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Atomic processes in planetary nebulae

Manuel A. Bautista

Centro de Física, IVIC, P.O. Box 21827 Caracas 1010A, Venezuela
email: bautista@kant.ivic.ve

Abstract. Historically, Planetary Nebula research has been a ground for much development in atomic physics. In the last five years the combination of a generation of powerful observatories, the development of ever more sophisticated spectral modeling codes, and important efforts on mass production of high quality atomic data have led to important progress in our understanding of the atomic spectra of PNe. In this paper I review such progress, including identification of heavy species (beyond the iron peak elements), observations of hyperfine emission lines and analysis of isotopic abundances, fluorescent processes, and new techniques for diagnosing physical conditions based on recombination spectra. Finally I discuss the new trends on the research of atomic processes in PNe.

Keywords. atomic processes, atomic data, line: formation, line: identification, radiation mechanisms: general, planetary nebulae: general

1. Introduction

Throughout history we find that there is a close relationship between astronomical research and the study of atomic processes and atomic data for spectroscopy, solar physics and Planetary Nebulae (PNe) being two distinctively important areas for development. In such a mature subject as PNe progress comes through a combination of various factors. On the one hand, nearly all modern observational research in PNe involves some kind of spectra, whose interpretation requires some understanding of the atomic processes involved and handling of atomic data. The level of understanding of such processes and data required for various applications ranges from phenomenological and statistical studies of commonly prominent lines in some types of PNe, to compilation of raw atomic data for direct inspection (such as line finding lists), to modeling of synthetic spectra attempting to fit the observed spectra. On the other hand, the accuracy and quantity of atomic models describing various features in observed spectra have evolved with time, driven by great advances in ground- and space-based observatories, computer technology and experimental techniques. At present there are models and data accurate enough for satisfactory analysis of at least the most prominent features in the PNe spectrum. Also the advent of on-line databases and spectroscopy tools has revolutionized the dissemination of results of atomic physics research. Thus, the scope for the study of atomic processes in PNe is only limited by the quality of observed spectra, in terms of spatial and spectral resolution and statistical quality to measure very accurate fluxes and detect weak lines.

A review of atomic processes spans an audience that includes specialists in the study of atomic systems with tools capable of providing models and atomic data, astronomers seeking to understand the reliability and accuracy of their modeled spectra, and those who use the models and data to compare synthetic spectra with observations, diagnose the physical conditions and compute chemical abundances of nebulae. The atomic physics tools have been reviewed in several other publications, including previous proceedings of this series of conferences (e.g. Nahar 2003), thus for the sake of brevity they will not be reviewed here. Instead, I will discuss novel atomic processes and new atomic species identified in spectra of PNe within the last five years, since the last symposium of this series. Also, I will review the available atomic models and data in terms of their potential for reliable diagnostics of physical conditions and determinations of chemical abundances.

The physical conditions in PNe, which are of interest here, are those of photoionized plasmas as observed in the ultraviolet (UV), optical, and infrared (IR) bands, unlike X-ray spectra which result from coronal mechanically heated gas. This band of shorter wavelengths will not be discussed here. A good review on this subject can be found in Kallman & Palmeri (2006).

The present review is organized according the nuclear charge of atomic species, starting with hydrogen and helium, and following with the second and third row elements, the iron-peak ions, and then onto the heavier elements. I then finish the paper with a discussion of various general issues of interest.

2. Hydrogen

The spectrum of hydrogen in H II regions has been studied extensively for quite some time. In principle the spectrum is determined by the recombination rates into each level and the subsequent radiative cascades. Such a process is accurately modeled in two idealistic situations, the so called "case A" in which all lines are optically thin and "case B" which assumes that the optical depth of Lyα goes to infinity. Two complications arise beyond these approximations: (1) a detailed solution to the radiative transfer of Lyα photons including the effects of self-absorption, removal and collisionally induced transitions between the $2s$ and $2p$ states, and (2) when the electron temperature and density of the plasma are high enough for effective collisional excitations onto $n > 2$ states.

Dennison, Turner & Minter (2005) discuss the first of these problems and proposed an observational test. They claim that radio-observatories will soon be able to detect the $2s_{1/2} - 2p_{1/2}$ and $2s_{1/2} - 2p_{3/2}$ lines at 1.1 GHz and 9.9 GHz respectively. Dennison *et al.* explain that removal of Lyα photons by dust would limit the pumping of H atoms into the $2p$ states, and under these conditions the $2s_{1/2} - 2p_{1/2}$ transition will appear in stimulated emission and the $2s_{1/2} - 2p_{3/2}$ line will appear in absorption. In general, the relative strengths of these two lines should serve as diagnostics of the populations of the $2s$ and $2p$ states and the responsible processes. Further, Dennison *et al.* suggest that removal by dust is the dominant mechanism acting on Lyα photons in H II regions, which if correct would circumvent the need to solve the radiative transfer problem.

In regards to collisional excitation of hydrogen, Péquignot & Tsamis (2005) study the evolution of calculated collision strengths for $1s \to n = 3, 4, 5$. They point out large variations in the theoretical values up to the last calculation of Anderson *et al.* (2000). Péquignot & Tsamis compare their observations for the PN G135.9+55.9 with predictions of models using various collisional data sets. They find that the collision strengths of Anderson *et al.* yield the most consistent results, yet these may have not reached ultimate accuracy.

3. Helium

Modeling the He I recombination spectrum has become increasingly reliable, with an accuracy on line emissivities of the order of ∼1% (see Bauman *et al.* 2005; Benjamin, Skillman & Smits 1999, 2002). Then, given high-quality spectroscopic data it is now possible to use the He I lines as temperature diagnostics. Zhang *et al.* (2005a) write parametric forms for He I line ratios vs. temperature and conclude that the best diagnostic is obtained from the $\lambda7281/\lambda6678$ ratio. The results of the diagnostics have an intrinsic uncertainty of ~1000 K at around 10 000 K owing to optical depth effects on the He I $\lambda3889$ ($2s\ ^3S \rightarrow 3p\ ^3P^o$) line. When comparing the results from the $\lambda7281/\lambda6678$ ratio with those from $\lambda7281/\lambda5876$ a systematic error of (~500 K) arises, which may be related to the uncertainty on the optical depth of the $\lambda3889$ line, or perhaps from some other source. Interestingly, in a sample of 48 PNe the helium temperature is systematically lower than that obtained from the hydrogen Hβ decrement by an average of 4000 K.

Lee, Kang & Byun (2001) presented Raman-scattering as a likely mechanism for detecting He II emission in bipolar PNe where the high ionization region may be obscured (e.g. M2-9). According to their estimates a relatively small column density of neutral hydrogen surrounding the nebula would be enough to Raman-scatter He II $6p \rightarrow 2s$ to yield emission features at around 6545Å. In addition, the hydrogen Hα line acquires a $\Delta\lambda^{-2} = (\lambda - \lambda_{H\alpha})$ profile. Although the true origin of the Hα line in M2-9 is still subject of controversy the Raman-scattering process in PNe deserves further investigation.

4. Second and third row elements (C-Ar)

Density and temperature diagnostics in PNe are commonly based on line ratios among collisionally excited lines. The best known density diagnostics are [S II] $\lambda6717/\lambda6731$ and [O II] $\lambda3729/\lambda3726$ that are sensitive to densities of the order of 10^3 cm^{-3}, [Cl III] $\lambda5517/\lambda5537$ for $N_e \sim 10^4$ cm^{-3}, and [Ar IV] $\lambda4711/\lambda4740$ for $N_e \sim 10^4 - 10^5$ cm^{-3}.

The [O II] ratio that arises from transitions among the $^4S_{3/2}$ ground level and the $^2D_{5/2}$ and $^2D_{3/2}$ levels was a subject of controversy for the last few years. It was commonly assumed that LS-coupling was a valid approximation for terms of the ground configuration of the O^+ system, thus the ratio of collision strengths from the ground levels to the $^2D_{5/2}$ and $^2D_{3/2}$ levels was given by the statistical weights, i.e. 1.5. However, McLaughlin & Bell (1998) claimed to have found relativistic effects that yielded a ratio of the collision strengths of 1.93, with profound effects on N_e determinations for low surface brightness H II regions. Such claims were contested by evidence from the extensive literature survey of Copetti & Writzl (2002) and the observational campaign of Wang *et al.* (2004). The issue seems settled now with a new calculation by Pradhan *et al.* (2006), that accounts for all dominant relativistic effects and confirms the earlier predictions of the LS-coupling approximation. The spectroscopic survey of Wang *et al.* (2004) also served to test the A-values for dipole forbidden transitions of [O II]. They find that the transition probabilities of Zeippen *et al.* (1982) best fit the observations, the differences being of only a few percent, while the results of later calculations by Zeippen (1987) and Wiese *et al.* (1996) both look problematic.

Wang *et al.* also compared the electron densities obtained from various line ratios and obtained very good agreement between N_e([O II]), N_e([S II]), and N_e([Cl III]). By contrast N_e([Ar IV]) values yield densities systematically higher than those from the other diagnostics, which sheds some doubts on the accuracy of the N_e([Ar IV]) A-values.

An important development in atomic spectroscopy has been the detection of hyperfine-induced spectra from various ions, which allows for the determination of isotopic abundances with implications for stellar interiors and evolution and cosmology. Brage, Judge & Proffitt (2002) with the STIS instrument on the Hubble Space Telescope identified the hyperfine-induced $2s2p\ ^3P^o_0 \rightarrow 2s^2\ ^1S_0$ line of N IV at 1487.89 Å, together with the magnetic quadrupole ($2s2p\ ^3P^o_2 \rightarrow 2s^2\ ^1S_0$) and intercombination ($2s2p\ ^3P^o_1 \rightarrow 2s^2\ ^1S_0$) lines within the same multiplet. In the absence of coupling between the nucleus and the spin of the electronic level the $\Delta J = 0$ transition would not take place, but both stable isotopes of N have non-zero nuclear spin (^{14}N with spin 1 and ^{15}N with spin 1/2) and both have about the same transition rate. From the observations Brage *et al.* were able to confirm the theoretical transition rate for the first time for any low ionization species.

The same multiplet from C III, isoelectronic with N IV, lies around 1909.6 Å and was observed by Palla *et al.* (2002) in NGC 3242. Carbon has two stable isotopes, ^{12}C and ^{13}C with nuclear spins 0 and 1/2 respectively. Then, Palla *et al.* determined an upper limit to the ^{13}C hyperfine induced transition which combined with the measurements of the magnetic quadrupole and intercombination lines of ^{12}C yield an isotopic ratio ^{12}C/^{13}C in agreement with standard stellar models. This determination together with previous observations of ^{3}He in the same PN have important implications on stellar nucleosynthesis.

Along the same lines, Rubin *et al.* (2004) studied the ^{12}C/^{13}C ratio in a sample of 41 PNe, using spectra retrieved from the IUE archives. For one of these objects, NGC 2440, the ^{13}C hyperfine induced transition was clearly observed and a firm isotopic ratio was estimated.

The hyperfine splitting of the [Al VI] $^3P_1 \rightarrow {}^3P_2$ transition at 3.66μm was observed by Casassus *et al.* (2005) with the Phoenix instrument on Gemini South. The nuclear spins of the two stable isotopes, I=5 for ^{27}Al and I=5/2 for ^{26}Al, by coupling to electronic total angular momentum yield five well defined components out of a total of nine closely spaced lines. Angular momentum algebra leads to different spectra from both isotopes, which Casassus *et al.* compared to observations to establish an upper limit on the ^{26}Al/^{27}Al abundance ratio.

5. The iron-peak elements

Fe and iron-peak elements are important constituents of PNe. Depending of the excitation of the nebula, iron is frequently seen in stages from Fe I to Fe VII. The observed ions of nickel span about the same range. Other less abundant elements of the group are occasionally identified as well. Within the IRON Project we have devoted much effort to the computation of data and construction of spectral models for these ions. A summary of the data is presented in Fig. 1.

Of all these species Fe II is by far the most studied. It yields rich and complex spectra that can be excited by a variety of different mechanisms, i.e. electron impact excitation, photo-excitation by continuum radiation, fluorescence by H I Lyα and/or O VI λ1032 radiation. In moderately dense plasmas ($N_e \sim 10^7$ cm^{-3}) the populations of high levels involved in fluorescence are redistributed by collisionally induced transitions through highly excited pseudo-metastable levels (Bautista, Rudy & Venturini 2004). Furthermore, proper modeling of Fe II spectra requires large systems, approaching one thousand levels and complete and accurate atomic data. Some doubts still prevail in regard to whether current Fe II models have reached necessary accuracy. More work is still in progress along these lines by various groups like the IRON Project, the FERRUM Project at Lund University, and the group at the University of Queen's Belfast. At this point it is worth mentioning the work of Williams *et al.* (2003) who compared the abundance ratio Fe^+/Ni^+ in IC 418 as obtained from UV resonant absorption lines, Fe II λ1260.5 and Ni II λ1317.2, as opposed to the determination from optical forbidden lines in emission. They get a large discrepancy between Fe^+/Ni^+ >25 from absorption lines and Fe^+/Ni^+=5 from emission lines. However, their calculation from the [Ni II] λ7378 line was incorrect because they assumed that this line was excited by collisional excitation directly from the ground state, yet we find that a more important excitation channel comes from second excited level $3d^9\ ^2D_{3/2}$. A proper calculation yields Fe^+/Ni^+ several times greater than their previous value, consistent with the result from the absorption lines.

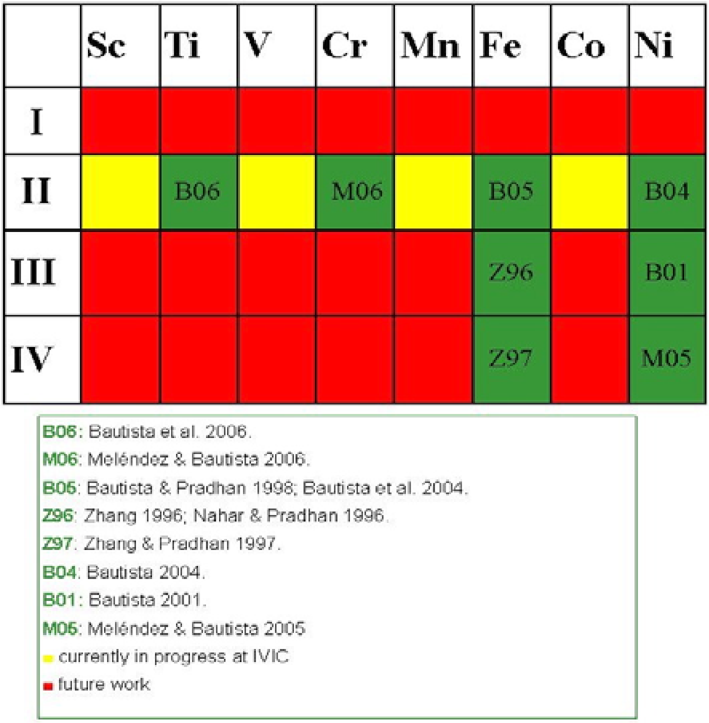

Figure 1. Spectral models for low ionization iron-peak species

6. Neutron capture elements

One of the frontiers of spectroscopy of PNe is the study of n-capture elements presumably synthesized by the AGB progenitor of the nebula. The progress on this area since the seminal work of Péquignot & Baluteau (1994) has been slow owing to the need for high spectral resolution (> 10 000) and the absence of atomic data and models. Despite the difficulties, Dinerstein (2001) was able to identify lines of [Kr III] and [Se IV] in the K-band of the near infrared spectra of NGC 7027 and IC 5117. To date these lines have been identified in almost a hundred PNe (Sterling & Dinerstein 2005).

On the theoretical side, the calculation of collisional data for heavy species represents an important challenge because intermediate coupling representations are inappropriate in many cases, at the same time as relativistic effects become too large to treat in the Breit-Pauli representation. Thus, researchers must turn to fully relativistic codes in the Dirac formalism. Recently, Badnell *et al.* (2004) were able to put the Dirac Coulomb R-matrix package of (Ait-Tahar *et al.* 1996) on the same footing as the traditional Breit-Pauli R-matrix codes as developed by the IRON/RmaX team. Nonetheless, these sort of calculations are still far from routine work, owing to the size of the atomic representations in JK -coupling.

7. Additional considerations

This review would not be complete without pointing out some important general issues of relevance to the present subject as well as recently developed tools for atomic spectroscopy.

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The accuracy of recombination rate coefficients was in recent years an important source of concern for modelers for their effects on calculations of ionic fractions. The issue, however, seems to have reached a point of stability as different theoretical methods, e.g. the unified R-matrix approach of Nahar and Pradhan and the Thomas-Fermi-Dirac approach in the version of Badnell and collaborators (Badnell *et al.* 2003), begin to yield consistent results and to release large amounts of data. Such theoretical results also seem to comply with recent experimental determinations (e.g. Fogle *et al.* 2005). A warning must be raised though regarding low temperature dielectronic recombination, that is dominated by near threshold autoionizing channels, whose positions are difficult to get accurately from theory. More experimental work on this area is needed to benchmark current and forthcoming data (e.g. Böhm *et al.* 2005).

On its origins, one of the explicit objectives of the IRON Project was to provide a complete and reliable set of data for positive ions of interest in nebular infrared spectroscopy. A comprehensive review of these data is presented by Badnell *et al.* within the present proceedings. The entire dataset produced by the IRON Project will soon be available through TIPbase (Mendoza 2000).

A very useful tool for nebular spectroscopy, the EMILI package for emission line identification, has been developed by Sharpee *et al.* (2003). This tool should expedite the analysis of high spectral resolution and signal-to-noise spectra, and enable the identification of faint poorly known features.

During the development of the present symposium there was considerable discussion on the presence of electromagnetic fields associated to the central star and some structures of PNe. Furthermore, it is worth pointing out that such fields could have profound effects on dielectronic recombination (DR). Electric fields increase the dielectronic recombination rates as they mix high-l autoionizing states, that normally do not contribute to recombination, with lower l states yielding larger autoionizing rates. Further enhancements occur in the presence of magnetic fields perpendicular to the electric field (Robicheaux & Pindzola 1997). Experimental determinations of DR of O VI show enhancements of up to a factor of 2 on the DR rate when an external electric field of 340 V/cm is applied. But, electric fields need not be external, as strong microfields are naturally produced in dense plasmas, although under these conditions the enhancements due to the field are partly compensated by the lowering of the continuum effect. For example, in a 10^9 cm^{-3} plasma the effective DR rate for C IV is increased by 40% (Badnell *et al.* 1993).

8. Conclusions

The question of what fractions of Lyα photons are self-absorbed and removed by dust in photoionized regions is rather important, as the treatment of hydrogen spectra in photoionization modeling is one of the main limitations to their accuracy. There are also various questions in regard to heating and photo-evaporation of grains in PNe. Thus, the work of Dennison *et al.* (2005) is fundamental for entering a new level of detailed understanding of PNe and H II regions. Likewise, similar techniques, as for the H I spectrum, are desirable for He II to understand optical depth effects on the λ3889 line.

The work of Zhang *et al.* (2005a,b) on temperature diagnostics from He I lines is very important, yet the large differences, $\sim$ 4000K, between the results of these diagnostics and the T(H I) are difficult to understand. The low He I temperatures, if confirmed, would open a whole new set of questions in regards to the structure and evolution of PNe.

As atomic models have become available for essentially all of the most prominent species in spectra of PNe it is important to systematically check on the consistency of

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density and temperature determinations out of those species. This would allow us to determine whether the atomic data have reached ultimate accuracy. A flag of warning must be raised, however, in regard to neutral species and ions with ionization potentials below that of hydrogen because their spectra could be affected by photo-excitation by continuum radiation. Such is the case of N I (Bautista 1999) that Copetti & Writzl (2002) tried to analyze on the same grounds as ionized species.

The iron and iron-peak ions are as important as ever, particularly Fe II, which is prominent throughout astronomy, beyond PNe research. These ions, however still pose great challenges to current theoretical and experimental techniques.

The importance to modern astronomy of studying isotopic abundances and n-capture elements can hardly be overstressed. Yet, such work imposes extreme demands on spectroscopic instruments and astronomers. Carefully coordinated efforts between atomic physicists, astronomers, and instrument designers would be desirable on this subject.

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