Ionized Gaseous Nebulae Abundance Determination from the Direct Method

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Abstract

This tutorial explains the procedure used to analyze an optical emission-line spectrum produced by a nebula ionized by massive star formation. Particularly, the methodology used to derive physical properties, such as electron density and temperature, and the ionic abundances of the most representative elements whose emission lines are present in the optical spectrum is described. The main focus is on the direct method, which is based on the measurement of the electron temperature to derive the abundances, given that the ionization and thermal equilibrium of the ionized gas is dominated by the metallicity. The ionization correction factors used to obtain total abundances from the abundances of some of their ions are also given. Finally, some strong-line methods to derive abundances are described. Such methods are used when no estimation of the temperature can be derived, but which can be consistent with the direct method if they are empirically calibrated.

Key words: ISM: abundances – galaxies: abundances – galaxies: star formation

Online material: color figures

1. Introduction

The determination of chemical abundances is one of the goals of the analysis of the emission-line spectra produced by the ionization of a gas cloud by massive stars. By deriving the relative amount of metals in the gas, it is possible to give valuable constraints to the past chemical enrichment and star formation history, as these elements can only be produced by nucleosynthesis in the star cores before their ejection into the interstellar medium. The relations between metallicity and other observational properties in the studied objects have important implications in different scales and environments. For instance, the integrated metallicity of star-forming galaxies correlates with stellar mass or star formation rate. Its distribution across galactic radii in spiral galaxies depends on the evolution of the disks, the search for the fraction of primordial helium can constrain other important cosmological parameters (e.g., Peimbert et al. 2002, 2007), and in planetary nebulae or envelopes or massive stars the study of chemical abundances allows us to analyze stellar evolution.

The processes of massive star formation irradiate light at all wavelengths, including the energetic UV and X-ray able to pull up the electrons in the atoms of the surrounding gas clouds. As a consequence, the gas atoms are excited and ionized, forming a plasma with free electrons, protons, and ions. When the protons and ions recapture the free electrons of the resulting plasma, they re-emit the radiation under the form of bright lines as the electrons fall from level to level towards their ground state orbiting around nuclei. These electron recombinations are in equilibrium with the constant process of photoionization. As the typical electron temperature of the nebular plasma is of the same order than the photons at the optical wavelength, the lines emitted by the gas are prominent and many times dominate the luminosity of the ionized gas and even of entire starburst galaxies. Figure 1 shows a typical emission-line optical spectrum of a H II region. Table 1 lists the most prominent emission lines with their respective wavelengths.

Among the different emission lines found in an H II region spectrum, there are the recombination lines (RLs), which are weakly dependent on the nebular internal temperature. Most of the brightest lines emitted by the lightest elements (H, He) are of this type. In the case of metals (i.e., all elements heavier than He), RLs provide more precise abundance determinations (i.e., with a precision better than 5%) but they are very weak (i.e., around 10^{-4} times fainter than H\beta 4861 Å), thus they are difficult to measure in weak or distant objects. Instead, collisional excited lines (CELs) are much brighter and more easily detected in optical spectra. These lines correspond to transitions that are forbidden owing to their very low quantum probabilities, but which dominate the cooling of the gas under the extremely low densities of the gas in these nebulae. The intensities of these CELs depend exponentially on the temperature. In principle, the temperature can be determined from appropriate line intensity ratios which, however, require the detection and measurement of intrinsically faint (or absent) auroral lines. This is particularly the case for regions with high metal content—for which the cooling produced by the metals is very efficient and the lines are no longer detected—and also for distant H II regions and
regions with low surface brightness. Table 1 also lists the nature of the emission lines usually observed in the optical spectrum, attending to RLs, nebular CELs, and auroral CELs.

In those cases where no auroral lines are measured with confidence in the optical spectrum, other methods based on the strong nebular line intensities are used. However, one must take into account that in many cases calibrations are obtained from photoionization models for which the uncertainties are difficult to quantify and lead to absolute metallicity values not always compatible with the values obtained from the direct method. See, for instance, Kewley & Ellison (2008) to see differences between direct method metallicities and other obtained from strong-line methods based on models. In contrast, see Dors et al. (2011) or Pérez-Montero (2014) to see other sets of models that lead to chemical abundances that are not systematically higher than those derived from the direct method.

In any case, even when the electronic temperature can be determined with high precision, there are some problems limiting the confidence on the attained results following the direct method. Those problems include: (1) the effect of the internal ionization structure on multiple zone models (Pérez-Montero & Díaz 2003); (2) temperature fluctuations across the nebula (Peimbert 2003); (3) collisional and density effects on the ionic temperatures (Luridiana et al. 1999); (4) neutral gas zones affecting the determination of ionization correction factors (ICFs)(Peimbert et al. 2002); (5) the ionization structure is not adequately described by present models (Pérez-Montero & Díaz 2003); and (6) possible photon escape affecting low ionization lines in the outer regions of the nebula (Castellanos et al. 2002). The first three effects can introduce uncertainties regarding the derived O abundance of some 0.2, 0.3, and 0.4 dex, respectively, depending on the degree of excitation. The uncertainties associated to the rest of the enumerated problems have not yet been quantified.

In this tutorial, some very basic instructions to derive physical properties and ionic chemical abundances following the direct method are given. There are two basic assumptions behind these calculations: (1) the gas is ionized by hot massive stars whose spectral every distribution can be modelized by a black-body and (2) all the emission from the ionized gas, including its complete ionization structure (i.e., from the innermost layer irradiated by the star up to the photodissociation region, where the gas is neutral or the outer edge is reached) is well traced by the observed spectrum.

For this work, all $n_e$, $T_e$ and ionic abundances were re-calculated using expressions derived using non-linear fittings to the results obtained from the emission-line analysis software PYNEB v0.9.3 (Luridiana et al. 2012) as described below and with the most updated sets of atomic coefficients. The expressions were obtained using arbitrary sets of input emission-line intensities covering the most common conditions; some of them can be also found in Pérez-Montero (2014) or Dors et al. (2016). These formulae are provided to ease the reproducibility of the calculations, the error analysis, and their applicability for large data samples using different software.

### 2. Emission-line Measurement and Extinction

Once an optical spectrum is conveniently reduced, calibrated, and extracted, the analysis of the emission lines must lead to the measurement of their integrated fluxes in units of erg s$^{-1}$ cm$^{-2}$, reddening corrected and usually relative to an H$eta$ line, usually H$eta$.

The main source of uncertainty associated with the derived physical properties are related with the error of the fluxes of the lines. The measure of these fluxes can be either done manually (e.g., using the IRAF TASK SPLOT) or using other automatic routines that fit a Gaussian function to the line profile. These programs can integer the intensity of each line over a local continuum. The errors of the fluxes measured in this way can be calculated with the expression from Gonzalez-Delgado et al. (1994):

$$\sigma_f = \sigma_c \cdot \sqrt{N + \frac{EW}{\Delta}},$$

where $\sigma_f$ is the error of flux of the line; $\sigma_c$ represents the standard deviation in a box near of the measured emission line and represents the error in the position of the continuum; $N$ is the number of pixels in the measure of the flux of the line; $EW$ is the equivalent width of the line; and $\Delta$ is the dispersion of the wavelength in angstroms per pixel If a Gaussian function fitting is used to integer the fluxes This expression should be added quadratically to the uncertainty of the fitting, as well as with other known sources of uncertainty, as flux calibration error. The use of any automatic routine to measure emission-line fluxes should consider all these sources of uncertainty in the final error balance.

A previous treatment of the underlying stellar continuum can help to reduce the uncertainty, above all if the recombination H and He lines are clearly affected by stellar absorption. Hence,

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**Figure 1.** Optical spectrum of the Galactic H II region S-156 as taken with the ISIS spectrograph mounted on the William Herschel Telescope (WHT) (Fernández-Martín et al. 2017)
Table 1
List and Properties of the Most Prominent Optical Emission Lines, Including Wavelength, Ion, Nature (RL for Recombination Line, CEL (n) for Nebular Collisional Line, and CEL (a) for Collisional Auroral Line) and Extinction Coefficient Using the Law by Cardelli et al. (1989)

| λ (Å) | Ion       | Class | f(λ) | λ (Å) | Ion       | Class | f(λ) |
|-------|-----------|-------|------|-------|-----------|-------|------|
| 3726.0 | [O II]  | CEL (n) | 0.322 | 5875.6 | He I | RL | 0.203 |
| 3728.8 | [O II]  | CEL (a) | 0.322 | 6300.3 | [O I] | CEL (n) | 0.263 |
| 3868.8 | [Ne III] | CEL (n) | 0.291 | 6312.1 | [S III] | CEL (a) | 0.264 |
| 3967.5 | [Ne III] | CEL (n) | 0.266 | 6363.8 | [O I] | CEL (n) | 0.272 |
| 3970.0 | He II | RL | 0.256 | 6548.1 | [N II] | CEL (n) | 0.295 |
| 4068.7 | [S II]  | CEL (a) | 0.239 | 6563.0 | He I | RL | 0.298 |
| 4076.4 | [S II]  | CEL (a) | 0.237 | 6583.5 | [N II] | CEL (n) | 0.304 |
| 4102.0 | He I     | RL | 0.229 | 6678.0 | He I | RL | 0.313 |
| 4340.0 | He I     | RL | 0.157 | 6716.6 | [S II] | CEL (n) | 0.318 |
| 4363.2 | [O II]  | CEL (a) | 0.149 | 6730.8 | [S III] | CEL (n) | 0.320 |
| 4471.5 | He I     | RL | 0.115 | 7065.0 | He I | RL | 0.364 |
| 4668.1 | [Fe III] | CEL (n) | 0.058 | 7135.8 | [Ar III] | CEL (n) | 0.378 |
| 4686.0 | He II    | RL | 0.050 | 7319.5 | [O II] | CEL (a) | 0.398 |
| 4711.3 | [Ar III] | CEL (n) | 0.042 | 7330.2 | [O II] | CEL (a) | 0.400 |
| 4713.1 | He I     | RL | 0.042 | 9017.4 | H I P10 | RL | 0.390 |
| 4740.1 | [Ar IV] | CEL (n) | 0.038 | 9068.6 | [S III] | CEL (n) | 0.594 |
| 4861.0 | H II     | RL | 0.030 | 9231.5 | H I P9 | RL | 0.605 |
| 4958.9 | [O III] | CEL (n) | 0.026 | 9530.6 | [S III] | CEL (n) | 0.625 |
| 5006.9 | [O III] | CEL (n) | 0.038 | 9548.6 | H I P8 | RL | 0.626 |
| 5754.6 | [N II]  | CEL (a) | 0.185 |        |        |       |      |

an appropriate subtraction of this emission before the measurement of the emission lines is convenient using fitting of synthetic stellar populations (e.g., STARLIGHT, Cid Fernandes et al. 2005).

Another important source of uncertainty that can affect the resulting abundances from the direct method is owing to extinction correction. The gas is mixed with dust grains that absorb and scatter part of the optical emission to re-emit it in the infrared affecting the relative emission line fluxes. Hence, each one of the intensities measured in this way must be reddening corrected. The physical law that describes the extinction of a certain emission line at a certain λ in units of Å is

\[ F_0(\lambda) = 10^{-\tau_\lambda} \cdot F_{\text{obs}}(\lambda) = 10^{(1+c(H\beta)) \cdot f(\lambda) - f_{\text{obs}}(\lambda)}, \]

where \( F_0 \) is the corrected emission line flux; \( F_{\text{obs}} \) is the measured flux and \( \tau_\lambda \) is the optical depth at a certain wavelength; \( c(H\beta) \) is the reddening constant, that defines the amount of extinction at the wavelength of H\beta. Finally, \( f(\lambda) \) is the extinction law, what defines the behavior of the extinction as a function of wavelength. The left panel of Figure 2 shows different extinction laws, including Cardelli et al. (1989), for the Milky Way, Gordon et al. (2003) for the Large Magellanic Cloud, or Calzetti et al. (2000) for starburst galaxies. These laws present differences above all in the ultraviolet part of the spectrum. Table 1 shows the values of \( f(\lambda) - f(H\beta) \) according to Cardelli et al. (1989), assuming a value of \( R_V = 3.1 \) (i.e., \( R_V \) is defined as the ratio \( A_V/(A_V - A_B) \) and \( A_V \) and \( A_B \) are the extinctions in mag for bands V and B, respectively).

The reddening constant \( c(H\beta) \) can be calculated from the decrement of Balmer of the stronger recombination lines of hydrogen. We can write this expression to calculate the reddening correction as a function of the H\beta flux as

\[ \frac{I_0(\lambda)}{I_0(H\beta)} = \frac{I_{\text{obs}}(\lambda)}{I_{\text{obs}}(H\beta)} = 10^{-c(H\beta)(f(\lambda) - f(H\beta))}. \]

Then, \( c(H\beta) \) can be derived comparing the observed flux ratios between the most prominent hydrogen recombination lines and the theoretical expected values, which depend on density and temperature. Table 2 lists the expected values between the flux of H\beta and other H I lines as predicted using data from Storey & Hummer (1995) in the case B (i.e., photons are absorbed as soon as they are emitted). Using this same data set, López-Sánchez et al. (2015) provide a polynomial fitting of the theoretical Balmer ratios as a function of temperature in units of K for a fixed density of 100 cm\(^{-3}\). The resulting fittings are the following:

\[ \frac{I(H\alpha)}{I(H\beta)} = 10.35 - 3.254 \cdot \log T_e + 0.3457 \cdot (\log T_e)^2 \]

\[ \frac{I(H\gamma)}{I(H\beta)} = 0.0254 + 0.1922 \cdot \log T_e - 0.0204 \cdot (\log T_e)^2 \]

\[ \frac{I(H\delta)}{I(H\beta)} = -0.07132 + 0.1436 \cdot \log T_e - 0.0153 \cdot (\log T_e)^2 \]
although other ratios for different atomic data can also be found in Osterbrock & Ferland (2006).

The reddening constant can then be derived using a linear fitting, as in Figure 2, or for doublets of lines as of Hα and Hβ when the other recombination H I lines are very faint. Because the calculation of reddening depends on temperature and density, if the derived temperature deviates much from the adopted value, it is better to make an iterative analysis to check the consistency of the calculated extinction. When the resulting reddening constant is negative, it is usually assumed that no dust attenuation is produced and no reddening correction is applied to the relative emission lines.

The uncertainty associated with the reddening correction must be taken into the account in the errors of the emission lines and conveniently propagated into all the physical magnitudes we calculate. Nevertheless, one way to minimize this uncertainty is to correct a given emission line relative to its closest H I line in wavelength and then using the theoretical ratio to Hβ.

In the case of integrated spectra from galaxies or extragalactic H II regions, one has to take care that the mechanism of ionization is not different than massive stars (e.g., active galactic nucleus (AGN), shocks, and post-AGB stars) with a spectral energy distribution that can make the ionization equilibrium to be different. In these cases, the derivation of the extinction, the physical properties, or the chemical abundances using this prescription is not possible. Normally, AGNs can be identified by means of X-ray emission or the use of adequate diagnostic diagrams (e.g., BPT Baldwin et al. 1981; see also Kewley et al. 2006). See Sánchez et al. (2015) for a description of other methods of selection of star-forming regions.

Figure 2. Left: different extinction laws including Cardelli et al. (1989) (solid black line), Gordon et al. (2003) for the LMC (black dashed line), and Calzetti et al. (2000) (red dashed line). Right: linear fittings to the theoretical-to-observed H I emission lines to obtain the reddening constants in four knots of star formation in the galaxy IIZw71 (Pérez-Montero et al. 2009).

(A color version of this figure is available in the online journal.)

Table 2

| Ratio       | n_e = 100 cm⁻³ |             |             |             | n_e = 1000 cm⁻³ |             |             |
|-------------|----------------|-------------|-------------|-------------|----------------|-------------|-------------|
|             | 7500 K          | 10,000 K    | 15,000 K    | 20,000 K    | 7500 K         | 10,000 K    | 15,000 K    | 20,000 K    |
| Hα/Hβ       | 2.93            | 2.86        | 2.79        | 2.75        | 2.92           | 2.86        | 2.78        | 2.74        |
| Hγ/Hβ       | 0.464           | 0.468       | 0.473       | 0.475       | 0.465          | 0.469       | 0.473       | 0.475       |
| Hδ/Hβ       | 0.256           | 0.259       | 0.262       | 0.264       | 0.256          | 0.259       | 0.263       | 0.264       |
| P10/Hβ      | 0.0189          | 0.0184      | 0.0177      | 0.0172      | 0.0189         | 0.0184      | 0.0177      | 0.0172      |
| P8/Hβ       | 0.0376          | 0.0356      | 0.0350      | 0.0339      | 0.0376         | 0.0366      | 0.0350      | 0.0339      |


3. Electron Temperature and Density

The thermal and density structure of H II regions can be obtained by means of the measurement of the fluxes of their emission lines. The direct method relies completely on the measurement of at least one auroral emission line, and the radial thermal structure can be derived using as many measured temperatures as possible or assuming the temperature of the different zones from the measured values. In Figure 3, we see two examples of thermal structure, one owing to photoionization models and the other to the measurement of different line diagnostics in a \( t \) \( \rightarrow \) \( n \) diagram. The relation between these temperatures is not many times simple and it depends on factors such as density profile, dust-to-gas ratio, and geometry of the gas (matter or density-bounded), so the most accurate method is to get as many temperature diagnostics as possible to derive consistently the chemical abundances of each ion.

One simple sketch of the thermal inner structure is the one proposed by Garnett (1992) assuming three different zones: (1) the high-excitation zone, which is the innermost, and corresponds to \( t(\text{O III}) \) (\( t_h \)); (2) the low-excitation zone, which is the outermost, and corresponds to electron temperatures such as \( t(\text{O II}) \), \( t(\text{S II}) \), or \( t(\text{N II}) \) (\( t_l \)); and (3) the intermediate excitation zone, which appears between these two and it is mainly represented by \( t(\text{S III}) \) (\( t_m \)).

Another limitation to calculate the physical properties is the dependence of the derived electron temperatures on density and vice versa. This is usually overcome using an iterative method if the assumed initial conditions deviate much from the results, or using diagnostic diagrams as the one shown in right panel of Figure 3.

This section describes the expressions to derive them from the strongest collisional lines usually observed in the optical spectrum.

3.1. Oxygen

The \( T_e \) of [O III] can be calculated from the emission-line ratio,

\[
R_{O3} = \frac{I(4959) + I(5007)}{I(4363)},
\]

given that, according to Osterbrock & Ferland (2006), temperature can be obtained from the ratio of collisional transitions that have a similar energy but occupy different levels. In this calculation, it is not required to measure the two strong [O III] lines as there is a theoretical ratio between them (\( I(5007) \approx 3 \cdot I(4959) \)). The fitting between the ratio and the electronic temperature was obtained using the program PYNEB assuming a five-level atom and the following non-linear fitting for \( n_e = 100 \text{ cm}^{-3} \):

\[
t([\text{O III}]) = 0.7840 - 0.0001357 \cdot R_{O3} + \frac{48.44}{R_{O3}}
\]

in units of \( 10^4 \text{ K} \), valid in the range \( t = 0.7\text{–}2.5 \) and using collisional strengths from Aggarwal & Keenan (1999). This fitting gives precisions better than 1% for \( 1.0 < t([\text{O III}] < 2.5 \) and better than 3% for \( 0.7 < t([\text{O III}] < 1.0 \). It was calculated for a density of \( 100 \text{ cm}^{-3}, \) but considering a density of \( 1000 \text{ cm}^{-3}, \)
reduces the temperature only in a 0.1%. This relation with the resulting fitting can be seen in left panel of Figure 4.

For \([\text{O II}]\) the quotient for the electron temperature is calculated from

\[
R_{O2} = \frac{I(3726) + I(3729)}{I(7319 \text{ Å}) + I(7330 \text{ Å})}.
\]  

(9)

One has to be careful in this case, because the \([\text{O II}]\) auroral lines might be contaminated by recombination emission. Such emission, however, can be quantified and corrected, according to Liu et al. (2001), as such contribution can be fitted (for 0.5 \(\leq t \leq 1.0\)) by the function

\[
I_R(7319 + 7330) / I(H\beta) = 9.36 \cdot t^{0.44} \cdot \frac{O^{2+}}{H^+}.
\]  

(10)

Moreover, the ratio of the \([\text{O II}]\) lines is strongly dependent on the electron density. Ideally, one should know the \([\text{O II}]\) density from the ratio \(I(3726 \text{ Å})/I(3729 \text{ Å})\) but very frequently we lack resolution to separate the doublet in which case one has to resort to the \([\text{S III}]\) density, also representing the low-excitation zone. The fitting obtained is

\[
t([\text{O II}]) = a_0(n) + a_1(n) \cdot R_{O2} + \frac{a_2(n)}{R_{O2}},
\]  

(11)

which also gives \(t\) in units of \(10^4\) K and where the coefficients are, respectively,

\[
a_0(n) = 0.2526 - 0.000357 \cdot n - 0.43, \\
a_1(n) = 0.00136 + \frac{0.00481}{n}, \\
a_2(n) = 35.624 - 0.0172 \cdot n - \frac{25.12}{n},
\]  

(12)

being \(n\) the electron density in units of cm\(^{-3}\) and using the collisional coefficients from Pradhan et al. (2006) and Tayal (2007). The fittings were made in the range \(t = 0.8-2.5\) in units of \(10^4\) K with an uncertainty better than 2%. The resulting fittings for different electron densities can be seen in right panel of Figure 4.

Often, the auroral \([\text{O II}]\) lines are not observed with good S/N or they are outside our observed spectral range. In that case, it is practical to use some relation based on photoionization models in order to infer \(t([\text{O II}]\) from \(t([\text{O III}]\). For instance, the relation

\[
t([\text{O II}]) = \frac{2}{t([\text{O III}])^{-1} + 0.8},
\]  

(13)

which is based on Stasińska (1990) models is frequently accepted. However, such an expression neglects the dependence of \(t([\text{O II}]\) on the density, consistent with the dispersion for the objects for which both temperatures have been derived from observations as can be seen in left upper panel of Figure 5.
the same panel are shown fittings to grids of models, presented in Pérez-Montero & Díaz (2003), with different electron densities. The density-dependent calibration obtained in this case and given in Hägele et al. (2006) is

\[ t([\text{O II}]) = \frac{1.2 + 0.002 \cdot n + \frac{1.2}{n}}{t([\text{O III}])-1 + 0.08 + 0.003 \cdot n + \frac{2.5}{n}}. \]  

(14)

3.2. Sulfur

The [S II] line ratio is commonly used to determine electron density for the low-excitation zone. It is generally assumed that the nebula has constant density, although there is growing evidence for the existence of a density profile instead.

Fortunately, the high-excitation species have diagnostic ratios that are almost no density sensitive.

Electron densities are necessary for the derivation of chemical abundances of ions of the type np², such as O⁺. These densities were derived using the following emission-line ratio:

\[ R_{S2} = \frac{I(6716)}{I(6731)}. \]  

(15)

The following expression is proposed to derive the electron density

\[ n_e([\text{S II}]) = 10^{3} \cdot \frac{R_{S2} \cdot a_{0}(t) + a_{1}(t)}{R_{S2} \cdot b_{0}(t) + b_{1}(t)}. \]  

(16)
with \( n_e \) in units of cm\(^{-3} \) and \( t \) in units of 10\(^4 \) K. Using the appropriate fittings and PYNEB with collision strengths from \cite{Tayal2010} gives these polynomial fittings to the coefficients

\[
a_0(t) = 16.054 - 7.79/t - 11.32 \cdot t,
\]
\[
a_1(t) = -22.66 + 11.08/t + 16.02 \cdot t,
\]
\[
b_0(t) = -21.61 + 11.89/t + 14.59 \cdot t.
\]  
\( b_1(t) = 9.17 - 5.09/t - 6.18 \cdot t. \quad (17) \)

This expression fits the density calculated by PYNEB better than a 1% for temperatures in the range \( 0.6 < t_e < 2.2 \) and densities in the range \( 10 < n_e < 1000 \). Here, \( t \) is generally \( t[O \text{ III}] \), although an iterative process could be used to calculate it with \( t[\text{S II}] \) given that this temperature, like \( t[O \text{ III}] \), a type np\(^3 \) ion, is density dependent. The ratio used in this case is

\[
R_{S2}^t = \frac{I(6717) + I(6731)}{I(4068) + I(4076)}. \quad (18) \]

For the [S II] auroral lines it is enough to measure one of them, as they are related by a fixed theoretical ratio, \( I(4068) \text{ Å} \approx 3 \cdot I (4076) \text{ Å} \). We can calculate in this way the [S II] temperature:

\[
t([\text{S II}]) = a_0(n) + a_1(n) \cdot R_{S2}^t + \frac{a_2(n)}{R_{S2}^t} + \frac{a_3(n)}{R_{S2}^t}, \quad (19) \]

where

\[
a_0(n) = 0.99 + \frac{34.79}{n} + \frac{321.82}{n^2},
\]
\[
a_1(n) = -0.0087 + \frac{0.628}{n} + \frac{5.744}{n^2},
\]
\[
a_2(n) = -7.123 + \frac{926.5}{n} - \frac{94.78}{n^2},
\]
\[
a_3(n) = 102.82 + \frac{768.852}{n} - \frac{5113}{n^2}. \quad (20) \]

also fitted with the coefficients by \cite{Tayal2010} in the range \( t = 0.8 \) to 2.5 in units of \( 10^4 \) K and \( n_e \) up to 500 cm\(^{-3} \) with a precision better than 2%.

When the [S II] auroral lines are not available it is usually assumed that \( t([\text{S II}]) \approx t[O \text{ II}] \). There is evidence, however, suggesting a somewhat lower value. From the models used in \cite{Perez-Montero2003}, it is obtained a lineal fitting:

\[
t([\text{S II}]) = 0.71 \cdot t([\text{O II}]) + 0.12 \quad (21) \]

for a 100 cm\(^{-3} \) number density. For lower densities, this expression seems to be valid. In any case, for the few objects for which we have a simultaneous measurement of both temperatures, the dispersion is quite large as can be seen in lower left panel of Figure 5 for H\( \alpha \) galaxies.

Direct measurements of the [S III] temperature become possible with the availability of the collisional lines in the near-IR:

\[
R_{S3} = \frac{I(9069) + I(9532)}{I(6312)}. \quad (22) \]

This expression can be simplified in case of lacking one of the near-IR lines, knowing that \( I(9532 \text{ Å}) \approx 2.44 \cdot I(9069 \text{ Å}) \). With this ratio, it is possible the corresponding temperature with the following fitting in the range \( t = 0.6–2.5 \) using the collision strengths from \cite{Hudson2012}.

\[
t([\text{S III}]) = 0.5147 + 0.0003187 \cdot R_{S3} + \frac{23.64041}{R_{S3}}, \quad (23) \]

with a precision better than 1% in the range \( 0.6 < t ([\text{S III}]) < 1.5 \) and better than 3% up to values \( t([\text{S III}]) = 2.5 \). These values enhance in less than a 3% when the considered density goes from 100 to 1000 cm\(^{-3} \).

As discussed in \cite{Garnett1992}, \( t([\text{S III}]) \) is in between the temperatures of \( [\text{O III}] \) and of \( [\text{O II}] \) and allows us to calculate the \( \text{S}^{2+} \) abundance from just the 6312 Å line in high-metallicity objects. In case that the \( [\text{S III}] \) cannot be measured, it is possible to derive \( t([\text{S III}]) \) from \( t([\text{O III}] \) and vice versa. The empirical fitting given by \cite{Hagele2006} is

\[
t([\text{S III}]) = (1.19 \pm 0.08) \cdot t([\text{O III}]) - (0.32 \pm 0.10), \quad (24) \]

which can be seen in left lower panel of Figure 5.

### 3.3. Nitrogen

The \( T_e \) of \([\text{N II}]\) can be calculated using the ratio

\[
R_{N2} = \frac{I(6548) + I(6583)}{I(5755)} \quad (25) \]

which, with the corresponding fitting leads to the expression

\[
t([\text{N II}]) = 0.6153 - 0.0001529 \cdot R_{S2} + \frac{35.3641}{R_{N2}}, \quad (26) \]

also in units of \( 10^4 \) K in the range \( t = 0.6–2.2 \) using collision strengths from \cite{Tayal2011}. This fit gives a precision better than 1% in the range \( 0.7 < t([\text{N II}]) < 2.2 \), and better than 3% in the range \( 0.6 < t([\text{N II}]) < 0.7 \). It was calculated for a density of 100 cm\(^{-3} \), but for a density of 1000 cm\(^{-3} \), the temperature is reduced in less than a 1%.

The nebular lines of \([\text{N II}]\) are very close to H\( \alpha \), so they sometimes appear blended to this line; therefore, it is not possible to measure both of them. In this case, it is often assumed the following theoretical relation between them, \( I(6583) \approx 2.9 \cdot I(6548) \). Besides, the auroral line of \([\text{N II}]\) is affected by recombination emission, which can be corrected using the next expression proposed by \cite{Liu2001}:

\[
\frac{I_8(5755)}{I(H\beta)} = 3.19 \cdot r^{0.30} \cdot \frac{N_2^2}{H^+} \quad (27) \]

in the range between 5000 and 20,000 K.
Unfortunately, the auroral line has very low signal-to-noise ratio (S/N), so it is usually considered the approximation \( t([\text{N} III]) \approx t([\text{O} II]) \) as valid. This relation is confirmed by photoionization models, but is quite sensitive to density and the inner ionization structure of the nebula and it is possible to reach values closer to \( t([\text{S} III]) \) in some cases; therefore, in all cases it cannot be taken without any sort of uncertainty.

Another possibility is to calculate \( t([\text{N} II]) \) directly from \( t([\text{O} III]) \) using the expression derived using photoionization models by Pérez-Montero & Contini (2009), as can be seen in lower right panel of Figure 5:

\[
\frac{1.85}{t([\text{O} III])^{-1} + 0.72} \quad (28)
\]

### 3.4. Balmer Temperature

The Balmer temperature is an alternative to other temperatures calculated using collisionally excited lines. It depends on the value of the Balmer jump (BJ) in emission (i.e., the continuum nebular emission at a bluer wavelength than the Balmer series). To measure this value, it is necessary to fit the continuum in both sides of the discontinuity (\( \lambda_B = 3646 \, \text{Å} \)). An example of the measurement of the BJ in an the optical spectrum of an H II galaxy can be seen in Figure 6.

The contribution of the underlying stellar population affects, between other factors, to the emission of hydrogen lines near from the BJ. The increment in the number of lines at shorter wavelengths produces blends between them that trend to reduce the level of the continuum at a redder wavelength of the discontinuity, so it is necessary to take into the account all this in the final uncertainty.

Once measured, the BJ and the Balmer temperature (T(Bac)) is measured from the quotient of the flux of the jump and the emission of the line H11 by means of the expression given in Liu et al. (2001):

\[
T(Bac) = 368 \times (1 + 0.259y^+ + 3.409y^{++}) \times \left( \frac{BJ}{H11} \right)^{3/2}
\]

where \( y^+ \) and \( y^{++} \) are the ionic abundances of helium once and twice ionized, respectively, and BJ is in ergs cm\(^{-2}\) s\(^{-1}\) Å\(^{-1}\).

### 3.5. Other Temperatures and Densities

There are other collisional excited lines for other ions in the optical spectrum, but their corresponding temperatures or densities cannot be directly measured using the appropriate emission line ratios in the optical or their auroral lines are too weak to be detected. This is the case for [Ar IV], for instance, for which we can derive the density in the inner nebula, or the temperatures of the rest of ions for which the corresponding auroral line are not available in the observed spectral range, or there is not enough S/N to detect their recombination lines. In this case, it usually takes some assumptions about the gas structure, and the position of each species is associated to another ion whose temperature is known. This is the case of the next ions, assuming the three-zone temperature sketch proposed by Garnett (1992):

\[
t([\text{Ne} III]) \approx t([\text{Fe} III]) \approx t(\text{He II}) \approx t([\text{Ar IV}])
\]

\[
\approx t([\text{O} III]) \approx t_h \quad (30)
\]

\[
t([\text{Ar} III]) \approx t([\text{S} III]) \approx t_m \quad (31)
\]

\[
t([\text{S} II]) \leq t([\text{N} II]) \approx t([\text{O} II]) \approx t_l. \quad (32)
\]

### 4. Ionic and Total Chemical Abundances

In what follows, the expressions used to derive the chemical abundances of the ions whose emission lines can be measured in the optical spectrum will be described. These formulae use the appropriate electron densities and temperatures obtained in the determination of the thermal structure of the gas. Most of the fittings follow equations with the same mathematical relations as those proposed by Pagel et al. (1992).

In addition, to derive total chemical abundances, the ionization correction factor for each species will be also described. ICFs are used to calculate total abundances from the observed ions of that element in the optical range, which usually do not fulfill all the ionic stages present in the gas:

\[
\frac{N(X)}{N(H)} = ICF(X_{obs}) \cdot \frac{N(X_{obs})}{N(H^+)} \quad (33)
\]
4.1. Helium

Helium lines, as equal as hydrogen ones in the visible spectrum, have a recombination nature and they are generally strong and numerous, although many of them are usually blended with other lines. Besides, they are affected by absorption of underlying stellar population by fluorescence or by collisional contribution.

The total He abundance can be calculated in the optical spectrum using lines of He I and He II. Following the same equations as those described in Olive & Skillman (2004), once subtracted, the stellar absorption and reddening correction has been carried out and the abundance of He$^+$ can be derived for each He I RL as

$$y^+(\lambda) = \frac{I(\lambda)}{I(H\beta)} \cdot \frac{F_{\lambda}(\lambda, n, t)}{f_{\lambda}(n, t, \tau)},$$

(34)

where $F_{\lambda}(\lambda, n, t)$ is the theoretical emissivity scaled to H$\beta$ and $f_{\lambda}$ is the optical depth function. It generally uses the strongest lines, including He I $\lambda\lambda$ 4471, 5876, 6678, and 7065 Å, and then $y^+$ is calculated using a weighted mean; however, a precise determination of He abundance requires the use of as many lines as possible (see Peimbert et al. 2002).

Using PYNEB with the atomic data from Porter et al. (2013), the theoretical emissivities related to H$\beta$ can be calculated:

$$F_{4471} = (2.0301 + 1.5 \cdot 10^{-5} \cdot n) \cdot t^{0.1463-0.0005n},$$

$$F_{5876} = (0.745 - 5.1 \cdot 10^{-5} \cdot n) \cdot t^{-0.226-0.0011n},$$

$$F_{6678} = (2.612 - 0.000146 \cdot n) \cdot t^{0.2355-0.155n},$$

$$F_{7065} = (4.329 - 0.00246 \cdot n) \cdot t^{-0.368-0.0017n}$$

(35)

with $t$ in units of $10^4$ K and $n$ in units of cm$^{-3}$ and calculated for temperatures between 8000 and 25,000 K and densities between 10 and 1000 cm$^{-3}$. The precision of the fittings is better than 1% in all cases. Normally, it takes the temperature of [O III], as it is the most precise. The optical depth functions can be taken from Olive & Skillman (2004), but these are only important for high-extinction objects, and when it is required, a very precise measurement of this abundance (e.g., for the search for the primordial helium abundance).

The abundance of He$^2+$ can be calculated using the He II 4686 Å line and a high-excitation temperature by means of the recombination coefficients by Storey & Hummer (1995) using the following expression:

$$y^{2+} = \frac{I(4686)}{I(H\beta)} \cdot 0.0416 \cdot t^{-0.146}$$

(36)

calculated in the same range as He I emissivities.

Then, the total He abundance can be derived the addition of the abundances of the two ions

$$y = y^+ + y^{2+},$$

(37)

where $y$ is the relative abundance of helium (He/H), $y^+$ is the abundance of He$^+$, and $y^{2+}$ is the abundance of He$^{2+}$.

4.2. Oxygen

The chemical abundance of O$^+$ can be derived with the relative intensity of [O II] 3726, 3729 Å emission lines to H$\beta$, and the corresponding temperature using the following expression obtained from fittings to PYNEB using the default collision strengths from Pradhan et al. (2006) and Tayal (2007):

$$12 + \log \left( \frac{O^+}{H^+} \right) = \log \left( \frac{I(3726) + I(3729)}{I(H\beta)} \right)$$

+ 5.887 + \frac{1.641}{t_H} - 0.543 \cdot \log(t_t)

+ 0.000114 \cdot n_e,$$

(38)

with a precision better than 0.01 dex in the temperature range $0.7 < t(O^+) < 2.5$ and density of 100 cm$^{-3}$. For a density of 1000 cm$^{-3}$, the precision is better than 0.02 dex.

Alternatively, Kniazev et al. (2003) suggest the use of the 7319,7330 Å doublet in those objects observed with a setup that does not cover the 3727 [O II] line:

$$12 + \log \left( \frac{O^+}{H^+} \right) = \log \left( \frac{I(7320) + I(7330)}{I(H\beta)} \right)$$

+ 7.21 + \frac{2.511}{t_H} - 0.422 \cdot \log(t_t)

+ 10^{-3.40} n_e (1 - 10^{-3.44} \cdot n_e).$$

(39)

Regarding O$^2+$, its chemical abundance was derived using the relative intensity of [O III] 4959, 5007 Å emission lines to H$\beta$ and the corresponding temperature using the following expression obtained from fittings to PYNEB:

$$12 + \log \left( \frac{O^{2+}}{H^+} \right) = \log \left( \frac{I(4959) + I(5007)}{I(H\beta)} \right) + 6.1868$$

+ \frac{1.2491}{t_H} - 0.5816 \cdot \log(t_H)$$

(40)

with a precision better than 0.01 dex in the temperature range $0.7 < t(O^{2+}) < 2.5$. A change in the density from 10 to 1000 cm$^{-3}$ implies a decrease of less than 0.01 dex in the derived abundance.

The total oxygen abundance can be approximated by

$$\frac{O}{H} = \frac{O^+ + O^{2+}}{H^+},$$

(41)

given that due to the charge exchange reaction, the relative fractions of neutral oxygen and hydrogen are similar:

$$\frac{O^0}{O} = \frac{H^0}{H}.$$}

(42)

However, in some high-excitation spectra where the He II 4586 Å is seen, it can be considered that part of the O is under
the form of O$^3+$. In that case, it can be assumed that

$$\text{ICF}(O^+ + O^2+) = 1 + \frac{y_2^+}{y^+}. \quad (43)$$

### 4.3. Sulfur

The abundances are obtained from the 6717 and 6731 Å lines for S$^+$, and by the 9069 and 9532 Å lines for S$^{2+}$, although for the latter, the 6312 Å line can also be used using the following expressions:

$$12 + \log\left(\frac{S^+}{H^+}\right) = \log\left(\frac{I(6717) + I(6731)}{I(H\beta)}\right)
+ 5.463 + \frac{0.941}{t_i} - 0.37 \cdot \log(t_i) \quad (44)$$

and

$$12 + \log\left(\frac{S^{2+}}{H^+}\right) = \log\left(\frac{I(9069) + I(9532)}{I(H\beta)}\right)
+ 5.983 + \frac{0.661}{t_m} - 0.527 \log(t_m). \quad (45)$$

In case the near-IR [S III] lines cannot be measured but the auroral line at 6312 Å is available with good S/N, it is possible to derive S$^{2+}$ abundances from the expression:

$$12 + \log\left(\frac{S^{2+}}{H^+}\right) = \log\left(\frac{I(6312)}{I(H\beta)}\right)
+ 6.695 + \frac{1.664}{t_m} - 0.513 \cdot \log(t_m). \quad (46)$$

These were derived using the same collisional coefficients as used for the derivation of expressions for temperature. The fittings have a precision better than 0.01 dex in the temperature range $0.7 < t < 1$. The ICF for sulfur takes into account the S$^{3+}$ abundance, which cannot be determined in the optical range. A good approximation is given by Stasińska (1978):

$$\text{ICF}(S^+ + S^{2+}) = \left[1 - \left(\frac{O^{2+}}{O^+ + O^{2+}}\right)^\alpha\right]^{-1/\alpha}. \quad (47)$$

Although it is customary to write this expression as a function of the O$^+/$(O$^+ + O^{2+})$ ionic fraction, we reformulated it in terms of O$^{2+}/$(O$^+ + O^{2+})$ because the errors that are associated to O$^{2+}$ are considerably smaller than for O$^+$, and for a sample of objects with observed [S IV] line at 10.5 μm, it was derived $\alpha \approx 3.27$ (Dors et al. 2016).

### 4.4. Nitrogen

We can calculate N$^+$ abundance from the 6548 and 6583 Å lines. The expression to calculate N$^+$/H$^+$ abundance using these lines and assuming a low-excitation temperature is

$$12 + \log\left(\frac{N^+}{H^+}\right) = \log\left(\frac{I(6548) + I(6583)}{I(H\beta)}\right)
+ 6.291 + \frac{0.90221}{t_i} - 0.5511 \cdot \log(t_i) \quad (48)$$

with a precision better than 0.01 dex in the temperature range $0.6 < t < 2.2$. It decreases less than 0.01 dex when the considered density goes from 100 to 1000 cm$^{-3}$.

One can calculate quite precisely the total abundance of Nitrogen assuming that

$$\frac{N^+}{N} = \frac{O^+}{O}, \quad (49)$$

owing to the similarity of ionization potentials of O$^+$ and N$^+$, which leads to the corresponding ICF:

$$\text{ICF}(N^+) = \frac{O}{O^+}. \quad (50)$$

The ratio N$^+$/O$^+$ can be derived directly from the expression

$$\log\left(\frac{N^+}{O^+}\right) = \log\left(\frac{I(6583) + I(3726) + I(3729)}{I(H\beta)}\right)
+ 0.493 - 0.025 \cdot \frac{0.687}{t_i} - 0.1621 \cdot \log(t_i). \quad (51)$$

### 4.5. Neon

Ne has [Ne III] prominent emission lines in the blue part of the spectrum and can be a good tracer of metallicity, as it is not depleted into dust grains. Because one of the emission lines (3968 Å) usually appears blended with and H I recombination line (H7), the Ne$^{2+}$ ionic abundance can be derived using the following expression and the electron temperature of the high-excitation zone (usually t([O III])):

$$12 + \log\left(\frac{Ne^{2+}}{H^+}\right) = \log\left(\frac{I(3968) + I(6583)}{I(H\beta)}\right)
+ 6.947 - \frac{1.614}{t_h} - 0.4291 \cdot \log(t_h), \quad (52)$$

with a precision better than 2% in the range of temperature from 0.6 to 2.2 in units of 10$^4$ K. The collisional coefficients are from McLaughlin et al. (2000).

The ionization correction factor for neon can be calculated according to the expression given by Pérez-Montero et al. [2016].
where \( x = O^{2+}/(O^+ + O^{2+}) \). This expression deviates from the classical approximation \( Ne/O \approx Ne^{2+}/O^{2+} \) used to derive total neon abundances.

### 4.6. Argon

For argon, we use the \([\text{Ar} \text{III}] 7137 \text{ Å} \) line. It is possible to measure the lines of \([\text{Ar} \text{IV}] \) at 4713 and 4740 Å, as well. Nevertheless, the first of them usually appears blended with another line of \( \text{HeII} \) at 4711 Å that is difficult to correct, so it is better to use the second and brighter to calculate the ionic abundance of \( \text{Ar}^{3+} \),

\[
12 + \log \left( \frac{\text{Ar}^{3+}}{H^+} \right) = \log \left( \frac{I(7135)}{I (H \beta)} \right) + 6.100 + \frac{0.86}{t_m} - 0.404 \cdot \log(t_m)
\]

(54)

\[
12 + \log \left( \frac{\text{Ar}^{3+}}{H^+} \right) = \log \left( \frac{I(4740)}{I (H \beta)} \right) + 6.306 + \frac{1.232}{t_h} - 0.703 \cdot \log(t_h),
\]

(55)

both with a precision better than 2\% in the fitting in the same temperature range than in Ne using the collisional coefficients from Galavis et al. (1995) for \( \text{Ar}^{2+} \) and Ramsbottom & Bell (1997) for \( \text{Ar}^{3+} \).

As in the case of neon, the total abundance of argon can be calculated using the ionization correction factors (ICF(\( \text{Ar}^{2+} \)) and the ICF(\( \text{Ar}^{2+} + \text{Ar}^{3+} \)) given by Pérez-Montero et al. (2007). The first one can be used only when we cannot derive a value for \( \text{Ar}^{3+} \). The expressions for these ICFs are

\[
\text{ICF}(\text{Ar}^{2+}) = 0.596 + 0.967(1 - x) + \frac{0.077}{(1 - x)}
\]

(56)

\[
\text{ICF}(\text{Ar}^{2+} + \text{Ar}^{3+}) = 0.928 + 0.364(1 - x) + \frac{0.006}{(1 - x)}
\]

(57)

where \( x = O^{2+}/(O^+ + O^{2+}) \).

### 4.7. Iron

The abundance of Fe is usually derived from the absorption stellar features, but there are some high-excitation \([\text{Fe} \text{III}] \) lines that can be used to derive \( \text{Fe}^{2+} \) abundances in the ionized gas-phase. For instance, from 4658 Å from PYNEB it is obtained:

\[
12 + \log \left( \frac{\text{Fe}^{2+}}{\text{H}^+} \right) = \log \left( \frac{I(4658)}{I (H \beta)} \right) + 6.288 + \frac{1.408}{t_h} - 0.203 \cdot \log(t_h)
\]

(58)

using the collisional coefficients of \( \text{Fe}^{2+} \) from Zhang (1996) in the range \( t = 0.8–2.5 \). The ICF to derive the total Fe abundance was proposed by Rodríguez & Rubin (2004):

\[
\text{ICF}(\text{Fe}^{2+}) = \left( \frac{O^+}{O^{2+}} \right)^{0.09} \left[ 1 + \frac{O^{2+}}{O^+} \right].
\]

(59)

### 5. Strong-line Methods Calibrated Using the DM

In absence on any of the auroral lines, it is not possible to obtain the electron temperature and hence to derive the thermal structure and the ionic and total abundances of the elements whose lines can be measured in the optical spectrum. However, some of the other nebular CELs can be measured and used as indicators of the chemical content of the gas.

As quoted above, many of the calibrations of these so-called strong-line methods have been made in the literature attending to different criteria or calibration sample, so it is difficult to assess if they are compatible. The most important rule to follow is to try to be consistent if a comparative analysis is to be made. This section describes the different strong-line methods calibrated with large samples of objects with a previous determination of the electron temperature, so that they are in principle, compatible with the direct method. For the sake of consistency, only those calibrations calculated using the same methodology as described in the above sections are cited; using a very similar sample of objects, they were selected only with criterion having at least one measured electron temperature, and can be ionized by massive star formation with no restriction on the resulting chemical abundances. However, it is worth mentioning the existence of other calibrations based on the direct method such as Pilyugin et al. (2010), Pilyugin & Grebel (2016), or Marino et al. (2013), among others.

#### 5.1. Calibrations of the Electron Temperature

Sometimes it is possible to derive an electron temperature and its corresponding ionic abundance. Nevertheless, the total abundance cannot be calculated, because the lines corresponding to other excitation lines cannot be measured. This is the case of \( O/\text{H} \) when the \([\text{OII}] 3727 \) Å lines are out of the spectral range or their corresponding auroral lines at 7319 and 7330 Å are too faint.

In this case, the total oxygen abundance can be estimated directly from the \([\text{OIII}] \) electron temperature as proposed by Amorín et al. (2015), which can be seen in left panel of
Figure 7. Left panel: empirical relation between electron temperature and total oxygen abundance (Amorín et al. 2015). Right panel: relation between oxygen abundance and the R23 parameter from the sample of objects in Pérez-Montero & Contini (2009) and non-linear fittings for the lower and upper branches assuming the average excitation in each range. (A color version of this figure is available in the online journal.)

Figure 7:

\[ 12 + \log(O/H) = 9.22(\pm0.03) - 0.89(\pm0.02) \cdot t([O \text{ III}]), \]

(60)

with a dispersion of 0.15 dex. This expression can also be used to derive the temperature from a strong-line derivation of O/H.

5.2. Parameters based on [O II] and [O III] lines

The most widely used parameter based on oxygen lines that can be related to metallicity is R23 given by Pagel et al. (1979):

\[ R23 = \frac{I(3727)}{I(H\beta)} + \frac{I(4959, 5007)}{I(H\beta)}. \]

(61)

However, there are some known limitations to give a calibration of this parameter with O/H. The main limitation is that the relation is double-valued: R23 grows with O/H for low-Z and decreases for high-Z, as the main source of cooling when the temperature is lower are hydrogen recombination lines. In the so-called turnover region (around $12 + \log(O/H) \approx 8.0–8.3$, as can be seen in right panel of Figure 7), the dispersion is very high and it is very difficult to provide an accurate determination.

For this tutorial and for the sake of consistency, I provide fittings to the sample of objects with a direct determination of O/H in Pérez-Montero & Contini (2009), following the same functional expressions given by Kobulnicky et al. (1999) based on R23 and on the excitation as a function of the ratio of [O II] and [O III]. The fittings for both branches at an average excitation in each branch are shown in Figure 7.

In the upper branch ($12 + \log(O/H) > 8.25$),

\[ 12 + \log(O/H) = 8.656 - 0.411 \cdot x - 0.586 \cdot x^2 + 0.469 \cdot x^3 - y \cdot ( -0.224 + 0.309 \cdot x + 0.741 \cdot x^2 + 0.722 \cdot x^3 ), \]

(62)

where $x = \log(R23)$ and $y = \log([O \text{ II}]3727/[O \text{ III}]4959 + 5007)$. The dispersion of this fitting is taken as the standard deviation of the residuals to the abundances from the direct method is 0.17 dex.

For the lower branch ($12 + \log(O/H) < 8.0$),

\[ 12 + \log(O/H) = 7.247 - 1.196 \cdot x + 4.078 \cdot x^2 - 2.194 \cdot x^3 - y \cdot (1.076 - 3.735 \cdot x + 5.671 \cdot x^2 - 2.947 \cdot x^3), \]

(63)

with a dispersion of 0.14 dex.

In cases where the [O III] are not observed owing the studied spectral range, Pérez-Montero et al. (2007) propose to use the empirical relation with [Ne III] at 3968 Å ($=[O \text{ III}] 5007/15.37$) and also used a hydrogen recombination line at a blue wavelength, such as Hγ or Hδ.

5.3. Parameters based on [N II] lines

The simplest strong-line ratio used to derive O/H using [N II] lines is the N2 parameter, defined by Storchi-Bergmann...
et al. (1994):

\[
N2 = \log \left( \frac{I(6583)}{I(H\alpha)} \right). \tag{64}
\]

Notice that, contrary to R23, the log is in the definition of the parameter. This parameter has the advantage of being totally independent on reddening correction or flux calibration uncertainties. The linear fitting proposed by Pérez-Montero & Contini (2009) gives

\[
12 + \log(O/H) = 9.07 + 0.79 \cdot N2, \tag{65}
\]

valid for all the range of metallicity with a dispersion of 0.34 dex. This relation can be seen in Figure 8. This is usually used to decide to the branch of the R23 parameter, but the dispersion is very high owing to a large dependence on ionization parameter and also because of the dispersion in the O/H-N/O relation.

The dependence on \(\log U\) can be reduced through the definition of the O3N2 parameter (Alloin et al. 1979):

\[
O3N2 = \log \left( \frac{I(5007)}{I(H\beta)} \cdot \frac{I(H\alpha)}{I(6583)} \right). \tag{66}
\]

The linear fitting proposed by Pérez-Montero & Contini (2009) leads to

\[
12 + \log(O/H) = 8.74 - 0.31 \cdot O3N2 \tag{67}
\]

with a dispersion of 0.32 dex, but for \(O3N2 > 2.0\) as the O3N2 parameter is constant for lower metallicities, as can be seen in Figure 8.

Among other strong emission line ratios the parameter N2O2,

\[
N2O2 = \log \left( \frac{I(6583)}{I(3727)} \right), \tag{68}
\]

can be used to derive N/O, as can be seen in Figure 8. The linear fitting proposed by Pérez-Montero & Contini (2009) gives

\[
\log(N/O) = 0.93 \cdot N2O2 - 0.20 \tag{69}
\]

with a dispersion of 0.24 dex for all N/O values. A similar parameter for a lower wavelength baseline is the N2S2 parameter,

\[
N2S2 = \log \left( \frac{I(6583)}{I(6717, 6731)} \right), \tag{70}
\]

whose linear fitting gives

\[
\log(N/O) = 1.26 \cdot N2S2 - 0.86 \tag{71}
\]

with a dispersion of 0.31 dex according to Pérez-Montero & Contini (2009).

5.4. Parameters Based on [SII] and [SIII] Lines

Strong-line methods based on sulfur emission lines provide accurate oxygen abundances when the red and near-IR spectral optical range is observed and measured. This is based on the fact that both O and S are primary elements, hence the S/O ratio is not expected to vary. Following an analogous definition as for oxygen lines, Vilchez & Esteban (1996) defined the S23 parameter based on [S II] and [S III] lines as

\[
S23 = \frac{I(6717, 6731) + I(9099, 9532)}{I(H\beta)} \tag{72}
\]

The polynomial fitting proposed by Pérez-Montero & Díaz (2005) to derive total oxygen abundance is

\[
12 + \log(O/H) = 8.15 + 0.85 \cdot x + 0.58 \cdot x^2, \tag{73}
\]

where \(x = \log(S23)\). This can be used up to solar metallicity (i.e., \(12 + \log(O/H) = 8.69\)) with a dispersion of 0.20 dex as the standard deviation of the residuals to the O/H derived from the direct method. This relation can be seen in left panel of Figure 9. Similarly, Pérez-Montero et al. (2006) propose a fitting to derive total sulfur abundances:

\[
12 + \log(S/H) = 6.62 + 1.860 \cdot x + 0.382 \cdot x^2, \tag{74}
\]

with a dispersion of 0.185 dex in the range of \(-1.0 \lesssim \log(S23) \lesssim 0.5\).

For high metallicities, Pérez-Montero & Díaz (2005) propose a polynomial fitting to a combination of both S12 and R23, as can be seen in right panel of Figure 9. This fitting gives

\[
12 + \log(O/H) = 9.09 + 1.03 \cdot x - 0.22 \cdot x^2, \tag{75}
\]

where \(x = \log(S23/R23)\) and the fitting to the objects has a dispersion of 0.27 dex.

6. Summary

This paper reviewed the procedure to analyze the optical emission-line spectrum from a gaseous nebula ionized by massive star formation. Both recombination lines emitted from H and He, and collisionally excited emission lines from metallic ions can be used to derive the physical properties and the ionized and total abundances using the so-called direct method. To do so, it has been provided expressions derived from the software PYNeb (Luridiana et al. 2012) under typical conditions observed in H II regions and using the most updated sets of atomic coefficients.

The direct method relies on the determination of the electronic temperature using the emission-line ratios between strong nebular lines and faint auroral emission lines. It is also assumed that the complete ionization structure is comprised in the observed spectrum. In this situation, one can calculate the thermal and density radial structure of the distribution of ionized gas, measuring as many temperatures as possible and solving their dependence on density. Alternatively, one can
assume relations between zone temperatures from empirical or model-based relations. Then the ionic abundances for the corresponding emission lines observed in the spectrum can be derived. Finally, the total chemical abundances are calculated by means of ionization correction factors that are used to derive the abundances of the ions not seen in the observed spectrum.

In case no auroral lines are observed in the optical spectrum, one can resort to strong-line methods based on the measurement of the nebular lines. These methods lead formally to determinations of the abundances that are much less accurate than the direct method, due to additional dependencies of the involved lines on other functional parameters (e.g., Pérez-Montero & Díaz 2005). However, most the important thing is that any comparison between abundances derived from the direct method and from strong-line calibrations is done consistently. This can happen for data sets in which the auroral

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**Figure 8.** Relations between strong-line parameters based on [N II] emission lines and ionic ratios from Pérez-Montero & Contini (2009). From left to right and from top to bottom: N2 with O/H, O3N2 with O/H, N2O2 with N/O, and N2S2 with N/O.

(A color version of this figure is available in the online journal.)
lines are not observed in all points. In this case, using strong-line methods calibrated empirically or using models consistent with the direct method are convenient.

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Figure 9. Left: relations and calibrations between the total oxygen abundance and the S23 parameter. Right: S23/R23 parameter from Pérez-Montero & Díaz (2005).
