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On the chlorine abundance in H II regions

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Abstract

Chlorine (Cl) is a chemical element of the group of the halogens and is between the 17th and the 20th most abundant elements in the Solar System. It is thought to be produced from the capture of a proton or neutron by specific alpha-element isotopes during both hydrostatic and explosive oxygen burning, though some contribution may come from Type Ia supernovae. Cl lines are quite rare in stellar spectra, so most of the information available about its abundance comes from analyzing the emission lines of ionized nebulae, especially the collisionally excited lines of Cl^{2+} ([Cl III] $\lambda\lambda$ 5518,5538). Our goal is to accurately determine the Cl abundance in H II regions, and gather more information about its nucleosynthetic origin. For this work we used a sample of observations that encompasses the deepest spectra of H II regions available in the literature, from both the Milky Way and other galaxies in the local Universe, covering a range of oxygen (O) abundances, $12 + \log(O/H)$, from 7.18 to 8.70. As a first step, we determine the most representative electron temperature of the zone of the nebulae where the Cl^{2+} ion lies. To this aim we used a grid of photoionization models and diagnostics valid for other ions, as that parameter cannot be determined directly through [Cl III] lines. We then computed the total Cl abundance using different sets of ionization correction factors to account for the contribution from unseen ionization stages.

1 Introduction

H II regions are nebulae photoionized by the ultraviolet radiation from young, massive Oand B-type stars, with effective temperatures ranging between 28,000 and 50,000 K. These nebulae are key to understanding the present-day chemical composition of the interstellar medium, shaped by stellar nucleosynthesis and Galactic chemical evolution. By studying their emission line spectra, we can derive both the physical conditions of the gas —such as electron density and temperature (n_e, T_e) — and the elemental abundances.

This study focuses on chlorine (Cl), a halogen group element, which is approximately the 17th most abundant element in the Solar System [1]. Cl is mainly analyzed in H II regions, because its spectral lines are extremely rare in stellar spectra, making nebular emission lines the main source of abundance data. The [Cl III] lines at 5517 and 5537 Å, the brightest Cl lines in the optical range, are typically used to determine the Cl abundance.

Under typical nebular conditions, Cl^{2+} is the main contributor to the total Cl abundance, with smaller contributions of Cl^+ and Cl^{3+} . The lines of these last two ions, such as [Cl II] λ 9123 and [Cl IV] λ 8046, are only detectable in the deepest spectra. In most cases, only [Cl III] lines are available, so ionization correction factors (ICFs) are needed to account for the unseen ions. Additionally, the T_e of the Cl^{2+} zone cannot be easily determined, so we rely on temperature relations and diagnostics for other ions to estimate it. This is the main aim of our study.

2 Photoionization models and observational sample

To achieve the objectives of this project, we used photoionization models to simulate the spectra of H II regions and compute their physical properties. Specifically, we employed the BOND photoionization model grid [9], available in the *Mexican Million Models database* (3MdB) [8], and applied a series of constraints to select the most appropriate models for our observational sample. The analysis of the model outputs was conducted using the PYNEB package [6], which calculates $n_{\rm e}$, $T_{\rm e}$, and ionic abundances from the modeled spectra.

In addition to our primary goal, we aim to verify the applicability of certain temperature relationships to observational data. For this, a sample of 148 H II regions and 120 star-forming galaxies with detected [Cl III] lines has been used. This sample constitutes the largest sample of ionized nebulae with reliable determinations of Cl abundances. We include our own observations (see compilation in [7]) and additional high-quality spectra from the literature. For each region, we reported line intensities and recomputed $n_{\rm e}$, $T_{\rm e}$ and ionic and elemental abundances.

To determine the Cl^{2+} abundance, we initially used $T_e(S^{2+})$, due to their similar ionization potentials. However, when no [S III] diagnostic lines are available, we used a temperature relationship [3]. This brought us back to the models and our main goal: identifying a reliable temperature relationship for Cl^{2+} . Instead of relying on S^{2+} , we explored a relationship between $T_e(Cl^{2+})$ and $T_e(O^{2+})$ and $T_e(N^+)$ obtained from the models, chosen because the ionization potential of Cl^{2+} is intermediate between to those of O^{2+} and N^+ , and $T_e(O^{2+})$ is typically measured with high accuracy through the classical [O III] $\lambda\lambda4959,5007\lambda4363$ line ratio in most H II regions.

3 Temperature relationships

To derive the temperature relationship we are looking for, we used the photoionization model grid to plot $T_{\rm e}({\rm Cl}^{2+})$ against $T_{\rm e}({\rm O}^{2+})$ and $T_{\rm e}({\rm N}^+)$, as shown in Figs. 1a and 1b, respectively. The observed behavior is: N⁺, which represents regions with lower ionization, fits better at lower temperatures, while O²⁺ provides a better fit in higher ionized regions.



Figure 1: $T_{\rm e}({\rm Cl}^{2+})$ vs. (a) $T_{\rm e}({\rm O}^{2+})$ and (b) $T_{\rm e}({\rm N}^+)$ obtained from photoionization models. The points are color-coded by its ionization degree. The red line is a linear fit to the points. In the bottom panel, we show the values of the standard deviation, σ , to the fit in bins of 1000 K. The mean value of σ is shown inside the red box.

The key conclusion from this analysis is that neither temperature seems to be appropriate for the whole range of ionization degrees, leading us to propose a representative temperature (T_{rep}) , defined as:

$$T_{rep} = T_{\rm e}({\rm N}^+) \cdot \left(1 - \frac{{\rm O}^{2+}}{{\rm O}}\right) + T_{\rm e}({\rm O}^{2+}) \cdot \frac{{\rm O}^{2+}}{{\rm O}}$$
(1)

This captures the trend observed in Fig. 1: for lower ionization degrees, $T_{\rm e}({\rm N}^+)$ has more weight, while $T_{\rm e}({\rm O}^{2+})$ dominates at higher ionization. Re-plotting with this new temperature yields Figure 2, which shows an improved behavior across ionization extremes and a significantly reduced standard deviation. Henceforth, we will compare results from our observational sample using this representative temperature.

4 Cl abundances

Once we have calculated the appropriate physical conditions, the next step is to complete the chemical abundance analysis of our observational sample using PyNEB [6]. We started with the determination of the Cl^{2+} ionic abundance. We then calculated the total Cl abundance using two different ICF schemes [2, 4], one of which directly calculates the Cl/O ratio. This



Figure 2: $T_{\rm e}({\rm Cl}^{2+})$ vs. $T_{rep}({\rm O}^{2+})$, from photoionization models. Color-code, lines and panels are equivalent to those shown in Fig. 1.

ratio is of interest because, Cl and O are both thought to be formed in hydrostatic and explosive oxygen burning in massive stars. Moreover, previous studies suggest that this ratio should remain constant and close to the solar value [5].

We first plotted the $\text{Cl}^{2+}/\text{O}^{2+}$ ratio as a function of the ionization degree for our sample, alongside the functions of the different ICFs, for both $T_{\rm e}(\text{S}^{2+})$ and $T_{\rm rep}$ (see Figs. 3a and 3b, respectively). The results show that the ICF from [2] is valid across the full ionization range, while the ICF proposed by [4] becomes applicable only when the ionization degree exceeds 0.2. However, at higher ionization degrees, the ICF of [4] fits the observational trend better, while the ICF from [2] does not.

Finally, using the ICF equations, we calculated and plotted the Cl/O ratio as a function of the ionization degree, resulting in the plots shown in Fig. 4. We observe that $T_{\rm rep}$ tends to reduce the data dispersion, and that the ICF from [4] gives smaller amplitudes in the Cl/O variations as a function of ionization degree, except at the highest ionization degrees. The peak on the right-hand side, more pronounced with $T_{\rm rep}$, could be due to the relationship between the temperature and ionization degree. Using $T_{\rm e}(S^{2+})$ introduces this dependence when calculating the total Cl abundance, while $T_{\rm rep}$ introduces it at the Cl²⁺ abundance calculation stage, which might increase the dispersion in these points and, thus, the overall dispersion of the mean value. The key takeaway is that none of the combinations fully eliminates the dependence on either temperature or ionization degree.



Figure 3: $\text{Cl}^{2+}/\text{O}^{2+}$ as a function of the ionization degree, calculated using: (a) $T_{\rm e}(\text{S}^{2+})$, and (b) $T_{\rm rep}$ for the observational sample. In both figures, the blue points correspond to star forming galaxies, while the black ones are H II regions. The dashed horizontal line marks the Solar Cl/O used as a reference, and the dotted lines display the curves of the different ICFs tested.

5 Preliminary conclusions and future work

The preliminary conclusions of this study are, first, that the proposed representative temperature $(T_{\rm rep})$ is valid for representing the region where ${\rm Cl}^{2+}$ is located. Second, despite our expectations, none of the combinations of ICF and temperature used in this analysis completely eliminates the dependence on either temperature or ionization degree. Lastly, and most importantly, as we will describe in detail in future publications, the results seem to rule out significant contributions apart from the hydrostatic and explosive oxygen burning in massive stars in the nucleosynthesis of chlorine.

As for next steps, we plan to further investigate the ionization degree dependence introduced by the chosen temperature. Additionally, we are exploring alternative temperature relationships applicable to other ions, which is a key focus of our ongoing work.

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Figure 4: Cl/O as a function of the ionization degree for the sample objects. The left and right columns correspond to the ICF by [2] and [4], respectively. The top and bottom rows show the results for $T_{\rm e}({\rm S}^{2+})$ and $T_{\rm rep}$, respectively. Blue points correspond to star forming galaxies and black ones to H II regions. The dashed horizontal line marks the mean Cl/O of the points, the red diamonds show the mean values for 0.2 wide bins, and the golden triangle indicates the Solar Cl/O used as a reference.

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