JOINT EUROPEAN TORUS

JET–P(91)57

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Preprint of a paper to be submitted for publication in proceedings of
NATO Advanced Research
Workshop on Recombination, 7th - 9th October 1991

APPLICATIONS OF RECOMBINATION

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ABSTRACT

The influence of recombination on modelling and spectral diagnostics of laboratory and astrophysical plasmas is described. The generalised collisional-radiative approach is presented as a method for sound application of recombination to the wide range of plasma experiments. Some practical issues in making use of fundamental studies of recombination in applications are discussed.

## 1. INTRODUCTION.

This paper is concerned with recombination of free electrons with atomic ions. The applications of recombination to be described are in the study and analysis of various types of ionised plasmas. Although other recombination processes such as charge exchange can be very important in, for example, neutral beam heated plasmas they are not the subject of discussion in this work. In all studies of plasmas it is certainly necessary to know the ionisation state of the species in the plasma and probably also the total radiated power. We might introduce the term, 'the standard model', to describe a plasma collisionally excited by electrons, in equilibrium, at low density, in which free electron recombination balances collisional ionisation. That is

$$N_e N^{(z+1)} \alpha(z+1 \rightarrow z) = N_e N^{(z)} S(z \rightarrow z+1) \qquad [1]$$

with $N_e$, the electron density, $N^{(z)}$, the number density of the element X in charge state z, $\alpha$, the recombination coefficient and S the ionisation coefficient. In the standard model recombination does not take place on boundary surfaces and charge transfer processes with other atoms or ions do not play a role. The $\alpha$ and S apply in a non- stationary state as

$$\begin{aligned} \frac{\partial N^{(z)}}{\partial t} + \nabla . \Gamma^{(z)} = & N_e N^{(z-1)} S(z-1 \rightarrow z) \\ & - N_e N^{(z)} \{\alpha(z \rightarrow z-1) + S(z \rightarrow z+1)\} \\ & + N_e N^{(z+1)} \alpha(z+1 \rightarrow z) \end{aligned} \qquad [2]$$

The line integrated photon emissivity for the transition $X_i^{(z)} \rightarrow X_j^{(z)}$ may be written formally as

$$I(z,i \rightarrow j) = \int q_{eff}^{excit}(i \rightarrow j) N_e N_1^{(z)} dl + \int q_{eff}^{recom}(i \rightarrow j) N_e N_1^{(z+1)} dl \qquad [3]$$

identifying that contributions arise driven from the ground state by excitation and from the ionised state by recombination. Evidently $q_{eff}^{recom}$ is connected with $\alpha$ but only on that part leading to the emission of the specific line. In the usual spectral monitoring of plasmas, it is the low resonance lines which are observed. For these the recombination part is generally negligible. So the emission depends on $\alpha$ only through the fractional abundances $N_1^{(z)}/N_{tot}$. The practical study of the spectrum line $i \rightarrow j$ itself may be complicated by uncertainties in cross-section data, cascading and branching and the emitting region may not be well localised in the plasma. Equally the recombination coefficient $\alpha$ is properly an effective coefficient of which radiative and dielectronic recombination may be the main ingredients but modified in the plasma. This disconnection between the fundamental recombination and the realities of observation in a plasma has had the consequence that theory and experiment are not well integrated in this area. Faults in theoretical values of $\alpha$ may not recognised as such but interpreted in terms of some plasma behaviour. Calculated recombination coefficients are absorbed into a mass of other data from which there is no return to the fundamental process specialist. Clearly more satisfaction is to be found in applications if while continuing to produce $\alpha$'s for modellers, some direct tie to spectral diagnostics can be made which reveal more of the makeup of $\alpha$ and specifically exploits it in the pursuit of the more elusive parameters of the plasma.

With a given distribution of ionisation stages at some time or position in a plasma, we can associate a temperature $T_Z$ which is the electron temperature at which the standard distribution matches the actual distribution, at least for the dominant stages. From the electron point of view the plasma is *ionising* if $T_e > T_Z$ and is *recombining* if $T_e < T_Z$. This is not to say that the plasma is necessarily changing with time. Evidently recombining plasmas emphasise the importance of the recombination coefficients and the contribution to spectral features from recombination is increased. Turning this round, if we can diagnose that a plasma is recombining, this is a valuable piece of diagnostic information on the plasma. Plasmas which are unbalanced in this sense have diagnostic opportunities which depend more sharply on particular portions of the descriptive atomic reaction database. Imbalance occurs for reasons including:

Photoionisation by an external radiation field sustaining the ionisation state of the plasma $\rightarrow$ *recombining*

Heating of electrons and/or ions by waves or shocks $\rightarrow$ *ionising*

Adiabatic expansion cooling $\rightarrow$ *recombining*

Radiative cooling $\rightarrow$ *recombining*

Transport across thermal gradients $\rightarrow$ *recombining* or *ionising*.

As pointed out earlier, spectroscopy of plasmas has tended to focus on the lowest resonance lines of the dominant emitting ions as most representative of the thermal state of the plasma. However for diagnostic studies, even within the constraint of $T_e \sim T_Z$, there is much to be gained by more varied spectral observations. Particularly transitions from higher n-shells, comparison of transitions from different spin systems, observations of closed shell ions with high first excitation energies and satellite lines favour recombination contributions and recombination diagnostics (see McWhirter and Summers, 1984, for a general discussion).

## 2. RECOMBINATION IN ACTION IN PLASMAS.

In this section a number of rather different plasmas are described. They are drawn from astrophysics, X-ray laser physics and magnetically confined fusion plasmas. Some of the plasmas have advantages for recombination of the type discussed in the previous section. The development is ordered in a manner to show recombination entering into plasma studies with increasing complexity.

### 2.1. Gaseous nebulae.

The archetypal nebulae studied for many years are diffuse nebulae such as Orion and planetary nebulae such as NGC7027. These nebulae have hot embedded stars, $T^{\times} \sim 50000 - 100{,}000\,{}^{o}K$, whose diluted, effectively black body radiation field provides the energy input to the nebula. Photoionisation maintains a relatively high state of ionisation, with ions such as $H^{+}$, $C^{+}$, $C^{+2}$, $O^{+}$ and $O^{+2}$ present. The electron temperature remains low. For example, a diffuse nebula may have $T_e \sim 10^3 K$ and $N_e \sim 10^2 - 10^4 cm^{-3}$. The nebula is usually optically thick in Lyman radiation but transparent to all other. Forbidden lines emitted in transitions within the ground configuration are excited by electrons, but the energies are too low to excite allowed lines from higher quantum shells. The latter are formed entirely by recombination.

Consider firstly hydrogen. In calculating the Balmer series decrement of hydrogen, the population of a principal quantum shell is determined by the direct radiative recombination to the level, the lifetime of the level and by cascading from higher levels. It is convenient to express the populations of the excited levels in terms of the ratio to Saha-Boltzmann values, $b_n$, (called 'b-factors', Menzel and Peckeris, 1935).

$$N_n = N_e N^{+} \left\{ \frac{\pi a_0{}^2 I_H}{kT_e} \right\}^{3/2} \frac{\omega_n}{2\omega^{+}} \exp\left(\frac{I_n}{kT_e}\right) b_n \qquad [4]$$

Results in the so called 'depopulated Case B' (Baker and Menzel, 1938) are shown in figure 1. Principal quantum shells up to 15 may be considered (Seaton, 1959). More carefully, separate nl-shells are examined (Burgess, 1958).

The observations of microwave radio recombinations lines such as 109$\alpha$ drew attention to very high n-shells ($\sim$ 100). Evidently, the pure recombination cascade calculations were not appropriate for this, since the free electrons do become effective in causing redistribution amongst these very high n-shell populations, and in coupling the populations to the free electron Maxwellian. Figure 1 also illustrates the b-factors taking this into account. Masing in these radio recombination lines coupled with the varying line widths with n-shell (Salem and Brocklehurst, 1979) provide a depth probe of diffuse nebulae. There are many such lines of *HI*, *HeI* and *CI* available for such studies (see Gordon and Walmsley, 1990; Rolfsema and Goss, 1991).

Turning to complex ions such as $O^{+}$ and $O^{+2}$ in diffuse nebulae, the lower level allowed lines are again entirely radiative recombination and cascade determined.

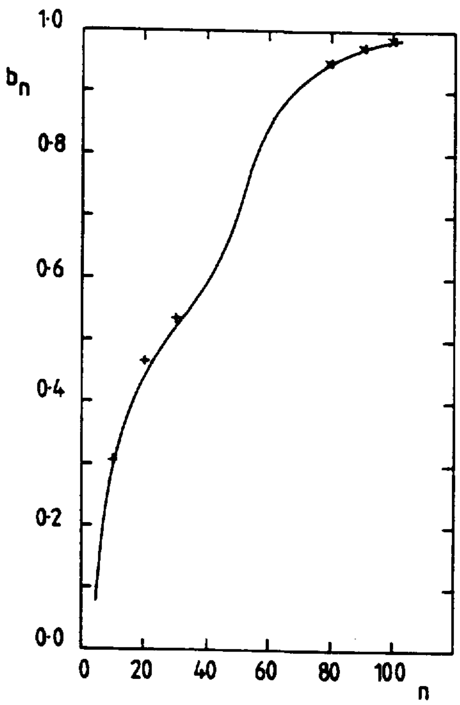


Fig. 1. $H^0$ b-factors. $T_e = 5 \times 10^3 K$, $N_e = 10^4\ cm^{-3}$.
*plus*, Seaton (1959) radiative solution - Case B ; *cross*, Dyson (1969) - Case B ; *solid*, Burgess and Summers (1976), $T_r = 5 \times 10^4 K$, $W = 10^{-20}$ - Case A.

Much more effort is required though to obtain the separate recombination coefficients to each term and all the transition probabilities for the cascade. Burgess and Seaton (1960a, 1960b) provided approximate methods for the recombination coefficients and introduced the ideas of cascade matrices and effective recombination coefficients and effective emission coefficients which include the effects of cascade. In practise careful consideration has to be given to variation of optical depth in different lines, fluorescent mechanisms etc.

In the complex ion studies for planetary nebulae, dielectronic recombination was originally assumed switched off, however anomalies in observations of certain lines such as $CIII$ 2297Å and in ionisation equilibria have prompted reappraisal. There are a number of resonances of $C^{+2}$, namely, $2p4p$, $2p4d$ and $2p4f$ within 0.1 Rydberg of the ionisation threshold which are accessible, ie. $C^{+3}(2s) + e \rightarrow C^{+2}(2pnl)$. Radiative decay of the outer electron is important and in particular the radiative chain $2p4d\,^1F \rightarrow 2p^2\,^1D \rightarrow 2s2p\,^1P$. The total dielectronic recombination coefficient can exceed the the total radiative recombination coefficient at $T_e \geq 10^4\ K$ (Storey, 1981). Introduce the b-factor for the resonant state as

$$N^{(z)}(i, \rho') = N_e N^{(z+1)}(\rho) \left\{ \frac{\pi a_0^2 I_H}{kT_e} \right\}^{3/2} \frac{\omega(i, \rho')}{2\omega(\rho)} \exp\left(\frac{I_{i,\rho'}}{kT_e}\right) b_{i,\rho'} \qquad [5]$$

with $\rho$ denoting the initial recombining parent ion state, $\rho'$, the excited parent ion state and $I_{i,\rho'}$ (negative), the resonant energy. Then

$$b_{i,\rho'} = \frac{A_a}{A_a + A_r} \qquad [6]$$

Because of the low electron temperature, the expontial factor cuts off very sharply to higher n-shells, and for the lowest n-shells $b \rightarrow 1$. So Auger rates do not need to be calculated at least in the first approximation but only the radiative transition probabilities to obtain the dielectronic rates (see also Nussbaumer and Storey, 1987; Rudy et al, 1991). Dielectronic recombination is not in its fully developed form here.

## 2.2. The solar corona.

The solar corona, in quiet sun conditions, has $T_e \sim 10^6\ K$ and $N_e \sim 10^8\ cm^{-3}$, but with the electron temperature rising to $\sim 10^7\ K$ in solar flares. At such high temperatures dielectronic recombination is the dominant recombination process for many highly ionised ions (depending on charge state and parent excitation energies). Figure 2 contrasts total dielectronic and radiative recombination coefficients for $Fe^{+14} + e$. The importance of dielectronic recombination in the solar corona was pointed out by Burgess (1964) who showed how to evaluate the rate coefficient correctly at high temperature. The inclusion of dielectronic recombination in the ionisation balance of the solar corona markedly improved the agreement between ionisation balance and Doppler temperatures (Burgess and Seaton, 1964).

It is of particular note that dielectronic recombination when fully active is effective in populating very highly excited states of the recombined ion. Quantum shells up to 1000 may contribute to the total effective recombination coefficient and require quite elaborate calculations. Such atoms are very large, easily influenced by fields and other particles, and vulnerable to destruction by futher ionising collisions with electrons (Burgess and Summers, 1969). Neglect of such effects, the usual practise in the solar corona, is acceptable only for the more highly charged ions and at fairly low density. The solar corona often approximates closely to the standard model, although ionising and recombining plasmas are encountered in the impulsive and decay phases of flares. The recombination shows itself through the ionisation balance alone for most observations except for dielectronic satellite lines.

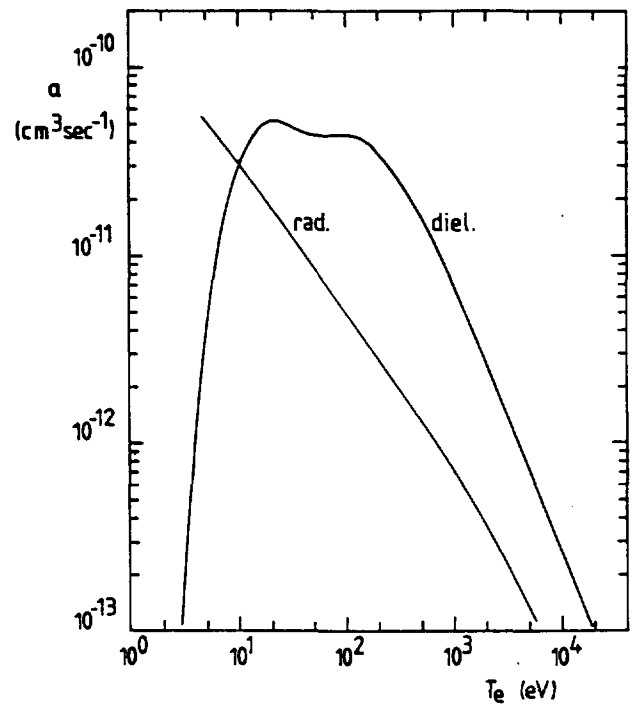


Fig. 2. $Fe^{+15} + e$ recombination at low density.
*diel.*, dielectronic coefficient summed over all levels ; *rad.*, radiative recombination coefficient summed over all levels.

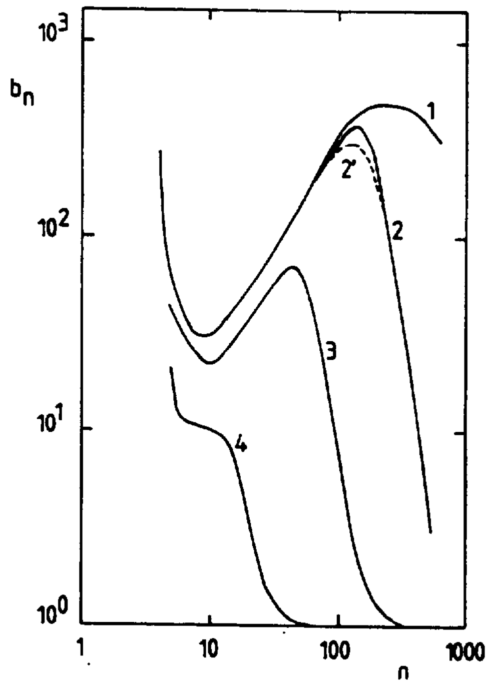


Fig. 3. $Fe^{+14}$ b-factors.
*curve 1*, $N_e = 10^4\ cm^{-3}$ ; *curve 2*, $N_e = 10^8\ cm^{-3}$ ; *curve 2'*, $N_e = 10^8\ cm^{-3}$, $T_r = 5600K$, $W = 0.5$ ; *curve 3*, $N_e = 10^{12}\ cm^{-3}$ ; *curve 4*, $N_e = 10^{16}\ cm^{-3}$.

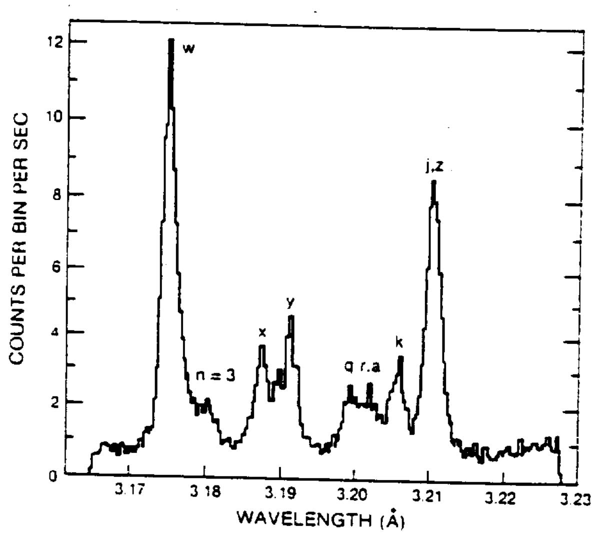


Fig. 4. The spectral vicinity of $CaXIX(1s^2\ {}^1S - 1s2p\ {}^1P)$.
Data from the Bent Crystal Spectrometer (BCS) on the Solar Maximum Mission Satellite. April 30, 1980 2033:50 - 2034:06 UT.

The most important satellite lines are those of the form $1s2l2l' - 1s^2 2l''$ to the helium-like resonance line $1s^2\,^1S - 1s2p\,^1P$. They have been intensely studied for many ions in many laboratory plasmas as well as in the corona. These lines, which are the stabilising emission in the dielectronic process (some can also be produced by inner shell excitation) are illustrated for CaXIX in figure 4. They yield information on electron temperature, non-Maxwellian distributions and transient ionisation state. Evidently, such lines and ionisation equilibria are critical to arguments of coronal abundances (Phillips and Feldman, 1991).

## 2.3. Laser produced plasmas.

Initial interest in production of dense, hot plasmas by high power laser illumination of targets has become very much concentrated in the two areas of laser compression and X-ray lasers. In the latter, a laser produced plasma is used as the amplifying medium with two schemes used to pump the upper population: (a) collisional excitation of closed shell medium Z ions , (b) recombination excitation of H-like and Li-like ions. The aim is to achieve lasing below the carbon K absorption edge, at 43.76 Å.

The first results showing gain for the collisionally pumped case were reported for Ne-like selenium ($Se^{+24}$) (Matthews et al, 1985) and used an exploding foil technique. Conditions with $N_e \sim 10^{20} cm^{-3}$ , $T_e \sim 500 - 1000 eV$ were produced. The inversions were obtained between the $2p^5 3p$ and $2p^5 3s$ terms shown in figure 5. The $J=0 \rightarrow 1$ gain was anomalously low and led to extended studies. It appears that dielectronic recombination is also a major process altering the gains by 20- 45 % (Whitten et al, 1986). Studies have been extended to $Y^{+29}$ at 132 Å and $Mo^{+32}$ at 156 Å and to the nickel-like system (MacGowan et al, 1987; see also Walling, 1991 for a general discussion).

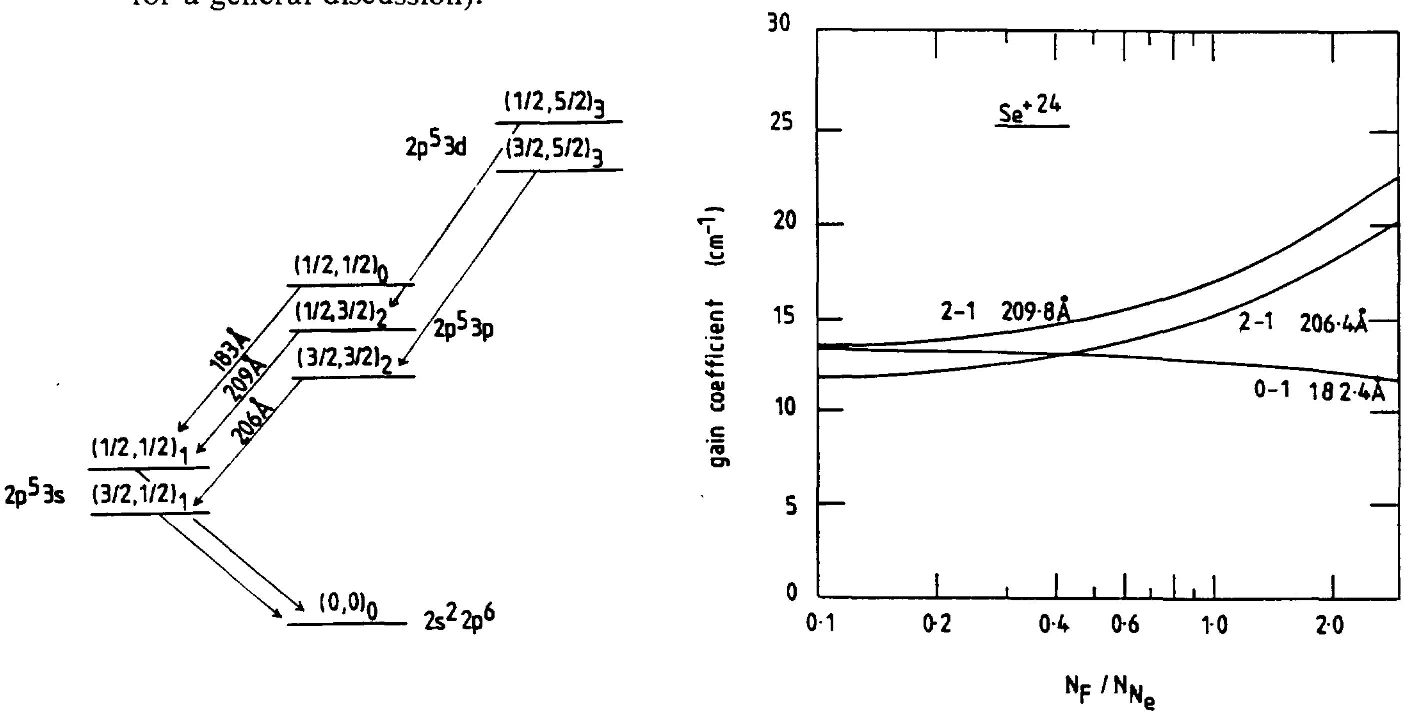


Fig. 5. (a) Level structure of $Se^{+24}$ showing the principal transitions involved in the X-ray laser scheme.
(b) Variation of gain coefficients due to dielectronic recombination $N_F$ is the $Se^{+25}$ abundance and $N_{Ne}$ is the $Se^{+24}$ abundance.

The dielectronic calculations required for such many electron systems are complex and usually performed in a fully relativistic Dirac representation.

The recombination X-ray laser schemes depend on the rapid expansion and adiabatic cooling of a plasma (for example from a carbon fibre irradiated by light from a glass laser) to produce inversion. Gain lengths $\sim 4$ cm$^{-1}$ have been obtained in $C^{+5}$ $n = 3 - 2$ at 182.0 Å. Many similar schemes are possible in ions including $F^{+8}$, $Na^{+10}$, $Al^{+10}$. In the high plasma densities of such experiments three-body recombination dominates radiative and dielectronic recombination (Keane et al., 1989; see Key, 1991 for a general discussion). It is the opposite extreme from that of the nebulae described earlier. Most plasmas are in the collisional-radiative regime between these two limits. A fast radiatively cooling and recombining plasma can also produce inversions. A two-component plasma can fruitfully be used where one species (higher Z) maximises the cooling, and gain is obtained at a convenient wavelength in a second (lower Z) species (Keane and Suckewer, 1991). Clearly, complete models of such plasmas must include radiation transport, hydrodynamics and laser-plasma interactions.

## 2.4. Fusion plasmas.

In modern magnetically confined fusion experiments such as JET (The Joint European Torus) achievable plasma parameters include $T_e \lesssim 10keV$ and $N_e \lesssim 10^{14} cm^{-3}$. Key factors involved in limiting fusion performance include radiant losses and fuel (deuterium/tritium) dilution. Impurities are responsible for both of these and indeed, the control of impurities is the main problem facing fusion. Impurities in fusion plasmas arise from the materials of the vessel walls (eg. nickel in JET), from special plasma facing surfaces, such as limiters and X-point strike zones and from unavoidable and accidental contaminants (eg. oxygen) (Behringer et al., 1989). The state of ionisation of the various impurities must be explored and evaluated. Impurities are generally released from bounding surfaces by sputtering, ionise rapidly as they migrate inwards into the core plasma, ultimately returning to the periphery again in energetic highly ionised states. Diffusing into the unconfined plasma region (scrape-off-layer) they travel rapidly to the limiting surfaces where the deposition/ sputtering cycle is repeated (Summers, 1988). Ions of species such as nickel are fairly close to ionisation equilibrium in the core of the plasma. Helium-like lines and associated satellites are commonly observed (eg. Beiersdorfer et al., 1989; Zastrow et al, 1990). Note also that non-Maxwellian electron distributions (eg. in electron cyclotron resonance heating) alters line ratios (Bartiromo et al, 1985) giving further diagnostic opportunities. However towards the periphery there are large temperature gradients (markedly so in high confinement modes of operation) giving non-equilibrium diffusive conditions (see Peacock, 1984 for a general discussion). Evidently extensive recombination data is required for the description and modelling of impurities in such conditions.

It is found to be advantageous to have bounding surfaces composed of or coated with light species such as beryllium (Summers et al, 1991), carbon or boron. Also, the trend in fusion research is towards active control of impurities by construction of pumped divertors. These are intended to create a flow in the scrape-off-layer which will entrap impurities and carry them into a separate divertor chamber. High density and strong radiative cooling in the divertor will establish low temperatures in the divertor and thereby minimise sputtering. Conditions will be dynamic. Ions flowing into the divertor will experience a dense recombining environment.

It is well known that metastable states of certain ions can have populations comparable with ground states in a plasma (McWhirter and Summers, 1984). The equilibrium population of $C^{+2}(2s2p\ ^3P)$ in a plasma at electr.n temperature

$T_e = 15eV$ and electron density $N_e = 10^{10}\,cm^{-3}$ relative to the ground state $C^{-2}(2s^2\,{}^1S)$ is 2.5. Also for $C^{+2}$ in a state of flux inwards from the limiter of the JET tokamak, the ratio is altered to typically $\sim$ 1. and does not correspond to an equilibrium ratio at the local electron temperature. The ionisation rate coefficient from a metastable state is different from that of the ground state. Also dielectronic recombination starting from a metastable parent ion may be very small compared with that starting from a ground state. The effective recombination rate coefficient for $Ni^{+17}$ (a sodium-like ion) $N_e = 5 \times 10^{13}\,cm^{-3}$ and $T_e = 500eV$ is 50% less than the rate coefficient at zero density, while the effective ionisation rate coefficient of $Be^{+0}(2s^2\,{}^1S)$ at $T_e = 25eV$ and $N_e = 3 \times 10^{12}\,cm^{-3}$ is 50% larger than the direct rate coefficient at zero density. These changes are because secondary collision processes involving formation and destruction of ions in highly excited states contribute to the effective coefficients. In all these cases, the fundamental zero density coefficients which are modified by the secondary processes would be expected to be accurate to 30% and so omission or simplistic treatment of the metastable and density effects can prejudice accurate original data. Current spectroscopy seeks to investigate the more complex plasma conditions by exploiting these atomic features.

Note that the influence of charge transfer from neutral hydrogen has not been discussed. It has wide ranging effects on ionisation equilibrium and spectral line emission, especially in neutral beam heated plasmas. It must be included in a complete picture of atomic behaviour in tokamaks (Boileau et al., 1989).

## 3. THE COLLISIONAL-RADIATIVE APPROACH FOR APPLICATIONS.

From the previous discussion, it is evident that complete theoretical description of recombination for both modelling and diagnostic application in the general plasma poses somewhat incompatible requirements. Very high quantum shells must be included to describe dielectronic recombination and the influences of collisions and fields on it adequately. Yet a refined view of emitting states of complex ions is necessary for spectroscopic studies. Also, parent states and metastable recombined states must be treated meaningfully in evolving as well as equilibrium plasmas. The main problem issues here are :

(i) Metastable states

(ii) Finite density plasma

(ii) High and low level resolutions

At JET, we have approached these issues from generalised collisonal- radiative theory and have been developing associated methods which we believe are accurate and flexible in application yet preserve the fundamental atomic physics.

### 3.1. The collisional-radiative model.

The basic model was established by Bates et al. (1962) (see also Burgess and Summers, 1976). The ion in a plasma is viewed as composed of a complete set of levels indexed by i and j and a set of radiative and collisional couplings between them denoted by $C_{i,j}$ (an element of the 'collisional-radiative matrix' representing transition from j to i) to which are added direct ionisations from each level of the ion to the next ionisation stage (coefficient $q_i^{(i)}$ ) and direct recombinations to each level of the ion from the next ionisation stage (coefficient $r_i$ ). There is no loss of generality in the present discussion in ignoring other ionisation stages provided couplings to and from them are only via ground states. For each level, there is a total loss rate coefficient for its population denoted by

$$C_{i,i} = -\sum_{j \neq i} C_{j,i} - N_e q_i^{(i)} \qquad [7]$$

so that the populations, $N_i$ are determined by

$$\begin{bmatrix} C_{1,1} & C_{1,j} \\ C_{i,1} & C_{i,j} \end{bmatrix} \begin{bmatrix} N_1 \\ N_j \end{bmatrix} + N_e N^+ \begin{bmatrix} r_1 \\ r_i \end{bmatrix} = \frac{d}{dt} \begin{bmatrix} N_1 \\ N_i \end{bmatrix} \qquad [8]$$

The ground state part has been explicitly partitioned off. In this picture, the recombined ion ground state index is 1 and the sole recombining ion state is denoted by +. These states alone are assumed significantly populated. Excited level populations (that is $N_i$ for $i > 1$ ) are small in comparison. Meaningful effective recombination and ionisation coefficients are obtained from such equations by considering the relaxation times of the populations. Excited populations relax rapidly whereas the ground and ionised state populations relax much more slowly in general. On dynamical timescales longer or of the order of ground population relaxation timescales, a quasi-static assumption may be made in which excited populations ($i > 1$) are supposed in equilibrium with the instantaneous ground and + populations. That is setting

$$\frac{dN_i}{dt} = 0 \; : \; i \neq 1 \qquad [9]$$

and eliminating the $N_i$, the collisional-dielectronic ionisation coefficient is

$$S_{cd} = C_{1,1} - C_{1,j} C_{j,i}^{-1} C_{i,1} \qquad [10]$$

and the collisional-dielectronic recombination coefficient is

$$\alpha_{cd} = r_1 - C_{1,j} C_{j,i}^{-1} r_i \qquad [11]$$

Physically, the collisional-dielectronic coefficients give the contributions to the effective growth rates for the ground state populations due to recombination from and ionisation to the state +. so that the time dependent equation for the ground population becomes

$$\frac{dN_1}{dt} = -N_e S_{cd} N_1 + N_e N^+ \alpha_{cd} \qquad [12]$$

The ionisation balance of Summers(1973) adopted this approach with the excited state populations combined into principal quantum shell populations (the 'bundle-n' method) and used 'matrix condensation' (Burgess and Summers, 1969) to allow very large numbers of principal quantum shells to be included in the calculations.

The problems mentioned earlier are apparent. Populated metastable states can exist and there is no real distinction between them and ground states. We use the term 'metastables' to denote both ground and metastables states and index them by $\rho$ for the recombined ion, and by $\sigma$ for the recombining ion. Therefore the ion of charge state z has metastable populations $N_\rho^{(z)}$ and the recombining ion population, $N^+$, must be subdivided into the set $N_\sigma^{(z+1)}$. We sometimes call the recombining ion metastable states 'parent' states. There is a practical problem. Evidently, discussion of metastables requires a detailed specific classification of the level structure of ions (for example LS or LSJ resolution) whereas to cope with the very many principal quantum shells participating in the calculations of collisional-dielectronic coefficients at finite density necessitates a grosser viewpoint (such as 'bundle-n'). Furthermore, addressing line radiation, each ion tends to have a limited set of low levels principally responsible for the dominant spectrum line emission for which the 'bundle-n' approach is too imprecise, that is, averaged energies, oscillator strengths and collision strengths do not provide a good representation. Note also that key parent transitions for dielectronic recombination span a few low levels for which precise atomic data is necessary.

In the recombined ion, parentage gives approximate quantum numbers, that is, levels of the same n divide into those based on different parents. Lifetimes of levels of the same n but different parents can vary strongly (for example through secondary autoionisation). Also the recombination population of such levels is generally from the parent with which they are classified.

We therefore recognise three sets of non-exclusive levels of the recombined ion

(i)*Metastable levels* - indexed by $\rho$

(ii)*Low levels* - indexed by i,j,...., in a resolved coupling scheme, being the complete set of levels of a principal quantum shell range $n_0 \leq n \leq n_1$, including relevant metastables and spanning transitions contributing substantially to radiative power or of interest for specific observations.

(iii)*Bundle-n levels* - segregated according to the parent metastable upon which they are built and possibly also by spin system.

Viewed as a recombining ion, the set (i) must include relevant parents and set (ii) must span transitions which are dielectronic parent transitions. Time dependence matters only for the populations of (i), high precision matters only for group (ii) and special very many level handling techniques matter only for group (iii).

## 3.2. Progressive condensation and matrix expansion.

To satisfy the various requirements and to allow linking of population sets at different resolutions, a series of manipulations on the collisional-radiative matrices are performed (Summers, 1977; Summers and Hooper, 1983). The old expressions (1) and (2) are the most immediate of these.

To illustrate this, suppose there is a single parent metastable state. Consider the collisional-radiative matrix for the recombined ion and the right hand side (see equation(1)) in the bundle-n picture, and a partition of the populations as $[n,\ n']$ with the $n'$ such that $n_0 \leq n' \leq n_1$ and $n$ such that $n > n_1$. Elimination of the $N_n$ yields a set of equations for the $N_{n'}$. We call this a 'condensation' of the whole set of populations onto the $n'$ populations. The coefficients are the effective loss coefficients from the $n'$, the effective cross-coupling coefficients between the $n'$ and the effective recombination coefficients into the $n'$, which now include direct parts and indirect parts through the levels n. Exclusion of the direct terms prior to the manipulations yields only the indirect parts. Call these $C^{indir}_{n',n''}$ and $r^{indir}_{n'}$. We make the assumption that $C^{indir}$ and $r^{indir}$ may be 'expanded' over the resolved low level set using statistical weight factors alone, since the collisional mixing of substate populations with $n > n_1$ is generally large. The expanded indirect matrix $C^{indir}_{i,j}$ and $r^{indir}_i$ where $i$ and $j$ span the resolved low level set (ii) are then combined with higher precision direct couplings $C^{dir}_{i,j}$ and $r^{dir}_i$ so that

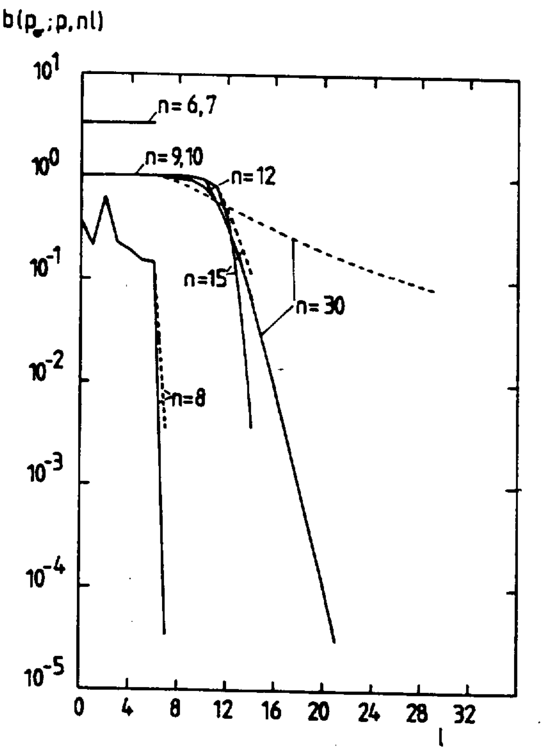


Fig. 6. $Cr^{+12}$ b-factors for doubly excited states.
Initial parent $p_\sigma$ is $2s^2 2p^6 3s$, and the excited parent $p$ is $2s^2 2p^6 3p$. $T_e = T_p = 1.69^6 K$, $N^e = 2 \times N_p$, $Z_p = 2$. *solid*, $N_e = 2.0^{11}\ cm^{-3}$ ; *dashes*, $N_e = 2.0^{13}\ cm^{-3}$ (Summers et al., 1987).

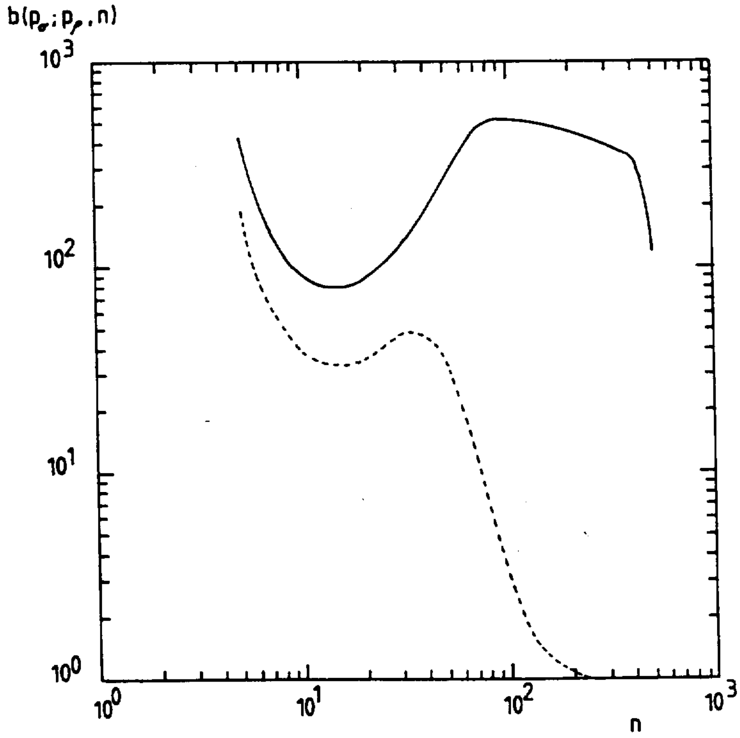


Fig. 7. $Ni^{+16}$ b-factors for singly excited states.
Initial parent $p_\sigma$ is $2s^2 2p^6 3s$, and the final parent is $p$ is $2s^2 2p^6 3s$. $T_e = T_p = 2.89^6 K$, $N_e = 2 \times N_p$, $Z_p = 2$. *solid*, $N_e = 2.0^0\ cm^{-3}$ ; *dashes*, $N_e = 2.0^{13}\ cm^{-3}$.

$$C_{i,j} = C_{i,j}^{dir} + C_{i,j}^{indir}$$
$$r_i = r_i^{dir} + r_i^{indir} \qquad [13]$$

If there is more than one recombining ion metastable state (indexed by $\sigma$) then the procedure must be performed for each parent and possibly spin system separately to assemble the final $C_{i,j}$. $r_i$ is replaced by its generalisation $r_{\sigma,i}$ and equations (8) are replaced by

$$\begin{bmatrix} C_{\rho,\rho'} & C_{\rho,j} \\ C_{i,\rho'} & C_{i,j} \end{bmatrix} \begin{bmatrix} N_{\rho'}^{(z)} \\ N_j^{(z)} \end{bmatrix} + N_e [N_\sigma^{(z+1)}] \begin{bmatrix} r_{\sigma,\rho} \\ r_{\sigma,i} \end{bmatrix} = \frac{d}{dt} \begin{bmatrix} N_\rho^{(z)} \\ 0 \end{bmatrix} \qquad [14]$$

where the metstables of the recombined and recombining ions have been partitioned off explicitly. The process may be continued (without the statistical expansion) condensing the low level set onto the metastable set. The generalised collisional-dielectronic coefficients are the result. The time dependent and/or spatial non-equilibrium transport equations which describe the evolution of the ground and metastable populations of ions in a plasma use these generalised coefficients. Following solution, the condensations can be reversed to recover the the complete set of excited populations and hence any required spectral emission.

The progressive condensation described above can be viewed as simply one of a number of possible paths which might be preferred because of special physical conditions or observations such as
*high bundle n → intermediate bundle nl → low LS resolved → metastables*
*high bundle n → low Stark resolved → ground*

Four types of bundling and condensation are distinguished in the JET work

(i) *Ground parent, spin summed bundle n → lowest n shell*
(ii) *Parent + spin separated bundle n → lowest spin system n shell*
(iii) *Parent + spin separated bundle n → low LS resolved → metastable states*
(iv) *Low LS resolved → metastable states*

Type (i) corresponds to the approach used in Summers (1974). (iv) corresponds to the usual population calculation for low levels in which normally recombination and ionisation are ignored. Then it establishes the dependence of each population on excitation for the various metastables only together with equilibrium metastable fractional populations and metastable cross-coupling effective rate coefficients. We illustrate these procedures with the series of figures 6,7,8 and 9.

## 4. PRACTICAL CONSIDERATIONS.

In seeking to advance the use of refined calculations and measurements of recombination in applications, there are two further considerations. These are

(i) Established practice

(ii) Data fill-in

Pioneering work in the fifties and sixties on transition probabilities (Bates and Damgaard, 1949), radiative recombination Burgess and Seaton, 1960b), dielectronic recombination (Burgess, 1965), collisonal ionisation (Seaton, 1964; Lotz, 1967,1968; Burgess, 1964) electron impact excitation (Seaton, 1962, Van Regemorter, 1962) left a legacy of simple, semi-empirical formulae for these various processes. These were of remarkably good accuracy (typically within a factor of two).

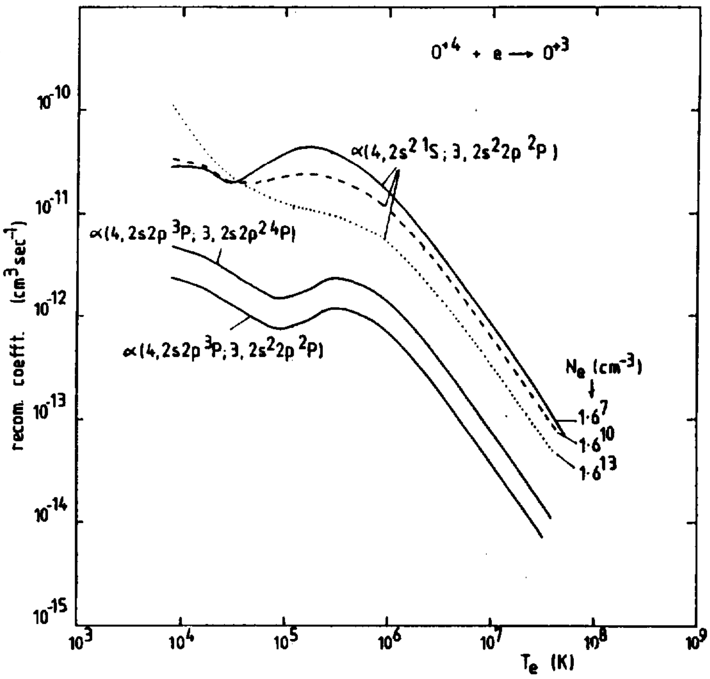


Fig. 8. $O^{+4} + e$ effective recombination coefficients.
Curves are labelled as $\alpha(z+1, p_\sigma; z, m_\rho)$ where $z+1$ is the recombining ion charge, $p_\sigma$ is the initial parent and $m_\rho$ is the final metastable.

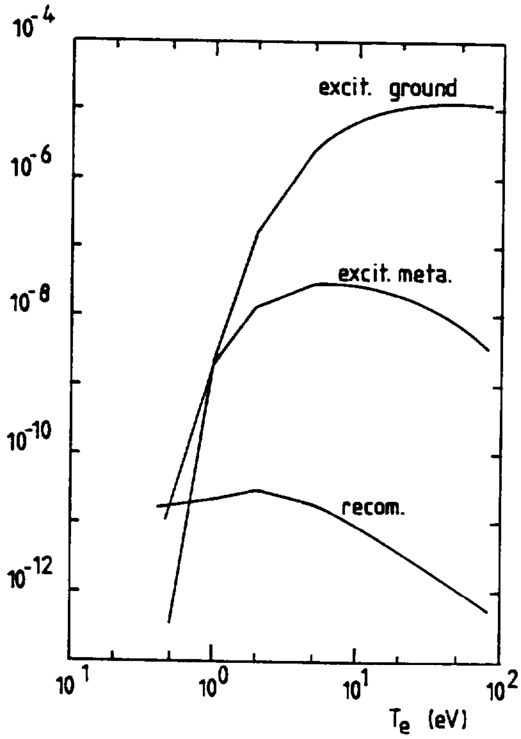


Fig. 9. $Be^0(2s4s\,^1S)$ populations. The population expansion coefficients in $N_i = N_e(F_{i,g}N(2s^2\,^1S) + F_{i,m}N(2s2p\,^1P) + F_{i,+}N^+(2s\,^2S))$ are given. $N_e = 10^{11}\ cm^{-3}$.

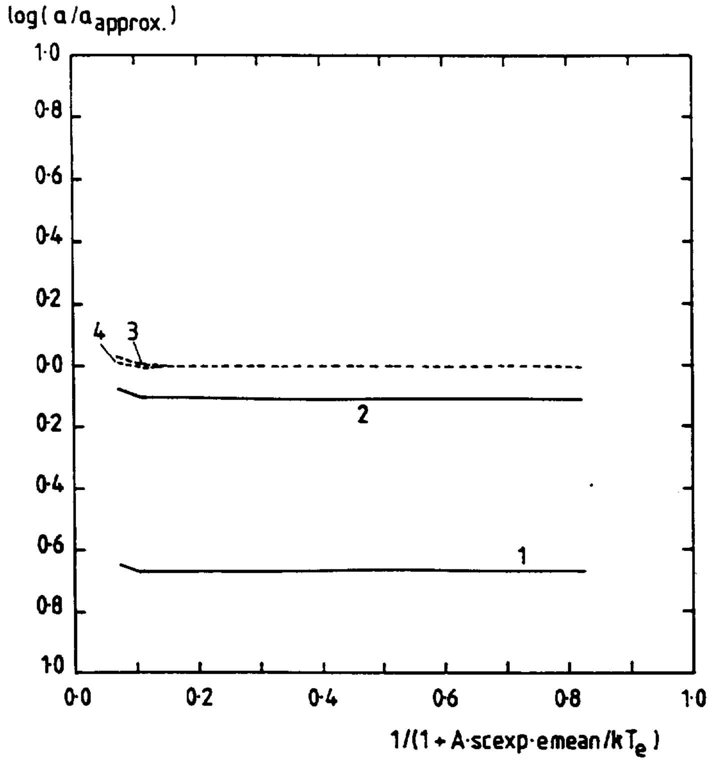


Fig. 10. $O^{+5} + e$ dielectronic recombination.
Analysis of Badnell (1990 - unpublished; see also Badnell and Pindzola, 1989) data for the inner shell parent transition in a reduced plot. *Curve 1*, initial GF comparison ; *Curve 2*, initial GP comparison ; *Curve 3*, final GF comparison ; *Curve 4*, final GP comparison. $A = 1.0$, *scexp* $= 2.0$, *emean* $= 41.5$ *Rydbergs.*

They were also general purpose, that is applied with some ease to arbitrary ions. Such formulae were enthusiastically used in the description of the ionisation state of astrophysical and laboratory plasmas from the middle sixties and are to the present day deeply established in most plasma physics modelling. Although many improvements have made over subsequent years, they have mostly been specific to one or two ions and have not easily allowed a global correction. The simple formulae have continued to dominate especially in the area of data fill-in. For many ionisation stages of many elements, there is no precise data yet completeness for modelling is necessary. The simple formulae allow this data fill-in, indeed, often since incorporation of best data may be awkward, it is bypassed in favour of the simpler methods. In recognition of this problem, it worthwhile to give some attention to simple formulae and the practicalities of incorporation of good data. It is helpful to see the simple formulae as *approximate forms* for the accurate data, also to identify empirical but physically based adjustments of the approximate forms by which they represent the accurate data better. At JET (Summers and Wood, 1988) we make use of approximate forms for all data types including cross-sections, recombination coefficients etc. each of which incorporates at most two adjustable parameters. By suitable choice of these parameters, hopefully slow variation along isoelectronic sequences can be obtained. Forming the ratio of accurate data to a fitted approximate form is helpful since the ratio remains close to unity. Errors or mistypings are readily spotted in a plot of the ratio, and interpolation of accurate data is improved by interpolating the ratio. This approach together with the 'reduced plots', we find helpful for data preparation and entry into our databases.

## 4.1. Dielectronic recombination.

We illustrate the above approach for dielectronic recombination only here and note that the basic approximate form is the 'Burgess zero-density General Formula' (Burgess, 1965). There are two further points. Most high quality dielectronic data is provided as total zero density rate coefficients as a function of temperature, or possibly in a reduced coefficient form. Secondly, as discussed in the previous section, the zero density coefficient is not appropriate in many plasmas, yet knowledge of the nl-shell distribution of capture is necessary for a proper density dependent correction to be made. Now the Burgess General Formulae may be inaccurate through a fault in the ratio $A_a A_r/(A_a + A_r)$ ( a temperature independent adjustment is appropriate ), or through inaccuracy in the mean satellite energy $\overline{E}$ adopted in the formula ( a temperature dependent fault with the correction appearing properly in the $\exp(-\overline{E}/kT_e)$).

In his work developing dielectronic recombination, Burgess prepared a fast algorithm for evaluation of the separate recombination coefficients into arbitrary nl-subshells based on the Correspondence Principle method This code, called the 'Burgess General Program (GP)' is to be distinquished from the Burgess zero density General Formula, GF. In this approach Auger rates are computed by extrapolating Bethe approximation collision strength data to below threshold. The lowest partial waves in Bethe approximation give substantial overestimates and so are multiplied by correction factors which have some universality. Correction factors can be specified for a series of parent transition types based on more elaborate calculations. Viewing the GP, summed over all nl-shells as an second approximate form to be adjusted to best available data, it is apparent that the Bethe corrections are the main source of error. We use default Bethe correction factors for various parent transition types and allow and adjustment of them involving a single parameter. Such comparisons and adjustments are shown for one case in figure 10. Then best data is converted to preferred temperature ranges, simple improvement of the GF provided when formula use is preferred in an application, and further density influence calculations are enabled. The three adjustments, namely *scale* and *edisp* for GF and *corfac* for GP are slowly varying with z and can be used for global isoelectronic sequence adjustment.

# 5. CONCLUSIONS.

Some of the applications of recombination to ionised plasmas have been described. These have been presented ito a progression of complexity in the atomic modelling of the behaviour of the recombination in the plasma.

To effect this modelling, a particular approach based on generalised collisional radiative theory has been explored and illustrated.

Some of the practical difficulties encountered by atomic physics recombination specialists in interacting with the applied community have been pointed out and some avenues suggested.

This paper is based on experience at the Joint European Torus. An implementation of the various ideas is in use there, called the 'Atomic Data and Analysis Structure'.

ACKNOWLEDGEMENTS.

HPS is on secondment to the Joint European Torus Experiment from the University of Strathclyde. WD holds a Science and Engineering Research Council CASE studentship.

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## Appendix I

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At 1st June 1991