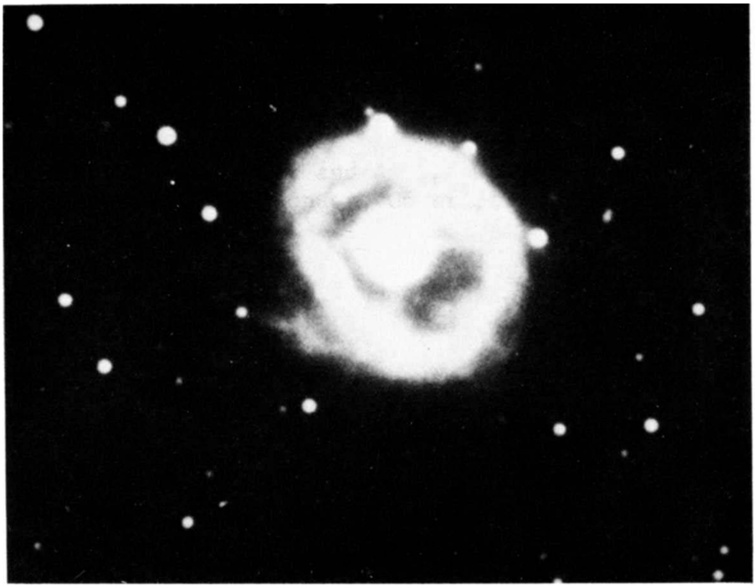

SESSION III

PHYSICAL PROCESSES

ADVANCES IN STUDIES OF PHYSICAL PROCESSES

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1. EXCITATION OF FORBIDDEN LINES

The forbidden lines in planetary nebulae are due to transitions between energy levels belonging to configurations ns^2np^q with $q = 1$ to 5, and with $n = 2$ ([O II], [O III], ...) or $n = 3$ ([S II], [S III], ...). For electron impact excitation of these levels, the expansion

$$\Psi = \sum_i A_i \psi_i \theta_i \tag{1}$$

is used for the wave function of the (electron and Target) system, where: ψ_i is a wave function for the target; θ_i a function for the colliding electron; and A_i an operator for vector-coupling and antisymmetrisation. The functions ψ_i satisfy systems of coupled integro-differential equations. Solution of the equations is referred to as the ID approximation. The main recent advances have been: (a) to use accurate target functions ψ_i and; (b) to include in (1) functions ψ_i belonging to excited configurations. Two independent computer programs have been used, RMATRX [1] and IMPACT [2].

(a) Calculations for [C I], [N I] and [O I].

Accurate calculations for C, N and O have been made using RMATRX [3]. The expansion (1) is taken to include states which allow for polarization of the target by the colliding electron. The results obtained have been integrated over Maxwell velocity distribution to give excitation rates [4].

(b) Calculations for $2s^22p^q$ positive ions.

Accurate calculations for $2s^22p^q$ ions have been made using IMPACT; excitation rates have been published for [N II], [O III], [Ne II] and [Ne III] [5] and for [O II] [6]. Calculations are being made at UCL for [Ne IV] and [Ne V]. Calculations for [N II] have been made using both IMPACT and RMATRX: there is good agreement [7]. Inclusion of

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states in (1) belonging to $2s2p^{q+1}$ configurations gives resonances in collision strengths which come close to forbidden line excitation thresholds for more highly ionized systems.

(c) Calculations for $3s^23p^q$ systems.

Available results for $3s^23p^q$ systems are much less accurate than those for $2s^22p^q$ systems. For most cases, only the distorted wave (DW) approximation has been used [8, 9]. For a few cases, ID calculations have been made, but with inclusion in (1) of only those states which belong to the $3s^23p^q$ configurations [10]. Recent work [6] for [S II] shows: (a) reasonable agreement between ID and DW calculations; (b) satisfactory agreement with earlier ID calculations [10], and: (c) much less satisfactory agreement with earlier DW calculations [8]. It is expected that coupling to higher configurations, such as ns np^{q+1}, will be more important for n = 3 than for n = 2. No detailed calculations have yet been completed but a systematic study of S ions has been started at UCL.

2. TRANSITION PROBABILITIES FOR np^3 $^2D_{5/2} \rightarrow {}^4S$, $^2D_{3/2} \rightarrow {}^4S$

In many nebulae the intensity ratios

$$r\ (N_e) = I(^2D_{5/2} \rightarrow {}^4S)/I(^2D_{3/2} \rightarrow {}^4S), \tag{2}$$

in spectra such as [O II], [S II] and [Cl III], are sensitive to electron density. In the limit of $N_e \rightarrow 0$, r is proportional to the ratio of excitation rates, which in turn is equal to the ratio of statistical weights: this gives r(0) = 1.5. At high densities (collisional de-excitation rates faster than radiative rates) the levels $^2D_{5/2}$, $^2D_{3/2}$ are populated in the ratio of their statistical weights and hence

$$r(\infty) = 1.5\ A(^2D_{5/2} \rightarrow {}^4S)/A(^2D_{3/2} \rightarrow {}^4S). \tag{3}$$

The sensitivity of r to N_e arises from the fact that the two transition probabilities are not equal; whereas $A(^2D_{5/2} \rightarrow {}^4S)$ is mainly due to electric quadrupole radiation, $A(^2D_{3/2} \rightarrow {}^4S)$ is mainly due to magnetic dipole radiation and is larger than $A(^2D_{5/2} \rightarrow {}^4S)$. It should also be noted that the transition probabilities are particularly small for np^3 configurations (because there are no diagonal matrix elements of the spin-orbit interaction): if it were not for this fact $r(N_e)$ would not be sensitive to N_e at the low densities typical of most planetary nebulae.

Twenty years ago, Seaton and Osterbrock [11] obtained for [O II] a best calculation value of r (∞) = 0.43 compared with the smallest measured value (for IC 4997) of 0.35±0.04 which was taken to be the observed value of r(∞). They remarked that "It would seem that further improvements in the theory could be made only by taking configuration interaction explicitly into account". More recent observations [12] have confirmed the earlier work: $r(\infty) = 0.36 \pm 0.02$ from observations of bright knots in NGC 7027. Very large configuration-interaction calculations have now been made [13]: they give $r(\infty) = 0.43$ in agreement with the earlier calculations. Thus a discrepancy between theory and observation still persists. A similar problem has been noted [14] for [N I], for which theory gives $r(\infty) = 0.64$ and observations give $r(\infty) \leqslant 0.51$.

The discrepancy is probably due to neglect of higher-order terms in the expression for the magnetic dipole transition operator. The leading terms are

$$\underset{\sim}{\mu} = \frac{-e}{2mc} (\underset{\sim}{L} + 2\underset{\sim}{S}), \qquad (4)$$

corresponding to the magnetic moment. In the solar uv, spectrum lines are observed due to transition $2\,^3S \rightarrow 1\,^1S$ in helium-like ions [15]. These transitions are not allowed with the operator (3) but are allowed when higher-order relativistic terms are included in the magnetic dipole operator [16]. For most forbidden transitions not involving a change in the principal quantum numbers these smaller terms can probably be neglected, but they may not be negligible for the delicate case of the np^3 configurations. Further calculations are therefore being made[17].

3. HYDROGENIC RECOMBINATION SPECTRA

(a) Infra-red wavelengths.

Level populations $N_{n\ell}$, expressed in terms of factors $b_{n\ell}$, have been computed as functions of T_e and N_e and used to obtain emissivities for H I Balmer and Paschen lines [18]. This work has now been extended to give emissivities for Brackett lines [19].

Consider the Brackett/Balmer ratios for lines with the same upper level,

$$I(n \rightarrow 4)/I(n \rightarrow 2). \qquad (5)$$

In the limit of high densities it can be assumed that $N_{n\ell} = (2\ell + 1)N_n/n^2$ (i.e., that $b_{n\ell} = b_n$ independent of ℓ) and hence that the ratios (4) depend only on ratios of transition probabilities. In planetary nebulae the densities are not sufficiently high for this to be a good approximation. Table 1 gives the ratio (4) for $N_e = 0$, 10^4 cm^{-3} and ∞, and $T_e = 10^4$ K.

TABLE 1

H I Brackett/Balmer ratios [19],

$I(n \rightarrow 4)/I(n \rightarrow 2)$, for $T_e = 10^4 K$

n N_e =	0	10^4 cm^{-3}	∞
5	0.179	0.166	0.114
6	0.184	0.173	0.124
8	0.177	0.172	0.129
10	0.174	0.171	0.130
20	0.171	0.154	0.132

(b) Radio wavelengths.

It is now established that maser action and pressure broadening must be taken into account in interpreting observations or radio recombination lines from planetaries and from denser H^+ regions [20,21] . A computer program has been published [22] for the calculation of continuum spectra, line-to-continuum ratios and line profiles for spherically symmetric models.

4. PERMITTED LINES OTHER THAN THOSE OF H I, He I AND He II

Spectra of planetary nebulae contain many weak permitted lines, other than those of H I, He I and He II. There are three possible excitation mechanisms: (a) fluorescent excitation by uv lines (Bowen mechanisms); (b) fluorescent excitation by stellar uv ("Case C" mechanism), and ; (c) recombination. Grandi [23] has made calculations which are approximate but of sufficient accuracy to estimate which mechanism is dominant for each observed line. Lines excited by stellar uv will give little information on conditions in the nebulae but may give information on the stellar uv radiation field (it may usually be assumed that absorption of radiation will be complete within the Doppler width of the uv absorption lines). Lines excited by recombination can give important information on ion abundances; the recombination lines of C are of particular interest [23, 24, 25, 26] . Pengelly [27] has made calculations for the recombination spectra of C II, C III and CIV. Since this reference is not easily available, we give in Table 2 his results for the effective recombination coefficients of lines which are almost certainly produced by recombination. For most of these lines excitation by stellar uv is unimportant because the upper state has an electron with large orbital angular momentum. There is then practically no difference between calculations for Cases A and B (Case B assumes self-absorption in transitions to the ground state).

For the line C III 3p $^3P \rightarrow 3s\ ^3S$, λ 4650, excitation by stellar uv is unimportant because the multiplicity (spin) is different from that of the ground state, $2s^2\ ^1S$. For this line there is a large difference between calculations for Cases A and B (for Case B it is assumed that there is self-absorption in lines to the triplet ground state, $2s2p\ ^3P$). The observed relative intensities [28] of C III λλ 4070, 4187 and 4647 in NGC 7027 are consistent with the assumption that Case A applies for C III triplets.

TABLE 2

Effective Recombination Coefficients$^{(a)}$

for C ions [24].

					$10^{13} \times \alpha(\mathrm{eff})$ (α in $cm^3\ s^{-1}$)		
Ion	Ground state	Line	λ(Å)		$T_e = 5\times10^3$	1×10^4	2×10^4
C II	$1s^22s^22p\ ^2P$	$4f\ ^2F \rightarrow 3d\ ^2D$	4267		4.82	2.52	1.17
C III	$1s^22s^2\ ^1S$	$5g\ ^3G \rightarrow 4f\ ^3F$	4070		6.48	2.18	1.47
		$5g\ ^1G \rightarrow 4f\ ^1F$	4187		2.16	1.06	0.49
		$3p\ ^3P \rightarrow 3s\ ^3S$	4650$^{(b)}$	(Case B	40.2	24.5	14.5
				(Case A	5.55	3.90	2.49
C IV	$1s^22s\ ^2S$	$6h\ ^2H \rightarrow 5g\ ^2G$	4659		15.1	7.24	3.24

Notes: (a) The effective recombination coefficient, α(eff), for a line is such that the number of photons emitted per unit volume per unit time is $N(X^+)N_e\ \alpha(\mathrm{eff})$ where $N(X^+)$ is the number density of recombining ions.

(b) Components at λλ 4647, 4650, 4651.

(a) Photo-ionization.

There has never been entirely satisfactory agreement between the observed spectra of planetaries and those computed for photo-ionization models. Before concluding that all discrepancies are a consequence of real nebulae being more complicated than model-makers have assumed, it is necessary to consider the accuracy of the atomic data used in the computations. In many cases there may be substantial errors in the photo-ionization cross sections which have been adopted.

Advances in techniques of electron collision computations enable much more accurate photo-ionization calculations to be made [29]. Wave function expansions of the type discussed in § 1 are used both for the initial bound state and for the final continuum state. Accurate calculations using RMATRX have been made for neutral C and O [30] and neutral N [31]. Similar calculations for O I oscillator strengths and O photo-ionization have been made using IMPACT [32]. The two calculations for oxygen are in close agreement.

These calculations show that the photo-ionization cross sections contain complicated resonance structures. Further systematic work is in progress. The results for ions should be of value for obtaining improved models both for the ionization structures of the nebulae and for the atmospheres of the central stars.

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DISCUSSION

Aller: In calculation of A values for 2s2p $^1P^\circ$ - $5s^2\,^1D$ transitions in CIII, NIV, OV and 5s5p $^1P^\circ$ - $5s^2\,^1S$ of SrI, the results depend strongly on wave functions. In CIII and OV for example, good results are obtained with Hartree-Fock wave functions with superposition of configurations. In CIII you get poor results unless superpositions are used, whereas in SrI satisfactory results are found with Hartree-Fock wave functions alone. Coulomb wave functions give poor results. Thus, sometimes Hartree-Fock wave functions suffice but in other instances superposition of configurations is needed also.

Seaton: This is precisely the point I was making. It is necessary in a lot of this work to worry about these things unless a more elementary treatment can be shown to give the correct result.

Nussbaumer: There are new calculations on CIII including 2s2p $^1P^\circ$ - $2p^2\,^1D$. We show that an already reasonable 3-configuration calculation gives a line strength S = 6.18 for that transition, but S = 4.30 for a 15-configuration basis and 4.21 for a 57-configuration basis.

Kaler: There is empirical evidence for discrepancies in the calculations, particularly for [NeIV] and [ClIV]. The [NeIV] lines are brighter than predicted, as are [ClIV] lines, the latter by perhaps half an order of magnitude. The [ArV] lines are also suspect.

Seaton: The miracle is that the actual rate coefficients have not changed very much. You could very well have situations with some resonance spike coming in. If you miss out on that resonance, you are easily down by factors of 2 or 3. Calculation on [NeV] is in fairly advanced stages of production work. [NeIV] is next on the list.

Garstang: How does the relative importance of the relativistic and non-relativistic contributions to the [OII] ^2D-^4S transition probabilities vary along the isoelectronic sequence? Do you think the correction would be important in [NeIV]?

Seaton: I think it applies to all those systems, but I haven't thought about whether it gets bigger along the sequence.