Lifetime of the $1s2p3d\ ^4F_{9/2}$ metastable state of Li-like ions

Mau Hsiung Chen
Lawrence Livermore National Laboratory, Livermore, California 94550

Bernd Crasemann
Department of Physics and Chemical Physics Institute, University of Oregon, Eugene, Oregon 97403
(Received 15 December 1986)

The metastable highest-spin $^4F_{9/2}$ state among $1s2p3d$ configurations of three-electron ions has unique characteristics. The decay rates of this state have been calculated relativistically by the multiconfiguration Dirac-Fock approach for ions with atomic numbers from $Z=6$ to 42. The major decay channels are found to be Auger transitions made possible by the Breit interaction, as well as $2s$-$2p$ and $3p$-$3d$ electric dipole, $2s$-$3d$ electric quadrupole, and $1s$-$2p$ magnetic quadrupole x-ray emission. The Auger rate scales as $Z^{4.6}$, the $2s$-$2p_{3/2}$ $E1$ radiative decay rate as $Z^{2.8}$, the $2s$-$3d_{5/2}$ $E2$ rate as $Z^{6.5}$, and the $1s$-$2p_{3/2}$ rate as $Z^{8.5}$. The differential metastability among the $1s2p3d\ ^4F$ fine-structure states caused by the effect of relativity is noted.

I. INTRODUCTION

The $1s2p3d\ ^4F_{9/2}$ state of doubly excited three-electron ions is unique among the ^{4}F states of these systems. For the other $1s2p3d\ ^4F_J$ ($J=\frac{3}{2},\frac{5}{2},\frac{7}{2}$) states, Auger decay and electric-dipole radiative transitions are forbidden in LS coupling, but these channels are opened through spin-orbit coupling with doublet states[1] and thus become the dominant decay mechanisms. The effects of relativity play a major role in the decay of these states.[1–3] Quite different are the decay characteristics of the $^4F_{9/2}$ state of three-electron systems, which is immune to the spin-orbit interaction. In this paper, we report on an investigation of the decay modes and lifetime of this highest-spin ^4F state. Leading decay modes are found to be radiationless transitions, electric-dipole transitions in which the principal quantum number does not change, $1s$-$2p$ magnetic-quadrupole, and $2s$-$3d$ electric-quadrupole transitions.

The other states of the $1s2l2l'$ and $1s2l3l'$ configurations of Li-like ions have been studied previously.[1–4]

II. THEORETICAL CALCULATIONS

The Auger transition probability from an initial state i with wave function ψ_i to a final state f with wave function ψ_f, in the frozen-orbital approximation, is[5]

$$T=\frac{2\pi}{\hbar}\left|\left\langle\psi_f\left|\sum_{\alpha<\beta}V_{\alpha\beta}\right|\psi_i\right\rangle\right|^2\rho(\epsilon)\ , \quad (1)$$

where $\rho(\epsilon)$ is the energy density of final states.

The two-electron operator $V_{\alpha\beta}$ in Eq. (1) is taken to be the sum of the Coulomb and Breit operators,[6–9] which in atomic units is

$$V_{12}=\frac{1}{r_{12}}-\boldsymbol{\alpha}_1\cdot\boldsymbol{\alpha}_2\frac{\cos(\omega r_{12})}{r_{12}}+(\boldsymbol{\alpha}_1\cdot\boldsymbol{\nabla}_1)(\boldsymbol{\alpha}_2\cdot\boldsymbol{\nabla}_2)\frac{\cos(\omega r_{12})-1}{\omega^2 r_{12}}\ , \quad (2)$$

where the $\boldsymbol{\alpha}_i$ are Dirac matrices, and ω is the wave number of the exchanged virtual photon.

The spontaneous transition probability for a discrete transition $i\rightarrow f$ in multipole expansion is given in perturbation theory by[10]

$$W_{fi}=\frac{1}{2J_i+1}\sum_L\frac{2\pi}{2L+1}\,|\langle f||T_L||i\rangle|^2\ . \quad (3)$$

In the multiconfiguration Dirac-Fock (MCDF) model,[8] a physical state i with total angular momentum JM is expanded in terms of n configuration state functions (CSF) as

$$\psi_i(JM)=\sum_{\lambda=1}^{n}C_{i\lambda}\Phi(\Gamma_\lambda JM)\ . \quad (4)$$

Here, the mixing coefficients $C_{i\lambda}$ are obtained by diagonalizing the energy matrix

The reduced multipole matrix element in Eq. (3) can be expressed in terms of a CSF basis as[11,12]

$$\langle f||T_L||i\rangle=\sum_{\alpha=1}^{n_i}\sum_{\beta=1}^{n_f}C_{i\alpha}C_{f\beta}\sum_{p,q}d_{pq}^L(\beta,\alpha)\langle p||T_L||q\rangle\ . \quad (5)$$

Here, the $d_{pq}^L(\beta,\alpha)$ are the CSF-dependent angular factors. The one-electron reduced matrix elements $\langle p||T_L||q\rangle$ of electric and magnetic types are defined in Ref. 10.

The energy levels and bound-state wave functions were calculated using the MCDF model with an extended average-level (EAL) scheme[6] which minimizes the statistically averaged energy of all the levels. In the present work, separate EAL calculations were performed for $1s2l3l'$ and $1s^23l$ states. The final Auger state is represented by a $1s^2$ single configuration. The transverse Breit and radiative corrections were taken into account through first-order perturbation theory.[9]

TABLE I. The Transition energies (in eV) and rates (in sec^{-1}) for the $1s2p3d\,^4F_{9/2}$ metastable state of Li-like ions. Numbers in square brackets indicate powers of ten, e.g., 3.78[7] = 3.78×10^7.

Z	Auger energy	Radiative energy 2s-2p	3p-3d	1s-2p	2s-3d	Auger rate	Radiative rate 2s-2p	3p-3d	1s-2p	2s-3d
6	277.90	5.48	1.42	301.96	49.05	1.45[5]	5.53[7]	3.78[7]	1.88[4]	7.92[5]
7	385.73	6.53	1.77	423.39	70.48	3.76[5]	6.65[7]	4.84[7]	7.80[4]	2.42[6]
8	510.99	7.61	2.12	565.30	95.72	8.09[5]	7.90[7]	5.91[7]	2.60[5]	6.19[6]
9	653.73	8.71	2.48	727.85	124.77	1.54[6]	9.29[7]	7.01[7]	6.92[5]	1.37[7]
10	813.97	9.84	2.84	910.78	157.64	2.69[6]	1.09[8]	8.12[7]	1.76[6]	2.82[7]
12	1 187.10	12.26	3.60	1 338.36	234.90	6.73[6]	1.48[8]	1.05[8]	8.64[6]	9.44[7]
14	1 630.70	14.95	4.40	1 848.52	327.62	1.42[7]	2.02[8]	1.29[8]	3.26[7]	2.58[8]
18	2 730.93	21.61	6.18	3 118.21	559.93	4.59[7]	3.94[8]	1.86[8]	2.75[8]	1.29[9]
22	4 118.55	30.94	8.28	4 723.78	855.89	1.13[8]	8.13[8]	2.57[8]	1.48[9]	4.63[9]
26	5 798.64	44.41		6 670.37	1 217.19	2.36[8]	1.74[9]		5.94[9]	1.33[10]
30	7 777.49	63.84		8 964.35	1 645.93	4.40[8]	3.85[9]		1.94[10]	3.28[10]
36	11 323.09	109.05		13 074.01	2 421.14	9.56[8]	1.22[10]		8.73[10]	1.04[11]
42	15 590.54	181.88		18 015.51	3 364.52	1.83[9]	3.76[10]		3.10[11]	2.76[11]

II. RESULTS AND DISCUSSION

In Table I we list transition energies and rates for Auger decay of the $1s2p3d\,^4F_{9/2}$ state and for radiative decay of this state by $2s$-$2p$ $E1$, $3p$-$3d$ $E1$, $1s$-$2p$ $M2$, and $2s$-$3d$ $E2$ transitions, calculated from the MCDF model. The radiative rates of electric multipoles were calculated in the Coulomb gauge.[13] Because the $^4F_{9/2}$ state is the only one in the $1s2l2l'$ and $1s2l3l'$ manifolds with total angular momentum $J=\frac{9}{2}$, it is a rather pure state not affected by spin-orbit interaction. The Auger transition $1s2p3d\,^4F_{9/2}\rightarrow 1s^2\epsilon h$ is forbidden via Coulomb interaction. This Auger transition is, however, made possible by the Breit interaction.

For $Z\lesssim 12$, the dominant decay routes for the $^4F_{9/2}$ state are the $1s2p3d\,^4F_{9/2}\rightarrow 1s2s3d\,^4D_{7/2}$ $E1$ and $1s2p3d\,^4F_{9/2}\rightarrow 1s2p3p\,^4D_{7/2}$ $E1$ transition. For $Z\gtrsim 15$, the $1s2p3d\,^4F_{9/2}\rightarrow 1s2s2p\,^4P_{5/2}$ $E2$ transition becomes the most important decay branch. For $Z>20$, the $1s2p3d\,^4F_{9/2}\rightarrow 1s^23d\,^2D_{5/2}$ $M2$ transition is as important as $2s$-$3d$ $E2$ transitions (Fig. 1).

The Auger transition caused by the Breit interaction

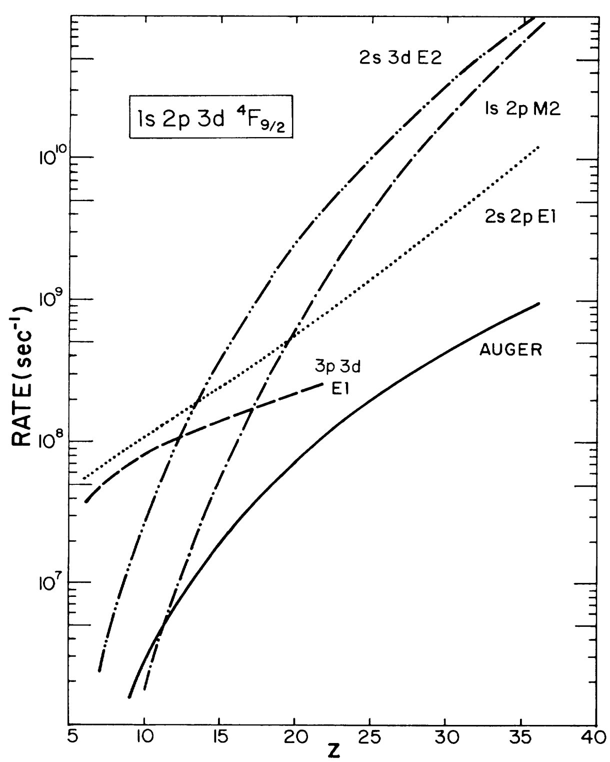

FIG. 1. Decay rates for the $1s2p3d\,^4F_{9/2}$ state, as functions of atomic number.

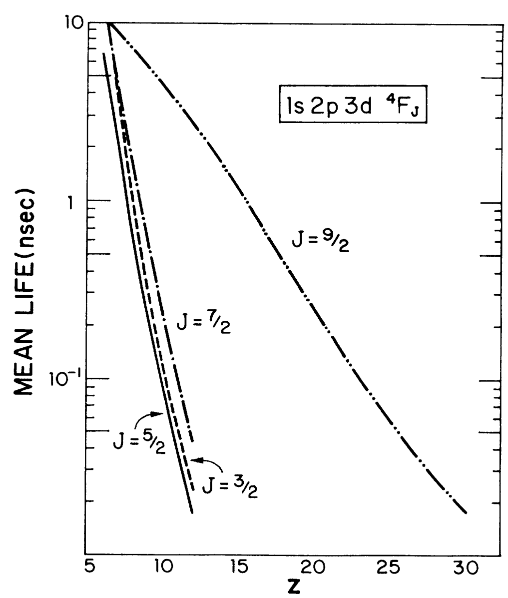

FIG. 2. Lifetimes of the $1s2p3d\,^4F$ fine-structure states, as functions of atomic number.

scales as $Z^{4.6}$; this represents a much stronger Z dependence than that of allowed Auger transitions due to the Coulomb interaction, which scale with the first power of Z. The radiative rates are found to scale as $Z^{2.8}$ for $2s$-$2p_{3/2}$ $E1$, $Z^{6.5}$ for $2s$-$3d_{5/2}$ $E2$, and $Z^{8.5}$ for $1s$-$2p_{3/2}$ $M2$ transitions.

In Fig. 2, the lifetimes of the $1s2p3d\,^4F$ fine-structure states are compared. The Auger and radiative rates for ^4F_J states with $J=\frac{3}{2}$, $\frac{5}{2}$, and $\frac{7}{2}$ were taken from Ref. 1. The lifetimes of the $^4F_{3/2}$, $^4F_{5/2}$, and $^4F_{7/2}$ states might be uncertain by as mush as a factor of 2 in the low-Z region. The lifetime of the $^4F_{9/2}$ state is found to be about two orders of magnitude longer than that of the other ^4F fine-structure states at $Z=12$. The disparity in the lifetimes of the fine-structure states of the low-Z ions is caused by the effect of relativity. The differential metastability of the fine-structure states has been observed in the other quartet states of Li-like ions.[2,3,14] Experimental tests of the present theoretical predictions could probably be carried out by beam-foil spectroscopy of low-Z ions;[14,15] more extensive experimental possibilities will arise with the advent of suitable heavy-ion storage rings.[16]

ACKNOWLEDGMENTS

We gratefully acknowledge the computational work of Mei Chi Chen. We thank William F. Ballhaus, Jr., Director of the NASA Ames Research Center (ARC), for permission to use the computational facilities of the Center, and thank the ARC Computational Chemistry and Aerothermodynamics Branch, particularly David M. Cooper, for their hospitality. In the Lawrence Livermore National Laboratory, this work was performed under the auspices of the U. S. Department of Energy under Contract No. W-7405-ENG-48. In the University of Oregon, this research was supported in part by the National Science Foundation through Grant No. PHY-8516788 and by the U. S. Air Force Office of Scientific Research under Contract No. F49620-85-C-0040.

[1] M. H. Chen, At. Data. Nucl. Data Tables **34**, 301 (1986).
[2] M. H. Chen, B. Crasemann, and H. Mark, Phys. Rev. A **24**, 1852 (1981); **26**, 1441 (1982); **27**, 544 (1983).
[3] C. P. Bhalla and T. W. Tunnell, Z. Phys. A **303**, 199 (1981).
[4] L. A. Vainshtein and U. I. Safronova, At. Data Nucl. Data Tables **21**, 49 (1978); **25**, 311 (1980).
[5] W. Bambynek, B. Crasemann, R. W. Fink, H.-U. Freund, H. Mark, C. D. Swift, R. E. Price, and P. Venugopala Rao, Rev. Mod. Phys. **44**, 716 (1972).
[6] M. H. Chen, B. Crasemann, and H. Mark, Phys. Rev. A **25**, 391 (1982).
[7] B. Crasemann, M. H. Chen, and H. Mark, J. Opt. Soc. Am. B **1**, 224 (1984).
[8] I. P. Grant, B. J. McKenzie, P. H. Norrington, D. F. Mayers, and N. C. Pyper, Comput. Phys. Commun. **21**, 207 (1980).
[9] B. J. McKenzie, I. P. Grant, and P. H. Norrington, Comput. Phys. Commun. **21**, 233 (1980).
[10] I. P. Grant, J. Phys. B **7**, 1458 (1974).
[11] J. Hata and I. P. Grant, J. Phys. B **14**, 2111 (1981).
[12] M. H. Chen, Phys. Rev. A **31**, 1449 (1985).
[13] M. H. Chen and B. Crasemann, Phys. Rev. A **18**, 2829 (1983).
[14] A. E. Livingston and H. G. Berry, Phys. Rev. A **17**, 1966 (1978).
[15] P. Richard, R. L. Kauffmann, F. F. Hopkins, C. W. Woods, and K. A. Jamieson, Phys. Rev. A **8**, 2187 (1973).
[16] K. W. Jones, B. M. Johnson, M. Meron, B. Crasemann, Y. Hahn, V. O. Kostroun, S. T. Manson, and S. M. Younger, Comments At. Mol. Phys. (to be published).