SOME ATOMIC PARAMETERS PERTINENT TO STUDIES OF NEBULAR IONIZED PLASMAS

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In order to predict emission line and continuum intensities and assess plasma diagnostics for gaseous nebulae, it is necessary to have accurate atomic parameters. In some instances the requirements for accuracy are very severe. A variety of data is required:

- 1) Coefficients of continuous absorption;
- 2) Direct and dielectronic recombination coefficients;
- 3) Transition probabilities for permitted lines, so we can accurately predict both recombination line intensities and fluorescent phenomena (e.g., **OI** λ8446);
- Transition probabilities for forbidden and intercombination lines; 4)
- 5) Collision cross sections for levels which give rise to:
 - a) resonance transitions,
 - b) intercombination lines,c) forbidden lines;
- 6) Charge-exchange cross sections.

Time limitations permit me to discuss just a few points. The importance of choosing good wave functions is illustrated by comparing observed and predicted f-values for some permitted lines as in the following example due to S. J. Czyzak:

Ion	λ	Transition	Exp.	Theory
<u>C 111</u>	2297	$2s2p^{1}P^{\circ} - 2p^{2} TD$	0.187 0.47ª	0.27b 0.19c
οv	1371	$2s2p^{1}P^{\circ} - 2s^{2} {}^{1}D$	0.147 0.32 ^a	0.18 ^b 0.15 ^c

^acoulombic wave functions; ^bHFX= Hartree-Fock wave functions with exchange; CHFX + superposition of configurations

Czyzak notes that Fermi-Thomas (FT) or Fermi-Thomas-Direc (FTD) wave functions tend to improve for heavy atoms. In the FT or FTD method, you can vary a parameter in a particular potential, but the HFX method minimizes the energy with no constraints on the form of expression for the function. Relativistic corrections are needed for heavy ions.

From the standpoint of practical calculations, the objection has been raised that in the HFX method you need to use separate radial wave functions for each level of a given configuration, thus greatly increasing the burden of the computation.

As a second example, I'd like to discuss the nebular-type transitions in a p^3 configuration. As the electron density increases, the intensity ratio of the two nebular-type transitions approaches a limiting value which depends only on the ratio of the A-values:

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$$\mathbf{r}(\infty) = \frac{\mathbf{I}({}^{2}\mathbf{D}_{5/2} - {}^{4}\mathbf{S}_{3/2})}{\mathbf{I}({}^{2}\mathbf{D}_{3/2} - {}^{4}\mathbf{S}_{3/2})} = \frac{\omega({}^{2}\mathbf{D}_{5/2})}{\omega({}^{2}\mathbf{D}_{3/2})} \frac{\mathbf{A}(\dots)}{\mathbf{A}(\dots)} = \frac{\mathbf{A}({}^{2}\mathbf{D}_{5/2} - {}^{4}\mathbf{S}_{3/2})}{\mathbf{A}({}^{2}\mathbf{D}_{3/2} - {}^{4}\mathbf{S}_{3/2})}$$

Observationally, this limiting value can be found in nebulae of high density. The classic example is found in the ratio of 3726/3729 [O II] lines. The observational limit is near 0.35, but since the 1940s and until very recently, theory has failed to reproduce this result. Eissner and Zeippen conclude that the ordinary magnetic dipole operator (L + 2S) does not always give a "safe" answer in intermediate coupling. A recent calculation by Zeippen (1982) includes: configuration interaction, semiempirical term energy corrections, "special" radial wave functions, and relativistic corrections to the magnetic dipole operator. With these improvements, he obtained $r(\infty) = 0.35$.

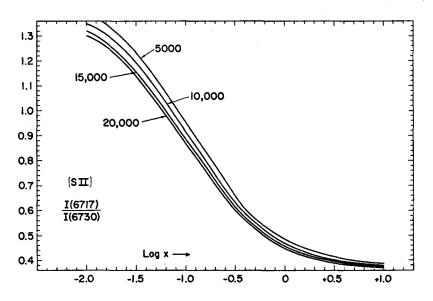
A similar analysis can be carried out for [N I], for which the A-values were first calculated by Ufford and Gilmour many years ago. Zeippen finds $r(\infty) = 0.54$. From observations with the shectograph on the 2.5-m telescope at Mt. Wilson, S. J. Czyzak and I found a limiting value very near 0.54 from a number of relatively dense planetary nebulae. This result is in excellent agreement with Zeippen's prediction.

For ions of the $3p^3$ configuration, the situation is not entirely satisfactory. Nebular line ratios have been measured for [S II], [CL III], and [Ar IV], both with the shectograph at the coudé of the 2.5-m telescope and with the ITS and Cassegrain scanner on the 3-m Shane telescope at Lick Observatory. Theoretical limiting values $r(\infty)$ given by Mendoza and Zeippen (1982) may be compared with limiting observed ratios as follows:

	<u>[S II]</u>	[Cl III]	[Ar IV]
Theory (Mendoza and Zeippen)	0.44	0.22	0.122
Observed (Aller and Czyzak)	0.41	0.28	(0.12::)

The [Ar IV] $\lambda4711$ is difficult to separate from He I $\lambda4713$; the shectograph observations for IC 4997 yield a ratio of about 0.12

One of the reasons for laying great emphasis on these A-values calculations and also on the cross sections for collisional excitation of metastable levels is that



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ratios of the nebular-type transitions in p^3 ions are useful for determining electron densities. In the figure we plot the 6717/6730 ratio for [S II] for values of the electron temperature ranging from 5000°K to 20,000°K as a function of log x, where x = 0.1 N_E//T_E. At low values of electron density, the ratio is determined primarily by the ratio of collision strengths for the two levels of ²D, and lies near 1.5. At intermediate densities, the ratio depends on both the collision strengths and A-values, while at high densities the A-value ratio determines I(6717)/I(6730). It is clear from this figure that at electron densities in excess of about 3000 cm⁻³ the derived value of N_E is strongly dependent on the adopted A-values. These curves were calculated with A-values given by Czyzak and Krueger (1963) which gave r(∞) = 0.38, which may be a little low. A more recent calculation by Czyzak (1982) with greatly improved wave functions suggests that further refinements must be considered.

Further clues are supplied by the intensity ratios of the auroral-type transitions in [Ar IV]. The A-values calculated by Mendoza and Zeippen and by Czyzak are in good agreement for these transitions but both fail to fit the observations. Furthermore, the ratio of the intensities of the auroral and nebular-type transitions suggests densities that are too high.

I have chosen the $3p^3$ configuration as an example of a situation where A-values and collision strengths are urgently needed for diagnoses of nebular plasmas, but where the necessary calculations appear to be of extreme difficulty. The small number of observational checks that can be carried out suggests that much more work needs to be done on this problem.

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