HII-CHI-mistry: A new model-based method to derive chemical abundances consistent with the direct method

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Abstract

In this contribution it is described the method HII-CHI-mistry to derive ionic chemical abundances of oxygen and nitrogen and the ionization parameter from emission-line optical spectra ionized by massive stars. This method is based on a χ^2 approach comparing the most prominent collisional emission lines with the results from a grid of photoionization models covering a wide range of possible solutions. The results of this method are totally consistent with the derivation of the abundances from the direct method. In case of absence of any emission-line ratio sensitive to the electron temperature, the method assumes an empirical law between $12 + \log(O/H)$ and $\log U$ that also leads to a solution in all metallicity regimes in agreement with the direct method. A similar approach is used in case that any emission-line ratio sensitive to the nitrogen-to-oxygen ratio is not attained and [NII] are used to derive oxygen abundance.

1 Introduction

Deriving metallicities from the line-spectrum emitted by HII regions is not an issue trivial to solve when only collisional lines are available and an estimate of the electron temperature cannot be obtained. There is a known disagreement between the empirical calibrations of the strong-line methods (e.g. R23, N2, O3N2) and photoionization models (e.g. [4]). Besides, not all strong-line methods have a single dependence with the metallicity and they are not equally efficient for all ranges, so they are not appropriate for the study of Z in datasets over a great variation of their properties that have to be analyzed consistently (i.e. gradients of metallicity across disks, mass-metallicity relation).

Another problem arises when one tries to derive oxygen abundances using strong-line methods based partially on [NII] lines (e.g. N2, O3N2, N2O2). Nitrogen-to-oxygen ratio can have a large dispersion around the predictions of closed-box chemical evolution models as

oxygen is ejected into the ISM mainly by massive stars and nitrogen by low and intermediate-mass stars. In addition, the behaviors of O/H and N/O can be very different when gas outflows or inflows appear in scene [2]. Therefore, a previous estimate of N/O is necessary when these methods are used to derive O/H [9].

In this way, a new method based on models should address some of the limitations of similar approaches investigated so far, including a realistic assessment of the disagreement with the chemical abundances from the direct method under the same set of input assumptions, the same ionizing spectral energy distribution, the same gas geometry, or the same atomic data. A model-based recipe has the advantage over other empirical calibrations that it can be equally calibrated in all metallicity ranges for sets of available emission lines over different spectral ranges, but the models should also cover a wide range of input conditions including those ratios of chemical abundances relevant for the abundance calculation, such as N/O, as explained above. The method HII-CHI-mistry [10] has been designed to address these queries and it is described in the following sections.

2 Description of the HII-CHI-mistry method

A large grid of photo-ionization models was calculated to obtain emission-lines under different input assumptions. The models were calculated using the code `CLOUDY` v.13.03 [3], assuming a thin shell gas sphere of constant density around a ionizing POPSTAR [7] spectral energy distribution of an instantaneous star-forming burst of 1 Myr at the same metallicity of the gas. A standard Milky-way value for the dust-to-grain ratio was assumed in all models. All chemical abundances, except N, were scaled in solar proportions to O, which has values $12 + \log(O/H)$ from 7.1 up to 9.1 in bins of 0.1 dex, while $\log(N/O)$ was varied from -2.0 up to 0.0 in bins of 0.125 dex. Finally the ionization parameter was varied from $\log U = -4.0$ up to -1.5. This gives place to a total of 3 927 models, that can be retrieved from the 3 MdB database [8] [1]

A weighted χ^2 method is applied to derive the abundances and $\log U$ from a observed set of reddening corrected [OII] 3727Å, [OIII] 4363, 5007 ÅÅ, [NII] 6584 Å, and [SII] 6717,6731ÅÅ emission-line fluxes relative to Hβ by comparing the corresponding emission-lines ratios (O_j) with the same values predicted by the models (T_j):

$$\chi_i^2 = \sum_j \frac{(O_j - T_{ji})^2}{O_j} \tag{1}$$

In a first step, N/O and its uncertainty are estimated using as observables those emission-line ratios sensitive to this abundance ratio (i.e. N2O2, N2S2)

$$\log(N/O)_f = \frac{\sum_i \log(N/O)_i/\chi_i}{\sum_i 1/\chi_i} \tag{2}$$

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[1]The Mexican Million Models Database can be found in `https://sites.google.com/site/mexicanmillionmodels/`. The models of HII-CHI-mistry have reference HII_CHIm.
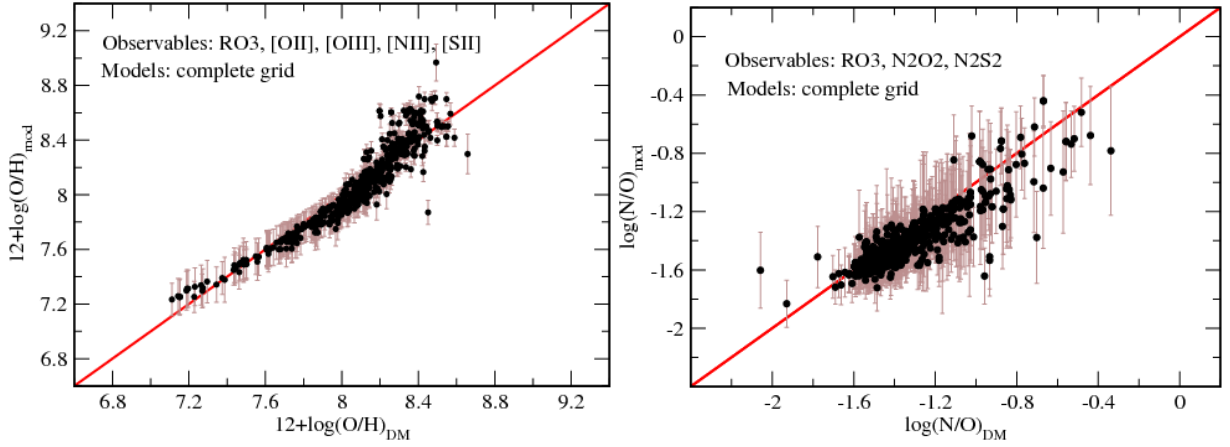
Figure 1:   At left, comparison between the oxygen total abundance obtained from HII-CHI-mistry using all available emission lines and from the direct method for the sample of objects described in the text. The red solid line represents the 1:1 relation. At right, same plot for $\log(N/O)$.

$$(\Delta \log(N/O))^2 = \frac{\sum_i \log((N/O)_f - \log(N/O)_i)^2/\chi_i}{\sum_i 1/\chi_i} \tag{3}$$

In a second step, O/H and $\log U$ are derived with a grid constrained in the N/O closest to the value derived in the previous step. In this way, [NII] can be used to derive metallicities.

$$12 + \log(O/H)_f = \frac{\sum_k (12 + \log(O/H))_k/\chi_k}{\sum_k 1/\chi_k} \tag{4}$$

$$\log U_f = \frac{\sum_k \log U_k/\chi_k}{\sum_k 1/\chi_k} \tag{5}$$

This procedure has been programmed in python language in a publicly available script called `HII-Chi-mistry` in the web page `http://www.iaa.es/~epm/HII-CHI-mistry.html`.

3   Comparison with the direct method

In order to compare the results from the HII-CHI-mistry method with the abundances derived from the direct method, it has been used the sample of objects with a direct estimate of the electron temperature from collisional emission lines made by [6]. Electron densities, temperatures and ionic abundances were re-calculated using sets of atomic coefficients consistent with the photoionization models and the software `PyNeb` [5].

The comparison between the abundances derived using HII-CHI-mistry and those obtained from PyNeb leads to an excellent agreement both for O/H and N/O (see Fig. 1) when all emission lines are available, including those in the electron-temperature sensitive ratio
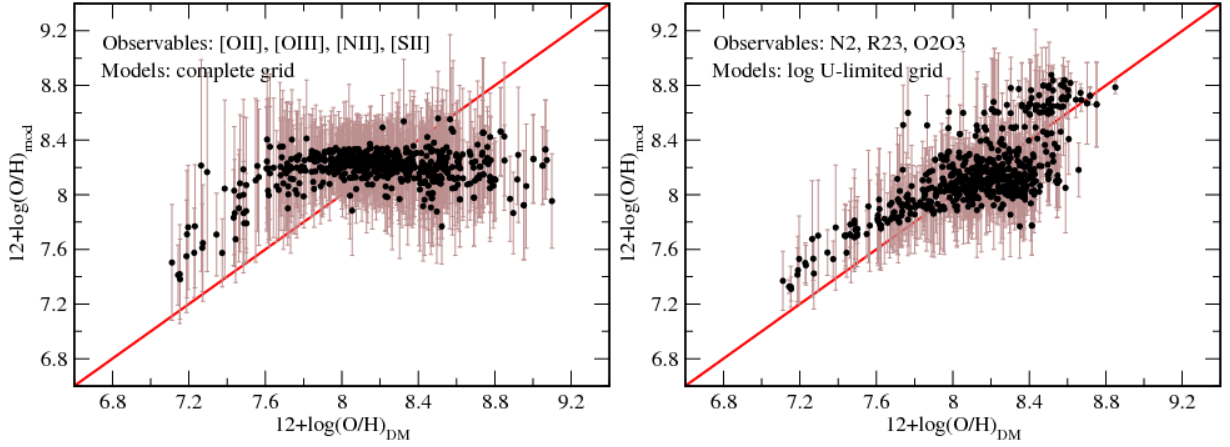
Figure 2: Comparison between oxygen abundance from HII-CHI-mistry and the direct method. At left, when no [OIII] 4363 Å emission line is considered and all models of the grid are used in the calculation. At right, same comparison when a constrained grid in the Z–$\log U$ space is used.

[OIII] 5007/4363 ÅÅ. The dispersion is higher at high Z probably owing to the uncertainty of the assumed relation between the high- (t3) and low-excitation (t2) electron temperatures, as t2 is not usually measured. Anyway, no offset between the abundances derived from models and from the direct method is found, contrary to other widely used model-based recipes.

However, if the [OIII] 4363 Å is not considered in the calculation of O/H, what is quite common in faint/distant and metal-rich objects, no reliable estimation of the metallicity can be achieved even if the space of possible models has been previously constrained in N/O (see left panel of Fig. 2). This means that if no additional assumptions are made and no observational information is available about the electron temperature a reliable estimation of O/H cannot be reached.

Alternatively, the space of parameters of the grid can be limited by considering an empirical law between O/H and $\log U$ (see left panel of Fig. 3). This relation, possibly due to an evolutionary sequence, points to a higher ionization parameter for those metal-poor objects and, on the contrary, higher $\log U$ for metal-rich ones. Nevertheless, before using this relation to constrain the models, It must be kept in mind that this law is somehow arbitrary and not necessarily always valid for all families of objects. Ideally, on should know what specific Z–$\log U$ law to apply for a specific kind of object. Applying this constrained grid in absence of [OIII] 4363 Å emission lines, consistent chemical abundances are obtained, as seen in right panel of Fig. 2, although O/H is slightly overestimated by the models for low Z, but in this regime the auroral [OIII] line is usually well detected. This procedure method leads to trustable Te-consistent abundances in wide ranges of Z.

A similar strategy can be followed in case of absence of a observed emission-line ratio sensitive to N/O (e.g. N2O2, N2S2) if one wants to use [NII] emission lines to obtain the oxygen abundance. As can be seen in left panel of Fig. 4, no reliable oxygen abundance can
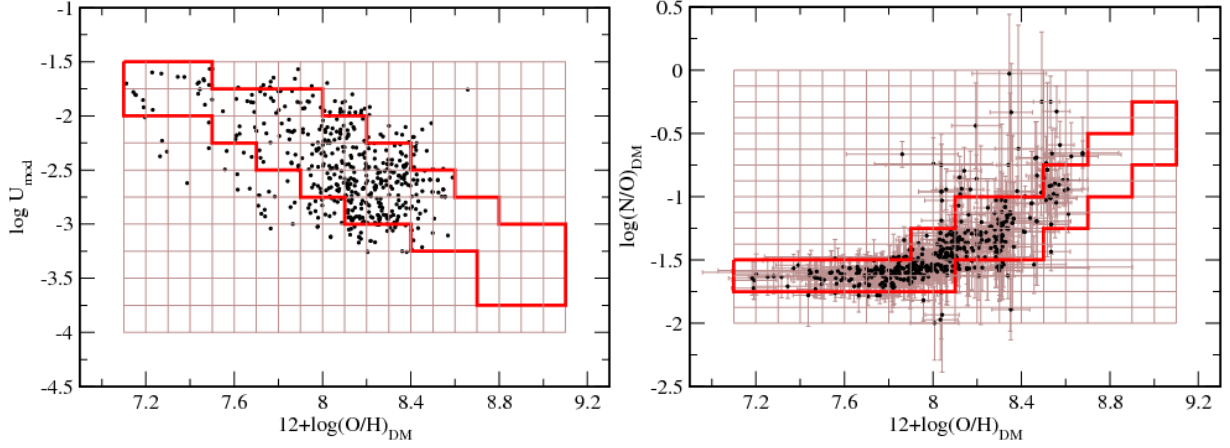
Figure 3: At left, relation between total oxygen abundance and ionization parameter for the sample studied in this work. The solid red line encompasses the most probable combination of parameters occupied by the objects. At right, empirical relation between $12 + \log(O/H)$ and $\log(N/O)$ with the region occupied by the grid of models in case of no available observational information to constrain N/O.
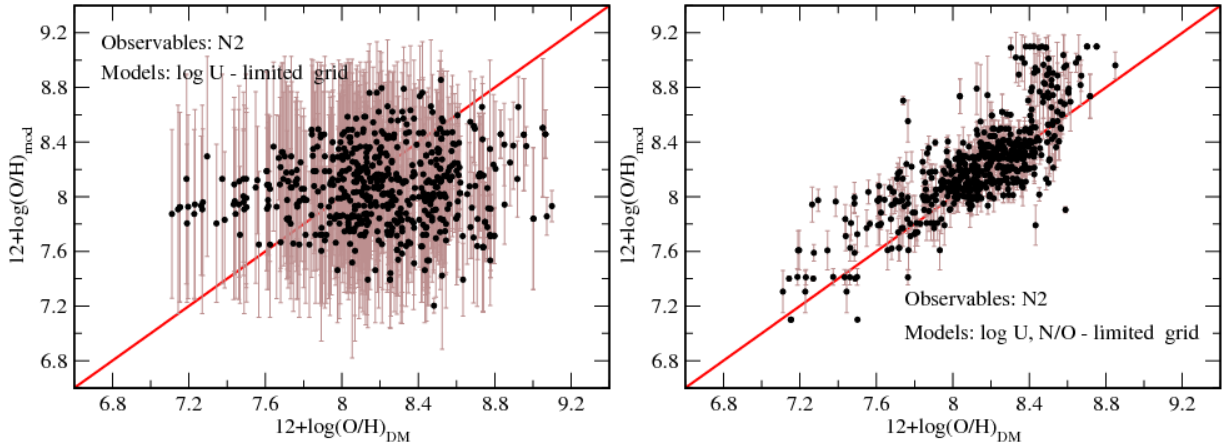

Figure 4: Comparison between oxygen total abundances obtained from HII-CHI-mistry and from the direct method. At left, results using only $[NII]/H\beta$ and no previous estimated of $\log(N/O)$. At right, same comparison with a grid of models with an initial assumption about the grid of models in the O/H-N/O space.

be obtained from [NII]/Hβ if no previous constraints have been assumed in the *O/H-N/O* space. By doing so using an empirical law, as shown in right panel of Fig. 3, we recover a good agreement with the abundances obtained from the direct method. However, as pointed out above with the *O/H*–log *U* relation, this can lead to mistakes in the derivation of *O/H* if the object cannot follow the expected relation, as can happen in objects with extreme star formation rates triggered by massive inflows of pristine gas (e.g. [1]).

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