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Dielectronic recombination of Fe^{22+} and Fe^{21+}

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Abstract. We calculate dielectronic recombination rate coefficients for the Be-like and B-like ions Fe^{22+} and Fe^{21+} using a multiconfiguration *LS*-coupling expansion and allowing for $\Delta n_c = 0$ and $\Delta n_c = 1$ autoionising transitions into the continuum of excited states. The effect of intermediate coupling is also investigated and found to be less than 10%. We use AUTOSTRUCTURE—a general program for the calculation of multiconfiguration *LS*-coupling or intermediate-coupling autoionisation transition rates (incorporating SUPERSTRUCTURE)—to calculate the dielectronic recombination rate coefficient for the 1-2 and 2-3 core transitions. Together with the Burgess general formula for the 2-2 transition, we obtain about 95% of the total dielectronic recombination rate coefficient for the ground state and look at its effect on the ionisation balance for a steady-state plasma. We also confirm the recent findings of Smith *et al* that the effect of $\Delta n_c = 0$ secondary autoionisation is much less significant for highly charged ions than was suggested by Jacobs *et al*.

1. Introduction

The process of resonant capture followed by radiative stabilisation, dielectronic recombination, is of great importance in the study of laboratory and astrophysical plasmas, particularly for highly stripped ions, and has recently been reviewed by Hahn (1985). For cases where the stabilising radiative transition rate A_r is much less than the autoionisation transition rate A_a (e.g. for $\Delta n_c = 0$ core transitions), the general formula of Burgess (1965) is accurate to 30% and better. For $\Delta n_c \neq 0$ core transitions in highly charged ions, $A_a \ll A_r$ and dielectronic recombination takes place mainly via capture to the lowest few levels and the Burgess GF is unreliable other than for 1-2 core transitions (Badnell 1986a).

To calculate dielectronic recombination rate coefficients we need to be able to generate easily large numbers of radiative and autoionisation transition rates for arbitrary atomic configurations with the minimum of input data. The code SUPERSTRUCTURE (see Eissner *et al* 1974, hereafter referred to as EJN) admirably serves the purpose for the radiative transition rates. From this code we have developed AUTOSTRUCTURE which also calculates configuration-mixing *LS*-coupling or intermediate-coupling autoionisation rates (Badnell 1985). We use this code to calculate dielectronic recombination rate coefficients for the 1-2 and 2-3 core transitions in Be-like and B-like iron.

McLaughlin *et al* (1985) have presented results for the Be-like target ion Fe^{22+} using an angular-momentum-averaged coupling scheme followed by a single-configuration *LS*-coupling calculation. Jacobs *et al* (1977, 1980 and references therein) have made comprehensive calculations of dielectronic recombination rate coefficients for all stages of ionisation of a number of atoms. They only consider 'no-coupling' *S*-coupling dipole autoionising transitions. However, the $2s \rightleftharpoons 3d \rightarrow 2p$ process is also

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important. Jacobs *et al* (1977) also include the effect of autoionisation into the continuum of excited states. However, it appears that their results are unreliable for highly ionised systems due to their neglect of a cut-off to exclude autoionisation into excited states that are energetically inaccessible (Jacobs 1985, Smith *et al* 1985).

Intermediate-coupling effects, while important for A_a, A_r and thus individual dielectronic satellites, are not expected to have too important an effect on the total dielectronic recombination rate for highly stripped ions (residual charge greater than 20). This is because the change from *LS* coupling to intermediate coupling redistributes the existing flux and does not open up any significant new radiative channels (see Badnell 1986a for an investigation of Fe^{24+}). The same is also true to a certain extent for the change from a single-configuration calculation to a multiconfiguration one. Intermediate coupling can be important though for atoms that are only a few times ionised due to the opening up of significant new autoionising channels ($A_r \ll A_a$ now). This has been looked at by Griffin *et al* (1985) for some Li-like ions while McLaughlin and Hahn (1984) have looked at configuration mixing only.

There are no purely experimental results for the total dielectronic recombination rate of highly charged ions although observations of satellites to resonance lines can provide a part estimate for some H-like and He-like targets (see, for example, Bitter *et al* 1984, 1985, TFR Group *et al* 1985a, b).

In § 2 we describe the theory behind the calculation of the autoionisation rates by AUTOSTRUCTURE. In § 3 we present and discuss our results for the dielectronic recombination of Fe^{22+} and Fe^{21+} via 1-2 and 2-3 core transitions. We also present the 2-2 dielectronic recombination results of the Burgess (1965) GF, the ionisation rates from the GF of Burgess and Chidichimo (1983) and radiative recombination rates from Woods *et al* (1981) to enable us to look at the ionisation balance for a steady-state plasma.

2. Theory

The total dielectronic recombination rate coefficient for a given initial state i is given by (see e.g. Burgess 1966)

$$\alpha_d(i;\text{tot}) = \left(\frac{4\pi a_0^2 I_H}{kT}\right)^{3/2} \sum_j \frac{w(j)}{2w(i)} \frac{\Sigma_\kappa A_r(j\to\kappa)\,\Sigma_l A_a(j\to i, E_c l)\,e^{-E_c/kT}}{\Sigma_\kappa [A_r(j\to\kappa)+\Sigma_l A_a(j\to\kappa, E_c l)]}$$

where E_c is the energy (in rydbergs) of the continuum electron, which is fixed by the position of the resonances; $w(j)$ is the statistical weight of the $(N+1)$-electron intermediate state, $w(i)$ the statistical weight of the N-electron target ion; and $(4\pi a_0^2 I_H/k)^{3/2} = 4.1414\times10^{-16}\,\text{cm}^3$.

2.1. Autoionisation transition rates

The autoionisation transition probability rate, A_a, is given in first-order perturbation theory by (see e.g. Cowan 1981)

$$A_a(b-f) = \frac{2I_H}{\hbar}|\langle f|H|b\rangle|^2 \tag{2.1}$$

where $I_H/\hbar = 2.067\,07\times10^{16}\,\text{s}^{-1}$.

2.1.1. LS coupling. We evaluate bound-continuum matrix elements of the form (in

the notation of EJN)

$$\langle \Lambda SL|H_{\rm nr}|\Gamma S'L'\rangle = \delta_{SS'}\delta_{LL'}\langle \Lambda SL|C\gamma SL\rangle\langle C\gamma SL|H_{\rm nr}|B\beta S'L'\rangle\langle B\beta S'L'|\Gamma S'L'\rangle \tag{2.2}$$

where $\langle B\beta SL|\Gamma SL\rangle$ diagonalises the $(N+1)$-electron Hamiltonian (see equation (2) of EJN), $B = n_1'l_1' \ldots n_{N+1}'l_{N+1}'$ denotes the $(N+1)$-electron configuration, β is a degeneracy label and Λ, Γ label the new basis. $\langle \Lambda SL|C\gamma SL\rangle$ diagonalises the N-electron target Hamiltonian, $C = n_1l_1 \ldots n_Nl_NE_cl_c$, where the same E_cl_c orbital is coupled to each target configuration and γ is another degeneracy label.

Diagonalising the Hamiltonian corresponds to satisfying the variational

$$\delta[\langle p|H - E|p'\rangle] = 0 \tag{2.3}$$

for the off-diagonal elements, where p and p' label the trial wavefunctions and the configuration expansion for the trial wavefunctions is always truncated, i.e. the basis is not complete.

2.1.2. Intermediate coupling. We evaluate

$$\langle \Lambda SLJ|H_{\rm BP}|\Gamma S'L'J'\rangle = \delta_{JJ'}\langle \Lambda SLJ|C\gamma SLJ\rangle \times \langle C\gamma SLJ|H_{\rm BP}|B\beta S'L'J'\rangle\langle B\beta S'L'J'|\Gamma S'L'J'\rangle \tag{2.4}$$

where $H_{\rm BP} = H_{\rm nr} + H_{\rm rc}$ is the Breit-Pauli Hamiltonian (see equation (43) of EJN), $\langle B\beta S'L'J|\Gamma S'L'J\rangle$ diagonalises the $(N+1)$-electron Breit-Pauli Hamiltonian and $\langle \Lambda SLJ|C\gamma SLJ\rangle$ diagonalises the N-electron target Breit-Pauli Hamiltonian.

We now note the following points.

(i) The eigenenergies of the doubly excited terms/levels of the $(N+1)$-electron ion are related to the eigenenergies of the N-electron target by

$$E(N+1) = E(N) + E_c \tag{2.5}$$

where E_c is the energy of the continuum electron. In the evaluation of $E(N)$ we assume that the target ion is unperturbed by the continuum electron. In the evaluation of $E(N+1)$ we assume that there is no interaction of the $(N+1)$-electron ion with the target ion plus continuum electron. In intermediate coupling we additionally neglect relativistic corrections to the energy of the continuum electron (see Jones 1975).

(ii) We have

$$|C\gamma SLJM\rangle = \langle SLM_SM_L|JM\rangle|C\gamma SLM_SM_L\rangle \tag{2.6}$$

and the matrix elements of the Hamiltonian are diagonal with respect to, and independent of, M_S, M_L and M and thus these labels have been dropped.

(iii) As with SUPERSTRUCTURE, only the one-body terms (mass variation, Darwin and spin-orbit) and the two-body fine-structure terms (spin-orbit, spin-other-orbit and spin-spin) are retained in the Breit-Pauli Hamiltonian. The two-body non-fine-structure terms (Darwin, contact spin-spin and orbit-orbit) are neglected (see EJN for discussion).

2.2. Accuracy

Sources of error that are the same as for SUPERSTRUCTURE include the use of a limited configuration expansion, the use of distorted-wave orbitals in a statistical model potential and the use of a non-relativistic or Breit-Pauli Hamiltonian (minus two-body non-fine-structure terms).

An additional source of error lies in the use of representative continuum functions. For a given doubly excited complex with eigenenergies $E(N+1)$, energy conservation implies that the energy of the continuum electron E_c is given by (2.5) where $E(N)$ is the energy of the target ion. The eigenenergies $E(N+1)$ of each term/level within a complex are only approximately the same. E_c can be chosen optimally to satisfy (2.5) for the most strongly autoionising term/level when one is interested in dielectronic recombination. One can also use more than one continuum orbital for a given l. Roughly, one can expect a 5% error in E_c to result in a 5% error in A_a.

Details and tests of the program AUTOSTRUCTURE may be found in Badnell (1985).

2.3. Radiative transition rates

The radiative transition probability rates are calculated exactly as in Eissner *et al* (1974). Only dipole radiative rates were used in the calculation of the results presented below.

3. Results and discussion

3.1. Fe^{22+}

In figure 1 we present our results for the dielectronic recombination rate coefficient of Fe^{22+}. The results for the 2-2 core transition were evaluated from the Burgess (1965) GF using the oscillator strengths and energy levels of Fuhr *et al* (1981), and at 1.16×10^7 K they lie 10% above the results of a numerical calculation by Merts *et al* (1976) and 20% below those of McLaughlin *et al* (1985). The work of McLaughlin *et al* (1985) supersedes that of an earlier paper by Hahn *et al* (1980a) which underestimated the contribution from high n, particularly for $\alpha_d(2\text{-}2)$ (see also LaGattuta and

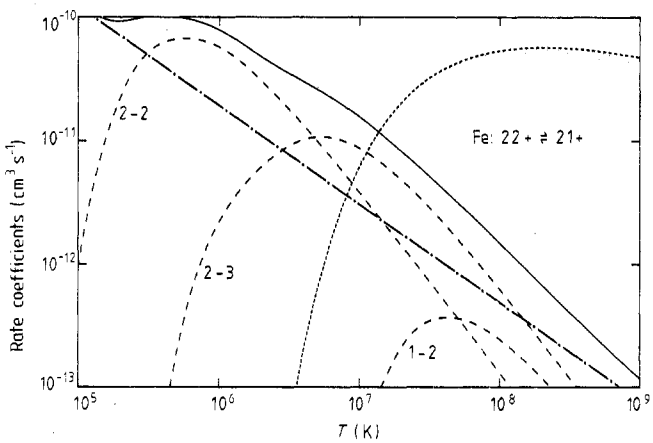
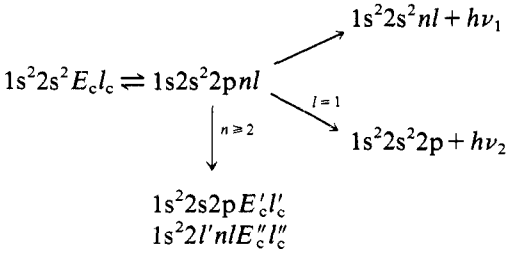


Figure 1. Recombination and ionisation rate coefficients for Fe^{22+} and Fe^{21+}:----, dielectronic recombination rate coefficients for the 1-2, 2-3 (this work) and 2-2 (Burgess 1965 GF) core transitions; – · – · –, radiative recombination rate coefficient (Woods *et al* 1981); ——, total recombination rate coefficient for Fe^{22+}; · · · · ·, ionisation rate coefficient for Fe^{21+} (Burgess and Chidichimo 1983 GF).

Hahn 1983). Results for the 1-2 and 2-3 core transitions were evaluated as described in § 2 using the following configurations:

1-2 core transition

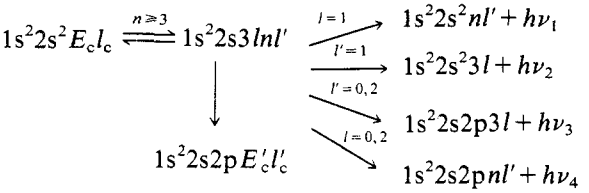


We note that $1s2s^22pns,\ nd \rightarrow 1s2s^22p^2 + h\nu$ is also possible, but that it is not stable against autoionisation and also

$$A_r(1s2s^22pns,\ nd \rightarrow 1s2s^22p^2) \ll A_r(1s2s^22pns,\ nd \rightarrow 1s^22s^2ns,\ nd)$$

and so we neglect it. Results were calculated separately for each value of n up to $n=5$, and for $n>5$ the sum over n was completed using the n^{-3} asymptotic dependence of A_a. At $n=5$ the results of the direct calculation agreed to within 5% of the results of scaling from $n=4$.

2-3 core transition



We have included all multipole autoionising transitions and dipole radiative transitions and we allow for autoionisation into the continuum of the excited $1s^22s2p$ configuration. The $1s^22s2pnl'$ configuration is not stable against autoionisation for $n>8$ (for the singlet parent, see Corliss and Sugar 1982) and since

$$A_r(1s^22s2pnl' \rightarrow 1s^22s^2nl') \ll A_a(1s^22s2pnl' \rightarrow 1s^22s^2E_cl_c)$$

we cut off the sum over n at $n=8$ for this path. Results were calculated separately for each value of n up to $n=8$, and those paths which required results for $n>8$ were calculated using the n^{-3} scaling. Dielectronic recombination via the non-dipole 2s-3s,3d autoionising transitions accounts for two-thirds of the 2-3 total.

Jacobs *et al* (1977) have calculated α_d(2s-3p) also allowing for dipole autoionisation into the continuum of excited states. However, we find that $1s^22s3p(^1P)nl \rightleftharpoons 1s^22s3s(^1S)E_cl_c$ is only energetically possible for $n>19$ and that this process has little effect since less than 1% of α_d(2-3) could come from $n>19$. Also, $1s^22s3dnl \rightleftharpoons 1s^22s3sE_cl_c$ is possible for $n>13$ (for the singlet parents) but the sum over n has already been truncated at $n=8$ for this path (see above). At $T=10^7$ K we find that our results for $\alpha_d(i;\text{tot})$ are a factor of 2.5 greater than those of Jacobs *et al* (1977) obtained from the fit by Woods *et al* (1981). The ratio of the two sets of results for only the dipole 2-3 transitions is only slightly smaller, namely 2.3. As the residual charge decreases, the dipole results of Jacobs *et al* (1977) can be expected to become

more reliable (see Smith *et al* 1985) while the error due to their neglect of non-dipole autoionising transitions will also decrease, since the non-dipole transitions become less important, but it will still remain significant (see Badnell 1986b).

We note that Corliss and Sugar (1982) list the $1s^2 2s3s\ ^1S_0$ level as being 9783 000 cm^{-1} above the $1s^2 2s^2\ ^1S_0$ ground level, as taken from Boiko *et al* (1977) who in fact identify the 9030 200 cm^{-1} line as arising from the $2s2p\ ^1P_1$-$2s3s\ ^1S_0$ transition. Bhatia and Mason (1981) do not accept this classification as it would place the $2s3s\ ^1S_0$ level above the $2s3d\ ^1D_2$ and $2s3p\ ^1P_1$ levels. We have extended their intermediate-coupling calculation to include the 1 : 1 : 3 : 3 complex as well as the $1s^2 2s4s$ and $1s^2 2p4p$ configurations and obtain $2s2p\ ^1P_1$-$2s3s\ ^1S_0 = 8223\ 500\ cm^{-1}$ as opposed to 8232 200 cm^{-1} by Bhatia and Mason (1981); also, Fawcett (1984) obtained 8210 900 cm^{-1} using the Hartree–Fock relativistic code of Cowan (1981). We believe that the 9030 200 cm^{-1} line observed by Boiko *et al* (1977) arose from the $2s2p\ ^1P_1$-$2p3p\ ^1S_0$ transition, for which we obtain 9030 900 cm^{-1}, and thus the $2s3s\ ^1S_0$ level in Corliss and Sugar (1982) should be labelled $2p3p\ ^1S_0$.

McLaughlin *et al* (1985) have evaluated $\alpha_d(2\text{-}3)$ in an *LS*-corrected angular-momentum-averaging scheme and their results ($\alpha_d(2\text{-}3) = 9.7 \times 10^{-12}\ cm^3\ s^{-1}$) lie about 20% above ours ($\alpha_d(2\text{-}3) = 7.9 \times 10^{-12}\ cm^3\ s^{-1}$) at $T = 1.16 \times 10^7$ K. McLaughlin *et al* (1985) allow for radiative decays of the outer electron to levels which are not stable against autoionisation (see Gau and Hahn 1980), but the inclusion of this cascade effect reduces $\alpha_d(2\text{-}3)$ by no more than 10% (see Gau *et al* 1980, Hahn 1985). However, McLaughlin *et al* (1985) and Hahn *et al* (1980a) assume that the $1s^2 2s2pnl$ configuration is stable against autoionisation for all n when in fact this is only true for $n \leqslant n_0$. This assumption does not result in a large error for Fe^{22+} since $n_0 = 8$; in fact our results increase by about 20% ($\alpha_d(2\text{-}3) = 9.6 \times 10^{-12}\ cm^3\ s^{-1}$ at $T = 1.16 \times 10^7$ K) if we assume that the $1s^2 2s2pnl$ configuration is stable for all n; but as the residual charge decreases, n_0 decreases (e.g. for O^{4+}, $n_0 = 3$) and the error due to this assumption becomes more serious (see Badnell 1986b for a detailed investigation of the Be sequence).

A further contribution to $\alpha_d(i; \text{tot})$ comes from 2-n core transitions for $n > 3$, but since the $1s^2 2s4ln'l'$ configuration can autoionise to $1s^2 2s3l''E_c l_c$ for $n' > 4$ its contribution is suppressed compared with that from the 2-3 core transition. We estimate that we have included 95% of the total dielectronic recombination rate in our calculations. McLaughlin *et al* (1985) include contributions from 2-4 core transitions but do not allow for 4-3 secondary autoionisation (see also Gau *et al* 1980, LaGattuta and Hahn 1983) and so overestimate its contribution, which is, however, small.

In figure 1, as well as the dielectronic recombination rate coefficients, we also include the radiative recombination rate coefficient $\alpha_r(Fe^{22+} \rightarrow Fe^{21+})$ of Woods *et al* (1981) and the ionisation rate coefficient $q(Fe^{21+} \rightarrow Fe^{22+})$ evaluated from the general formula of Burgess and Chidichimo (1983). For a steady-state plasma $(\alpha_d + \alpha_r)N(22+) = qN(21+)$ where $N(z)$ is the population number density of the ion with residual charge z. The population number densities for the two ions become equal at $T = 1.36 \times 10^7$ K, an increase of about 30% in the value obtained without including $\alpha_d(2\text{-}3)$ (and $\alpha_d(1\text{-}2)$) in $\alpha_d(i; \text{tot})$.

Jacobs *et al* (1977) obtained a temperature of 1.0×10^7 K for $N(22+) = N(21+)$ using the Lotz (1968) formula for the ionisation rate coefficient. Meanwhile, Jordan (1969, 1970) obtained a value of 1.6×10^7 K using Seaton's (1964) ionisation formula. Jordan (1969) also used the Burgess (1965) GF for $\alpha_d(2\text{-}3)$ as well as for $\alpha_d(2\text{-}2)$. However, the Burgess GF overestimates $\alpha_d(2\text{-}3)$ by a factor of 1.6 at this temperature. Both Jacobs *et al* (1977) and Jordan (1969) also modified the formula they used for

the ionisation rate coefficient to allow for the process of inner-shell excitation followed by autoionisation, which is also allowed for by the Burgess and Chidichimo (1983) GF.

3.2. Fe^{21+}

In figure 2 we present our results for the same processes as in figure 1 but this time for Fe^{21+}. Again, the results of the Burgess (1965) GF for $\alpha_d(2\text{-}2)$ lie 10% above those of Merts *et al* (1976). For the 1-2 core transition we use the same configurations as in § 3.1, now with a 2p orbital attached. Merts *et al* (1976) found that the results of their numerical calculation for $\alpha_d(1\text{-}2)$ were a factor of 2 smaller than those of the Burgess GF. However, the temperature ($T = 1.16 \times 10^7$ K) at which they made the comparison in their paper corresponds to $E/kT = 5$, i.e. at the limit of the applicability of the GF at low temperatures. At $T = 4 \times 10^7$ K we find that our results for $\alpha_d(1\text{-}2)$ are only a factor of 1.34 smaller than those of the GF and in line with the expected error of the GF. Meanwhile, at $T = 1.16 \times 10^7$ K our results for $\alpha_d(1\text{-}2)$ lie 5% above those of Merts *et al* (1976).

For the 2-3 core transition we again use the configurations of § 3.1, with a 2p orbital attached. The $1s^2 2s 2p^2 nl'$ configuration is not stable against autoionisation for $n > 8$ (^2D parent) or $n > 7$ (^2S, ^2P parents) and again we cut off the sum here for this path. Also, the secondary autoionisation path $1s^2 2s 2p 3lnl' \rightleftharpoons 1s^2 2s^2 3lE_c l_c$ is energetically possible for $n > 8$ and so we cut off the sum here for this path. Now, we must also include the additional configurations corresponding to

$$1s^2 2s^2 2p E_c l_c \rightleftharpoons 1s^2 2s^2 3lnl' \begin{cases} \xrightarrow{l=0,2} 1s^2 2s^2 2p nl' + h\nu_1 \\ \xrightarrow{l'=0,2} 1s^2 2s^2 2p 3l + h\nu_2. \end{cases}$$

Dielectronic recombination via non-dipole autoionising transitions now accounts for only one-third of the 2-3 total.

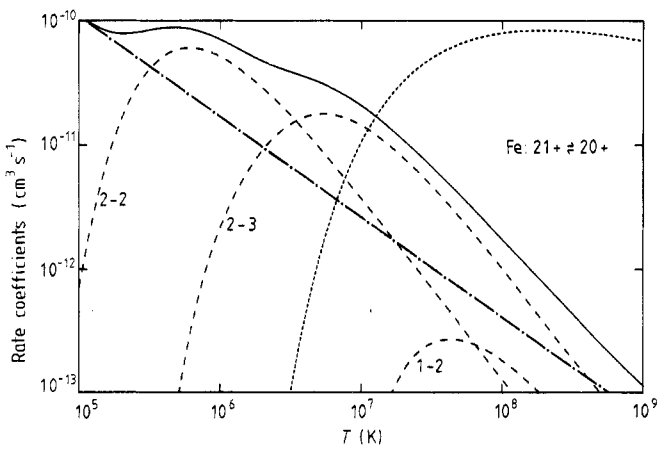


Figure 2. Recombination and ionisation rate coefficients for Fe^{21+} and Fe^{20+}: ----, dielectronic recombination rate coefficients for the 1-2, 2-3 (this work) and 2-2 (Burgess 1965 GF) core transitions; - · - · -, radiative recombination rate coefficient (Woods *et al* 1981); ——, total recombination rate coefficient for Fe^{21+}; · · · ·, ionisation rate coefficient for Fe^{20+} (Burgess and Chidichimo 1983 GF).

We can also include excited configurations of the form $1s^22p^23lnl'$, although they only contribute to the dielectronic process through mixing. Omitting these mixing configurations for $n=3$ reduces the contribution to $\alpha_d(2\text{-}3)$ by less than 1%. We can also treat the $1s^22s^23lnl'$ and $1s^22s2p3lnl'$ configurations separately and for $n=3$ this reduces the contribution by 3%. For $n>4$ we do treat them separately. Using a smaller configuration expansion, we have also calculated results for $n=3$ in intermediate coupling and they are about 7% larger than the *LS*-coupling results calculated with the same expansion.

Merts *et al* (1976) have calculated $\alpha_d(2s\text{-}3p)$ including only dipole autoionising transitions and neglecting secondary autoionisation, and consequently their results are a factor of 2 smaller than our results for $\alpha_d(2s\text{-}3l)$. On performing a calculation similar to that by Merts *et al* (1976), we obtained a result for $\alpha_d(2s\text{-}3p)$ that was only 20% smaller than theirs.

As with Fe^{22+}, $\Delta n_c=0$ secondary autoionisation has little or no effect on our results for $\alpha_d(2\text{-}3)$ for Fe^{21+}. However, our results for $\alpha_d(i;\text{tot})$ at $T=10^7$ K are only a factor of 1.5 greater than those of Jacobs *et al* (1977) and are almost the same if we compare only the dipole 2-3 transitions. This is surprising given the difference for Fe^{22+}. There is further evidence that the error due to the neglect of a cut-off by Jacobs *et al* (1977) is not negligible. Smith *et al* (1985) have looked at the dielectronic recombination of the Ne-like ion Fe^{16+} and obtain a value of $\alpha_d(2\text{-}3)=1.3\times10^{-11}$ cm^3 s^{-1} at $T=1.16\times10^7$ K, in very close agreement with the results of Hahn *et al* (1980b). From the fit of Woods *et al* (1981), or directly from figure 2 of Jacobs *et al* (1977), we find $\alpha_d(2\text{-}3)=4.9\times10^{-12}$ or 4.6×10^{-12} cm^3 s^{-1}, a factor of about 2.7 smaller than Smith *et al* (1985). These results are purely for 2p-3s,3d transitions and the difference between the two can be directly attributed to the neglect of a cut-off by Jacobs *et al* (1977). Jacobs *et al* (1980) have also calculated similar results for Ca and Ni ions. As expected from the z-scaling properties of $\alpha_d(i;\text{tot})$, we find a smooth trend in their results for Be-like Ca, Fe and Ni. The same is not true for the B-like ions; their results for B-like Fe (Jacobs *et al* 1977) are anomalously large compared with their results for B-like Ca and Ni (Jacobs *et al* 1980) and could account for the above discrepancy.

From figure 2 we see that the population number densities $N(21+)$ and $N(20+)$ become equal at $T=1.26\times10^7$ K, approximately 40% higher than it would be if $\alpha_d(2\text{-}3)$ were omitted from $\alpha_d(i;\text{tot})$. The inclusion of $\alpha_d(2\text{-}3)$ in the total recombination coefficient for $Fe^{(22-n)+}$ becomes increasingly important as n increases and, of course, at $n=6$, Ne-like iron, $\alpha_d(i;\text{tot})\simeq\alpha_d(2\text{-}3)$. Jordan (1969, 1970) obtained a temperature of 1.1×10^7 K for $N(21+)=N(20+)$; the Burgess (1965) GF now overestimates $\alpha_d(2\text{-}3)$ by a factor of 1.9 at this temperature.

4. Conclusions

We have described a general method for the calculation of autoionisation transition rates from low-lying states within a multiconfiguration *LS*-coupling or intermediate-coupling expansion. We have applied the resulting program AUTOSTRUCTURE to the calculation of dielectronic recombination rate coefficients for $\Delta n_c\neq0$ core transitions in Fe^{22+} and Fe^{21+} allowing for autoionisation into the continuum of excited states. We deduce that the neglect of a cut-off on n for $\Delta n_c=0$ secondary autoionising transitions leads to appreciable errors in the results of Jacobs *et al* (1977, 1980) for highly charged ions. Also, the inclusion of non-dipole autoionising transitions is

particularly important for Be-like ions. The program AUTOSTRUCTURE should be useful for future work looking at the effect of inner-shell excitation autoionisation in high-temperature plasmas and dielectronic recombination at low temperatures.

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