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Abundances from emission lines in ionized nebulae

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Abstract: This contribution, presented at the 2016 conference on Atomic Spectra and Oscillator Strengths for Astrophysical and Laboratory Plasmas (ASOS12), shows how atomic physics contributes in the interpretation of emission-line spectra observed in astronomical nebulae, and discusses a few unsolved issues where atomic physics might play a role, although other possible explanations are indeed possible. It is limited to the determinations of chemical abundances, the most sought after information derived from emission lines.

Résumé français:

Cette contribution, présentée lors de la conférence de 2016 sur les spectres atomiques et les forces d'oscillateur pour les plasmas de laboratoire et les plasmas astrophysiques (ASOS12), vise à montrer comment la physique atomique contribue à interpréter les spectres des raies d'émission observées dans les nébuleuses astrophysiques et à présenter quelques problèmes non résolus où la physique atomique pourrait jouer un rôle, bien que d'autres explications soient possibles. Ce texte est limité aux déterminations d'abondances, qui sont les principales informations dérivées des raies d'émission.

1. Introduction

The principles of abundance determinations from emission-line nebulae are the same for planetary nebulae (PNe), H II regions, ring nebulae, and nova envelopes. PNe are actually the best objects to discuss the relevant atomic physics because their spectra are the richest in the number of both ions and lines belonging to specific species. Also, the geometry of PNe is far simpler than that of H II regions facilitating reliable photoionization modelling.

2. Abundance derivations in emission-line nebulae and stellar atmospheres

The first thing to note in stellar atmospheres is that iron is generally the most important element, and it is its abundance which generally defines the 'metallicity'. In PNe iron lines are weak, and the measured iron abundance is only associated to the amount in the gas phase while most of the iron is locked in dust grains whose chemical composition cannot be derived directly. In PNe the strongest lines – apart from those of hydrogen – are due to oxygen ions. Oxygen plays a dominant role in the cooling processes of the nebular gas. In the astrophysical jargon, oxygen is a 'metal' (just like all the elements heavier than hydrogen and helium), and since the oxygen mass fraction in the Universe is roughly equal to the sum of rest of the 'metals', it has become common practice in nebular astrophysics to identify the oxygen abundance with the 'metallicity'. This causes some misunderstandings between the stellar and nebular communities as oxygen and iron are not produced by the same nuclear processes and arise from stars of different masses; thus they do not evolve in lockstep in the interstellar medium of galaxies.

Traditionally, abundances in PNe are derived from the intensities of a few collisionally excited emission lines, while in stars they are obtained from the equivalent widths of (usually many) absorption

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lines. In general, emission lines are not affected by radiation transfer effects (except for resonance lines that all lie in the UV), and thus the ionic abundance ratios can be determined *directly* from the line intensity ratios. It must be emphasized that, for abundance determinations, nebular spectra need to be properly flux calibrated in the entire spectral range and corrected for interstellar extinction.

In the derivation of abundances in nebulae, the most important atomic parameters are the collision strengths while in stellar atmospheres they are the oscillator strengths. Nb., if nebular abundances are derived from recombination lines instead of collisionally excited emission lines, the results rely not on collision strengths but on the recombination rate coefficients. Other parameters also play a role in nebular abundances determinations, although to a lesser degree as will become clearer below.

3. Basic abundance determination in ionized nebulae

3.1. Ionic abundances

The abundance of an ion X^{+i} with respect to H^+ is obtained from the relation

$$X^{+i}/H^+ = \frac{I_\lambda(X^{+i})/I_{H\beta}}{j_\lambda(X^{+i})(T_e, n_e)/j_{H\beta}(T_e)}, \quad (1)$$

where $I_\lambda(X^{+i})$ is the dereddened intensity ratio of a line emitted by this ion with respect to that of $H\beta$, and $j_\lambda(X^{+i})(T_e, n_e)/j_{H\beta}(T_e)$ is the ratio of the line emission coefficients. T_e and n_e are respectively the electron temperature and density which are assumed constant in the emission zone. Their values are obtained from the intensity ratios of lines emitted by the same ion and sensitive to the electron temperature and/or density.

In the case of collisionally excited lines (CELs), the emission coefficients are proportional to the collision strengths, and have a strong temperature dependence if the excitation energy is high with respect to the thermal energy of the electrons. They also depend at high densities on the radiative transition probabilities when collisional deexcitation competes with radiative deexcitation. The emission coefficients of recombination lines (RLs), on the other hand, are all roughly inversely proportional to the electron temperature and are thus only weakly dependent on density. More information can be found in any textbook dealing with ionized nebulae (e.g. Osterbrock & Ferland, 2006).

In practice there are often several line pairs in a spectrum that allow estimates of the electron density n_e and temperature T_e , and appropriate values to the ionization state of the ion of interest should be used. In many instances, the observational data are not enough to allow this, and the final choice is a personal matter guided by experience.

3.2. Total abundances

Once ionic abundances have been determined, elemental abundances are obtained by correcting for unobserved charge states using the so-called ionization correction factors (ICFs).

The first ICFs, based on species with comparable ionization potentials, can be quite inaccurate. Reliable ICF prescriptions are based on photoionization models constructed using accurate photoionization cross sections, recombination rate coefficients, and charge-exchange coefficients. The reliability of the photoionization models does not depend only on the atomic data as other ingredients are also important such as the spectral energy distribution of the ionizing radiation field, the geometry, and the density distribution law.

During the past two decades, abundances in PNe have been computed using ICFs from Kingsburgh & Barlow (1994) that were based on (unpublished) tailored photoionization models for a dozen PNe.

Recently, using a large grid of *ab initio* photoionization models with the CLOUDY package (Ferland et al. 2013), Delgado Inglada et al. (2014) have produced an ICF database to compute O, N, Ne, S, Ar, Cl, and C abundances. For the first time, ICF uncertainties have been estimated which in this paper

are rather ‘generous’, but the authors are working on more realistic estimations. Following the same approach, ICFs are now being computed for Co, Cr, Mg, and Mn.

Sterling et al. (2015) have independently computed ICFs for Se and Kr, two *n*-capture elements, adding them to CLOUDY. For Rb, Cd, and Ge, Sterling et al. (2016) proposed ICFs based on ionization potentials since the atomic data necessary to compute the ionization of those elements with photoionization codes are not yet available.

3.3. A public tool to compute abundances

Recently, Luridiana et al. (2015) have published a Python computer tool, referred to as PyNeb, to derive ionic and elemental abundances in nebulae. For each ion, this package includes atomic data from all known sources allowing a comparison of results based on different data sets.

3.4. Elements detected in PNe

Thanks to the use of deep spectroscopy, the list of elements with detected lines has impressively increased in the last decades. Presently it involves H, He, C, N, O, F, Ne, Na, Mg, Si, P, S, Cl, Ar, K, Ca, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Ga, Ge, Se, Br, Kr, Rb, Cd, and Xe. The atomic data necessary to fully take advantage of these observations are gradually becoming available but there is still room for work.

Abundance determination for these elements in PNe allows:

- The study of nucleosynthesis in low mass stars
- The tagging of the chemical composition of the ISM of galaxies $10^8 - 10^{10}$ yr ago
- The study of grain formation and destruction in the atmospheres of evolved stars
- The testing of the atomic data.

4. Atomic data for abundance determinations in emission-line nebulae

4.1. How to choose the right atomic data set

Assessing the accuracy of computed atomic data is a very difficult matter. It is not always the most recent atomic physics calculation with the most sophisticated method that yields the most accurate data.

It is sometimes possible to use nebula observations to rank a certain atomic data set. This was, for example, the case of a study of abundances in PNe in the galaxy NGC 300 (Stasińska et al. 2013). For these nebulae, the only available density diagnostic was the [S II] doublet. Many of the observed [S II] ratios were above the high-density limit when using the atomic data of Tayal & Zatsarinny (2010), and for some objects the oxygen abundances were found to be abnormally high. The [S II] atomic data were then checked by comparing the densities derived from the [S II] and [O II] ratios in a sample of galactic PNe observed with high resolution and high S/N (Wang et al. 2004). It was concluded that it was better to use the old transition probabilities from Mendoza & Zeippen (1982) rather than those from Tayal & Zatsarinny (2010) since the former led to more reasonable results.

4.2. Atomic data to rescue photoionization models

For abundance studies of *n*-capture elements in PNe, Sterling and collaborators needed to correct the abundances determined from observations for the presence of unobserved ions. For this purpose, they first computed the missing atomic data: charge-transfer rate coefficients for the low-charge ions of Ge, Se, Br, Kr, Rb, and Xe (Sterling & Stancil 2011); photoionization cross sections and radiative and dielectronic recombination rate coefficients for the first six ions of Se and Kr (Sterling & Witthoeft 2011) and Sterling (2011); photoionization, recombination, and collisional excitation of Rb and Br

ions (Kerlin et al. 2016); photoionization and recombination of Xe ions (Sterling & Kerlin 2016); and photoionization of Se^{++} (Macaluso et al. 2015).

4.3. Photoionization models to rescue atomic physics

A recent example is the work of Badnell et al. (2015) on the dielectronic recombination (DR) rate of S^{++} to S^+ . These authors noted that ‘accurate DR rates can be predicted when the positions of autoionizing states are known. Unfortunately such data are not available for most third- and higher-row elements’. They thus constructed photoionization models of the Orion nebula to reproduce the $[\text{Ne III}]:[\text{O III}]:[\text{O II}]:[\text{O I}]$ intensity ratios (O and Ne have accurate atomic data). Then, the S^{++} to S^+ DR rate coefficient was varied until the observed $[\text{S III}]/[\text{S II}]$ ratio was fitted. This allowed the empirical determination of the positions of autoionizing states. Theoretical calculations of the DR rates at other temperatures were then computed using these positions. A simple fit to the resulting rate coefficient at all temperatures was proposed to be incorporated in spectral synthesis codes. This method can be used to derive empirical DR rates for other ions.

5. Intriguing results concerning nebular abundances

5.1. The sulfur conundrum

Henry et al. (2012) noted that the S/O ratios presented different trends in PNe and H II regions that is not *a priori* expected. They examined several possible explanations:

- Incorrect ICFs
- DR effects on the sulfur ionization
- S depletion into dust and/or molecules
- S destruction or O production by AGB stars.

Incorrect ICFs were their preferred explanation, but

- the ICFs by Delgado-Inglada et al. (2014) do not solve the mystery,
- the work by Badnell et al. (2015) was motivated by this S conundrum although their new DR rates do not solve it either.

5.2. Oxygen enrichment in carbon-rich PNe

The oxygen abundance in PNe is traditionally used as a proxy of the interstellar medium metallicity at the time the PN progenitor stars were born. From a sample of PNe with high-quality optical spectra that allow reliable N, O, Ne, Cl, and Ar abundances, and IR spectra that indicate the presence of either C- or O-rich dust, Delgado Inglada et al. (2015) found that all (but one) of the PNe with C-rich dust show evidence of oxygen self-enrichment. To explain this fact, non-standard post-AGB nuclear synthesis models are required. This finding implies that oxygen is not always a reliable indicator of the original metallicity, and therefore, other elements such as Cl and Ar should be used instead.

5.3. The major problem with abundances in PNe: the so called abundance discrepancy

5.3.1. Abundances from recombination lines

In the last twenty years, many deep and high-resolution PNe spectra have been obtained allowing the detection of hundreds of recombination lines (see Garcia-Rojas 2016 for a review). These lines (apart from those of H and He) are all very weak (typically one thousandth of $\text{H}\beta$), but their interest arises

from their similar dependence on the electron temperature causing the abundance determination of the parent ions to be weakly affected by T_e uncertainties.

The RL abundances are systematically larger than the CEL abundances by factors larger than 10 in some cases (in H II regions, such discrepancies also exist, typically of a factor of 2). Over the years, it has been shown that this discrepancy is real and not due to calibration or measurement errors, line blending, the dereddening procedure, contamination of recombination lines by fluorescence or charge transfer, or inaccuracies in the atomic data.

5.3.2. Link between abundance discrepancy and temperature structure

The electron temperature of the ionized plasma can be determined not only by ratios of the auroral to nebular forbidden lines such as $[\text{O III}]\lambda 4363/[\text{O III}]\lambda 5007$ but also by the Balmer and Paschen discontinuities. It is generally found that T_{BJ} is smaller than $T_{[\text{O III}]}$ often by significant amounts, and that the abundance discrepancy factors are correlated with $T_{[\text{O III}]} - T_{BJ}$ (Wang & Liu 2007). Recent atomic data calculations (Bastin & Storey 2005) have allowed the use of recombination lines as temperature indicators (for example, using $\text{O II}\lambda 4649/4662$ in conjunction with $\text{O II}\lambda 4649/4069$). These recombination lines indicate temperatures of 1000–2500 K that are much smaller than the typical $T_{[\text{O III}]}$ temperatures of around 10 000 K.

Several possible interpretations of the abundance discrepancy are presently being disputed.

5.3.3. First interpretation: temperature fluctuations

This interpretation was initially proposed by Peimbert (1967) to explain the $T_{[\text{O III}]} - T_{BJ}$ discrepancy by assuming that the electron temperature was not uniform. Peimbert's formalism allows the derivation of the mean-square temperature fluctuation t^2 by assuming that the mean temperature and t^2 are equal in the O^{++} and H^+ zones. t^2 is generally found to be between 0 and 0.1 with a typical value of 0.04. Such values can also explain the abundance discrepancy if due to temperature fluctuations (e.g. García-Rojas & Esteban 2007).

Many possible causes have been invoked to explain temperature fluctuations:

- Deposition of mechanical energy
- Deposition of magnetic energy
- Density fluctuations
- Dust heating
- Shadowed regions.

Thus far, none of these by itself has been shown to produce temperature fluctuations to the required level so as to explain the abundance discrepancy.

5.3.4. Second interpretation: abundance inhomogeneities

Liu et al. (2000) were the first to suggest that metal-rich inclusions could explain the abundance discrepancies. Indeed, in the metal-rich (i.e. H-poor) zones, cooling is enhanced and lowers the electron temperature, favouring the emission of the recombination lines, while the collisionally excited lines are emitted in the high-temperature metal-poor zones. Yuan et al. (2011) were able to construct a bi-abundance photoionization model of the PN NGC 6153 which reproduces simultaneously the CELs and RLs.

What could be the possible origin of those metal-rich inclusions? Liu (2002) proposed the evaporation of solid bodies inside the PNe. This scenario was further elaborated in detail by Henney & Stasińska (2010) who showed that for it to work the following requirements should be fulfilled:

- The bodies must be larger than tens of meters to generate a low-temperature plasma during ablation;
- If considering the sum of the AGB and PN phases, the total mass of the solid body reservoir must exceed $10^{-4} M_{\odot}$ to reproduce the observed values of the abundance discrepancies, which is comparable to the most massive debris disks observed around solar-type stars;
- In addition, absence of efficient mixing during the pre-PN and PN stages is required to reproduce the observed ADFs.

5.3.5. Third interpretation: non-Maxwellian electron distribution

While it is assumed in all nebular studies that the free electrons follow a Maxwell–Boltzmann (MB) temperature distribution, Nicholls et al. (2012) suggested that deviations from this MB distribution could explain the abundance discrepancies. A κ -velocity distribution peaks at a lower velocity than the MB distribution with a longer tail at high velocities. This tail will increase the intensities of CELs for a given value of the kinetic temperature.

Assuming that O^{++} and S^{++} are found in the same zone, by comparing the apparent values of $T_{[O\ III]}$ and $T_{[S\ III]}$, it is possible to derive the value of κ and then estimate ionic abundances from the CELs for the appropriate value of κ ; however, this procedure requires available energy-tabulated collision strengths. Therefore, producers of atomic data should also publish such collision strengths in addition to MB-integrated collision strengths.

The κ -velocity distribution seems a very elegant and promising way to solve the abundance discrepancy in PNe and ionized nebulae in general. But, can it occur in such plasmas? Nicholls et al. (2012, 2013) argue that this is very likely: ‘ κ -like energy distributions can arise as a consequence of variations of physical parameters such as density, temperature, and electric and magnetic fields (Collier 1993) or whenever the population of energetic electrons is being pumped in a timescale shorter than the normal energy redistribution timescale of the electron population. Suitable mechanisms include [...] injection of high-energy electrons through the photoionization process itself.’

On the other hand, Ferland et al. (2016) strongly argue against the presence of κ -distributions in ionized nebulae: ‘The distance over which heating rates change is much longer than the distance suprathermal electrons can travel, and the timescale to thermalize these electrons is much shorter than the heating or cooling timescales. [...] Suprathermal electrons will have disappeared into the Maxwellian velocity distribution long before they affect the collisionally excited forbidden and recombination lines that are used for deriving abundances relative to hydrogen. The electron velocity distribution in nebulae should be closely thermal.’

6. Summary

Ionic abundances in nebulae can be obtained directly from emission line intensities. Their derivation depends on collision strengths if they are obtained from collisionally excited lines (and on transition probabilities in the high-density regime), and on recombination rate coefficients if they are obtained from recombination lines.

Elemental abundances require the use of ionization correction factors that are based on photoionization models. The relevant atomic parameters here are photoionization cross-sections, recombination coefficients, and charge exchange reaction rates.

Deep high-resolution spectroscopy of PNe allows the CEL abundance determination of 30 species. Atomic data are still needed for some of them.

There are two major unsolved problems in nebular astrophysics: the temperature discrepancy (the fact that different temperature indicators yield very different temperatures) and the CEL/RL abundance discrepancy. These two problems are most likely linked. Presently several possible solutions are hotly

debated: temperature fluctuations, bi-abundances, and deviation from MB electron velocity distributions. This lack of consensus implies that H II region and PN abundances are uncertain within at least a factor of 2 – unless one of the hypotheses is clearly dismissed.

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References

1. N. R. Badnell, G. J. Ferland, T. W. Gorczyca, D. Nikolić, G. A. Wagle, *ApJ*, 804, 100 (2015)
2. R. J. Bastin, P. J. Storey, *AIPC*, 804, 62 (2005)
3. M. R. Collier, *GeoRL*, 20, 1531 (1993)
4. G. Delgado-Inglada, M. Rodríguez, M. Peimbert, G. Stasińska, C. Morisset, *MNRAS*, 449, 1797 (2015)
5. G. Delgado-Inglada, C. Morisset, G. Stasińska, *MNRAS*, 440, 536 (2014)
6. G. J. Ferland, et al., *RMxAA*, 49, 137 (2013)
7. G. J. Ferland, W. J. Henney, C. R. O'Dell, M. Peimbert, *RMxAA*, 52, 261 (2016)
8. J. García-Rojas, *arXiv:1612.02568* (2016)
9. J. García-Rojas, C. Esteban, *ApJ*, 670, 457 (2007)
10. W. J. Henney, G. Stasińska, *ApJ*, 711, 881 (2010)
11. R. B. C. Henry, A. Speck, A. I. Karakas, G. J. Ferland, M. Maguire, *ApJ*, 749, 61 (2012)
12. A. Kerlin, D. A. Macaluso, M. Bautista, R. C. Bilodeau, A. Aguilar, A. L. D. Kilcoyne, I. Dumitriu, N. C. Sterling, *AAS*, 227, 238.03 (2016)
13. R. L. Kingsburgh, M. J. Barlow, *MNRAS*, 271, 257 (1994)
14. X.-W. Liu, P. J. Storey, M. J. Barlow, I. J. Danziger, M. Cohen, M. Bryce, *MNRAS*, 312, 585 (2000)
15. X.-W. Liu, *RMxAC*, 12, 70 (2002)
16. V. Luridiana, C. Morisset, R. A. Shaw, *A&A*, 573, A42 (2015)
17. D. A. Macaluso, A. Aguilar, A. L. D. Kilcoyne, E. C. Red, R. C. Bilodeau, R. A. Phaneuf, N. C. Sterling, B. M. McLaughlin, 2015, *PhRvA*, 92, 063424
18. C. Mendoza, C. J. Zeppen, *MNRAS*, 199, 1025 (1982)
19. D. C. Nicholls, M. A. Dopita, R. S. Sutherland, L. J. Kewley, E. Palay, *ApJS*, 207, 21 (2013)
20. D. C. Nicholls, M. A. Dopita, R. S. Sutherland, *ApJ*, 752, 148 (2012)
21. D. E. Osterbrock, G. J. Ferland, *Astrophysics of gaseous nebulae and active galactic nuclei*, (2006)
22. M. Peimbert, *ApJ*, 150, 825 (1967)
23. G. Stasińska, M. Peña, F. Bresolin, Y. G. Tsamis, *A&A*, 552, A12 (2013)
24. N. C. Sterling, H. L. Dinerstein, K. F. Kaplan, M. A. Bautista, *ApJ*, 819, L9 (2016)
25. N. C. Sterling, R. L. Porter, H. L. Dinerstein, *ApJS*, 218, 25 (2015)
26. N. C. Sterling, P. C. Stancil, *A&A*, 535, A117 (2011)
27. N. C. Sterling, M. C. Witthoeft, *A&A*, 529, A147 (2011)
28. N. C. Sterling, *A&A*, 533, A62 (2011)
29. N. C. Sterling, A. B. Kerlin, *AAS*, 227, 238.02 (2016)
30. S. S. Tayal, O. Zatsarinny, *ApJS*, 188, 32 (2010)
31. W. Wang, X.-W. Liu, Y. Zhang, M. J. Barlow, *A&A*, 427, 873 (2004)
32. H.-B. Yuan, X.-W. Liu, D. Péquignot, R. H. Rubin, B. Ercolano, Y. Zhang, *MNRAS*, 411, 1035 (2011)