+}$ and H $^+$ in this case).

4 TESTING BIMETALLICITY HYPOTHESIS

In the following, we explore the case where the nebula is made of two regions of very different abundances. Then, the H $\beta$ line is mainly emitted by the close-to-solar metallicity region I and the [O III] $\lambda$4363 recombination line is mainly emitted by a cold, metal-rich region 2; equation (4) leads to

$$\frac{I(4363)}{I(\beta)} = \frac{E_{4363} \alpha_{4363}(T_2) n(O^{3+})_2 n(e)_2 V_2}{E_\beta \alpha_\beta(T_1) n(H^+)_1 n(e)_1 V_1}, \quad (5)$$

where $E_{\lambda}$ is the energy of the line, $\alpha$, the recombination coefficient, $n$, the density (by number) of the ion X, and $V$, the effective volume.

In order to test the bimetallicity hypothesis, we need a model for the nebula, which should reproduce the measured spectrum. Then, we can use equation (4) to determine the physical conditions and chemical abundances from an observational point of view.
Figure 1. Examples of the fit to the emission lines. Upper panels for A46 and lower panels for NGC 6778. From left to right, the fits are for the O\II $\lambda\lambda$ 4649+50, the \[O III\] $\lambda$ 4363, and the \[O III\] $\lambda$ 4959 emission lines. Line fluxes are in arbitrary units.

Figure 2. Recombination coefficients of \[O III\] $\lambda$ 4363: RR computed by Pequignot et al. (1991) (blue line), DR by Nussbaumer & Storey (1984) (orange dashed line), the value obtained by the formula from Liu et al. (2000) (equation 1, green dot line), and our fit to RR + DR (equation 3, red dot-dashed line). The actual value of RR + DR is not shown, as it is not distinguishable from our fit. The BS60 values from Burgess & Seaton (1960) upper limits used in CLOUDY are also shown in purple.

where the subscripts 1 and 2 indicate a mean value over the regions 1 and 2, respectively.

Therefore, if $T_1$ and $T_2$ are very different, the simplification of the temperature-dependent power terms in the recombination coefficients of the two lines cannot be applied, nor do the $n_e$ ratio $n(e)_1/n(e)_2$ and the volume ratio $V_1/V_2$ cancel. These ratios cancel only if the same region of the nebula is considered to emit both lines. The abundance ratio $O^+/H^+$ only appears in a final relation if the implicit hydrogen densities $n(H)_1$ and $n(H)_2$ are the same.

$^2$In the general situation, both lines are emitted by both regions and the line intensities are obtained by summing contributions from regions 1 and 2, leading to an even more complex equation for the line ratio:

$$I(4363) \frac{E_{4363}}{E_\beta} \left[ I(4363)_1 + I(4363)_2 \right] = \frac{E_{4363}}{E_\beta} \left[ I(4363)_1 + I(4363)_2 + I(4363)_3 \right], \quad (6)$$

where $I(\lambda)_i = \alpha_\lambda(T_e) n(X)_i n(e)_i V_i$.

Gómez-Llanos & Morisset (2020) explored a case where an ADF($O^{3+}$) $\sim$ 8, determined from observations of NGC 6153, can be reproduced by models in which the actual abundance ratio between the two components (termed the abundance contrast factor or ACF) is as high as 600. In their annex, they even show that an ACF of 1000 could lead to an apparent ADF of 1!

As derived from equations (5) and (6), it is very difficult to determine the contribution to the emission of the \[O III\] $\lambda$ 4363 that comes from the recombination in cases where the gas has two phases of different metallicities, with the metal recombination contribution mainly coming from the H-poor region. Estimating the parameters (e.g. $T_e$ and $n_e$) of both regions needed in equation (5) is very hard, as for most objects the observed morphology does not allow to separate the emission coming from each region.

We have seen that, from a theoretical standpoint, it is almost impossible to correctly determine the contribution to the emission of the \[O III\] $\lambda$ 4363 line that originates from recombination. We can nevertheless attempt to obtain this contribution on an observational basis. In the following, we try to determine the recombination contribution by removing the contribution of the collisionally excited emission to the total emission.

Several authors have found that the spatial distribution of the \[O III\] $\lambda$ 4363 emission is very similar to that of the O\II $\lambda$ 4649 one, but very different from the \[O III\] $\lambda$ 5007, 4959 lines (Corradi et al. 2015; García-Rojas et al. 2016; Jones et al. 2016; Wesson et al. 2018). The observed behaviour is consistent with an increasing temperature towards the central parts of the PN, which is at odds with the fact that O\II ORL emission also peaks at the centre of the nebula, indicating that the cold, H-poor gas is located close to the central star (García-Rojas et al. 2016).

Adopting an $n_e$ of $10^3$ cm$^{-3}$, we estimate (using PYNEB, version 1.1.10) the spatial distribution of $T_e$ in Abell 46 and NGC 6778 from the line ratio \[O III\] $\lambda$ 4363/4959. This is shown in blue in the top left and right panels of Fig. 4, respectively. In Abell 46, we can see a noticeable increase of the temperature estimation towards the central parts of the PN, which is at odds with the fact that O\II ORL emission also peaks at the centre of the nebula, indicating that the cold, H-poor gas is located close to the central star (García-Rojas et al. 2016).

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panel, we show the $T_e$ map obtained from the ratio of both lines, assuming a constant density $n_e \sim 1000$ cm$^{-3}$. The $T_e$ map shows a roughly constant $T_e$ distribution, with an average $T_e$, weighted by the $\lambda 6312$ flux of $\sim 8150$ K, implying that $S^{+}$ recombination emission is not significantly enhanced. This is consistent with previous studies, which suggested that the phenomenon of highly enhanced recombination-line emission is restricted to second-row elements (Barlow et al. 2003; Wesson et al. 2018). Following this observational evidence and the bimetallicity hypothesis, we adopt a constant $T_e$ (red solid line in top panels of Fig. 4) for the close-to-solar region in Abell 46 and NGC 6778 of 10 000 and 8000 K (see above), respectively. The spatial distribution of the observed $\lambda 4363$ line is plotted in orange in the middle panels of Fig. 4 for Abell 46 (left) and NGC 6778 (right). To obtain the collisional contribution of $\lambda 4363$, we divide the observed emission of the line $\lambda 4959$ by the theoretical line ratio $\lambda 4959/\lambda 4363$ at the adopted constant temperature. The result is shown in green in the middle panels of Fig. 4. We then subtract this collisional contribution to the total observed flux of $\lambda 4363$ (orange line) to get the possible recombination contribution of $\lambda 4363$ from $O^{+}$ (red line). For comparison, we also show the spatial distribution of $\lambda 4449$ ORL (blue line) multiplied by a normalization factor. We can see that the residual spatial profile of $\lambda 4363$ (red line) resembles that of the $\lambda 4449$ ORL, indicating that the emissivity of the line is dominated by the recombination contribution. In the lower panels of Fig. 4, we show the spatial distribution of the recombination contribution to the total $\lambda 4363$, which reaches up to 70 and 50 per cent of the total emission for Abell 46 (left) and NGC 6778 (right), respectively.

The recombination contribution to the $\lambda 4363$ line may also be estimated using $O^{+}$ ORLs. Using Pequignot et al. (1991) via PYNEB, one can, for example, deduce $I(\lambda 4959)/I(\lambda 4363)$ increasing from 0.35 to 0.55 (0.45 to 0.7) when $T_e$ increases from 1000 to 20 000 K in case B (case A). Jones et al. (2016) report $I(\lambda 3760) = 0.61$ ($H \beta = 100$) for NGC 6778. One can estimate the intensity of the whole V2 multiplet $I(\lambda 3762+)$ to be $\simeq 1.00$, leading to a prediction of $I(\lambda 4363)$ from recombination to be of the order of 0.4–0.5. This is between 20 and 25 per cent of the observed $I(\lambda 4363) = 2.07$, close to what we obtain for the same PN (see Fig. 4).

5 DISCUSSION
In this paper, we explored the very crude hypothesis that the $T_e$ of the close-to-solar abundance gas in the central part of the nebula is the same as in the main nebula (the red line showing the adopted value in Fig. 4). This may not be the case. If one wants to increase
the precision in the determination of the \([\text{O III}] \lambda 4363\) recombination contribution, one needs to make a detailed photoionization model of the object. This requires a good atmosphere model for the ionizing source in order to correctly reproduce the heating of the nebula. One also may need to take into account the presence of dust and its properties, to accurately compute the balance between the heating and the cooling in the inner part of the nebula. This is totally out of the scope of the simple ‘proof of concept’ presented in this letter.

One can also question the precision of the atomic data involved in the different parts of the emission calculus, especially the RR at low temperature. Although the DR seems to vanish at low temperature (Fig. 2), it has recently been pointed out that the effect of ‘exotic’ atomic processes like Rydberg enhanced recombination (RER) could be very important in these regimes. RER could thus have an impact on the predicted ionization balance and, hence, on the derived ionic abundances (Nemer et al. 2019), changing \(n(\text{O}^+)\) in equation 5. The residual obtained in Section 4 and associated with the \(\text{O}^+\) recombination can also include a contribution from RER, as such an exact computation of the RER-based emission will be important in understanding the entirety of the \([\text{O III}] \lambda 4363\) emission.

Regarding observations, it is becoming increasingly clear that for a complete understanding of this problem, a combination of detailed photoionization models with deep IFU observations might improve the situation. In the case of extreme ADF PNe, where two different plasma components coexist, the Balmer and Paschen jumps might not be indicative of any real gas temperature, as they are only a weighted mean of two very different phases of gas. Similarly, the recombination lines (e.g. \([\text{O II} \text{ or H I}\]) are not telling us the value of the ionic abundance ratio \(\text{O}^{2+}/\text{H}^+\), as it is impossible to determine what fraction of \(\text{H}^+\) actually comes from the cold region. The exact weight of the H-poor zone can only be constrained through detailed photoionization models. From the comparison of theoretical models with observations, one can obtain the physical properties (\(T_e, n_e,\) mass, and abundances) of the two plasma components that reproduce the observed spectra. However, a detailed treatment of the physics has revealed that the ADF might be only a rough estimate of this discrepancy and is unlikely to provide ‘real’ information on the ORL/CEL abundance ratios (see Gómez-Llanos & Morisset 2020).

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DATA AVAILABILITY

The original data used in the paper are available under request to the authors.

REFERENCES

Barlow M. J., Liu X. W., Péquignot D., Storey P. J., Tsamis Y. G., Morisset C., 2003, in Kwok S., Dopita M., Sutherland R., eds, Proceedings of the 209th Symposium of the International Astronomical Union held at Canberra, Australia, 19-23 November, 2001, Planetary Nebulae: Their Evolution and Role in the Universe. 373

Burgess A., Seaton M. J., 1960, MNRAS, 120, 121

Corradi R. L. M., García-Rojas J., Jones D., Rodríguez-Gil P., 2015, ApJ, 803, 99

Ferland G. J. et al., 2017, Rev. Mex. Astron. Astrofis., 53, 385

Froese Fischer C., Tachiev G., 2004, At. Data Nucl. Data Tables, 87, 1

García-Rojas J., Corradi R. L. M., Monteiro H., Jones D., Rodríguez-Gil P., Cabrera-Lavera A., 2016, ApJ, 824, L27

García-Rojas J., Wesson R., Boffin H. M. J., Jones D., Corradi R. L. M., Esteban C., Rodríguez-Gil P., 2019, AAA Workshop Ser., 11, 33

Gómez-Llanos V., Morisset C., 2020, MNRAS, 500, 368, 1959

Luridiana V., Morisset C., Shaw R. A., 2015, A&A, 573, A42

Nemer A. et al., 2019, ApJ, 887, L9

Pequignot D., Petitjean P., Boisson C., 1991, A&A, 251, 680

Richer M. G., Georgiev L., Arrieta A., Torres-Peimbert S., 2013, ApJ, 773, 133

Richer M. G., Suárez G., López J. A., García Díaz M. T., 2017, AJ, 153, 140

Stasińska G., Tenorio-Tagle G., Rodríguez M., Henney W. J., 2007, A&A, 471, 193

Nemer A. et al., 2019, ApJ, 887, L9

Nussbaumer H., Storey P. J., 1984, A&AS, 56, 293

Peimbert M., 1967, ApJ, 150, 825

Peimbert M., Peimbert A., Delgado-Ingla G., 2017, PASP, 129, 082001

Peña M., Ruiz-Escobedo F., Rechy-García J. S., García-Rojas J., 2017, MNRAS, 472, 1182

Wesson R., Liu X. W., Barlow M. J., 2003, MNRAS, 340, 253

Wesson R., Liu X. W., Barlow M. J., 2005, MNRAS, 362, 424

Wesson R., Barlow M. J., Liu X. W., Storey P. J., Ercolano B., De Marco O., 2008, MNRAS, 383, 1639

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