

The impact of strong recombination on temperature determination in planetary nebulae

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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] 4363/4959 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 & Daltabuit 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).¹ Moreover, the mechanisms producing, and allowing for the survival of, temperature fluctuations in a photoionized plasma are still under debate (Peimbert, Peimbert & Delgado-Inglada 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

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¹An updated data base on the ADFs measured in H II regions and PNe by Wesson, R. can be found at <https://www.nebulousresearch.org/adfs/>

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] $\lambda 4363/\lambda 4959$ 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 1S_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

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

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

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

where $t = T_e/10^4$ K and considering $\alpha_{H\beta} \simeq 2.94 \times 10^{-14} \times t^{-0.80} \text{cm}^3 \text{s}^{-1}$.

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:

$$\alpha_{4363} \simeq 2.63 \times 10^{-13} \times t^{-0.6} + 1.4 \times 10^{-13} \times e^{-0.8/t}. \quad (3)$$

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

$$\frac{I(4363)}{I(\beta)} = \frac{\int_V E_{4363} \alpha_{4363}(T) n(O^{3+}) n(e) dV}{\int_V E_{\beta} \alpha_{\beta}(T) n(H^+) n(e) dV}, \quad (4)$$

where E_{λ} 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 1 and the [O III] $\lambda 4363$ recombination line is mainly emitted by a cold, metal-rich region 2; equation (4) leads to

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

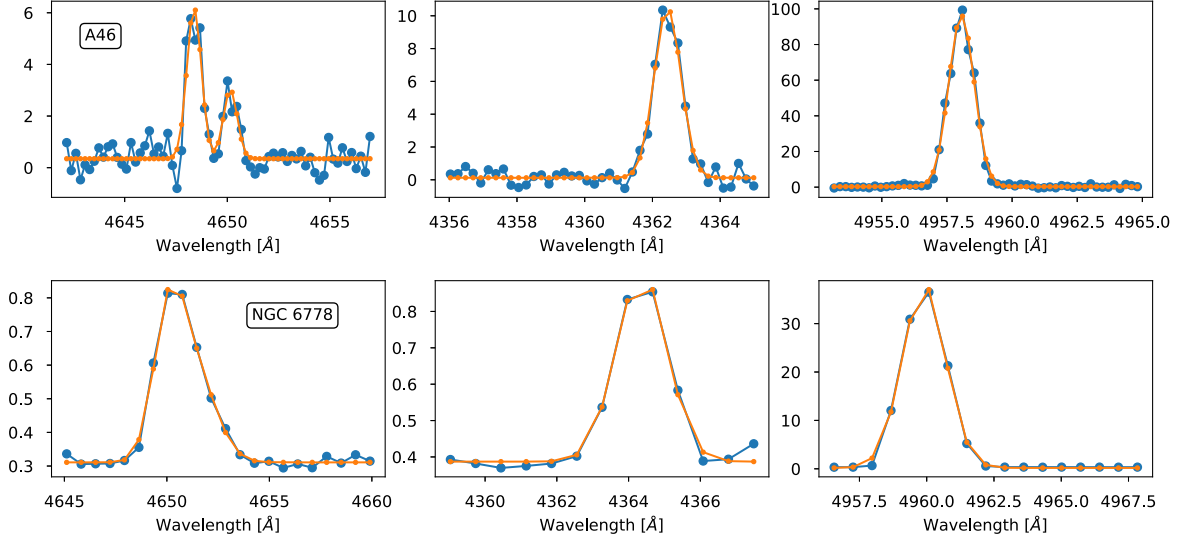


Figure 1. Examples of the fit to the emission lines. Upper panels for A46 and lower panels for NGC 6778. From left to right, the fits are for the O II $\lambda\lambda 4649+50$, the [O III] $\lambda 4363$, and the [O III] $\lambda 4959$ emission lines. Line fluxes are in arbitrary units.

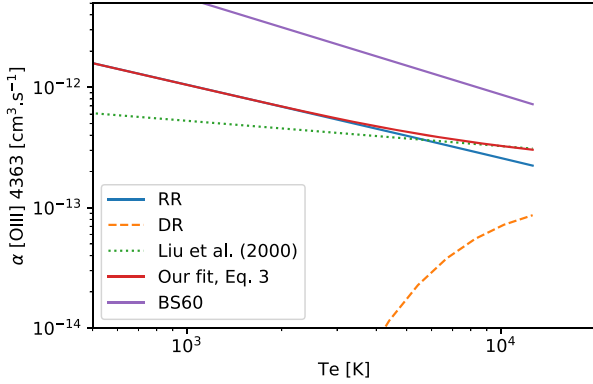


Figure 2. Recombination coefficients of [O III] $\lambda 4363$: RR computed by Pequignot et al. (1991) (blue line), DR by Nussbaumer & Storey (1984) (orange dashed line), the value obtained by the formula from Liu et al. (2000) (equation 1, green dot line), and our fit to RR + DR (equation 3, red dot-dashed 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.²

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^{3+}/H^+ only appears in a final relation if the implicit hydrogen densities $n(H)_1$ and $n(H)_2$ are the same.

²In 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:

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

where $I(\lambda)_i = \alpha_{\lambda}(T_i) n(X)_i n(e)_i V_i$.

Gómez-Llanos & Morisset (2020) explored a case where an $ADF(O^{2+}) \sim 8$, 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 centre of the object. In the left-hand and middle panels of Fig. 3, we show MUSE emission-line maps of the T_e -sensitive [S III] $\lambda 6312$ and [S III] $\lambda 9068$ CELs in NGC 6778 (García-Rojas, Boffin, Wesson et al., in preparation), and in the right-hand

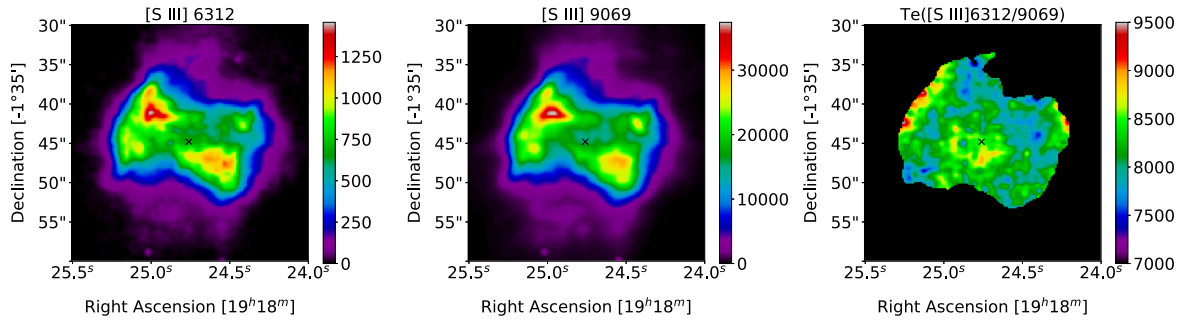


Figure 3. Left-hand and middle panels: MUSE emission line dereddened maps of the T_e -sensitive [S III] λ 6312 and [S III] λ 9068 CELs for NGC 6778, showing a very similar spatial distribution. The raw maps have been convolved with a Gaussian kernel with $\sigma = 1.5$ pixels. The ‘x’ marks the position of the central star in both maps. The colour bar shows the flux in units of 10^{-20} erg s $^{-1}$ cm $^{-2}$ Å $^{-1}$. Right-hand panel: T_e ([S III]) map computed with PYNEB from the extinction-corrected [S III] λ 6312/ λ 9068 line ratio (a cut is made for intensities lower than 10 per cent of the peak emission in [S III] λ 6312). The average T_e weighted by the flux of the λ 6312 line is ~ 8150 K.

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 [S III] λ 6312 flux of ~ 8150 K, implying that S $^{3+}$ 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 [O III] λ 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 [O III] λ 4363, we divide the observed emission of the line [O III] λ 4959 by the theoretical line ratio [O III] $\lambda\lambda$ 4959/4363 at the adopted constant temperature.³ 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 [O III] λ 4363 (orange line) to get the possible recombination contribution of λ 4363 from O $^{3+}$ (red line). For comparison, we also show the spatial distribution of O II λ 4649 ORL (blue line) multiplied by a normalization factor. We can see that the residual spatial profile of [O III] λ 4363 (red line) resembles that of the O II λ 4649 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 [O III] λ 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 [O III] λ 4363 line may also be estimated using O $^{3+}$ ORLs. Using Pequignot et al. (1991) via PYNEB, one can, for example, deduce $I([\text{O III}] \lambda 4363)/I([\text{O III}] \lambda 3762+)$ 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 $I([\text{O III}] \lambda 3760) = 0.61$ ($H\beta = 100$) for NGC 6778. One can estimate the intensity of the whole V2 multiplet $I([\text{O III}] \lambda 3762+)$ to be $\simeq 1.00$, leading to a prediction of $I([\text{O III}] \lambda 4363)$ from recombination to be of the order of 0.4–0.5. This is between 20 and 25 per cent of the

³This is obtained with PYNEB, from the ratio of emissivities $\epsilon(4959)/\epsilon(4363)$ using the adopted temperature of 8000 and 10 000 K for NGC 6778 and Abell 46, respectively, and a density of 10^3 cm $^{-3}$. The corresponding ratios are 117 and 51.

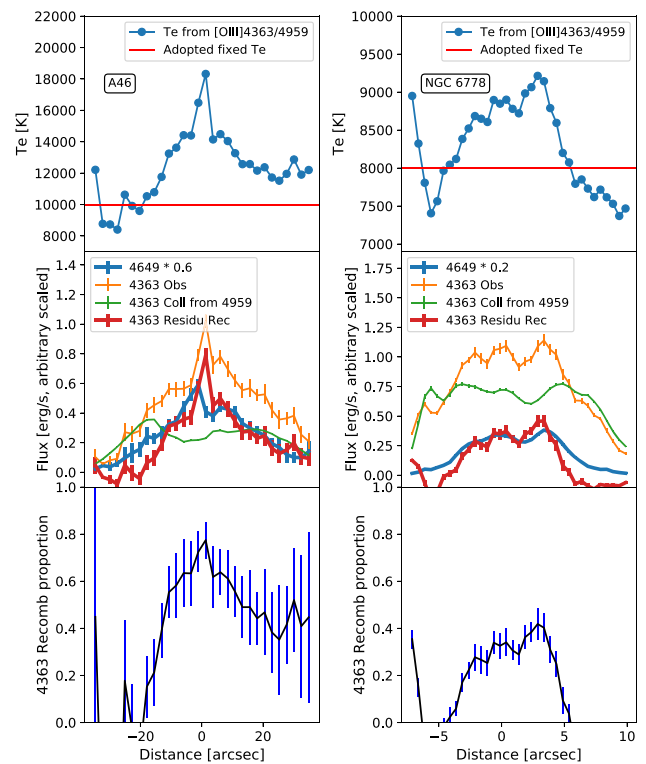


Figure 4. Top panels: T_e estimated from [O III] λ 4363/ λ 4959 ratio. The red line represents the adopted T_e . Middle panels: Spatial distribution of observed [O III] λ 4363 (orange), the expected profile of [O III] λ 4363 emitted by collision assuming the fixed T_e from the upper panels and the profile of [O III] λ 4959 (green), the residuals from subtracting the expected collisional [O III] λ 4363 profiles from the observed one (red), and for comparison the O II λ 4649 profile multiplied by a scale factor (blue). Lower panels: Relative contribution of recombination to the [O III] λ 4363 line.

observed $I([\text{O III}] \lambda 4363) = 2.07$, 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 [O III] λ 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 $n(\text{O}^{3+})$ in equation 5. The residual obtained in Section 4 and associated with the 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 [O III] λ 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. O II or H I) are not telling us the value of the ionic abundance ratio O^{2+}/H^+ , as it is impossible to determine what fraction of 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.

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