RECOMBINATION PROCESSES

P.J. Storey
Department of Physics and Astronomy,
University College London, Gower Street,
LONDON WC1E 6BT, England.

ABSTRACT

The role of resonances in the photoionization cross-sections of ions is discussed in relation to the radiative recombination coefficient. The calculation of dielectronic contributions to the recombination coefficient is reviewed for nebular conditions, and the importance of autoionizing states close to the first ionization threshold is illustrated. For those ions for which dielectronic recombination is not important at nebular temperatures, an assessment of the accuracy of the best available recombination coefficients is given.

1. RADIATIVE RECOMBINATION AND PHOTOIONIZATION

The most satisfactory approach to the calculation of recombination coefficients makes no distinction between 'radiative' and 'dielectronic' recombination. Consider the radiative capture process

$$X^{+m} + e \rightarrow X_b^{+m-1} + h\nu \qquad (1)$$

resulting in the bound state X_b^{+m-1} and the emission of a photon. Let the radiative capture cross-section be σ_{RC} and the cross-section for the inverse process of photoionization be σ_{PI}. The photoionization cross-section in general has the form of a smooth background interrupted by resonances. The resonances correspond to quasi-bound states of the recombined system X_a^{+m-1}, and Rydberg series of such states converge on the terms of the recombining system. The cross-sections for radiative capture and photoionization are connected by the Milne relation,

$$\sigma_{RC} = \frac{\omega_b}{2\omega_+} \frac{h\nu}{mc^2} \frac{h\nu}{\frac{1}{2}mv^2} \sigma_{PI} \qquad (2)$$

where ω are statistical weights and v is the electron velocity. The

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rate coefficient for radiative capture is then obtained by integrating σ_{RC} over the free electron velocity distribution. The resonances in the photoionization cross-section correspond to the 'dielectronic' component of the radiative recombination coefficient. The calculation of the total radiative recombination coefficient by this method requires the integration of the photoionization cross-section, including resonances, for all bound states, X_b^{+m-1}.

For the calculation of recombination coefficients at nebular temperatures, only free electron energies up to about 0.2 Rydbergs need be considered. If the photoionization cross-sections $\sigma_{PI}(X_b^{+m-1})$ are strongly enhanced by resonances in this energy range, there will be a significant dielectronic contribution to the radiative recombination coefficient. Such enhancements have been demonstrated for ions of C, N and O (Beigman and Chichkov, 1980, Storey, 1981).

2. H, He AND Li-LIKE IONS

No resonance effects are possible in hydrogenic ions. In He and Li-like ions, the formation of resonance states involves the excitation of an electron from the 1s shell and free electron energies which are not available at nebular temperatures. Dielectronic recombination can therefore be neglected for these ions. Seaton (1980) has reviewed the theory of recombination lines of H and He^+. I shall restrict myself to some comments on the accuracy, in nebular conditions, of currently used recombination coefficients.

2.1 Hydrogen Like

The most complete calculations of recombination coefficients for H are those of Brocklehurst (1970, 1971). The first of these two papers deals with high (principal quantum number, $n \geq 40$) states, making the assumption that the ℓ sub-states are populated according to their statistical weights, $2(2\ell+1)$. The second paper treats the low ($n \leq 40$) states and the populations of ℓ sub-states are calculated explicitly. Intensities of Balmer and Paschen lines are given. Giles (1977) has used unpublished level populations for hydrogen obtained by Brocklehurst to determine the intensities of the infra-red Brackett lines. All these calculations are for Case B of Baker and Menzel (1938). The computer codes of Brocklehurst have recently been revived by Hummer and Storey and generalised to deal with H, He and Li-like ions of arbitrary nuclear charge.

Photoionization cross-sections (and bound-bound transition probabilities) are in principle known exactly for hydrogenic ions and can, in practice, be calculated to any required precision. Brocklehurst (1970) estimates the error in these quantities to be less than 1% in his calculations. Rate coefficients for collisional redistribution of angular momentum and energy are known with less precision. Arguing that a 10% change in collision rates is equivalent to a 10% change in electron density, Brocklehurst (1971) infers a maximum uncertainty of 2% in the intensities

of the higher hydrogen Balmer lines. For lines originating from low ($n \lesssim 10$) states, there is no reason to suppose that the relative intensities given by Brocklehurst (1971) and Giles (1977) for hydrogen lines are in error by more than 1%.

Brocklehurst (1971) also gives intensities for the Pickering and Pfund series of He II. Note that in Table II of his paper, the column headings 10^4, 10^5, 10^6 cm^{-3} should read 10^6, 10^5, 10^4 cm^{-3}. Seaton (1978) has used scaling laws to determine the intensities of the UV Balmer and Paschen lines of He II, and to demonstrate that collisional redistribution of angular momentum is less effective in He^+ than in H. The scaling laws relating the radio recombination lines of He II to those of H I are discussed by Weisheit and Walmley (1977). New calculations for He^+ indicate that a) the results of Seaton (1978) are accurate to about 1% for the He II Balmer line intensities and about 3% for the Paschen lines. b) the uncertainty in the results of Brocklehurst (1971) is about 1%.

In He, the uncertainty due to collisional processes among the excited states is comparable to that for H discussed above. In the work of Brocklehurst (1972), the photoionization cross-sections for He are derived from quantum defect theory using experimental energies for the excited states. The uncertainties in these energies imply an error of less than 1% in the photoionization cross-sections near threshold, and in the resulting recombination coefficients.

3. COMPLEX IONS

3.1 Photoionization

Various approximations exist for the evaluation of photoionization cross-sections for complex ions (see for example the report by C. Mendoza in the present volume). If the wave functions for the X^{+m} + e system are calculated by a method, such as the close-coupling approximation, in which the interaction between open and closed channels is included, resonance effects are automatically incorporated. This approximation is incomplete in certain cicumstances. In a full treatment, the interaction of the ion with the quantised radiation field is included in the evaluation of the photoionization amplitude (Davies and Seaton, 1969). The cases considered here do not generally require this more sophisticated approach.

To a first approximation, the strength of background and resonance contributions to the photoionization cross-section for a bound state are determined by the parentage of that state. For example for states belonging to the $2s^2(^1S)n\ell$ series of C^+, such as $2s^2 3d\ ^2D$ (Figure 1), there is a strong background contribution, corresponding to photoionization to the $2s^2\ ^1S$ + e continuum, and weak resonance contributions from the $2s2p(^3P^o)n\ell$ series of resonances. The corresponding term diagram of C^+ is shown in Figure 2. For bound states with $2s2p(^3P^o)$ parentage, there is a weak background with prominent resonances. The terms in the ground

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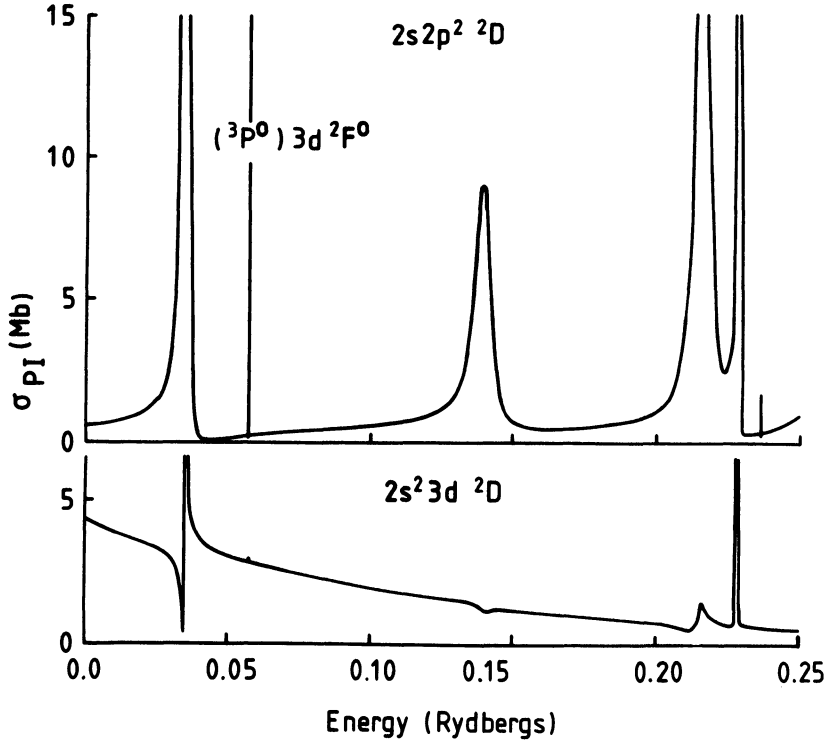

Figure 1. Photoionization cross-sections for C^+ $2s2p^2\ ^2D$ and $2s^23d\ ^2D$ close to the first ionization threshold.

complex ($2s^22p$, $2s2p^2$, $2p^3$), such as $2s2p^2\ ^2D$ have mixed parentage, and there can in general be large resonance contributions from many series. In C^+, the recombination coefficient for the $2s2p^2\ ^2D$ state, and for the ion, is dominated by the $2s2p(^3P^o)3d\ ^2F^o$ resonance.

For most ions of astrophysical interest, photoionization cross-section calculations which incorporate resonance effects have been made only for the ground and some low-lying metastable states. These calculations need to be extended at least to include all terms for which parentage considerations imply a large contribution from resonances. Calculations of this sort are in progress at UCL for C^+, C^{2+} and N^{2+}. An alternative approach consists of evaluating background photoionization cross-sections for parentage allowed processes using, for example the quantum defect method, and adding dielectronic contributions separately. Compilations of coefficients for the non-resonant part of the recombination coefficient have been made by Aldrovandi and Péquignot (1973, 1974, 1976) and Gould (1978). In both cases, a hydrogenic formulation is used from excited states, but the results of Gould are superior in that they make some

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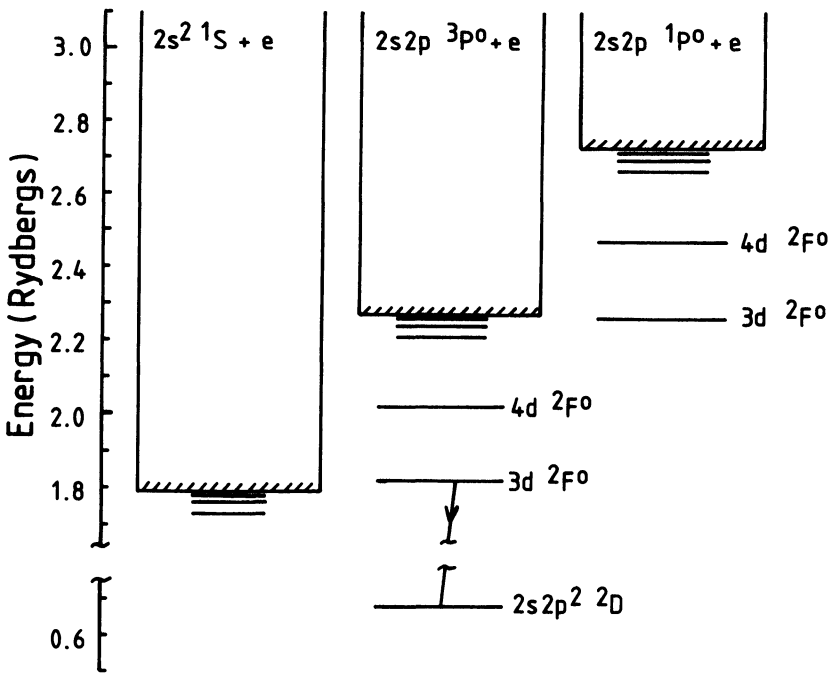

Figure 2. Autoionizing states in C^+.

allowance for their nonhydrogenic nature.

3.2 Dielectronic Recombination

The most widely used approach to the calculation of dielectronic recombination coefficients follows from considering the properties of the quasi-bound states X_a^{+m-1}. Provided angular momentum and parity selection rules are satisfied, these states may undergo a radiationless transition to a continuum state of the same energy,

$$X_a^{+m-1} \rightarrow X^{+m} + e \qquad (3)$$

Let the probability of this autoionization be $\Gamma_a^{(A)}$ (s^{-1}). The inverse process is dielectronic capture. In thermodynamic equilibrium, the rates of these two processes must be equal, so

$$N_{TE}(X_a^{+m-1})\ \Gamma_a^{(A)} = N_e\ N_{TE}(X^{+m})\ \alpha_c \qquad (4)$$

where α_c is the capture coefficient, and the population ratio

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$N_{TE}(X_a^{+m-1})$ / N_e $N_{TE}(X^{+m})$ is given by the Saha equation. In the non TE conditions which prevail in nebulae, the possibility of radiative decay of X_a^{+m-1} with total probability $\Gamma_a^{(R)}$ (s^{-1}) must also be included;

$$N(X_a^{+m-1}) \ (\Gamma_a^{(A)} + \Gamma_a^{(R)}) = N_e \ N(X^{+m}) \ \alpha_c \qquad (5)$$

Combining equations (4) and (5) gives

$$\frac{N(X_a^{+m-1})}{N_e N(X^{+m})} = \frac{N_{TE}(X_a^{+m-1})}{N_e N_{TE}(X^{+m})} \frac{\Gamma_a^{(A)}}{(\Gamma_a^{(A)} + \Gamma_a^{(R)})} = \frac{N_{TE}(X_a^{+m-1})}{N_e N_{TE}(X^{+m})} \ b(X_a^{+m-1}) \qquad (6)$$

where $b(X_a^{+m-1}) \equiv b_a$ is a measure of the departure of the population of the autoionizing state from its TE value. The rate of recombination to some bound state X_b^{+m-1}, $N(X_a^{+m-1}) \ \Gamma_{ab}^{(R)}$ can then be obtained once b_a and the transition probabilities $\Gamma_{ab}^{(R)}$ are known. The autoionizing state X_a^{+m-1} can be characterised by $(\gamma_p S_p L_p n s \ell; SL)$ where S,L are total spin and orbital angular momentum quantum numbers, $ns\ell$ are principal, spin and orbital angular momentum quantum numbers of the added electron and γ_p represents all other quantum numbers associated with the parent term p. It can be shown (eg Seaton and Storey, 1976) that, in atomic units, $\Gamma_a^{(A)}(n) = C/n^3$ where C is of order unity. In addition, $\Gamma_a^{(A)}$ tends to zero for ℓ large.

3.2.1 Burgess general formula. Burgess (1964) was concerned with electron temperatures characteristic of an ionization balance determined primarily by electron collisions, for which the free electron energies are comparable with the ionization potentials of the abundant ions. Burgess considered resonance series in which the parent term p is connected to the recombining ion ground state (p=1), by an optically allowed transition. He further assumed that the autoionizing states can only decay radiatively via the p→1 transition in the ion core, the highly excited added electron being considered as a 'spectator'. Following the core transition, the ion is left in a bound state. The total dielectronic recombination coefficient is then obtained by summing over all possible resonance states. Since $\Gamma_a^{(R)}$ is independent of a, the sum converges since $b_a \to 0$ as $\Gamma_a^{(A)} \to 0$ for n,ℓ large. In practice at high temperatures, states with $n \simeq 100$ and $\ell \leq 10$ are important. Burgess (1965) introduced a fit to the dielectronic recombination coefficient, intended for use at high temperatures, in which the energies of the resonance states relative to the first ionization limit are replaced by a constant energy close to the parent term energy difference, ΔE_{1p}, leading to the coefficient falling approximately as $\exp(-\Delta E_{1p}/kT)$ as $T \to 0$. For most ions of interest, $\Delta E_{1p} \gtrsim 0.5$ Rydberg for the first optically allowed transition, and at 10^4K, the general formula gives the dielectronic contribution to the recombination coefficient to be negligible.

3.2.2 Low temperatures. The use of the Burgess general formula is incorrect at nebular temperatures, because a) individual low-lying auto-

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-ionizing states are not included, b) for low-lying autoionizing states, the radiative probability $\Gamma_a^{(R)}$ may be enhanced by the decay of the outer electron, c)series of autoionizing states exist for which the p→1 transition is not permitted, which can also decay radiatively due to outer electron transitions. As an example consider recombination to form C^+. In the Burgess model, only the states $2s2p(^1P^o)n\ell$ are included. These are assumed to decay radiatively with the same probability as the C^{2+} $2s2p(^1P^o)\rightarrow 2s^2(^1S)$ transition. In practice, none of these states lie close enough to threshold to contribute significantly to the recombination coefficient. Members of the series $2s2p(^3P^o)n\ell$, however, do lie close to threshold and as mentioned above, the $2s2p(^3P^o)3d\ ^2F^o \rightarrow 2s2p^2\ ^2D$ transition dominates the recombination.

Consider a series of autoionizing states for which the p→1 transition is not permitted, connected to a common bound state , b, by radiative decay of the outer electron. The transition probability , in atomic units, is $\Gamma_{ab}^{(R)}=B\alpha^3z^4/n^3$, where B is of order unity, z is the recombining ion charge and α is the fine structure constant. For z,ℓ small, $\Gamma_a^{(A)}>>\Gamma_a^{(R)}$ so that $b_a(n)=1$, independent of n. The evaluation of the dielectronic recombination coefficient at low temperatures therefore involves only calculation of the radiative probabilities $\Gamma_{ab}^{(R)}$, since the populations of the autoionizing states are given by the Saha equation. In practice, the most important transitions are usually to the ground complex of the recombined ion, and configuration interaction is therefore important in representing the wave function of the lower state. The rate of recombination from the members of a series

$$N_{TE}(X_a^{+m-1})\ b_a(n)\ \Gamma_{ab}^{(R)} \propto n^{-3} \exp(-E_n/kT) \qquad (7)$$

where E_n is the energy of the autoionizing state relative to the first ionization threshold. The sum over a given series therefore converges rapidly and it is normally sufficient to consider only the first few terms explicitly. A correction for higher members can be obtained using the functional form of equation (7).

3.2.3 Recombination lines. At low temperatures, most of the dielectronic recombination involves radiative transitions between a few low--lying resonance states and one or two terms in the ground complex of the recombined ion. Frequently the bulk of the recombination passes through a single such term and a line is strongly enhanced. In the B-like ions, the $2s2p^2\ ^2D$ state is populated, giving rise to emission in λλ1335, 991, 789 in C^+, N^{2+} and O^{3+}. Similarly in the Be-like ions, λλ2297, 1718, 1371 arise from the $2p^2\ ^1D$ state in C^{2+}, N^{3+} and O^{4+}. Many other weaker recombination lines are also generated. In C III, in addition to the strongest lines at λλ1176, 2297, there is for example, a satellite line to C IV λ1550, $2p3d\ ^3F^o \rightarrow 2s3d\ ^3D$ at λ1577 and enhancement of the $2s3p\ ^3P^o \rightarrow 2s3s\ ^3S$ λ4650 transition. For these weaker lines to be utilised, a full treatment of recombination and cascade processes as outlined in section 3.1 is required.

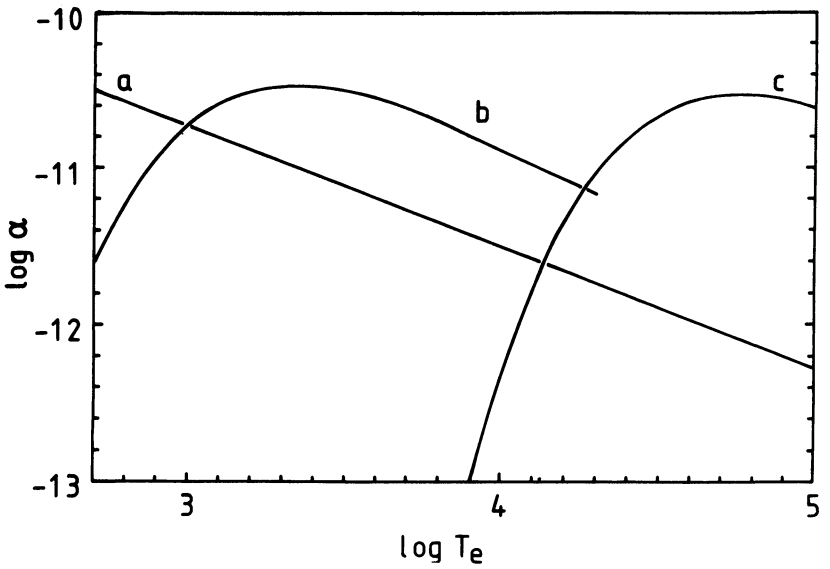

Figure 3. Recombination coefficients for C^{3+} + e as a function of electron temperature. See text for explanation.

3.2.4 Recent work. Since the early work of Burgess, various calculations of total dielectronic recombination coefficients have been made, but with the main emphasis on the solar ionization balance. Davis et al. (1977) demonstrate that the general formula may overestimate when autoionizing states lie energetically above a second or higher ionization threshold, due to the additional channels for autoionization. This effect is unlikely to be important at nebular temperatures. A series of papers have been published (Jacobs et al. 1977, 1979, 1980) incorporating this effect and in some cases giving dielectronic recombination coefficients down to 10^4K. The compilation of dielectronic recombination coefficients by Shull and Van Steenberg (1982) consists of fits to these results and to unpublished work of Jacobs for ions of C, N and O. Throughout this work, the assumptions of Burgess (1964), that the recombination only occurs via optically allowed transitions in the recombining ion, have been retained and consequently the coefficients are underestimates at low temperatures , sometimes by orders of magnitude. The same is true of the fits given by Aldrovandi and Péquignot (1973, 1974, 1976), derived from the Burgess general formula. Summers'(1974) extensive tabulations of total recombination coefficients also underestimate at nebular temperatures.

Dielectronic recombination coefficients which take account of the effects discussed in section 3.2.2 have been given by Beigman and Chichkov (1980) for $O^+ \rightarrow O$ recombination, and by Storey (1981) for the recombined ions C^+, C^{2+}, N^{2+}, N^{3+} and O^{4+}. Calculations have also been made for

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the remaining ions of C, N and O by Nussbaumer and Storey (1983). This work is described in a contributed paper. Storey (1981) also gives effective recombination coefficients for some of the stronger UV recombination lines. Figure 3 shows radiative recombination coefficients for $C^{3+} \rightarrow C^{2+}$ recombination. The non-resonant contribution to the coefficient (a), was calculated from the parameters given by Aldrovandi and Péquignot (1973). Curve (c) is the dielectronic contribution calculated from the Burgess general formula, also taken from Aldrovandi and Péquignot. The values given by Storey (1981), together with some unpublished results for T<7000K are curve(b). The total recombination coefficient is enhanced by about a factor of five at 10^4K by the proper inclusion of resonance effects. Curve (b) falls below (c) at higher temperatures, because the calculations of Storey do not include, in full, the series of autoionizing states in which a permitted transition in the recombining ion is involved. Preliminary calculations show that there is a similar enhancement for $Si^{3+} \rightarrow Si^{2+}$ recombination to that for $C^{3+} \rightarrow C^{2+}$. Work on the ions of Mg, Al and Si is in progress.

Once the electron temperature is low enough that $kT<E_L$, where E_L is the energy of the lowest resonance relative to the first ionization threshold, curve (b) in Figure 3 falls as $\exp(-E_L/kT)$. Below $T_L=E_L/k$, the approach used by Storey is unsuitable. The recombination coefficient can then only be determined correctly from the threshold behaviour of the photoionization cross-sections.

3.2.5 Coupling schemes. The discussion so far has been in terms of LS coupling, in which S, L and parity are conserved in the dielectronic capture process. Usually, for the autoionizing states of interest, $\Gamma_a^{(A)}/\Gamma_a^{(R)} = 10^3 - 10^6$. Relativistic interactions such as spin-orbit coupling, although weak for light ions of low ionization, may lead to $\Gamma_a^{(A)} \geq \Gamma_a^{(R)}$ for states which are excluded from an LS coupling model. Consider the case of $O^+ \rightarrow O$ recombination. Above the O^+ $^4S^o$ ground state lie singlet and triplet states of O. In LS coupling, none of the singlets and about two thirds of the triplets are populated by dielectronic capture. The recombination coefficient could be increased by about a factor of two if the spin-orbit interaction is sufficiently strong.

3.3 Summary

The best approach to the calculation of total radiative recombination coefficients at nebular temperatures at present is to add a) the values of Gould (1978) or of Aldrovandi and Péquignot (1973, 1974, 1976) for the non-resonant contributions, b) the values of Aldrovandi and Péquignot for dielectronic contributions from the Burgess general formula and c) the values of Beigman and Chichkov (1980), Storey(1981) and Nussbaumer and Storey (1983) for dielectronic contributions due to low-lying resonances. An ucertainty of about a factor of two has to be reckoned with for the resulting total radiative recombination coefficient.

Photoionization cross-sections which incorporate resonance effects now exist for the ground and some low-lying states of many ions. Work

is in progress to obtain recombination coefficients from the cross-sections. As further cross-sections become available, it will be possible to improve on current estimates of the important dielectronic contributions to the radiative recombination coefficient.

REFERENCES

Aldrovandi, S.M.V. and Péquignot, D., 1973. Astron. Astrophys., 25, 137.
Aldrovandi, S.M.V. and Péquignot, D., 1974. Rev. Bras. de Fis., 4, no 3, 491.
Aldrovandi, S.M.V. and Péquignot, D., 1976. Astron. Astrophys., 47, 321.
Baker, J.G. and Menzel, D.H., 1938. Astrophys. J., 88, 52.
Beigman, I.L. and Chichkov, B.N., 1980. J. Phys. B., 13, 565.
Brocklehurst, M., 1970. Mon. Not. R. astr. Soc., 148, 417.
Brocklehurst, M., 1971. Mon. Not. R. astr. Soc., 153, 471.
Brocklehurst, M., 1972. Mon. Not. R. astr. Soc., 157, 211.
Burgess, A., 1964. Astrophys. J., 139, 776.
Burgess, A., 1965. Astrophys. J., 141, 1588.
Davies, P.C.W. and Seaton, M.J., 1969. J. Phys. B., 2, 757.
Davis, J., Jacobs, V.L., Kepple, P.C. and Blaha, M., 1977. J. Quant. Spectrosc. Radiat. Transfer, 17, 139.
Giles, K., 1977. Mon. Not. R. astr. Soc., 180, 57P.
Gould, R.J., 1978. Astrophys. J., 219, 250.
Jacobs, V.L., Davis, J., Kepple, P.C. and Blaha, M., 1977. Astrophys. J., 215, 690.
Jacobs, V.L., Davis, J., Rogerson, J.E. and Blaha, M., 1979. Astrophys. J., 230, 627.
Jacobs, V.L., Davis, J., Rogerson, J.E., Blaha, M., Cain, J. and Davis, M., 1980. Astrophys. J., 239, 1119.
Nussbaumer, H. and Storey, P.J., 1983. Astron. Astrophys., to be submitted.
Seaton, M.J., 1978. Mon. Not. R. astr. Soc., 185, 5P.
Seaton, M.J., 1980. "Radio Recombination Lines", ed. P.A. Shaver (D. Reidel), 3.
Seaton, M.J. and Storey, P.J., 1976. "Atomic Processes and Applications", ed. P.G. Burke and B.L. Moiseiwitsch (North-Holland), chapter 6.
Shull, M.J. and Van Steenberg, M., 1982. Astrophys. J. Suppl., 48, 95.
Storey, P.J., 1981. Mon. Not. R. astr. Soc., 195, 27P.
Summers, H.P., 1974. Appleton Laboratory, IM 367.
Weisheit, J. and Walmsley, C.M., 1977. Astron. Astrophys., 61, 141.

PEIMBERT: I am very pleased to see that the computations of recombination coefficients have been repeated and that these are in very good agreement with the previous work by Brocklehurst. These data are needed to determine the pregalactic He/H abundance ratio which is of paramount importance in the study of cosmology and elementary particles. Are the results of the He I numerical study going to be available in the near future?

STOREY: Yes, work is in progress.

NUSSBAUMER: Could you comment on the work recently published in the Astrophys. J. by Shull and Van Steenberg on recombination coefficients.

STOREY: Their non-resonant ("radiative") contributions to the recombination coefficient are taken directly from the paper of Aldrovandi and Péquignot. The dielectronic contributions are from Jacobs and co-workers and are substantial underestimates at nebular temperatures.

PÉQUIGNOT: I am glad to learn that, at least at a qualitative level, the recombination of O^{++} to O^{+} and of N^{++} to N^{+} will be amplified, as indicated by recent models of NGC 7027 (Péquignot, Stasinska and Aldrovandi, 1982, unpublished). Empirical dielectronic recombination coefficients have already been used in a model of the Crab nebula (Péquignot and Dennefeld, 1982, in press).

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