Improvements on the Determination of (PNe) Nebular Abundances

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Outline:

- Why PN (H II region) abundances?
- Deriving nebular abundances
- Uncertainties related with $X^+ / H^+ \ (X/H)$
- The problem of PN shapes vs ICFs
- Our PN 3D photo models vs ICFs
- Results: optical + IR spectra
  UV + optical + IR spectra
Why PN (HII region) abundances?

- PNe are useful probes of ISM composition
- PNe provide information about low- to intermediate-mass stellar nucleosynthesis
- PNe archive progenitor abundances of $\alpha$-element elements
- The $\alpha$-element abundances of the H II regions are a snapshot of current ISM
- While the $\alpha$-element abundances derived from PNe reflect the ISM at the time that the progenitor star formed

A few reviews:
- Kwitter & Henry (2012; IAUS 283) PNe abundances in the Galaxy + MCs
- Magrini, Stanghellini & Gonçalves (2012; IAUS 283) Local Group PNe (H II regions) beyond the MCs
- Stasinska 2002 (IAC Winter School 2002) PN + H II region abundances
Why PN (H II region) abundances?

Nucleosynthesis in AGB: (Herwig 2005)
Why PN (H II region) abundances?

Nucleosynthesis in AGB:

- From He and H, PNe produce an array of elements!!!
- Their primary production is He, C and N and neutron-heavy species like $^{22}\text{Ne}$
- O and Ne production is dominated by core collapse SNe, but at low metallicity (1/100 solar) PNe can dredge-up and have positive yields of both: O and Ne
- S and Ar are not produced by these stars
Why PN (H II region) abundances?

Nucleosynthesis in AGB:

And also

Zhang & Liu 2005
Sharpee et al. 2007
Liu 2012
Karakas & Lugaro 2012
Karakas 2009
Sterling & Witthoeft 2011
Sterling 2011, 2012
Maiorca et al 2012

- CELs from ions of extremely low abundance elements have been detected – Fluorine
- Many neutron-capture elements (Br, Kr, Xe, Rb, Ba, and Pb) are being measured
- Great effort to get atomic data for neutron-capture elements
  - So making possible to convert ionic abundances into elemental abundances
  - They provided, recently, ICF for Ge, Se, Br, Kr, Rb and Xe...
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Mainly two methods

1) **DIRECT (EMPIRICAL)**

Given the limited $\Delta \lambda$, only few lines of some ions can be measured:
- unseen ions must be corrected for: **ICF method**

- Despite the many problems, ICF for empirical abundance is frequently the only option available, and it does provide reasonable results

- The higher the $\lambda$ coverage the better the abundance determination: UV and IR, instead of only optical data, improve enormously the results

- Examples of ICFs are: **Kingsburgh & Barlow (1994)** for PNe
  **Mathis & Rosa (1991)** for HII regions
Deriving nebular abundances

Mainly two methods

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Based on photomodelling
Deriving nebular abundances

Mainly two methods

2) Empirical (ICF) abundances are the input abundances for a Photoionization model fitting
   – the empirical abundances are varied until the predicted line ratios (and emission line maps) match the observations

Stasinska (2002) has shown – for PN M2-5, with a too limited number of constraints – that acceptable photo models give two families of solutions, responding to the same observables. One gives $O/H \approx 2.4 \times 10^{-4}$ and other $O/H \approx 1.2 \times 10^{-3}$!

No solution is found – cases on which given the constraints of the gas distribution and ionizing star(s), one cannot reproduces the $[O \text{ III}] \lambda 4363/5007$ line (Peña et al. 1998; Luridiana et al. 1999; Stasinska & Schaerer 1999)

Abundances are not necessarily better determined from model fitting... But with sufficient number of constraints, it provides more accurate ICFs than using the simple formulae in the literature.
Deriving nebular abundances

What about the results one obtain with these methods?
What about the results one obtain with these methods?

Others will talk (already talked) about these results:
- W. Maciel – Galactic O/H and Ne/H gradients
- F. Matteucci – Models for the chemical evolution of galaxies
- In fact H II regions and PNe abundances are being used to constrain:
  (Magrini, Stanghellini & Gonçalves 2012)
  i) metallicity gradients of disk galaxies
  ii) chemical evolution models of dwarf LG galaxies
  iii) stellar nucleosynthesis at low metallicities (the O production in PNe)

Here I mention ONLY TWO important general results related with abundances determination in H II regions and PNe

- ADF (abundance discrepancy factor)
- SA (sulphur anomaly)
ADF – abundance discrepancy factor
Abundances derived using collisionally excited lines (CELs) differ from those of recombination lines (RLs) of the same elements (Peimbert et al. 1993)

→ RLs imply abundances higher than those implied by CELs
  – by factors around two in most cases
  – with some PNe showing much higher discrepancies (Liu 2006)

→ The emissivities of CELs have a stronger dependence on $T_e$ than those of RLs

→ Most proposed explanations rely
  – on the presence of low temperature H-poor inclusions that are rich in He and heavy elements in PNe (Liu 2006 and references therein),
  – on the presence of temperature variations, in a homogeneous medium, due to additional physical processes not included in photoionization models (Peimbert & Peimbert 2006, and references therein)
Deriving nebular abundances

ADF – abundance discrepancy factor

Hernández-Martínez et al. (2011)
– Empirical CELs and RL abundances as well as chemical evolution models of the dwarf galaxy NGC 6822
– An unsuccessful attempt to distinguish which of the two abundances (CELs or RLs) is more robust

O'Dell et al. (2013)
– Detailed analysis of the $T_e$ and $N_e$ in the Ring Nebula
– Their HST images show unprecedented small-scale ($< 3.5 \times 10^{15}$ cm) variations in $T_e$
– They strongly restricted the mechanism causing the large $t^2$ observed values to very small scales
Deriving nebular abundances

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THEREFORE, the ADF persists, but it is much better constrained!
Deriving nebular abundances

SA – sulphur anomaly
First described by Henry et al. (2004), refers to the observation that PN sulfur abundances are systematically lower than those found in most other interstellar abundance probes for the same O abundance (metallicity).
Deriving nebular abundances

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The S vs. O expected relation between given by a sample of H II regions and blue compact galaxies, H2BCG. PNe in the MWG, M31 disks, SMC fall below this track and exhibit much more scatter!

(Henry et al. 2012)
Deriving nebular abundances

SA – sulphur anomaly

Henry et al. (2012) tested a large range of hypotheses for explaining the SA

- NOT a single causal factor!
- Their best guess is that the eventual solution will involve the sulfur ICF.

Shaw et al. (2010) confirmed that SA persists when IR observations are also considered

- They derive the X/H from deep, high-dispersion optical spectra, as well as mid-IR spectra from the Spitzer, in the SMC.
- They pointed out that $S^{4+}$ is the sink, causing the SA, because the restricted morphology, and uniform density, in (over)simplified photo-models used for ICF-computation, severely underestimated the $S^{4+}$ contribution.
Deriving nebular abundances

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PROBABLY,

final solution to the SA involves the computation of ICF based on more realistic PN density distributions.
Deriving nebular abundances

**Softwares to derive empirical abundances**

The physical basis for line emission from ionized nebula has been well established for decades (Aller 1984; Osterbrock 1989; Osterbrock & Ferland 2006)

– The statistical equilibrium to obtains the level population and emissivities is usually resolved within the 5-level approximation (De Roberts, Dufour and Hunt 1987)

- Certain ratios of line emissivity are sensitive to $T_e$, others to $N_e$
- By using several diagnostics from ions with different IP, a simple physical model is inferred for an observed nebula, from which ionic abundances are obtained.

**Shaw & Dufour (1995) - nebular**

- Software tools for the IRAF/STSDAS environment to derive the physical conditions ($N_e$ and $T_e$) and ionic abundances ($X^i/H^+$)
- The package is based on the five-level program developed by De Robertis et al. (1987) and uses IRAF atomic data – WIDELY USED!
Deriving nebular abundances

Softwares to derive empirical abundances

Johnson et al. (2006) - ELSA
- A semi-automated nebular abundance package (written in C)
- It calculates plasma diagnostics and abundances from nebular emission lines
- An advantage is that it can read the output of the *splot* task for line fluxes
- “Recent” atomic data, mainly from Osterbrock & Ferland (2006) or from Mendoza (1983)

Leal-Ferreira, Gonçalves & Monteiro (2011) - 2D_Neb
- Another tool to derive the physical conditions, ionic abundances and total abundances
- Adaptation of *nebular* to easily deal with two-dimensional spatial maps (IDL routines)

![NGC 40 Ne[SII]](image1)
![NGC 40 He/H](image2)
Deriving nebular abundances

Softwares to derive empirical abundances

Wesson, Stock & Scicluna (2012) - NEAT

- Nebular Empirical Analysis Tool
- Determining $N_e$, $T_e$ and ionic abundances ($X^i/H^+$) from CEL and ORL
- Uses ICF schemes to obtain total abundances
- Uses Monte Carlo technique to robustly propagate uncertainties from line flux measurements through the derived abundances!!!
- Atomic data, documentation, code source in: http://www.sc.eso.org/~rwesson/codes/neat/

Luridiana, Morisset & Shaw (2012) - PyNeb

- A migration of the nebular from IRAF to Python
- It can be used from command line or the web
- It stores a vast repertoire of ICFs from the literature
- At run time, it allows to explore intermediate results, display atomic data, and change them
- The results can be computed numerically or displayed graphically...
Deriving nebular abundances

Softwares to derive empirical abundances

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- The results can be computed numerically or displayed graphically...
- [https://pypi.python.org/pypi/PyNeb/](https://pypi.python.org/pypi/PyNeb/)
Deriving nebular abundances

Photoionization codes

– They simultaneously solve the equations of statistical and thermal equilibrium, so treating the equations that balance ionization-neutralization processes, and heating-cooling processes of the nebular gas.

– In 3D stellar and diffuse radiation fields are treated self-consistently

– 1D the nebula is spherically symmetric

– 3D can treat non-spherical nebular geometry

ICFs in use currently were mostly obtained from the ionization structure of different 1D photo-codes (Kingsburgh and Barlow 1994; Kwitter & Henry 2001)
Deriving nebular abundances

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Most used photo codes for abundances

CLOUDY (Ferland 1998)

MOCASSIN (Ercolano et al. 2003, 05, 08)
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Uncertainties related with $X^{i+}/H^+(X/H)$

Atomic data

Luridiana & García-Rojas (2012)
– on the impact of the atomic data (for Sulphur, in a Herbig-Haro object):
  the peak density changes from about 5 000 to 15 000 cm$^{-3}$!
Uncertainties related with $X^{i+}/H^{+}(X/H)$

Atomic data

Luridiana & Garcia-Rojas (2012)

Accurately quantifying the effect of uncertainties is often difficult due to the complex ways in which different types of atomic data affect the calculations.

– 2010, in Tenerife, a workshop Uncertainties in Atomic Data and How They Propagate in Chemical Abundances

– They advise: “Users should always try to compare among different datasets before deciding for one”. This can be done using: [http://astroatom.wordpress.com](http://astroatom.wordpress.com)

Liu 2012 (IAUS 283)

– Reviewed the atomic processes in planetary nebulae

– On top of the improvements on the field, he discussed the potential of good atomic data to investigate the ADF and OII became available, making possible to study $T_{e}[O III]$ versus the H I Balmer jump, He I, NII and OII ones... In Hf 2-2 $T_{e}[OIII]$ is 1 order of magnitude higher than all the others $T_{e}$, implying the ORL originate from low $T_{e}$ H-deficient inclusions.
Uncertainties related with $X^{i+}/H^+(X/H)$

Spectral Coverage + Model Fitting

Otsuka et al. (2010)
Chemical abundance analysis of the extremely metal-poor ([Ar/H] < −2) halo PN BoBn 1 – Based on IUE archive data, Subaru/High-Dispersion spectra, VLT/UVES archive data, and Spitzer/IRS spectra.

- The ADF, apart from O, is explained by a temperature fluctuation model
- O ADF might be by a hydrogen-deficient cold component model
Uncertainties related with $X^{i+}/H^{+}(X/H)$

The spectral coverage + model fitting

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**CLOUDY model SED with the observation superposed.**

**THEREFORE,**
Better $\Delta \lambda$ allows to explain (better constrain) the problems!
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The problem of PN shapes vs ICFs

Shaw (2012; IAUS 283)
– Discussed the results of a series of papers starting with Stanghellini, et al. (2000)
– They extended to the MC Peimbert (1978), Peimbert & Torres-Peimbert (1983) ideas relating N and He abundances to PN morphological type
– There is a strong correlation of macro-morphology with N abundance (in the Galaxy; Corradi & Schwarz (1995) and also in the clouds.
The problem of PN shapes vs ICFs

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Taking the statistics of morphological PN type in the Galaxy

From MASH, IPHAS, etc:
905 PNe (true, likely and possible)

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Parker (2006)
The problem of PN shapes vs ICFs

THEREFORE,
the effect of the morphology on the PN abundances should be explored!

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The problem of PN shapes vs ICFs

Gonçalves et al. (2006)
– Our careful photoionization modeling of NGC 7009
– Convincingly proved that FLIERs are not nitrogen overabundant
– The empirical N/H, higher in the FLIERS than in the overall nebula, is an ICF illusion!

\[
\frac{ICF(N)}{O/ O^+} = \frac{N/N^+}{H^+}
\]

This ICF assumes that \(O/ O^+ = N/N^+\)
The problem of PN shapes vs ICFs

Gonçalves et al. (2006)
– Our careful photoionization modeling of NGC 7009
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$$ICF(N) = \frac{O}{O^+}$$

$$N/H = ICF(N) \frac{N^+}{H^+}$$

This ICF assumes that
$$O/O^+ = N/N^+$$

BUT the real ICF, from 3D model of NGC 7009 would be

$$O/O^+ = 0.73 N/N^+ \text{ Rim}$$
$$= 0.60 N/N^+ \text{ Fliers}$$
$$= 0.62 N/N^+ \text{ Neb}$$
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Our PN 3D photo models vs ICFs

Alexander & Balick (1997)
Gruenwald & Viegas (1998)
Morisset & Stasinska (2008)

**Range of Stellar/Nebular Parameters**

ContShape: blackbody

$50 \leq T_{\text{eff}} \leq 250 \text{ kK}$

$1 \times 10^3 \leq L_* \leq 2 \times 10^4 \, L_\odot$
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PN abundances:
Kingsburgh & Barlow (94)

<table>
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<tr>
<th>Parameter</th>
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<th>Value non-Type I</th>
<th>Change</th>
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<tbody>
<tr>
<td>He/H</td>
<td>0.12 ± 0.015</td>
<td>1.2 increased</td>
<td></td>
</tr>
<tr>
<td>O/H</td>
<td>(4.93 ± 2.22) \times 10^{-4}</td>
<td>same</td>
<td></td>
</tr>
<tr>
<td>N/H</td>
<td>(1.40 ± 0.88) \times 10^{-4}</td>
<td>increased by 3.8</td>
<td></td>
</tr>
<tr>
<td>C/H</td>
<td>(6.48 ± 5.35) \times 10^{-4}</td>
<td>decreased by 2.2</td>
<td></td>
</tr>
<tr>
<td>Ne/H</td>
<td>(1.25 ± 0.63) \times 10^{-4}</td>
<td>same</td>
<td></td>
</tr>
<tr>
<td>Ar/H</td>
<td>(2.42 ± 2.28) \times 10^{-6}</td>
<td>same</td>
<td></td>
</tr>
<tr>
<td>S/H</td>
<td>(8.08 ± 6.19) \times 10^{-6}</td>
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Our PN 3D photo models vs ICFs

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X/H: Type I and non-Type I

Geometry: round - R, spherical - E, bipolar - B

Ne: 3 000 cm\(^{-3}\)

Size: depends on morphology (radiation-bounded)

Tafoya et al (2009)

Bipolars have dense torus;
5 – 10 x denser than the lobes

\[\text{Ne}_{\text{torus}} = 6 \times \text{Ne}_{\text{lobes}}\]
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Results: optical + IR spectra

UV + optical + IR spectra
This is why it is hard to derive ICFs for bipolar and elliptical PNe.
Results: KB94\textsubscript{ICF} versus MOC\textsubscript{ICF}

Line intensities given by MOCASSIN for the 126 models are used to obtain He/H and ionic abundances, and then KB94's ICF.

MOC ionic fractions return the true ionization correction factors, MOC\textsubscript{ICF}.
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MOC ionic fractions return the true ionization correction factors, MOC_{ICF}

The KB94_{ICF}/MOC_{ICF} ratio will tell us which are the additional corrections we should apply to the KB94 scheme in order to derive more robust abundances for BIPOLARS and ELLIPTICALS! (Gonçalves, Wesson, Morisset, Barlow & Ercolano., in prep.)
KB94_{ICF} / MOC_{ICF} : NITROGEN

Optical + IR

![Graph showing KB94_{ICF}/MOC_{ICF} as a function of T_{eff} (10^3 K). The graph includes data points for BIPOLARS (circles) and ELLIPTICALS (squares). Type I = filled, non-Type I = empty.]
KB94$_{ICF} / MOC_{ICF} : \text{NITROGEN}$

Optical + IR

- **2$\times$10$^3$ $L_{\text{sun}}$**
  - Bipolars = Circles
  - Ellipticals = Squares
  - Type I = filled
  - Non-Type I = empty

- **1.1$\times$10$^4$ $L_{\text{sun}}$**
Optical + IR lines

KB94\textsubscript{ICF} / MOC\textsubscript{ICF} : NITROGEN
KB94_{ICF} / MOC_{ICF} : NITROGEN

Optical + IR lines

![Graph showing optical + IR lines vs. $T_{\text{eff}}$ (10^3 K)]

- BIPOLARS = CIRCLES
- ELLIPTICALS = SQUARES
- Type I = filled
- non-Type I = empty
KB94 ICIF / MOC ICIF : OXYGEN

Optical + IR

![Graph showing KB94 ICIF / MOC ICIF vs. $T_{\text{eff}}$ (10$^3$ K)].

- **BIPOLARS** = CIRCLES
- **ELLIPICALS** = SQUARES

Type I = filled
non-Type I = empty
Optical + IR

- $K_{B94}^{ICF} / M_{OICF}^{ICF}$

Graph:
- $T_{eff} (10^3 K)$
- $K_{B94}^{ICF} / M_{OICF}^{ICF}$

Legend:
- BIPOLARS = CIRCLES
- ELLIPTICALS = SQUARES

Type I = filled
Non-Type I = empty
Optical + IR

![Graph showing KB94 ICf / MOC ICf: SULPHUR vs. T_{eff} (10^3 K)]

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KB94 / MOC : ARGON

Optical + IR

![Graph](image-url)
Results: KB94\textsubscript{ICF} versus MOC\textsubscript{ICF}

Discrepancies in between ICF and true abundances

- Vary with $T_{\text{eff}}$ as much as with shape, and they also change with luminosity and chemical type.
- Are in general higher for bipolars than for ellipticals.
- In the worst cases, they amount to B (E):
  - up to 33 (19)$\%$ for N (under & over estimated)
  - up to 17 (13)$\%$ for O (under)
  - up to 40 (40)$\%$ for Ne (over)
  - up to 55 (50)$\%$ for S (under)
  - up to 28 (24)$\%$ for Ar (under & over)
Results: KB94 ICF versus MOC ICF

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  - up to 55 (50)\% for S (under)
  - up to 28 (24)\% for Ar (under & over)

What about if we include the UV spectrum in the analysis?
KB94$_{ICF}$/MOC$_{ICF}$: NITROGEN

Optical + IR

UV + Optical + IR

Missing ions: N$^{2+}$
N$^{3+}$

Missing ions: N$^{2+}$
(UV, but too faint)
KB94$_{ICF}$ / MOC$_{ICF}$: OXYGEN

Optical + IR

UV + Optical + IR

Missing ions: $O^{3+}$

$O^{4+}$
KB94_{ICF} / MOC_{ICF} : NEON

Optical + IR

UV + Optical + IR

Missing ions: Ne^{3+}
Ne^{4+} (optical, but too faint)
In conclusion

- Nebular abundance ratios are crucial to understand the interplay of the different populations in galaxies.

- One should carefully choose which elements to use as diagnostics of a galaxy's past and present time (since they depend on the galaxy metallicity).

- Uncertainties should be considered.

- The tools to derive empirical abundances need to be (and are being) improved.