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Variation of dielectronic satellite intensity factors with n for dielectronic recombination processes in selected lithium-like ions*

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Satellite intensity factors $F_2^*(\mathrm{s}\to\mathrm{f})$ have been calculated for the $1s^22s+\varepsilon l \to (1s^23l'nl'')^* \to 1s^22sml'''+h\nu$ dielectronic recombination processes of lithium-like V, Cu, Se, Ag and Ba ions. The relevant atomic parameters have been calculated explicitly for all intermediate resonance states $|\mathrm{s}\rangle \equiv |1s^23l'nl''SLJ\rangle$ with n=3–9 in the intermediate coupling scheme. The $1/n^3$ scaling, which has often been used in extrapolating $F^*(\mathrm{s}\to\mathrm{f})$ for $n \geq 4$, is tested against these values of $F_2^*(\mathrm{s}\to\mathrm{f})$.

Keywords: lithium-like ions, dielectronic recombination, satellite intensity factor
PACC: 3480D, 3280D, 3250H

Dielectronic recombination (DR) is the dominant electron–ion recombination channel in low-density high-temperature plasmas. Knowledge of DR rate coefficients is necessary for the understanding of astrophysical plasmas, for the development and diagnostics of laboratory fusion plasmas, and in connection with x-ray laser research.[1−4] As a consequence, there has been intense interest in computing DR rate coefficients in the past ten or more years. Computations have been performed, employing different atomic models.[5−8] But these calculations have been limited, however, to low-lying resonance states. It is very necessary to estimate approximately the satellite intensity factors in the measurement of the DR satellite spectrum.

Dielectronic recombination is a two-step resonant process. In the first step, an ion captures a free electron with simultaneous excitation of one of its electrons to a higher orbit. The resulting doubly-excited autoionizing state emits a photon and ends up in a low-lying state which is stable against autoionization. For lithium-like ions this process can be schematically represented as

$$1s^4 2s + \varepsilon l \to (1s^2 3l'nl'')^* \to 1s^2 2sml'' + h\nu. \quad (1)$$

Here the incoming free electron εl loses energy as it excites the 2s electron of the lithium-like ion in the initial state $|l\rangle \equiv 1s^22s\ {}^2S_{1/2}\rangle$ to either $3l'$ or nl'' orbits, and is itself captured to form the doubly-excited resonance state $|\mathrm{s}\rangle \equiv |1s^23l'nl''SLJ\rangle$. The state $|\mathrm{s}\rangle$ may now autoionize, re-emitting the electron, or it may decay radiatively to a lower energy state $|\mathrm{f}\rangle \equiv |1s^22snl''S'L'J'\rangle$. The former process represents the resonant electron–ion scattering, and the latter is the DR if the final state $|\mathrm{f}\rangle$ lies sufficiently low in energy and cannot autoionize.

Assuming a Maxwellian electron energy distribution, DR rate coefficients can be expressed as[10]

$$\alpha^{\mathrm{DR}}(\mathrm{s}\to\mathrm{f}) = \frac{1}{2}(2\pi\hbar^2/mkT_\mathrm{e})^{3/2} F_2^*(\mathrm{s}\to\mathrm{f}) \mathrm{e}^{-(\Delta E_{si}/kT_\mathrm{e})}, \quad (2)$$

where $\Delta E_{si} = E_s - E_i$ is the Auger electron energy, T_e is the electron temperature, and k is the Boltzmann constant. The function $F_2^*(\mathrm{s}\to\mathrm{f})$ in Eq.(2) is called the satellite intensity factor, and is given by

$$F_2^*(\mathrm{s}\to\mathrm{f}) = \frac{(2J_s+1)}{(2J_i+1)} \frac{\Gamma_a(\mathrm{s}\to i)\Gamma_r(\mathrm{s}\to\mathrm{f})}{\Gamma(\mathrm{s})}. \quad (3)$$

Here J_s and J_i are, respectively, the total angular momentum quantum numbers of the autoionizing states $|\mathrm{s}\rangle$ and the initial $|i\rangle$; $\Gamma_a(\mathrm{s}\to i)$ is the rate of autoionization of the state $|\mathrm{s}\rangle$; $\Gamma_r(\mathrm{s}\to\mathrm{f})$ is the rate for

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radiative transition; and $\Gamma(\mathrm{s})$ is the total decay rate for the state $|\mathrm{s}\rangle$ in all possible radiative and autoionizing channels.

There is an enormous number of intermediate resonance states $|\mathrm{s}\rangle$, hence the calculation of $F_2^*(\mathrm{s–f})$ for each possible $|\mathrm{s}\rangle$ using Eq.(3) is not practicable. Explicit calculations of satellite intensity factors and DR rate coefficients[3,4,10,11] have consequently been limited so far only to low-lying resonance states. An approximate $1/n^3$ scaling law, where n is the principal quantum number of the outermost occupied shell of the resonance state, has generally been used to extrapolate satellite intensity factors for higher ($n \geq 4$) resonance. As for large n states, the radiative rates do not change appreciably whereas the Auger transition rates decrease approximately as $1/n^3$. In this approximation, the satellite intensity factor $F_2^*(\mathrm{s–f})$ for a state $|\mathrm{s}\rangle$ of the $1\mathrm{s}2lml$ manifold is related to the intensity factor $F_2^*(\mathrm{s–f})$ of the $1\mathrm{s}2lnl$ manifold by

$$F_s^*(\mathrm{s}_m - \mathrm{f}) = (n/m)^3 F_2^*(\mathrm{s}_n - \mathrm{f}). \qquad (4)$$

The above approximation has been widely used in the literature, but has never been tested for large n against explicitly calculated values. The satellite intensity factors generally decrease with n, but we know little about the actual rate of convergence. The $1/n^3$ scaling law is supposed to be satisfactory only for large n, however, no serious quantitative analysis of this "largeness" has so far been attempted. We also note that, as n increases, the wavelengths of the satellite lines $1\mathrm{s}^2 3lnl' \rightarrow 1\mathrm{s}^2 2snl'$ approach the wavelengths of the resonance lines $1\mathrm{s}^2 3l \rightarrow 1s^2 2\mathrm{s}$. The experimental resolution is not usually sufficient to resolve the satellite lines originating from the high-lying resonance states. The $1/n^3$ approximation has been used to determine the "true" intensity of the resonance line, since the ratios of intensities of the satellite to resonance lines have important diagnostic applications.

The purpose of this paper is to report on the variations of satellite intensity factors with n for a few selected lithium-like ions for n=3–9 and to test the validity of the $1/n^3$ scaling approximation by comparing $F_2^*(\mathrm{s–f})$ functions from Eq.(4) with the explicitly calculated values.

We have employed the Hartree–Fock atomic model to generate the one-electron orbital. The antisymmetric configuration state functions $|i\rangle$ are constructed using Fano's ansatz.[12] Initial and final atomic states are expressed as a linear combination of $|i\rangle$ with the same J and parity. The x-ray and Auger transition rates for all possible channels are calculated numerically.

In Table 1 we list the satellite intensity factors $F_2^*(\mathrm{s–f})$ of a few selected satellite lines which originate from the DR process $1\mathrm{s}^2 2\mathrm{s} + \varepsilon l \rightarrow (1\mathrm{s}^2 3l'nl'')^* \rightarrow 1\mathrm{s}^2 2sml''' + h\nu$ as a function of n. The lithium-like ions considered in this table are of atomic numbers Z=23, 29, 34, 47 and 56. A complete list of $F_2^*(\mathrm{s–f})$ and the corresponding wavelengths of all possible satellites for lithium-like ions with $3 \leq n \leq 9$ and Z=23, 29, 34, 47 and 56 are being prepared for publication. According to $1/n^3$ scaling, $n^3 F_2^*(\mathrm{s–f})$ for each transition should approach a constant value as n increases. We have plotted $n^3 F_2^*(\mathrm{s–f})$ as a function of n in Fig.1 for several transitions of lithium-like vanadium. Figures 2 and 3 show the variation of a selected transition with n and the atomic number. The data in Table 1 and the curves of Figs.1–3 clearly suggest that the $1/n^3$ scaling is appropriate only after $n \approx 9$ for middle-Z elements, and after $n \approx 5$ for high-Z elements. The $1/n^3$ scaling law is the most appropriate for Z=29.

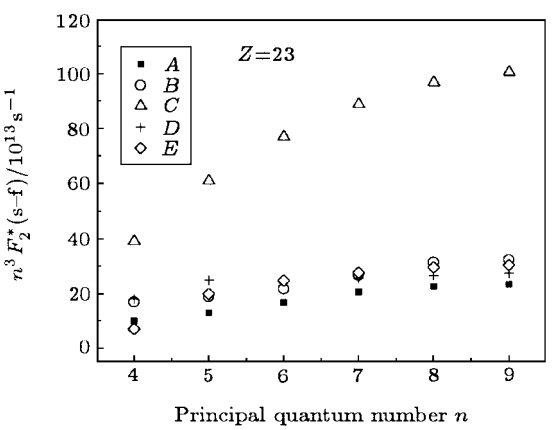


Fig.1. Satellite intensity factors multiplied by n^3 versus n for several selected transitions of Li-like vanadium. The lines are designated by the following notations: A, $1\mathrm{s}^2 3\mathrm{p}nd\ (^3\mathrm{F}_2) \rightarrow 1\mathrm{s}^2 2\mathrm{s}nd\ (^3\mathrm{D}_1)$; B, $1\mathrm{s}^2 3\mathrm{p}nd\ (^3\mathrm{F}_3) \rightarrow 1\mathrm{s}^2 2\mathrm{s}nd\ (^3\mathrm{D}_2)$; C, $1\mathrm{s}^2 3\mathrm{p}nd\ (^3\mathrm{F}_4) \rightarrow 1\mathrm{s}^2 2\mathrm{s}nd\ (^3\mathrm{D}_3)$; D, $1\mathrm{s}^2 3\mathrm{p}nd\ (^3\mathrm{P}_1) \rightarrow 1\mathrm{s}^2 2\mathrm{s}nd\ (^3\mathrm{D}_2)$; E, $1\mathrm{s}^2 3\mathrm{p}nd\ (^3\mathrm{P}_2) \rightarrow 1\mathrm{s}^2 2\mathrm{s}nd\ (^3\mathrm{D}_3)$.

Table 1. The satellite intensity factors F_2^*(s–f) in units of $10^{11}s^{-1}$ for a few prominent satellite lines of lithium-like ions with Z=23, 29, 34, 47 and 56. Dielectronic recombination is achieved for these satellite lines via the intermediate resonance states $|1s^2 3pnd SLJ\rangle$.

Transition	n=3	n=4	n=5	n=6	n=7	n=8	n=9
			Z=23				
$1s^2 3pnd(^3F_2) \rightarrow 1s^2 2snd(^3D_1)$	0.695	16.3	10.9	7.95	6.04	4.49	3.34
$1s^2 3pnd(^3F_3) \rightarrow 1s^2 2snd(^3D_2)$	7.93	26.2	15.0	10.1	8.01	6.30	4.53
$1s^2 3pnd(^3F_4) \rightarrow 1s^2 2snd(^3D_3)$	20.9	60.2	48.7	35.8	26.0	18.9	13.9
$1s^2 3pnd(^1P_1) \rightarrow 1s^2 2snd(^1D_2)$	107	106	91.9	79.5	69.7	61.5	54.7
$1s^2 3pnd(^3P_1) \rightarrow 1s^2 2snd(^3D_2)$	10.3	28.6	19.8	11.6	7.46	5.20	3.88
$1s^2 3pnd(^3P_2) \rightarrow 1s^2 2snd(^3D_3)$	10.6	10.1	15.9	11.6	8.15	5.93	4.25
			Z=29				
$1s^2 3pnd(^3F_2) \rightarrow 1s^2 2snd(^3D_1)$	1.89	21.5	19.3	13.6	9.16	6.24	4.36
$1s^2 3pnd(^3F_3) \rightarrow 1s^2 2snd(^3D_2)$	2.03	33.2	22.6	15.2	10.3	7.22	5.20
$1s^2 3pnd(^3F_4) \rightarrow 1s^2 2snd(^3D_3)$	64.4	120	91.3	60.9	40.2	26.9	18.6
$1s^2 3pnd(^1P_1) \rightarrow 1s^2 2snd(^1D_2)$	233	235	201	169	142	118	99.3
$1s^2 3pnd(^3P_1) \rightarrow 1s^2 2snd(^3D_2)$	8.68	34.6	21.6	13.5	9.15	6.56	4.94
$1s^2 3pnd(^3P_2) \rightarrow 1s^2 2snd(^3D_3)$	8.05	8.37	13.8	11.5	8.79	6.70	5.20
			Z=34				
$1s^2 3pnd(^3F_2) \rightarrow 1s^2 2snd(^3D_1)$	2.57	32.3	25.9	16.9	10.8	7.10	4.83
$1s^2 3pnd(^3F_3) \rightarrow 1s^2 2snd(^3D_2)$	87.6	45.0	24.8	14.6	9.03	5.90	4.05
$1s^2 3pnd(^3F_4) \rightarrow 1s^2 2snd(^3D_3)$	93.5	166	122	76.7	48.0	31.0	20.8
$1s^2 3pnd(^1P_1) \rightarrow 1s^2 2snd(^1D_2)$	336	370	315	257	206	165	133
$1s^2 3pnd(^3P_1) \rightarrow 1s^2 2snd(^3D_2)$	8.01	32.4	22.0	14.8	10.4	7.53	5.70
$1s^2 3pnd(^3P_2) \rightarrow 1s^2 2snd(^3D_3)$	7.18	6.88	12.6	11.4	9.04	7.02	5.50
			Z=47				
$1s^2 3pnd(^3F_2) \rightarrow 1s^2 2snd(^3D_1)$	2.66	45.6	33.5	20.3	12.4	7.87	5.26
$1s^2 3pnd(^3F_3) \rightarrow 1s^2 2snd(^3D_2)$	157	28.8	11.4	5.48	2.99	1.80	1.18
$1s^2 3pnd(^3F_4) \rightarrow 1s^2 2snd(^3D_3)$	104	224	159	93.6	55.8	34.8	22.8
$1s^2 3pnd(^1P_1) \rightarrow 1s^2 2snd(^1D_2)$	423	626	530	403	300	223	172
$1s^2 3pnd(^3P_1) \rightarrow 1s^2 2snd(^3D_2)$	7.71	23.8	20.2	15.1	11.0	8.13	6.25
$1s^2 3pnd(^3P_2) \rightarrow 1s^2 2snd(^3D_3)$	5.78	4.70	10.2	10.0	8.30	6.54	5.21
			Z=56				
$1s^2 3pnd(^3F_2) \rightarrow 1s^2 2snd(^3D_1)$	1.89	45.0	33.2	20.0	12.2	7.76	5.01
$1s^2 3pnd(^3F_3) \rightarrow 1s^2 2snd(^3D_2)$	31.9	13.4	4.80	2.19	1.16	0.693	0.393
$1s^2 3pnd(^3F_4) \rightarrow 1s^2 2snd(^3D_3)$	69.6	220	158	92.8	55.3	34.5	22.6
$1s^2 3pnd(^1P_1) \rightarrow 1s^2 2snd(^1D_2)$	380	640	547	409	298	230	167
$1s^2 3pnd(^3P_1) \rightarrow 1s^2 2snd(^3D_2)$	7.50	18.8	17.4	13.5	9.97	8.34	5.76
$1s^2 3pnd(^3P_2) \rightarrow 1s^2 2snd(^3D_3)$	5.25	3.59	8.37	8.54	7.17	6.23	4.59

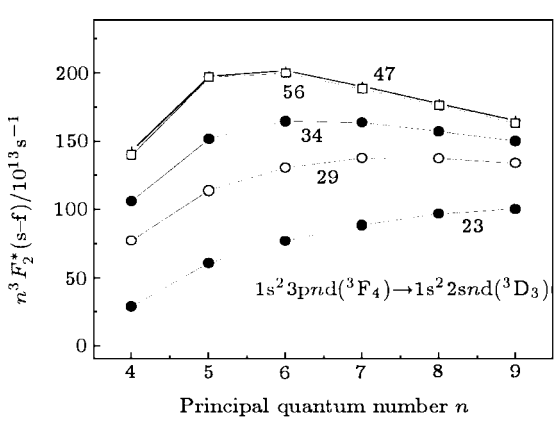


Fig.2. Satellite intensity factors multiplied by n^3 for a selected transition in Li-like ions as functions of n and atomic number of the ions.

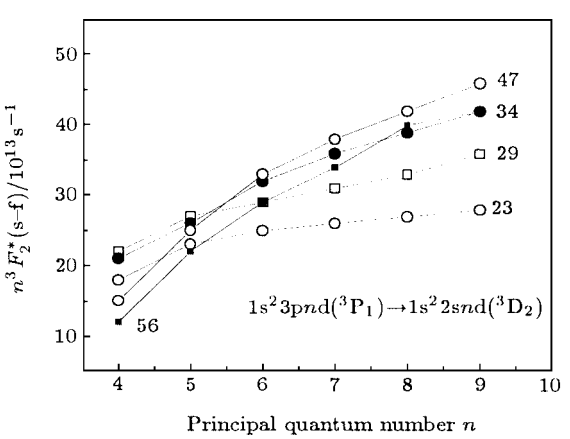


Fig.3. Satellite intensity factors multiplied by n^3 for a selected transition in Li-like ions as functions of n and atomic number of the ions.

We have compared the F_2^*(s–f) functions using Eq.(4) with the calculated values. It is seen that the reliability of $1/n^3$ scaling improves with n for all elements and for all transitions considered. However, the magnitude and sign of the scaling vary greatly with Z. For vanadium and silver, the $1/n^3$ scaling underestimates the calculated satellite factors F_2^*(s–f) for all transitions listed in Table 1. In high-Z elements the values of F_2^*(s–f) obtained from $1/n^3$ scaling for a particular transition may be smaller or larger than the calculated values. An $1/n^3$ scaling estimate of F_2^*(s–f) for the transition $1s^2 3pnd(^3F_4) \rightarrow 1s^2 2snd(^3D_3)$ for n=6 from its calculated value of n=5 yields 28.8, 52.8, 70.6, 92 and 91, respectively, for Z=23, 29, 34, 47 and 56, as compared to the values of 35.8, 60.9, 76.7, 93.6 and 92.8 from our explicit calculation. Thus, for vanadium and copper the results from $1/n^3$ scaling for $1s^2 3pnd(^3F_4) \rightarrow 1s^2 2snd(^3D_3)$ transitions are, respectively, 19.5% and 13.3% less than the calculated values, and for silver and barium the results from $1/n^3$ scaling for $1s^2 3pnd(^3F_4) \rightarrow 1s^2 2snd(^3D_3)$ transitions are, respectively, 2.7% and 1.9% more than the calculated values. We also find that for lithium-like ions with Z <34 the F_2^*(s–f) functions fall off at a slower rate than those obtained from Eq.(4) for all n up to n=9. For high-Z elements F_2^*(s–f) functions fall off at a much faster rate than the $1/n^3$ scaling from n=3 to n=4; for n >5 the calculated F_2^*(s–f) functions are in good agreement with the $1/n^3$ scaling. In conclusion, we have shown that the validity of the $1/n^3$ scaling for the satellite intensity factors, used both in DR rate calculations and plasma diagnostics,[13,14] depends on n and the atomic number of the ion, and also on the transitions involved.

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