Deexcitation of light Li-like ions in the $1s2s2p$ state

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Auger and x-ray emission rates have been computed relativistically for the $1s2s2p$ configuration of three-electron ions with $6 \leq Z \leq 10$. Results are compared with earlier calculations and with experiment.

I. INTRODUCTION

This paper is an addendum to recent work in which we computed relativistic Auger and x-ray emission rates of the $1s2s2p$ configuration of three-electron ions with nuclear charges $13 \leq Z \leq 92$.[1] Relativistic effects on the Auger rates were found to be as large as two orders of magnitude; multiplet flourescence yields were found to be substantially affected, and the Breit interaction was seen to reverse the fine-structure level order in some cases.[1]

It has become desirable to extend these relativistic calculations of the properties of $1s2s2p$ states to lighter ions ($6 \leq Z \leq 10$), because of the role that low-Z, highly stripped atoms play in astrophysical and plasma environments. Furthermore, light Li-like ions are more easily produced in the laboratory than heavy ones, and we hope that the present theoretical predictions may provide an incentive for additions to the exceedingly scant experimental literature on the subject. We do not, however, include ions lighter than $Z = 6$ because for these systems electron-electron correlations may become so important as to make the present treatment inadequate.

II. THEORY

We calculate Auger transition rates from perturbation theory, assuming frozen orbitals. The two-electron operator is that first formulated by Møller,[2] which includes the retarded Coulomb and current-current interaction. In the local-potential approximation, the Møller operator is equivalent to a Hamiltonian including the full Breit interaction.[3–5] The two-electron Auger matrix elements have been derived in Ref. 3, and applications to the present system are described in Ref. 1. The multiplet x-ray emission rates are calculated from first-order perturbation theory following the procedure of earlier calculations.[6–8]

The transition-rate computations are carried out in relativistic intermediate coupling, using j-j coupled basis states.[1,9] In order to examine the effects of the Breit interaction[10] on the fine-structure and multiplet transition rates, we have performed the intermediate-coupling calculations both with and without the Breit interaction in the energy matrices.[1]

Numerical computations were carried out with a generalized relativistic Auger code.[11]

III. RESULTS AND DISCUSSION

Energies. The calculated K-shell Auger and x-ray energies for $1s2s2p$ three-electron states of ions with atomic numbers $6 \leq Z \leq 10$ are listed in Table I. It should be noted that the effect of correlations on these energies, of the order of $\sim$1 eV, is not included. The present energies agree well (generally to within $\sim$1.5 eV) with results from Z-expansion theory.[12]

Radiative transition rates. X-ray transition rates from the present relativistic calculations in intermediate coupling are included in Table II. The electric dipole ($E1$) rates agree with results from Z-expansion theory[12] to better than 10% for all states. In both Vainshtein and Safronova's[12] and the present work, spin-orbit and Breit interaction were included in the intermediate-coupling energy matrix.

Nonrelativistic Hartree-Slater calculations in which only the spin-orbit energy is included in the intermediate-coupling energy matrix (HS-SO),[13] on the other hand, lead to significantly lower $E1$ x-ray emission rates: the difference is $\sim$18% for ^2P states and reaches a factor of 2 for $^4P_{1/2,3/2}$ states. Omission of the Breit interaction from the intermediate-coupling energy matrix may be the cause for this large discrepancy between the HS-SO[13] and present results for $E1$ x-ray emission rates from the $^4P_{1/2,3/2}$ states, since the radiative decay of these levels depends strongly on mixing with $^2P_{1/2,3/2}$ states.

Theoretical magnetic-quadrupole ($M2$) x-ray emission rates are compared in Fig. 1. Present results fall

TABLE I. Calculated K-shell Auger and x-ray energies (in eV) for states of the $1s2s2p$ configuration of Li-like ions of atomic number Z.

Z / State[a]	6 Auger	6 x ray	7 Auger	7 x ray	8 Auger	8 x ray	9 Auger	9 x ray	10 Auger	10 x ray
$^2P_{1/2}^{(+)}$	239.85	304.06	328.10	426.02	430.35	568.50	546.34	731.46	675.65	914.79
$^2P_{1/2}^{(-)}$	235.39	299.60	323.01	420.92	424.62	562.77	539.98	725.10	668.66	907.80
$^2P_{3/2}^{(+)}$	239.85	304.06	328.10	426.02	430.35	568.50	546.35	731.47	675.67	914.81
$^2P_{3/2}^{(-)}$	235.40	299.62	323.04	420.95	424.67	562.82	540.07	725.19	668.80	907.94
$^4P_{1/2}$	229.01	293.22	315.07	412.98	415.11	553.26	528.89	714.01	655.98	895.12
$^4P_{3/2}$	229.01	293.22	315.07	412.99	415.12	553.27	528.91	714.03	656.03	895.17
$^4P_{5/2}$	229.02	293.23	315.10	413.02	415.17	553.32	529.00	714.12	656.17	895.31

[a]The ^2P eigenstates, with energies in descending order, are designated by $^2P_{1/2}^{(+)}$, $^2P_{1/2}^{(-)}$; $^2P_{3/2}^{(+)}$, $^2P_{3/2}^{(-)}$.

~14% below rates from nonrelativistic Z-expansion theory.[14] This discrepancy for light ions can probably be ascribed to the neglect of correlations in the present work, rather than to relativistic effects: relativistic random-phase-approximation calculations[15] of $1s2p\,^3P_2 \rightarrow 1s^2\,^1S_0$ $M2$ rates agree with nonrelativistic Z-expansion results[16] to better than 2.5% at low Z.

The $M2$ x-ray emission rates calculated in the Dirac-Hartree-Slater (DHS) model by Cheng, Lin, and Johnson[17] are greater than predicted by Z-expansion theory.[14] The excess (~30% at $Z=6$) may be due to the use of eigenvalues to estimate x-ray energies: if we use eigenvalues to make x-ray-energy estimates, we obtain the same $M2$ rates with our present code as predicted in Ref. 17 (Fig. 1).

Auger rates. Auger decay rates of $1s2s2p$ three-electron ions are also listed in Table II. These relativistic intermediate-coupling results for ^2P states fall within ~20% of rates from nonrelativistic HS calculations,[13] but differ greatly from predictions based on Coulomb wave functions.[12]

Auger decay of the ^4P_J states via the Coulomb interaction is forbidden in LS coupling. The $^4P_{1/2,3/2}$ states can decay, however, by spin-orbit mixing with $^2P_{1/2,3/2}$ states, or through the spin-other-orbit, orbit-orbit, and spin-spin interactions which are part of the current-current interaction in the present treatment. The Auger rates of the $^4P_{1/2,3/2}$ states are very sensitive to the atomic model. A 7% error in transition energies can change the transition rates by an order

TABLE II. Theoretical Auger and x-ray emission rates (in a.u.[a]) for states of the $1s2s2p$ configuration of Li-like ions of atomic number Z.

Z / State	6 Auger	6 x ray	7 Auger	7 x ray	8 Auger	8 x ray	9 Auger	9 x ray	10 Auger	10 x ray
$^2P_{1/2}^{(+)}$	1.48(−3)	2.21(−6)	1.65(−3)	4.57(−6)	1.78(−3)	8.46(−6)	1.89(−3)	1.45(−5)	1.98(−3)	2.36(−5)
$^2P_{1/2}^{(-)}$	2.01(−4)	1.72(−5)	2.05(−4)	3.58(−5)	2.06(−4)	6.64(−5)	2.09(−4)	1.13(−4)	2.15(−4)	1.80(−4)
$^2P_{3/2}^{(+)}$	1.48(−3)	2.16(−6)	1.66(−3)	4.38(−6)	1.79(−3)	7.87(−6)	1.89(−3)	1.30(−5)	1.99(−3)	1.99(−5)
$^2P_{3/2}^{(-)}$	1.92(−4)	1.73(−5)	1.90(−4)	3.60(−5)	1.82(−4)	6.70(−5)	1.74(−4)	1.15(−4)	1.66(−4)	1.84(−4)
$^4P_{1/2}$	6.50(−9)	4.19(−11)	1.26(−8)	2.25(−10)	2.13(−8)	9.34(−10)	3.29(−8)	3.24(−9)	4.78(−8)	9.84(−9)
$^4P_{3/2}$	1.73(−9)	1.04(−10)	2.60(−9)	5.57(−10)	3.17(−9)	2.33(−9)	3.07(−9)	8.17(−9)	2.15(−9)	2.48(−8)
$^4P_{5/2}$	2.06(−10)	3.97(−13)	4.45(−10)	1.69(−12)	8.49(−10)	5.73(−12)	1.48(−9)	1.66(−11)	2.43(−9)	4.21(−11)

[a]1 a.u. $= 27.21$ eV/$\hbar = 4.134 \times 10^{16}$ sec^{-1}. Numbers in parentheses stand for powers of 10, e.g., $1.48(-3) = 1.48 \times 10^{-3}$.

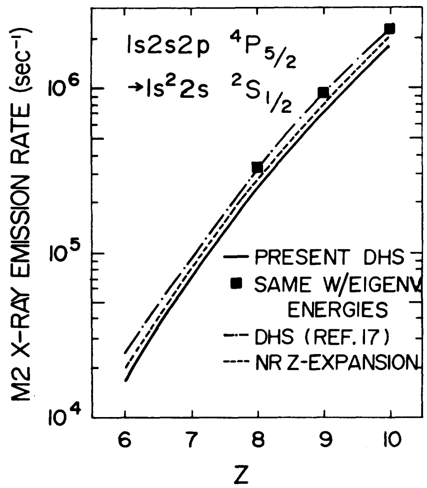

FIG. 1. Magnetic-quadrupole x-ray emission rates (per sec) of the $^4P_{5/2}$ state of $1s2s2p$ configurations of three-electron ions with atomic number Z. The present Dirac-Hartree-Slater results with exact transition energies (present DHS) are compared with DHS results from the present theory, but with eigenvalue transition energies, with DHS results of Cheng, Lin, and Johnson (Ref. 17), and with Z-expansion-theory results (Ref. 12).

of magnitude. Inclusion of the Breit interaction in the energy matrix of the intermediate-coupling calculation can produce an order-of-magnitude change in transition rates.

In Fig. 2 we compare the Auger decay rates of the $^4P_{1/2}$ and $^4P_{3/2}$ states as predicted in different approximations. The following observations can be made: (i) For light ions with $6 < Z < 10$, the magnetic interaction's contribution to the $^4P_{1/2,3/2}$ Auger decay rate exceeds that of spin-orbit mixing. For heavier elements ($Z > 30$), spin-orbit mixing becomes dominant. (ii) If the magnetic interaction is omitted from the mixing calculation and from the Auger matrix element in the present intermediate-coupling computations, then the resultant rates agree with those from nonrelativistic Hartree-Slater calculations including spin-orbit mixing.[13] Rates computed from Coulomb wave functions,[12] however, differ substantially. (iii) For the $^4P_{3/2}$ state, there is strong cancellation between the contributions from spin-orbit mixing and from the magnetic interaction.[18,19] Consequently, present Auger rates for the $^4P_{3/2}$ state are less reliable than for the $^4P_{1/2}$ state. (iv) Inclusion of the magnetic interaction in the mixing calculations substantially reduces the mixing between $^4P_{1/2,3/2}$ and $^2P_{1/2,3/2}$ states.

Lifetimes of the ^4P states. The present calculations predict $^4P_{5/2}$ lifetimes ~10% shorter than from Hartree-Fock computations with the Pauli approximation for relativistic effects,[18] and ~18% longer than previous DHS results.[17] The latter discrepancy is

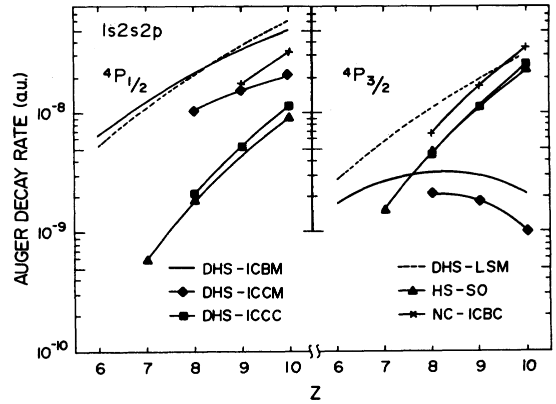

FIG. 2. Auger decay rates of the $^4P_{1/2,3/2}$ states of the $1s2s2p$ configuration of Li-like ions of atomic number Z. The present Dirac-Hartree-Slater computations in intermediate coupling, including Coulomb and magnetic interaction in both the energy matrices and the Auger transition matrices (DHS-ICBM) are compared with the following: DHS computations with only the Coulomb interaction in the energy matrix but also the magnetic interaction in the Auger matrix (DHS-ICCM); DHS computations with only the Coulomb interaction in both the energy and Auger matrices (DHS-ICCC); DHS computations in LS coupling, including contributions from the magnetic interaction in the Auger matrix elements (DHS-LSM); nonrelativistic Hartree-Slater calculations in intermediate coupling with spin-orbit mixing and Coulomb interaction in the Auger matrix (Ref. 13) (HS-SO); results of Z-expansion theory based on Coulomb wave functions (Ref. 12) (NC-ICBC).

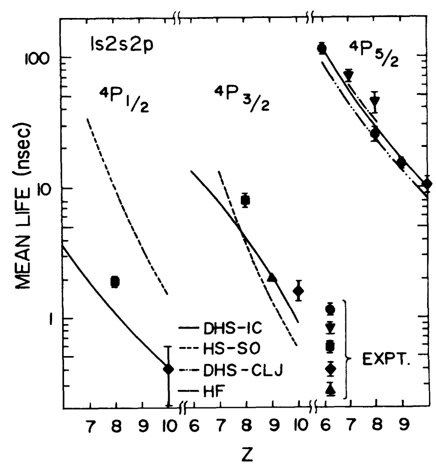

FIG. 3. Lifetimes (in nsec) of the ^4P states of $1s2s2p$ three-electron ions with atomic number Z. Predictions of the present Dirac-Hartree-Slater calculations in intermediate coupling including magnetic interaction (DHS-IC) are compared with the DHS calculations of Cheng, Lin, and Johnson (Ref. 17) (DHS-CLJ), with the Hartree-Fock computations of Manson (Ref. 18) (HF), and with nonrelativistic Hartree-Slater calculations including only the spin-orbit interaction (Ref. 13) (HS-SO). Experimental data included for comparison are from Ref. 27 (squares), Ref. 22 (diamonds), Ref. 26 (triangles), Ref. 21 (dots), and Ref. 20 (inverted triangles).

largely due to the transverse correction which is included in the present calculations of Auger matrix elements.[1] Present results agree well with measured lifetimes[20–22] (Fig. 3) and with the relativistic results of Bhalla and Tunnell.[23]

The $^4P_{1/2,3/2}$-state lifetimes are also displayed in Fig. 3. The present relativistic calculations predict a shorter lifetime for the $^4P_{1/2}$ state and a longer lifetime for the $^4P_{3/2}$ state, opposite to the predictions of nonrelativistic HS-SO calculations.[13] Some discrepancies are found between present results and those of a previous DHS calculation.[23] These are partly due to the fact that the Auger rates of $^4P_{1/2,3/2}$ states are extremely sensitive to the transition energy and the mixing coefficients between ^4P and ^2P states. Furthermore, the eigenvectors of $^4P_{1/2,3/2}$ states from the work of Goldsmith,[24] which were used in Ref. 23, have been found to produce a multiplet splitting between $^4P_{1/2}$ and $^4P_{3/2}$ that is an order of magnitude too large compared with results of other relativistic calculations[12,25] and the present work. Measured lifetimes[22,26,27] are included in Fig. 3, with the states identified in accordance with present theory. Agreement of the sparse data with present calculations is seen to be fair. The remaining discrepancies between calculated and measured $^4P_{1/2,3/2}$-state lifetimes are partly due to experimental uncertainties engendered by cascade contributions from the upper levels,[26,27] and partly theoretical vagaries caused by the strong dependence of the Auger rates on the atomic model.

The effects of full exchange and Coulomb correlation on the Auger decay rates of the ^4P states need yet to be explored. Accurate experimental data on lifetimes and fluorescence yields of these states are very much needed to guide further refinements of the theory.

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