Scaling of dielectronic-recombination data in fluorinelike ions

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Dielectronic data for state-specific F-like to Ne-like recombinations are obtained for elements between argon and krypton (and perhaps somewhat beyond). The data consist of energy levels, autoionization rates, radiative rates, and dielectronic-recombination branching ratios. Detailed calculations using a Hartree-Fock method that includes relativistic corrections, but no configuration interactions, were carried out for Ar^{9+} , Ti^{13+} , Fe^{17+} , and Se^{25+} . Three- and four-parameter fits were then made to these data enabling one to calculate dielectronic rates for all elements in the fourth row of the periodic table. These scaling relations provide checks on the accuracy of the numerical methods used to obtain the Ar, Ti, Fe, and Se data. Further checks are provided by comparisons made to other published work. The dielectronic-recombination rates presented in this paper are very important in the calculation of population inversions and x-ray laser gain within neonlike ionization stages.

I. INTRODUCTION

Dielectronic recombination (DR) is an important process for ionization balance¹ and x-ray laser^{2,3} calculations in plasmas with moderate- to high-Z ions. It can also provide valuable plasma diagnostics in high-temperature, moderately dense plasmas. The dielectronic satellite lines that appear on the long-wavelength side of the resonance lines as a result of these recombinations are often used for the measurement of electron temperature.⁴⁻⁷ However, most calculations to date of DR processes consist of case by case explicit calculations of the necessary atomic quantities such as energy levels, bound and continuum wave functions, and matrix elements involving these wave functions. These calculations are carried out using detailed relativistic or nonrelativistic atomic codes for each element of concern. With each case done individually, and especially when they are done in great detail, it is not possible to know with certainty whether numerical errors or discrepancies between calculations exist either in the behavior of the energy levels or matrix elements as one goes from one ion to another in the same isoelectronic sequence. However, on general theoretical grounds, one knows that all of the quantities entering into the calculation of DR rate coefficients should make a smooth transition into one another as one moves along an isoelectronic sequence.

Lazer⁸ has shown, by incorporating the atomic number Z as a dynamical variable, that radial wave functions in an isoelectronic sequence have a perturbation series expansion in powers of 1/Z. He used this theory to define screening constants that gave excellent approximations to the 1/Z expansion dependence of the term energies. Similarly Wiese⁹ has used the 1/Z power series expansion of the wave functions and energies to show that expansions of oscillator strengths in powers of 1/Z converge rapidly in the isoelectronic sequence. Generally only three terms are needed to accurately determine a large

number of oscillator strengths along an isoelectronic sequence of moderate-Z elements. Even though most authors take the autoionization rate to be independent of atomic number, one can show that autoionization rates scale with Z, like oscillator strengths, following the same arguments as in Ref. 9 for both bound and continuum wave functions, i.e., one can also employ three term power series to accurately determine such quantities. There is also a growing amount of published literature on the Z dependence of excitation¹⁰ and ionization¹¹ collision strengths and photoionization cross sections.¹²

Since isoelectronic scaling relationships exist for most of the atomic data that is needed to make accurate calculations of ionization equilibrium and plasma energetics, it is important that an accurate determination of the Z scaling of DR rates be made. The semiempirical formulas derived by Burgess¹³ and modified by Merts, Cowan, and Magee¹⁴ are often used as the principal tool to obtain estimates of how total ground-to-ground effective DR rates scale with atomic number. Even though these simple formulas sometimes predict rates that are close to those calculated by more detailed and accurate methods, where this close agreement occurs is itself unpredictable. Hahn¹⁵ obtained a scaling relation for DR rates by modi-fying the Burgess-Merts¹⁴ formula. He based his results on the detailed calculations of DR rates for Be and Ne sequences. However, he eliminated the energy scaling part of the problem by presenting his results only for temperatures which themselves scale as Z^2 .

Recent interest in improving the calculation of DR rates has been generated by the need for an improved understanding of the kinetics of soft x-ray lasers in and around neonlike ionization stages.^{16,17} Dielectronic recombination is a significant and direct contributor to the kinetics of neonlike selenium.^{2,18,19} DR processes help to create population inversions by preferentially populating the upper lasing levels in addition to the collisional excitations from the ground state. In order to ac-

curately calculate a gain for the x-ray laser transitions, therefore, it is necessary to obtain DR rate coefficients as well as resonance excitation rates directly into the n=3 excited states of the neonlike system and into each of the upper and lower levels.

Dielectronic recombination rate coefficients for F-like ions have been calculated by several authors. Roszman²⁰ used a single configuration, LS coupled, nonrelativistic Hartree-Fock method, while Chen²¹ adopted a fully relativistic multiconfiguration Dirac-Fock (MCDF) approach and carried out the calculation for moderate- to high-Z elements. Another relativistic calculation of DR rates for F-like Se²⁵⁺ was carried out by Hagelstein.²² However, he calculated DR rate coefficients by including only the very-low-lying 3/3/1' manifold of Ne-like states.

In most of these published works only total DR rate coefficients were presented and discussed. By contrast, in the calculations to be presented in this paper, a detailed and accurate set of DR rates into specific (n, l) singly excited states of neonlike ions will be made for the purpose of carrying out ionization dynamic studies of the neonlike system and of evaluating the effects of these dynamics on 3s-3p gain calculations. The total effective ground-toground rate can be obtained, if needed, by summing over these state specific rates. More importantly, the Z dependence of various DR data such as branching ratios, the energies of the autoionizing states, autoionization rates, and radiative rates will be determined. These scaling relations can be used to obtain DR rates and satellite line data for any ion from argon through krypton in the same F-like sequence with little effort.

We will investigate the Z dependence of DR rate coefficients and other related data of the fluorine isoelectronic sequence by calculating this data in detail for Flike Ar^{9+} , Ti^{13+} , Fe^{17+} , and Se^{25+} ions. One can then utilize either three-parameter, least-squares fits, or fourparameter interpolations of the data in order to obtain DR data from argon through krypton with a great saving in the amount of theoretical work. The DR data for Ar^{9+} , Ti^{13+} , Fe^{17+} , and Se^{25+} is calculated for a large number of intermediate resonance states using a singleconfigurational Hartree-Fock calculation with relativistic corrections (HFR method of Cowan²³). Approximate relativistic corrections are made to both the radial wave functions as well as to the singly and doubly excited state energies. We expect that this method of calculation will give more accurate results than previously calculated DR rates using single-configuration nonrelativistic wave functions or a simple angular momentum averaged pro-cedure.²⁴ On the other hand, the HFR method is less time consuming and less complex than fully relativistic calculations.^{21,22} Thus for calculating autoionization or DR rates for moderate-Z ions, our use of Cowan's HFR method of calculation is a very good compromise between insufficient accuracy on the one hand and excessive accuracy or computation time on the other.

A brief description of the general theory and of the formulas we used to calculate the DR rates is given in Sec. II. This section also contains a description of the numerical methods involved in the calculation as well as the atomic level structure for the singly and doubly excited states that was employed. Numerical results for DR rates and comparisons of our results with other theoretical work are presented in Sec. III. In Sec. IV the Z dependence of the rates, energies, and DR branching ratios is discussed and numerical results are presented. Finally, in Sec. V, a summary of the present work is given.

II. THEORETICAL CONSIDERATIONS

The net process of dielectronic recombination is generally considered a two step process. First, dielectronic capture of an electron by an ion occurs into a doubly excited state (the reverse of autoionization):

$$X_{i}(Z,N) + e^{-} \rightarrow X_{i}^{**} \quad (Z,N+1)$$
⁽¹⁾

where one of the bound electrons of the initial ion goes to an excited state and the free electron is also captured to an excited state. In the second step, the doubly excited state deexcites by radiative decay to different states of the recombined ion, which are below the ionization threshold and therefore stable against autoionization:

$$X_{i}^{**}(Z, N+1) \rightarrow X_{k}^{*}(Z, N+1) + h\nu$$
 (2)

The doubly excited state can also immediately decay by autoionization to the initial state or to any other possible excited state of the initial recombining ion. For a Maxwellian distribution of electrons, the DR rate coefficient $\alpha^{DR}(i,k)$ from an initial state $|i\rangle$ into a final bound state $|k\rangle$ is given by a sum over all dielectronic captures into the unbound autoionizing states $|j\rangle$:

$$\alpha^{\mathrm{DR}}(i,k) = \left(\frac{4\pi\mathcal{R}}{kT}\right)^{3/2} \frac{a_0^3}{2g_i} \sum_j F_{ijk} e^{-\varepsilon_j/kT}, \qquad (3)$$

where

$$F_{ijk} \equiv \frac{g_j A_{ji}^a A_{jk}^r}{\sum_{i'} A_{ji'}^a + \sum_{k'} A_{jk'}^r} .$$
(4)

Here g_i and g_j are the statistical weights of the initial and doubly excited states, respectively, a_0 is the Bohr radius, kT is the plasma electron temperature, ε_j is the energy of the free recombining electron, and \mathcal{R} is the Rydberg energy (13.6 eV). ε_j is, of course, also equal to the energy of the doubly excited state above the ionization limit of the recombining ion. A_{ji}^a and A_{jk}^r are the autoionization and radiative rates from state $|j\rangle$ to states $|i\rangle$ and $|k\rangle$, respectively. F_{ijk} , which we shall call DR branching ratios, are the individual terms from which the quantity F, defined by Cowan,²⁵ is obtained by a summation over all indices. They are useful physical quantities since they also provide a direct measure of the intensity of the Nelike satellite lines that are emitted by the fluorine-to-neon recombination processes:

$$I(j,k) = N_e E_{jk} \left[\frac{4\pi \mathcal{R}}{kT} \right]^{3/2} a_0^3 \frac{e}{2}^{-\epsilon_j/kT} \sum_i \frac{N_i}{g_i} F_{ijk} .$$
 (5)

In this formula, N_e is the electron density, N_i is the density of *F*-like initial states $|i\rangle$, and E_{jk} is the energy of the

satellite line $(=E_j^{**}-E_k^*)$.⁷ The calculations of F_{ijk} were carried out using the atomic code of Cowan²³ (RCG mod 9), which, as mentioned, determines matrix elements and state energies by the HFR method. In this code, states are defined at the submultiplet level and the differential Auger transition probabilities for doubly excited states are calculated from the perturbation expression

$$A_{ii}^{a} = (2\pi/h) |\langle (\gamma J_{i}), l_{i}, J_{t} | H | \gamma J_{i} \rangle|^{2} , \qquad (6)$$

where γJ_i defines the initial target state with total angular momentum J_i . The free electron has orbital angular momentum l_i , and the total target-electron angular momentum J_t necessarily is equal to the value J_j of the resonance capture state $|j\rangle$. After summing these partial rates over all orbital angular momentum states defined by l_i , one gets the autoionization rate from each level J_j of the doubly excited configuration.

The evaluation of the matrix element in Eq. (6) involves the evaluation of two-electron radial integrals with four radial wave functions, one of them being a continuum function. Similarly the radiative electric dipole transition probability from state $|j\rangle$ to a lower state $|k\rangle$ can be written as

$$A_{jk}^{r} = [4\omega_{jk}^{3}/3c^{3}(2J_{j}+1)]|\langle \gamma_{k}J_{k}||D||\gamma_{j}J_{j}\rangle|^{2}, \quad (7)$$

where $\gamma = a, \beta$ is used to designate all quantum numbers other than J, and D is the electric dipole operator for the electromagnetic interaction. When these J valued autoionization rates and radiative states are inserted into Eq. (4), with g_i equal to $(2J_i + 1)$, we obtain F_{ijk} .

The transition matrix elements in Eqs. (6) and (7) can be expressed as sums of terms involving the product of angular and radial integrals. When it is assumed that all singly excited final states $|k\rangle$ cascade freely to the ground state, a total DR rate coefficient can be calculated that is the sum of $\alpha^{DR}(i,k)$, over all levels $|i\rangle$ and $|k\rangle$. However, most published works report only total dielectronic recombination rates $\sum \alpha^{DR}(i,k)$ in which the summation extends over sublevels of the ground state configuration only and over all $|k\rangle$. When DR rate coefficients are calculated in this way, however, it is not possible to study the dynamical effect of multiplet collisional mixing on dielectronic recombination nor is it possible to determine the direct influence of DR pumping on x-ray laser gain calculations. In these situations, it is necessary to know the DR rate data to specific singly and doubly excited configurations and ultimately to each of the individual sublevel states. For these reasons, we focused our attention on the calculation of state-specific DR rate coefficient data and obtained total rates only as an optional second step.

While in some instances it is useful and important to work at either the multiplet or submultiplet level of states, which are defined by the indices $j \equiv (\gamma_j, J_j)$, in general this leads to the generation of a superabundance of atomic data and the performance of difficult many level ionization dynamic calculations for noncoronal plasmas. An alternative strategy for carrying out rate calculations is to work at the configuration state level and to determine the multiplet emissions from the configuration populations as a second step. Some of the basics of this approach are described in Ref. 26. It provides the motivation for the presentation of results in this paper. Thus, if we define $\gamma_j = a, \beta_j$, where a is an index denoting the electron configuration and β_j denotes the quantum numbers describing the angular momentum coupling of the state, then it is useful to calculate configuration branching ratios F_{abc} which are defined as follows:

$$F_{abc} = \sum_{\substack{\beta_i, \beta_j, \beta_k \\ J_i, J_j, J_k}} F_{a\beta_i J_i, b\beta_j J_j, c\beta_k J_k} \quad .$$
(8)

This definition of F_{abc} ensures, with the proper definition of ε_b , that the total DR rate calculated from F_{ijk} will agree with the same rates calculated from F_{abc} when the ground state configurations of the fluorine ion are in statistical equilibrium; namely, ε_b should be defined, in principle, by

$$e^{-\varepsilon_b/kT}F_{abc} = \sum_{\substack{\beta_i,\beta_j,\beta_k\\J_i,J_j,J_k}} F_{ijk}e^{-\varepsilon_j/kT} .$$
(9)

In general, the distribution of populations among the states of a multiplet is defined in terms of fractional populations $f_{\beta J}$ satisfying $\sum_{\beta J} f_{\beta J} = 1.^{26}$ Thus, for example, one can write

$$N_i = f^a_{\beta_i J_i} N_a \quad , \tag{10}$$

$$N_j = f^b_{\beta_j J_j} N_b , \qquad (11)$$

where, for the $2s^22p^5$ populations of the fluorinelike ion, one can assume a statistical distribution

$$f^{a}_{\beta_{i}J_{i}} = \frac{g_{i}}{\sum_{J} g_{i}} = \frac{g_{i}}{g_{a}} .$$

$$(12)$$

According to Eq. (5), however, which may be rewritten as $I(j,k) = N_j A_{jk}^r E_{jk}, N_j$ has the coronal form

$$N_{j} = N_{e} \left[\frac{4\pi \mathcal{R}}{kT} \right]^{3/2} \frac{a_{0}^{3}}{2} e^{-\varepsilon_{j}/kT} \sum_{i} \frac{N_{i}}{g_{i}} \left[\frac{F_{ijk}}{A_{jk}'} \right], \quad (13)$$

and $f_{\beta_j J_j}$ must be obtained from this equation. Since effective DR rates between multiplets must be defined in terms of the $f_{\beta_j J_j}$ by

$$\alpha^{\mathrm{DR}}(a,c) \equiv \sum_{\substack{\beta_i,\beta_k \\ J_i,J_k}} f_{\beta_i,J_i} \alpha^{\mathrm{DR}}(i,k) , \qquad (14)$$

it follows from Eqs. (8), (9), and (12) that $\alpha^{\text{DR}}(a,c)$ can be expressed in terms of F_{abc} in the same form as $\alpha^{\text{DR}}(i,k)$ was expressed in terms of F_{ijk} :

$$\alpha^{\mathrm{DR}}(a,c) = \left(\frac{4\pi\mathcal{R}}{kT}\right)^{3/2} \frac{a_0^3}{2g_a} \sum_b F_{abc} e^{-\varepsilon_b/kT}, \qquad (15)$$

where $g_a \equiv \sum_{\beta_i J_i} g_i$.

Similarly, if the emission I(b,c) between configuration

states is defined as $I(b,c) \equiv \sum_{(j,k)}' I(j,k)$, then I(b,c) may also be expressed in terms of F_{abc} when the energy splitting is ignored $(E_{jk} \rightarrow E_{bc})$ because of Eqs. (8), (9), and (12):

$$I(b,c) = N_e \left[\frac{4\pi\mathcal{R}}{kT} \right]^{3/2} a_0^3 e^{-\varepsilon_b/kT} \frac{E_{bc}}{2} \sum_a \frac{N_a}{g_a} F_{abc} . \quad (16)$$

As noted in Ref. 26, the extraction of a multiplet spectrum from a configuration spectrum requires that one know the fractional distribution $f_{\beta J}$ of populations among the multiplet states. For high enough densities, this distribution becomes a local thermodynamic equilibrium (LTE) statistical distribution. However, the underlying assumption of Eq. (3) is that the populations of the doubly excited multiplets are determined by F_{ijk} / A'_{jk} . Thus, the calculation of a satellite multiplet spectrum from configuration rate data and configuration populations will involve an iteration procedure and be more complicated than the procedure described in Ref. 26, but it should still, in principle, be doable.

For some problems, one must know how A_{ab}^{a} and A_{ab}^{r} behave as a function of Z in order to study the Z scaling of F_{abc} . Oscillator strengths or f numbers of radiative transitions are defined as

$$f_{kj}^{r} = \left[\frac{g_{j}}{g_{k}}\right] \left[\frac{m_{e}c}{8\pi^{2}e^{2}}\right] \lambda^{2} A_{jk}^{r} .$$
(17)

Because oscillator strengths and autoionization rates have similar expansions in powers of 1/Z, it is convenient by analogy to define a dimensionless f number for autoionization rates as

$$f_{ij}^{a} = \left[\frac{g_{j}}{g_{i}}\right] \left[\frac{m_{e}c}{8\pi^{2}e^{2}}\right] a_{0}^{2}A_{ji}^{a} , \qquad (18)$$

which, like f', is of order unity. λ is determined from the energy difference between the states of the transition, which scales as Z^{-2} . Thus, $Z^{-4}A'$ has a power series expansion like A^a , i.e., like f^a or f'. Therefore, the scaling of F_{abc} with Z depends on whether A^a or A' is the dominant rate. If for a range of Z, $A_{ba}^a \gg A_{bc}^r$, then F_{abc} will scale like A_{bc}^r , i.e., as Z^4 .

Figure 1 shows some of the energy level structure of the Ne-like and F-like states that was involved in our calculations. It contains only those doubly excited Ne-like states that produce the strongest six satellite lines in the F spectrum, i.e., only those transitions whose selenium F_{abc} values are greater than 5×10^{15} (s⁻¹) are shown. In order to calculate DR rate coefficients from F-like to singly excited Ne-like ions only two initial states are needed:

$$2s^2 2p^{5}(^2P)$$
 and $2s 2p^{6}(^2S)$.

These states recombine by $\Delta n \neq 0$ transitions (here Δn refers to the change of the principal quantum number of the main radiative transition) to the doubly excited neon-like states:

$$2s^{2}2p^{4}3ln'l'$$
, $2s^{2}2p^{5}3ln'l'$, $1s^{2}2p^{6}3ln'l'$,

where n' refers to the principal quantum number of the Rydberg electron. These states then stabilize by dipoleallowed radiative decay to the singly excited states,

$$2s^22p^5n''l'', 2s^2p^6n''l'',$$

the six most important of which are shown in Fig. 1. Radiative transitions involving higher multipoles are neglected in these calculations. For the initial ${}^{2}P$ state there are also $\Delta n = 0$ transitions. The autoionizing states for these transitions have configurations of the form $2s2p^{6}n'l'$, and these states stabilize by radiative decay both to the ground state $2s^22p^6$ and to lower-lying singly excited $2s^22p^5n'l'$ and $2s2p^6n''l''$ states. These transitions become energetically possible for an increasing number of Rydberg states as one moves from argon toward higher-Z ions such as selenium. Finally, we note that additional autoionization to the excited F-like states $2s^22p^43l$ and $2s^22p^53l$ was included in the calculation of F_{ijk} whenever these processes were energetically possible. As pointed out by Jacobs *et al.*,²⁷ the inclusion of these decay channels has a significant effect on the temperature where maximum equilibrium F-like abundance occurs due to a substantial reduction of the DR rates. Moreover, extreme care must be taken in calculating autoionization to excited states that lie very close and just below



FIG. 1. Energy level diagram for F-like and Ne-like states. It includes only the six doubly excited states, dielectronic captures, and radiative decays that produce the strongest satellite lines in the fluorine spectrum (with $F_{abc} > 5 \times 10^{15}$ (s⁻¹) for selenium). The autoionization and radiative transitions are numbered 1–6 and the doubly excited states are labeled with the numbers given in Table IV.

the doubly excited states because of numerical problems that can be encountered by including these open Auger channels. However, cascade autoionizations, i.e., radiative transitions to other autoionizing states were neglected in this present work since it was assumed that their effect in reducing the DR rate coefficient was small.

For $\Delta n \neq 0$ recombinations, the radiative rates A_{jk}^{r} and autoionization rates A_{jl}^{a} were calculated explicitly for $n \leq 10$ and $l \leq 6$. For states with n > 10, they were obtained by using a $1/n^{3}$ extrapolation of the $n \leq 10$ coefficients. For $\Delta n=0$, as mentioned above, autoionization becomes energetically possible for $n \geq n_0$ where n_0 varied from ion to ion $(n_0=5 \text{ for Ar}, 6 \text{ for Ti and Fe}, \text{ and}$ 7 for Se). We calculated the transition rates for $n_0 \leq n \leq 15$ and $l \leq 8$ for the $\Delta n=0$ recombinations. For states with n > 15, the radiative rates remain constant, whereas the autoionization rates can be obtained by the usual $1/n^3$ extrapolation procedure. For $\Delta n=0$ recombination, radiative decay from the Rydberg electron was found to contribute significantly to the DR rate coefficients at low temperatures.

Transition energies, radiative rates, and autoionization rates were calculated in the intermediate coupling and single configuration approximation. All autoionizing resonance states were treated as isolated, i.e., configuration interaction between autoionizing states was neglected. For each transition, the energy used was the center-ofgravity energy averaged over the multiplets of each of configuration. Continuum wave functions were calculated in the distorted wave approximation.

III. RESULTS

In this section, we will present both state-selective and total DR rate coefficients for F-like Ar, Ti, Fe, and Se and compare them with other published work. In order to make detailed gain coefficient calculations for the observed x-ray laser transitions, it is useful to average over the sublevels of the initial F-like configurations while retaining the submultiplet levels of the bound final states. Thus, one is led to begin DR rate coefficient calculations using a procedure that is midway between those given in Eqs. (3) and (14):

$$\alpha^{\mathrm{DR}}(a,k) = \sum_{\beta_i, J_i} f_{\beta_i J_i} \alpha^{\mathrm{DR}}(i,k) .$$
⁽¹⁹⁾

Again, $f_{\beta_i J_i}$ is given by Eq. (12). The summation in Eq. (3) was not actually carried out, however. Following Cowan we replaced each of the energies ε_j appearing in Eq. (3) with the center of gravity energy of each configuration b. This energy was denoted ε_b even though it will differ slightly from the average energy defined in Eq. (9). The DR rates $\alpha^{\text{DR}}(a,k)$, which are shown in Fig. 2, were obtained, therefore, from an equation like Eq. (15), except that the summation over the sublevels of the final 3p and 3s configurations were not carried out.

These rates and the ones that follow were obtained from the full and detailed calculations described in Sec. II, which included the extrapolation procedures for the autoionization rates, radiative rates, and multiplet ener-



FIG. 2. Dielectronic-recombination-rate coefficients from the ground state of F-like selenium to the observed upper $2p^{5}3p$ and lower $2p^{5}3s$ lasing levels of Ne-like selenium.

gies ε_b that were used to accurately extend the summation over *j* to high quantum numbers. The results of these summations were then assigned to lumped configuration states such as the two shown in Fig. 1.

The DR processes of Fig. 2 directly feed the five 3s and 3p states that participate in the observed lasing from Nelike selenium. An energy diagram for these states is given in Ref. 19. Figure 2 confirms the observation made in Ref. 2 that the 3p, J=2 states receive substantial population directly from the F-like ground state via dielec-



FIG. 3. Dielectronic-recombination-rate coefficients from the initial ${}^{2}P$ state of Ar⁹⁺ to the n=3 singly excited Ne-like states.



FIG. 4. Dielectronic-recombination-rate coefficients from the initial ²P state of Ti¹³⁺ to the n=3 singly excited Ne-like states.

tronic recombination. DR pumping of the lower lasing levels, on the other hand, is competitive only with the DR pumping rate into the J=0 3p state, and it is significantly smaller than the rates into the J=2, 3p states. This behavior, quantified in Fig. 2, conforms with another observation made in Ref. 2 that the gains of the $J=2\rightarrow 1$ transitions increase while that of the $J=0\rightarrow 1$ decreases slightly when the population ratio of the F-like to Ne-like ground state is increased.

When less detailed questions about the 3s-3p gain coefficients are asked, such as how the gain scales with



FIG. 6. Dielectronic-recombination-rate coefficients from the initial ${}^{2}P$ state of Se²⁵⁺ to the n=3 singly excited Ne-like states.

atomic number,¹⁸ it is often sufficient to combine the J states into configurations and to utilize the rate coefficients shown in Figs. 3–8. Configuration state calculations are justified whenever the submultiplet and multiplet states are strongly mixed collisionally. This condition is opposite to the one assumed in Ref. 18, where the gain calculations were scaled in the absence of 3p-3p collisions. These intraconfigurational collisions more evenly distribute populations among the 3p levels, and they tend to equalize the $J=2\rightarrow 1$ gains. As noted in Ref. 18, nearly identical gains have, in fact, been mea-



FIG. 5. Dielectronic-recombination-rate coefficients from the initial ${}^{2}P$ state of Fe¹⁷⁺ to the n=3 singly excited Ne-like states.



FIG. 7. Dielectronic-recombination-rate coefficients from the initial ${}^{2}S$ state of Fe¹⁷⁺ to the n=3 singly excited Ne-like states.



FIG. 8. Dielectronic-recombination-rate coefficients from the initial ${}^{2}S$ state of Se²⁵⁺ to the n=3 singly excited Ne-like states.

sured experimentally for the two $J=2\rightarrow 1$ lines, which supports the use of configuration state modeling.

Figures 3-6 show how the rate coefficients for DR from the ²P initial state into all of the n=3 excited states change as one progresses from argon to titanium, to iron, to selenium, respectively. Note that the ${}^{2}P$ rates into the $2s 2p^{6} 3l$ states tend to peak and to dominate only at low temperature, and that they peak more for the higher Zelements. In Figs. 7 and 8 we present rate coefficients to the n=3 singly excited Ne-like states of iron and selenium, respectively, for recombination from the ${}^{2}S$ initial state. It can now be seen that DR to the $2s2p^63l$ states is always higher than it is to the $2s^2 2p^5 3l$ states at temperatures where there is strong recombination to the neonlike system during ionization equilibrium. Note that recombination from the ²S state into the $2s2p^{6}3p$ and 3d states is competitive with recombination pumping into the $2s^22p^53p$ and 3d states from the ²P state. Thus, ²S recombinations should produce important cascade contributions to the pumping of the $2s^22p^53p$ and 3d states because of dipolar collisional mixing between the $2s2p^{6}3l$ and $2s^2 2p^5 3l$ states. Also note that recombination into the $2p^{5}3p$ and $2p^{5}3d$ states strengthens as one moves from Ar^{9+} to Se^{25+} while the $2p^{5}3s$ recombination remains relatively unchanged. Hence, recombination pumping will intensify as the atomic number of the plasma is increased from Z=18 to 34 in agreement with the gain calculations reported in Ref. 18. There it was found, in fact, that the 3s-3p gain peaks for elements around selenium.

To compare the calculations of this paper to those of other authors, it is necessary to add together all recombinations into the neon-like system to form a total rate for F-like to Ne-like dielectronic recombination. Comparisons will be made between total rates and between partial contributions to these rates from $\Delta n=0$ and

 $\Delta n \neq 0$ and from high and low Rydberg, intermediate state recombinations.

In Fig. 9, we compare the partial DR rate contributions from the 3lnl' configurations of Fe¹⁷⁺ and Se²⁵⁺ for total recombination from the ${}^{2}P$ state into the neonlike ion. The contributions of the partial rates that proceed through the 3/3l' and 3/4l' manifold are much stronger for Se^{25+} than for Fe^{17+} . Consequently, one infers that the DR rate coefficients converge faster for ions with higher Z values such as selenium than for lower Z elements like iron. This observation is also supported by the results reported in Ref. 21. However, one also knows that DR rates are reduced by autoionization into excited states of the recombining ion, and these transitions become much more significant for low Z ions.²⁷⁻²⁹ Since Coster-Kronig transitions such as $2p^{4}3dnl' \rightarrow 2p^{4}3lkl''$ and $2s2p^{5}3lnl' \rightarrow 2s^{2}2p^{4}3lkl''$ and $2s2p^{5}3l'kl''$ become energetically possible at lower values of n for lower-Z ions, one would expect, in fact, that partial contributions from high Rydberg states are relatively smaller for Fe^{17+} than for Se^{25+} , i.e., that DR rate coefficients converge slower for ions with higher Z values. However, as just noted, this is not true. The reason for this behavior is that the autoionization energies ε_b for selenium are larger than those for iron for the same transitions; therefore, the exponential factor in the DR rate coefficient sum has the net effect of producing relatively smaller higher Rydberg contributions for Se^{25+} than for Fe^{17+} at the same temperature.

In Figs. 10-12, we compare our DR rate coefficients for $\Delta n \neq 0$ transitions from the ²P state for Ar^{9+} , Fe^{17+} , and Se^{25+} with the calculations of Roszman²⁰ and Chen. ²¹ All of the results of Chen that are used in this paper for comparison are angular momentum averaged.



FIG. 9. Partial dielectronic-recombination-rate coefficients for $\Delta n \neq 0$ transitions for recombination from the initial ²P state of Fe¹⁷⁺ and Se²⁵⁺ by way of resonance capture through the intermediate states shown.

For both Ar^{9+} and Fe^{17+} , our rates remain higher than those of Roszman's (by 30-35 % at the peak value). On the other hand, our rates for Fe^{17+} and Se^{25+} are very close to Chen's (higher by less than 9% at the maximum value). Aside from a slight difference in the extrapolation procedures that are used to extend the doubly excited state sums to high Rydberg and high angular momentum numbers, the main differences between Roszman's calculations and ours is that (i) his is fully nonrelativistic while ours includes relativistic corrections to the energies and wave functions, and (ii) he used LS coupling, and we used intermediate coupling. Chen's calculations, on the other hand, are fully relativistic and use intermediate coupling. In addition, he includes configuration interactions among states in the same complex. Therefore, the observation that our results differ quite a bit from Roszman's while being, at the same time, in rather close agreement with Chen's is somewhat puzzling. For ions such as argon and even iron, relativity does not play an important role in the rate calculations. Nevertheless, based on the comparisons in Fig. 10, one would be led to conclude that relativity and intermediate coupling are more important than configuration interaction in the calculation of DR rates for moderate-Z ions.

If we compare $\Delta n \neq 0$ and $\Delta n = 0$ contributions to the total DR rates separately, the results are similar. To begin with, we see very different trends in each of the two cases when a comparison of our results is made with Roszman's.²⁰ While our DR rates for Ar^{9+} and Fe^{17+} are higher than Roszman's for the $\Delta n \neq 0$ transitions (see Fig. 10), for the $\Delta n = 0$ transitions, his results are much larger than ours. This is shown in Fig. 11. However, in both $\Delta n = 0$ and $\Delta n \neq 0$ cases, our DR rates are very close to Chen's and almost always higher for both Fe^{17+} and



FIG. 10. Dielectronic-recombination-rate coefficients for the $\Delta n \neq 0$ transitions for recombination from the initial ²P state of Ar⁹⁺, Fe¹⁷⁺, and Se²⁵⁺. \bullet , Ar⁹⁺ (Roszman, Ref. 20); +, Fe¹⁷⁺ (Roszman); \circ , Fe¹⁷⁺ (Chen, Ref. 21); \blacktriangledown , Se²⁵⁺ (Chen).



FIG. 11. Dielectronic-recombination-rate coefficients for the $\Delta n = 0$ transitions for recombination from the initial ²P state of Ar⁹⁺, Fe¹⁷⁺, and Se²⁵⁺. •, Ar⁹⁺ (Roszman, Ref. 20); +, Fe¹⁷⁺ (Roszman); *, Fe¹⁷⁺ (Chen, Ref. 21); \bigtriangledown , Se²⁵⁺ (Chen).

Se²⁵⁺. Since the autoionization energies are very small for the $\Delta n=0$ transitions, the DR rates peak at very low temperatures, and the DR rate coefficients become very sensitive to the autoionization energies for these low temperatures. It has been noted that the Coster-Kronig rates for $\Delta n=0$ transitions are also very sensitive to the continuum wave functions. Roszman²⁰ uses a local semiclassical exchange potential by replacing the exchange terms in



FIG. 12. Total dielectronic-recombination-rate coefficients for the $\Delta n \neq 0$ transitions from the initial ²P state of Fe¹⁷⁺. \bullet , Fe¹⁷⁺ (Roszman, Ref. 20); \odot , Fe¹⁷⁺ (Chen, Ref. 21).

		Ar ⁹⁺			Ti ¹³⁺	
Т	^{2}P	^{2}P		^{2}P	^{2}P	
(keV)	$(\Delta n = 0)$	$(\Delta n \neq 0)$	² S	$(\Delta n = 0)$	$(\Delta n \neq 0)$	² S
0.01	0.638			0.691		
0.02	3.562	0.076	0.135	3.463	0.004	0.009
0.03	5.786	0.730	1.051	6.405	0.110	0.210
0.04	6.631	2.462	2.942	8.196	0.583	0.973
0.05	6.706	5.227	5.376	8.976	1.597	2.431
0.06	6.438	8.600	7.871	9.110	3.176	4.470
0.08	5.603	15.433	12.003	8.549	7.694	9.495
0.10	4.784	20.858	14.609	7.651	13.170	14.618
0.15	3.298	27.255	16.506	5.630	25.651	23.808
0.20	2.412	27.725	15.586	4.257	33.064	27.685
0.25	1.854	26.049	13.400	3.338	36.207	28.382
0.30	1.479	23.792	12.407	2.699	36.785	27.556
0.50	0.756	15.985	7.847	1.418	30.874	21.069
0.60	0.589	13.341	6.451	1.113	27.293	18.188
0.80	0.394	9.733	4.618	0.751	21.416	13.851
1.00	0.287	7.468	3.533	0.550	17.176	10.940
1.50	0.160	4.464	2.142	0.309	10.894	6.834
2.00	0.106	3.039	1.493	0.205	7.641	4.780
3.00	0.060	1.734	0.938	0.115	4.493	2.868
4.00	0.041	1.155	0.722	0.077	3.035	2.023
5.00	0.032	0.840	0.628	0.057	2.224	1.580

TABLE I. The dielectronic-recombination-rate coefficients (in 10^{-12} cm³/sec) for Ar⁹⁺ and Ti¹³⁺ ions.

the Hartree-Fock calculations of the continuum wave function. This may somewhat explain the difference between our results and Roszman's for the $\Delta n=0$ transitions. Finally, in Fig. 12, we compare our total DR rate for

recombination from the initial ${}^{2}P$ state of Fe¹⁷⁺ with the

total rates of Roszman²⁰ and Chen.²¹ We notice that the total rates are in much better agreement with each other than the separate $\Delta n \neq 0$ and $\Delta n = 0$ contributions are, since the differences in one case compensate differences in the other. In fact, even though our total rate is again closer to Chen's than to Roszman's, all three rates tend

TABLE II. The dielectronic-recombination-rate coefficients (in 10^{-12} cm³/sec) for Fe¹⁷⁺ and Se²⁵⁺

ions.						
		Fe ¹⁷⁺			Se ²⁵⁺	
Т	^{2}P	^{2}P		${}^{2}P$	${}^{2}P$	
(keV)	$(\Delta n = 0)$	$(\Delta n \neq 0)$	² S	$(\Delta n = 0)$	$(\Delta n \neq 0)$	² S
0.01	6.748			12.631		
0.02	8.067			16.531		
0.03	9.202	0.011	0.024	16.718		
0.04	10.327	0.109	0.217	17.709	0.001	0.003
0.05	10.984	0.438	0.788	19.162	0.012	0.030
0.06	11.185	1.098	1.825	20.497	0.060	0.135
0.08	10.757	3.427	5.094	22.012	0.439	0.843
0.10	9.870	6.804	9.313	22.133	1.398	2.425
0.15	7.585	17.256	20.150	19.712	6.054	9.107
0.20	5.883	26.900	28.165	16.612	12.089	16.815
0.25	4.698	33.932	32.844	13.950	18.066	23.774
0.30	3.835	38.317	35.028	11.826	23.370	29.461
0.50	2.063	40.819	32.947	6.847	35.922	40.507
0.60	1.628	38.506	30.072	5.506	38.074	41.489
0.80	1.108	32.860	24.606	3.835	38.174	39.706
1.00	0.815	27.755	20.257	2.862	35.814	36.155
1.50	0.460	18.891	13.319	1.648	28.308	27.406
2.00	0.306	13.735	9.516	1.111	22.277	21.102
3.00	0.171	8.375	5.702	0.636	14.745	13.661
4.00	0.114	5.760	3.887	0.436	10.584	9.696
5.00	0.084	4.267	2.865	0.333	8.054	7.333

to have the same temperature behavior for temperatures greater than 200 eV, even while Roszman's rate always remains below the other two in value.

In Figs. 9-12 we made comparisons of total DR rates specifically from the ²P state of Ar⁹⁺, Fe¹⁷⁺, and Se²⁵⁺. Similar comparisons of the total rate from the ²S state can be made for these ions. We found that differences in the three ²S calculations were similar to those found in the ²P, $\Delta n \neq 0$ case. The data for making such detailed comparisons are listed in Tables I and II. In addition to the ²S data, these tables include data for $\Delta n=0$ and $\Delta n \neq 0$ recombinations from the ²P state for all four ions including Ti¹³⁺ in the temperature range $0.02 \leq T \leq 5$ keV.

IV. Z SCALING

The DR branching ratios defined in Eq. (8) are useful in rate equation calculations that involve only singly excited configuration states. The main features of the satellite spectrum (less the multiplet structure) can be inferred from Eq. (16) with N_a being provided by the rate equation calculation. The underlying assumption of the overall calculation is that the doubly excited submultiplet populations are not mixed collisionally, but that they are to be calculated from Eq. (13).

On the other hand, if one wanted to investigate the dynamics of the doubly excited configurations on the same footing as that of the singly excited states, and at higher plasma densities where the coronal approximation breaks down, then one would need to define autoionization and radiation rate coefficients that take into account the collisional mixing of the closely spaced, doubly excited, multiplet states. In this case, configuration-averaged transition rates A_{ba}^{a} and A_{bc}^{r} , would be defined in the conventional way:²³

$$A^{a}_{ba} \equiv \sum_{\beta_{j}J_{j},\beta_{j}J_{j}} f_{\beta_{j}J_{j}} A^{a}_{ji} , \qquad (20)$$

$$A_{bc}^{r} \equiv \sum_{\beta_{j}J_{j},\beta_{k}J_{k}} f_{\beta_{j}J_{j}} A_{jk}^{r} , \qquad (21)$$

where $f_{\beta J}$ would have the value

$$f_{\beta,J} \cong g_j / g_b , \qquad (22)$$

rather than the value that would be inferred from Eq. (13). One could then set up rate equations for the populations N_b utilizing these rates. They would be identical in form to those for N_j . Because of this form identity, Eqs. (15) and (16) would be derived directly from the rate equations for N_b , i.e., Eq. (22) will guarantee that the rate for dielectronic recombination from state a into b detail balances with A_{ba}^a in the same way that DR from i to j detail balances with A_{ju}^a . In this case, however, F_{abc} would be given by

$$F_{abc} = \frac{g_b A^a_{ba} A^r_{bc}}{\sum_{a'} A^a_{ba'} + \sum_{c'} A^r_{bc'}} .$$
(23)

Cowan comments in Ref. 23 (p. 557) that there is no



FIG. 13. Variation of autoionization f numbers as a function of Z. The six DR channels shown in this figure are those shown in Fig. 1 and are labeled correspondingly. The curves are three-parameter fits to the four calculated points shown for Ar^{8+} , Ti^{12+} , Fe^{16+} , and Se^{24+} ions.

reason to expect the two methods of calculating F_{abc} , which are given by Eqs. (8) and (23), to agree. However, one would expect the difference between them to be minimized if the value for $f_{\beta_i J_i}$ that is obtained from Eq. (13) were to be used to define the rates rather than Eq. (22).



FIG. 14. Variation of oscillator strengths as a function of Z. The six radiative decays represented in this figure are those shown in Fig. 1 and are labeled correspondingly. The curves are three parameter fits to the four calculated points shown for Ar^{8+} , Ti^{12+} , Fe^{16+} , and Se^{24+} ions.



FIG. 15. Variation of the energies of the six doubly excited states that are shown and labeled in Fig. 1 as a function of Z. The curves are three-parameter fits to the four calculated points shown of Ar^{8+} , Ti^{12+} , Fe^{16+} , and Se^{24+} ions.

The problem of scaling F_{abc} with atomic number is also different depending on whether F_{abc} is obtained from Eq. (8) or from Eq. (23). For dielectronic recombination from fluorinelike to neonlike ions, there are roughly 22 dominant channels (i.e., dominant F_{abc} 's) through which recombination occurs from the ground ²P state (a=1), and 17 dominant channels through which it occurs from the ²S excited state (a=2). From a rate equation point of

 TABLE III. Scaling coefficients for energies of singly excited

 Ne-like and F-like ground and first excited states.

с	State	b [*] ₀	b *	<i>b</i> [*] ₂
1	$2s^2 2p^5 3s$	1.898	-23.76	64.65
2	$2s^2 2p^5 3p$	1.928	-22.91	57.80
3	$2s^{2}2p^{5}3d$	1.943	-20.89	40.08
4	$2s2p^63s$	2.013	-21.93	72.17
5	$2s2p^{6}3p$	2.043	-21.15	65.86
6	$2s2p^{6}3d$	2.059	-19.21	49.12
7	$2s^{2}2p^{5}4l$	2.612	-32.34	85.21
8	$2s2p^{6}4l$	3.045	-39.37	189.7
9	$2s^2 2p^5 nl, n > 4$	3.167	-48.61	280.5
10	$2s^2 2p^5$	3.467	-47.13	147.9
11	2s 2p ⁶	0.1161	1.609	10.15

view for the doubly excited states, the scaling of F_{abc} , $\alpha^{\text{DR}}(a,c)$, and I(b,c) would be accomplished indirectly through the scaling of A_{bc}^r , A_{ba}^a , and ε_b . In turn, A^r and A^a will depend on Z through the energies ε_b and ε_c and the oscillator strengths f_{cb}^r and f_{ab}^a , which are defined by Eqs. (17) and (18) with a change of indices. We found that the variation of these latter quantities is well described by the following three term expansions:

$$f_{ab}^{a} \simeq (b_{0}^{a} + b_{1}^{a}/Z + b_{2}^{a}/Z^{2})_{ab} , \qquad (24)$$

$$f_{cb}^{\prime} \simeq (b_0^{\prime} + b_1^{\prime} / Z + b_2^{\prime} / Z^2)_{cb} , \qquad (25)$$

$$\varepsilon_b = Z^2 (b_0^{**} + b_1^{**} / Z + b_2^{**} / Z^2)_b , \qquad (26)$$

$$\varepsilon_{c} = Z^{2} (b_{0}^{*} + b_{1}^{*} / Z + b_{2}^{*} / Z^{2})_{c} , \qquad (27)$$

[where Eqs. (26) and (27) are in units of eV] for atomic

 b_{1}^{**} b_{2}^{**} b b** State $2s2p^{6}nl, n = 5, 10$ -0.234610.96 -64.431 $2p^{4}3s3p$ -32.692 0.3575 2.175 3 $2p^4 3s 3d$ 0.3738 4.083 -47.51 $2p^4 3p 3d$ 4 0.4037 4.827 -52.75 $2p^4 3d^2$ 5 0.4219 6.652 -67.22 $2p^{5}3s3p$ 0.4739 3.246 -19.206 7 $2p^{5}3p^{2}$ 0.5038 4.058 -24.578 $2p^{5}3p3d$ 5.749 -37.98 0.5216 9 $2p^{5}3d^{2}$ 0.5402 7.537 -52.08 $2p^{4}3s4l$ 10 1.043 -6.709 -8.48111 $2p^43p4l$ 1.065 -6.621-6.13512 2p⁴3d4l 1.092 -4.455-24.0713 $2p^{5}3s4l$ 1.157 -5.5914.508 14 $2p^{5}3p4l$ 0.8758 10.15 -148.815 $2p^{5}3d4l$ 1.209 -3.525-9.4072p⁶3p4l -3.30116 1.306 13.39 $2p^{4}3snl, n > 4$ 17 1.497 -14.1820.61 $2p^{4}3pnl, n > 4$ 18 1.524 -13.8320.57 19 $2p^{4}3dnl, n > 4$ 1.547 -12.046.697 $2p^{5}3snl, n > 4$ 20 1.950 -33.06281.2 21 $2p^{5}3pnl, n > 4$ 1.645 -12.6732.89 22 $2p^{5}3dnl, n > 4$ 1.999 -30.90266.6

TABLE IV. Scaling coefficients for energies of doubly excited Ne-like states.

numbers between argon and krypton: $18 \le Z \le 36$. Figures 13–15 display, for example, the three-parameter, least-squares fits to the oscillator strengths and doubly excited energies of the six DR channels that are displayed in Fig. 1. They also contain the Ar^{9+} , Ti^{13+} , Fe^{17+} , and Se^{25+} data points from which the curves were calculated. In general, the points fall on the curves with better than a few percent accuracy, but, as in most numerical calculations, there are exceptions to the rule as can be seen in Fig. 13. In such cases, one expects that the least-squares fit will reduce the error that is present in the original calculation.

The complete set of scaling coefficients $\{b_i^a\}, \{b_i^r\}, \{b_i^{**}\}, and \{b_i^*\}$ that were determined from the four Ar, Ti, Fe, and Se databases are listed in Tables III–V. The 18 dielectronic recombinations from the ground state and the 8 from the excited state, whose autoionization coefficients are listed in Table V, produce the dominant DR channels when they are coupled to the 35 radiative

decays whose coefficients are also given in Table V. In other words, when recombinations through these channels are added together, they constitute more than 95% of the total DR transition rate from the fluorinelike to the neonlike ion. These recombinations proceed through the 22 doubly excited states whose configurations are identified and numbered in Table IV. The energies of these states, together with the energy of the $2s2p^6$ excited state of the fluorinelike ion (which is given by the last entry in Table III), are measured from the ground $2s^2 2p^5$ state. The ionization energy of this state above the neonlike ground state is given by the 10th entry in Table III. The recombinations terminate on the nine singly excited states, which are labeled and numbered in Table III. The energies of these states are measured from the ground state of the neonlike ion.

A different scaling problem arises when F_{abc} is computed from F_{ijk} using Eq. (8). In this case, F_{abc} must be scaled directly, and its Z behavior is dependent on the

TABLE V. Scaling coefficients for radiative and autoionization f numbers for transitions from state b to states c and a, respectively.

-								
a ^a	Ь	с	b '_0	<i>b</i> ′ ₁	<i>b</i> ['] ₂	b ^a ₀	<i>b</i> ^{<i>a</i>} ₁	b ^{<i>a</i>} ₂
1	1	8	1.942	-102.8	1571.0	0.1634	18.00	-330.6
1	1	9	0.2854	-16.36	279.2			
1	2	2	0.1040	0.002	13.42	0.030 67	0.1983	- 8.098
1	3	1	-0.0778	130.4	-1610.0	0.007 283	-0.09177	1.405
1	4	2	3.185	6.887	-442.0	0.3382	-1.223	- 53.99
1	5	3	2.880	4.800	-382.1	0.6461	-4.298	-76.85
1	6	1	0.9634	-12.97	50.86	0.039 65	0.3894	-12.74
1	10	1	-0.6414	50.52	-493.2	0.012 65	-0.01638	- 1.546
1	11	2	0.5513	6.287	-93.35	0.1144	0.3310	-28.60
1	12	3	1.055	-18.58	163.3	0.6282	-4.767	-63.38
1	12	7	3.193	4.722	-368.6			
1	13	1	0.1087	2.688	-40.68	0.057 29	-0.063 66	-10.74
1	13	8	0.1278	-4.121	44.40			
1	14	7	0.9580	-14.81	77.88	0.037 42	-0.4439	-1.192
1	15	8	1.061	-3.362	-26.93	0.1221	-1.098	-10.45
1	17	9	0.2118	-6.342	109.0	0.011 35	-0.01225	-1.467
1	18	2	0.3403	4.659	-49.11	0.1040	0.2543	-24.93
1	19	3	1.403	-23.98	88.13	0.6513	-6.296	-46.10
1	19	9	3.736	-41.32	532.4			
1	20	8	0.3071	-14.43	174.9	0.087 33	-2.522	21.19
1	21	9	0.8178	-9.846	89.84	0.035 32	-0.2443	-4.470
1	22	8	4.993	-227.0	2777.0	0.043 21	-0.05812	-7.229
2	7	2	0.6347	-2.965	-40.81	0.1414	1.517	-47.15
2	8	3	0.7969	-14.00	108.4	0.4071	-1.586	-63.21
2	8	5	3.409	79.06	-1534.0			
2	9	6	3.440	7.536	-473.6	0.7757	-4.762	-96.57
2	14	2	0.2346	-2.883	6.365	0.2435	1.544	-72.97
2	14	5	1.525	-17.22	86.01			
2	15	3	0.2646	-3.933	18.83	0.7295	-4.241	-92.88
2	15	6	1.245	-18.09	126.2			
2	16	8	0.1101	-1.202	4.03	0.019 14	-0.2495	-0.236
2	21	2	0.2901	-5.348	28.0	0.2334	1.049	-63.65
2	21	5	1.066	4.291	-228.8			
2	22	3	0.4141	-9.868	66.96	0.3980	-3.334	-25.17
2	22	6	1.869	-47.78	390.5			

^a1 and 2 stand for the ground and the first excited states of fluorinelike ions.

relative strength of A^a and A^r . When $A^a \gg A^r$, $F_{abc} \sim A^r \sim Z^4(b_0^r + b_1^r/Z + \cdots)$; whereas, when $A^r \gg A^a$, $F_{abc} \sim A^a \sim b_0^a + b_1^a/Z + \cdots$. In order to accommodate both kinds of behavior, we found it convenient to express F_{abc} as the following four-coefficient polynomial:

$$F_{abc} = Z^{2} (b_{0}^{F} + b_{1}^{F} / Z + b_{2}^{F} / Z^{2} + b_{3}^{F} / Z^{3}) 10^{14}$$
(28)

(in units of sec⁻¹). The four coefficients were determined from the four calculated values of F_{abc} for Ar^{9+} , Ti^{13+} , Fe^{17+} , and Se^{25+} . These coefficients are presented in Table VI. They constitute the 39 dominant DR channels that combine to give 95% or more of the total DR rate for recombination between the F- and Ne-like ions.

Because Eq. (28) is not a least-squares fit, it reproduces the calculated Ar^{9+} , Ti^{13+} , Fe^{17+} , and Se^{25+} points when

Z=18, 22, 26, and 34, respectively. There are, however, three exceptions to this rule that are shown in Figs. 16 and 17. These figures illustrate several points. On one hand, all of the curves that are calculated from Eq. (28) using the coefficients in Table VI have the same smooth shapes as do the curves shown in Figs. 16 and 17. In each of the 36 nonexceptional cases, therefore, the argon, titanium, iron, and selenium points that were calculated give rise to smooth interpolations of the kind shown in Figs. 16 and 17. On the other hand, of the 39×4 calculated F_{abc} , only the one argon and the two titanium points shown in Figs. 16 and 17 were irregular and fell off of the smooth interpolating curves that are defined by the other nine points. Because similar behavior is seen in Figs. 13 and 14, one might conclude that the three anomalous points are the result of numerical error.

TABLE VI. Scaling coefficients for the DR branching ratios F_{abc} . Numbers in square brackets denote powers of 10.

-						
a	b	с	b ^F ₀	b ^F ₁	<i>b</i> ^{<i>F</i>} ₂	<i>b</i> ^{<i>F</i>} ₃
1	1	8	9.064[-3]	-4.311[-1]	7.063[0]	-3.972[1]
1	1	9	1.037[-2]	-5.610[-1]	1.183[1]	- 8.476[1]
1	2	2	7.526[-3]	-3.042[-1]	4.365[0]	-2.215[1]
1	3	1	-2.500[-2]	1.785[0]	-3.344[1]	1.864[2]
1	4	2	2.117[-1]	-6.629[0]	5.253[1]	2.102[1]
1	5	3	4.360[-1]	-1.703[1]	2.244[2]	-9.775[2]
1	6	1	1.141[-2]	-1.243[-1]	- 5.279[0]	7.330[1]
1	10	1	3.057[-3]	-2.821[-1]	9.033[0]	- 8.374[1]
1	11	2	8.172[-2]	-2.843[0]	3.132[1]	-9.713[1]
1	12	3	6.772[-2]	-1.787[0]	9.545[0]	4.109[1]
1	12	7	7.907[-2]	1.770[1]	-6.374[2]	5.533[3]
1	13	1	1.022[-2]	-4.545[-1]	7.005[0]	- 3.697[1]
1	13	8	9.498[-3]	-1.244[-1]	-3.063[0]	4.544[1]
1	14	7	-1.879[-2]	2.783[0]	-7.490[1]	5.778[2]
1	15	8	8.675[-3]	1.525[0]	-6.015[1]	5.524[2]
1	17	9	-4.993[-3]	8.364[-1]	-1.872[1]	1.233[2]
1	18	2	5.235[-2]	-1.267[0]	1.986[0]	9.011[1]
1	19	3	-2.605[-2]	4.129[0]	-1.146[2]	8.955[2]
1	19	9	-1.021[0]	1.024[2]	-2.468[3]	1.782[4]
1	20	8	6.741[-2]	-4.252[0]	9.178[1]	-6.670[2]
1	21	9	-1.603[-1]	1.294[1]	-2.939[2]	2.066[3]
1	22	8	9.452[-2]	-5.565[0]	1.135[2]	-7.865[2]
2	7	2	2.638[-2]	-7.598[-1]	4.703[0]	1.542[1]
2	8	3	7.806[-2]	- 3.999[0]	7.310[1]	-4.654[2]
2	8	5	7.768[-2]	-2.961[0]	3.627[1]	-1.338[2]
2	9	6	1.117[-1]	-3.531[0]	2.817[1]	1.267[1]
2	14	2	1.295[-2]	-5.664[-1]	9.193[0]	- 5.493[1]
2	14	5	1.128[-2]	-1.512[-1]	-3.026[0]	4.403[1]
2	14	7	-6.545[-2]	7.592[0]	-2.060[2]	1.664[3]
2	15	3	-9.406[-3]	1.309[0]	-3.726[1]	3.066[2]
2	15	6	8.753[-3]	4.098[-1]	-2.035[1]	1.917[2]
2	15	8	2.879[-2]	5.182[0]	-1.892[2]	1.635[3]
2	16	8	-3.762[-3]	6.047[-1]	-1.714[1]	1.384[2]
2	21	2	2.019[-3]	1.277[-1]	-6.024[0]	5.560[1]
2	21	5	-1.533[-2]	1.534[0]	-4.033[1]	3.188[2]
2	21	9	-8.895[-2]	9.723[0]	-2.503[2]	1.903[3]
2	22	3	-9.053[-3]	1.330[0]	- 3.979[1]	3.385[2]
2	22	6	6.393[-2]	-3.901[0]	8.365[1]	-6.138[2]
2	22	8	4.420[-1]	-2.619[1]	5.475[2]	- 3.911[3]



FIG. 16. Four-parameter polynomial curves for $F_{1,21,9}$ and $F_{1,22,8}$ are shown corresponding to the coefficients listed in Table VI. The four points shown for Ar^{9+} , Ti^{12+} , Fe^{16+} , and Se^{24+} were calculated.

V. SUMMARY

A number of important problems arise when formulating ionization dynamic calculations in the L shell of moderate-Z elements. One concerns the reliability and scalability of the atomic data that is used in the calculations. Another concerns the number of states to be utilized and the amount of atomic data to be generated to couple these states. One way to judge the reliability of



FIG. 17. Four-parameter polynomial curves for $F_{2,21,9}$ are shown corresponding to the coefficients listed in Table VI. The four points shown for Ar^{9+} , Ti^{12+} , Fe^{16+} , and Se^{24+} were calculated.

calculated data is to compare it, where possible, to the calculations of other researchers. Equally important, data for one element should be compared to data in the same isoelectronic sequence of other elements. These procedures have been successfully used in the past to calculate atomic energies, oscillator strengths, collision strengths, and photoionization cross sections. In this paper, we have extended these procedures to dielectronic recombination.

The kind of DR data that is needed depends on the problem under consideration. When the main problem is to determine the ionization balance and radiation loss rates of L-shell ionization stages, one can use configuration-averaged states in rate equation calculations as the most straightforward generalization of the average atom approach. One can then compute multiplet spectra and multiplet opacities as a supplemental step in the calculation.²⁶ X-ray laser calculations can also be carried out at this level of state simplification. Although they provide only average gain information, they allow detailed radiative hydrodynamics calculations to be carried out with a considerable savings in computer time. The atomic data we presented in this paper is geared to this approach. More detailed x-ray laser modeling requires more detailed atomic state structure. The reliability of the atomic data in this case can be checked against the configuration averaged data. Compare Figs. 2 and 6.

The results of our calculations for partial and total DR rate coefficients of val calculations for partial and total DR rate coefficients were compared with Roszman's²⁰ HF calculations for Fe^{17+} and Ar^{9+} and with Chen's²¹ fully relativistic calculations for Fe^{17+} and Se^{25+} . In all three calculations radiative cascades were neglected, i.e., radiative decays to states which are above the ionization limit and thus autoionize or again decay radiatively to a stable state. These cascades generally reduce the total DR rate coefficients by only a few percent.^{30,31} Lagatutta,³² however, has shown that radiative cascades have more pronounced effects on some ions than others in the same isoelectronic sequence. For example, when we included a few radiative channels just above the ionization limit in the Ar^{9+} calculation, it made a noticeable difference in some DR rate coefficients. The main differences between the three calculations appear to be in their inclusion or not of relativistic effects, intermediate angular momentum coupling, or configuration interactions. Chen's²¹ calculation included configuration interaction (CI) among the resonance states in the same complex; both the present calculation and Roszman's²⁰ calculation neglect such CI effects. These effects are expected to be small,²⁵ however. It has also been shown³³ that, even though configuration interactions have an important effect on DR rate coefficients for individual autoionizing states, their contribution to the total DR rate is quite small. This finding is also somewhat verified by the fact that our results for Fe^{17+} and Se^{25+} agree so well with Chen's. In fact, our results for the total DR rate, whenever compared, are much closer to Chen's than to Roszman's. This can be seen most clearly for Fe^{17+} where all three calculations can be compared. In trying to measure the effect of relativistic correction, we computed the DR rate roefficients for a few resonance states for Fe¹⁷⁺ using only the HF (no relativistic correction) method of Cowan. For the few cases that we tested, the effect was not significant. Thus the agreement between Chen's calculation and ours, in this case where relativity does not play an important role, gives us confidence in the atomic model that was used in this present work. Moreover, a difference in atomic models may be partly responsible for the differences in Rosman's and our total DR rate coefficients, since our calculation and Chen's were done using intermediate coupling, whereas Roszman used an LS coupled scheme.

We found generally that F-like DR data scales smoothly with atomic number between argon and krypton. Doubly and singly excited state energies, autoionization and radiative decay f numbers, and DR branching ratios all varied smoothly from one element to another. Except in a few cases, mostly in titanium, numerical inaccuracies in the calculations were not discernible. Inevitably, however, numerical difficulties do arise in complex calculations. Cowan discovered, for example, that one source of numerical error occurs when the energies of two configurations become close.³⁴ Whether similar, special case errors have occurred that will account for the behavior seen in Figs. 16 and 17 or whether this behavior is physical remains to be determined.

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