Excitation energies, polarizabilities, multipole transition rates, and lifetimes of ions along the francium isoelectronic sequence

U. I. Safronova*
Physics Department, University of Nevada, Reno, Nevada 89557, USA

W. R. Johnson†
Department of Physics, University of Notre Dame, Notre Dame, Indiana 46556, USA

M. S. Safronova‡
Department of Physics and Astronomy, 217 Sharp Lab, University of Delaware, Newark, Delaware 19716, USA

(Received 12 June 2007; published 5 October 2007)

Relativistic many-body perturbation theory is applied to study properties of ions of the francium isoelectronic sequence. Specifically, energies of the 7*s*, 7*p*, 6*d*, and 5*f* states of Fr-like ions with nuclear charges $Z=87-100$ are calculated through third order; reduced matrix elements, oscillator strengths, transition rates, and lifetimes are determined for 7*s*-7*p*, 7*p*-6*d*, and 6*d*-5*f* electric-dipole transitions; and 7*s*-6*d*, 7*s*-5*f*, and $5f_{5/2}$-$5f_{7/2}$ multipole matrix elements are evaluated to obtain the lifetimes of low-lying excited states. Moreover, for the ions $Z=87-92$ calculations are also carried out using the relativistic all-order single-double method, in which single and double excitations of Dirac-Fock wave functions are included to all orders in perturbation theory. With the aid of the single-double wave functions, we obtain accurate values of energies, transition rates, oscillator strengths, and the lifetimes of these six ions. Ground state scalar polarizabilities in Fr I, Ra II, Ac III, and Th IV are calculated using relativistic third-order and all-order methods. Ground state scalar polarizabilities for other Fr-like ions are calculated using a relativistic second-order method. These calculations provide a theoretical benchmark for comparison with experiment and theory.

DOI: 10.1103/PhysRevA.76.042504 PACS number(s): 31.15.Ar, 31.15.Md, 32.10.Fn, 32.70.Cs

I. INTRODUCTION

A detailed investigation of radiative parameters for electric dipole (*E*1) transitions in Fr-like ions with $Z=89-92$ was presented recently by Biémont *et al.* [1]. The electronic structure of Fr-like ions consists of a single *nl* electron outside of a core with completely filled $n=1$, 2, 3, 4 shells and 5*s*, 5*p*, 5*d*, 6*s*, and 6*p* subshells. In Fig. 1, we plot one-electron Dirac-Fock (DF) energies of *valence* 5*f*, 6*d*, and 7*s* states as functions of *Z*. We find that the valence 7*s* orbital is more tightly bound than the 5*f* and 6*d* orbitals at low stages of ionization ($Z=87-89$), while the 5*f* and 6*d* orbitals are more tightly bound for highly ionized cases ($Z\geq 90$). Competition between the 5*f*, 6*d*, and 7*s* orbitals leads to problems for calculations, making it difficult to obtain very accurate excitation energies and line strengths for the transitions between the low-lying 5*f*, 6*d*, and 7*s* states.

Relativistic Hartree-Fock and Dirac-Fock atomic structure codes were used in Ref. [1] to perform calculations of radiative transition rates and oscillator strengths for a limited number of transitions using the energies given by Blaise and Wyart [2], where experimental values were given for the 7*p*, 8*p*, *nd* (with $n=10-33$), and *ns* (with $n=12-31$) levels of neutral Fr, for 24 levels of Fr-like Th, and for seven levels of Fr-like Ac and U. Adopted energy level values in the *ns*, *np*, and *nd* ($n\leq 30$) series of neutral francium were presented by Biémont *et al.* [3]. Experimental measurements of energy levels of the 8*s* and 7*d* states in Fr I were reported recently in Refs. [4,5]. The experimental energies of 13 levels of Fr-like Ra were reported in the NIST compilation [6].

Lifetime measurements for neutral francium were presented in Refs. [7–11] for the 7*p*, 6*d*, 9*s*, and 8*s* levels. In those papers, experimental measurements were compared with *ab initio* calculations performed by Johnson *et al.* [12], Dzuba *et al.* [13,14], Safronova *et al.* [15], and Safronova and Johnson [16]. Third-order many-body perturbation theory was used in Ref. [12] to obtain the *E*1 transition amplitude for neutral alkali-metal atoms. The correlation potential method and the Feynman diagram technique were used in Refs. [13,14] to calculate *E*1 matrix elements in neutral

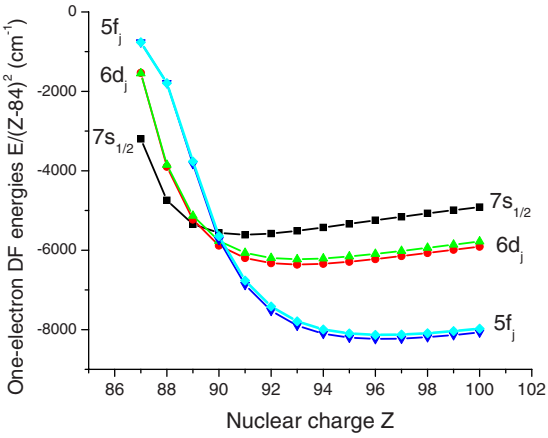

FIG. 1. (Color online) Dirac-Fock one-electron energies $[E/(Z-84)^2$ in $\mathrm{cm}^{-1}]$ for the $5f_j$, $6d_j$, and $7s_{1/2}$ states of Fr-like ions as functions of *Z*.

*On leave from ISAN, Troitsk, Russia; usafrono@nd.edu
†johnson@nd.edu; URL: www.nd.edu/~johnson
‡msafrono@udel.edu

francium and Fr-like radium. Atomic properties of the Th IV ion were studied by Safronova *et al.* [17] using a relativistic all-order method.

The present third-order calculations of excitation energies of the $7s$, $7p$, $6d$, and $5f$ states in Fr-like ions with nuclear charges $Z=87-100$ start from a closed-shell Dirac-Fock potential for the 86 electron radonlike core. We note that Th IV is the first ion in the francium isoelectronic sequence with a $[\mathrm{Rn}]5f_{5/2}$ ground state instead of the $[\mathrm{Rn}]7s_{1/2}$ ground state as for Fr I, Ra II, and Ac III. Correlation corrections become very large for such systems as was demonstrated by Savukov *et al.* [18], where the ratio of the second-order and DF removal energies for the $[\mathrm{Xe}]4f_{5/2}$ ground state in Ce IV and Pr V were 18% and 11%, respectively.

In the present paper, dipole matrix elements are calculated using both relativistic many-body perturbation theory, complete through third-order, and the relativistic all-order method restricted to single and double (SD) excitations. Such calculations permit one to investigate the convergence of perturbation theory and estimate the theoretical error in predicted data. To obtain lifetime predictions, multipole matrix elements for $7s$-$6d$, $7s$-$5f$, and $5f_{5/2}$-$5f_{7/2}$ transitions are also evaluated. Additionally, scalar polarizabilities for the $7s_{1/2}$ ground state in Fr I, Ra II, and Ac III are calculated using relativistic third-order and SD methods. Finally, scalar polarizabilities of the $5f_{5/2}$ ground state of Fr-like ions with nuclear charge $Z=91-100$ are calculated in second-order many-body perturbation theory (MBPT).

II. THIRD-ORDER AND ALL-ORDER MBPT CALCULATIONS OF ENERGIES

We start from the "no-pair" Hamiltonian [19]

$$H = H_0 + V_I, \tag{1}$$

where H_0 and V_I can be written in a second-quantized form as

$$H_0 = \sum_i \varepsilon_i a_i^\dagger a_i, \tag{2}$$

$$V_I = \frac{1}{2}\sum_{ijkl} g_{ijkl} a_i^\dagger a_j^\dagger a_l a_k. \tag{3}$$

Negative-energy (positron) states are excluded from the sums. The quantities ε_i are eigenvalues of the one-electron Dirac-Fock equations with a frozen core and g_{ijkl} is a two-particle Coulomb matrix element. Our calculations start from a V^{N-1} DF potential for a closed-subshell radonlike ion.

The all-order single-double (SD) method was discussed previously in Refs. [15,20–24]. Briefly, we represent the wave function Ψ_v of an atom with one valence electron as $\Psi_v \cong \Psi_v^{\mathrm{SD}}$ with

$$\Psi_v^{\mathrm{SD}} = \left[1 + \sum_{ma} \rho_{ma} a_m^\dagger a_a + \frac{1}{2}\sum_{mnab} \rho_{mnab} a_m^\dagger a_n^\dagger a_b a_a + \sum_{m\neq v} \rho_{mv} a_m^\dagger a_v + \sum_{mna} \rho_{mnva} a_m^\dagger a_n^\dagger a_a a_v\right]\Phi_v, \tag{4}$$

where Φ_v is the lowest-order atomic wave function, which is taken to be the frozen-core DF wave function of a state v. Substituting the wave function Ψ_v^{SD} into the many-body Schrödinger equation, with Hamiltonian given by Eqs. (1)–(3), one obtains the coupled equations for the single- and double-excitation coefficients ρ_{mv}, ρ_{ma}, ρ_{mnva}, and ρ_{mnab}. The coupled equations for the excitation coefficients are solved iteratively. We use the resulting excitation coefficients to evaluate multipole matrix elements and hyperfine constants. This method includes the contribution of important classes of MBPT corrections to all orders.

The SD valence E_v^{SD} energy does not include all third-order MBPT corrections. The missing part of the third-order contribution, $E_{\mathrm{extra}}^{(3)}$, is written out in Ref. [23] and must be calculated separately. We use our third-order energy code to separate out $E_{\mathrm{extra}}^{(3)}$ and add it to the E_v^{SD}. For notational simplicity, we drop the index v in the designations in the text and tables below.

Results of our energy calculations for low-lying states of Fr I–U VI are summarized in Table I. Columns 2–7 of Table I give the lowest-order DF energies $E^{(0)}$, second- and third-order Coulomb correlation energies $E^{(2)}$ and $E^{(3)}$, first-order Breit contribution $B^{(1)}$, second-order Coulomb-Breit $B^{(2)}$ corrections, and the Lamb shift (LS) contribution E_{LS}. The sum of these six contributions is our final third-order MBPT result $E_{\mathrm{tot}}^{(3)}$ listed in the eighth column. First-order Breit energies (column $B^{(1)}$ of Table I) include retardation, whereas the second-order Coulomb-Breit energies (column $B^{(2)}$ of Table I) are evaluated using the unretarded Breit operator. We list all-order SD energies in the column labeled E^{SD} and the part of the third-order energies omitted in the SD calculation in column $E_{\mathrm{extra}}^{(3)}$. We note that E^{SD} includes $E^{(2)}$, part of $E^{(3)}$, and dominant higher-order corrections. The sum of the six terms $E^{(0)}$, E^{SD}, $E_{\mathrm{extra}}^{(3)}$, $B^{(1)}$, $B^{(2)}$, and E_{LS} gives the final all-order results $E_{\mathrm{tot}}^{\mathrm{SD}}$ listed in the 11th column of the table.

As expected, the largest correlation contribution to the valence energy comes from the second-order term, $E^{(2)}$. This term is simple to calculate in comparison with $E^{(3)}$ and E^{SD} terms. Thus, we calculate the $E^{(2)}$ term with higher numerical accuracy than $E^{(3)}$ and E^{SD}. The second-order energy $E^{(2)}$ includes partial waves up to $l_{\max}=8$ and is extrapolated to account for contributions from higher partial waves (see, for example, Refs. [25,26]). As an example of the convergence of $E^{(2)}$ with the number of partial waves l, we consider the $5f_{5/2}$ state in U VI. Calculations of $E^{(2)}$ with $l_{\max}=6$ and 8 yield $E^{(2)}(5f_{5/2})=-33\,598$ and $-34\,756\ \mathrm{cm}^{-1}$, respectively. Extrapolation of these calculations yields $-35\,163$ and $-35\,227\ \mathrm{cm}^{-1}$, respectively. Therefore, we estimate the numerical uncertainty of $E^{(2)}(5f_{5/2})$ to be $64\ \mathrm{cm}^{-1}$. This is the largest contribution from the higher partial waves, since the numerical uncertainty of $E^{(2)}(6d)$ is equal to $34\ \mathrm{cm}^{-1}$, and the numerical uncertainty of $E^{(2)}(7s)$ is equal to $1\ \mathrm{cm}^{-1}$. The numerical uncertainty of the second-order energy calculation for all other states ranges from 1 to $5\ \mathrm{cm}^{-1}$. We use $l_{\max}=6$ in our third-order and all-order calculations, owing to the complexity of these calculations. Therefore, we use our high-precision calculation of $E^{(2)}$ described above to account for the contributions of the higher partial waves, i.e., we replace $E^{(2)}[l_{\max}=6]$ with the final high-precision second-order value $E_{\mathrm{final}}^{(2)}$. The contribution $E_{\mathrm{extra}}^{(3)}$ given in Table I accounts for

TABLE I. Zeroth-order (DF), second-, and third-order Coulomb correlation energies $E^{(n)}$, single-double Coulomb energies E^{SD}, $E^{(3)}_{\mathrm{extra}}$, first-order Breit and second-order Coulomb-Breit corrections $B^{(n)}$ to the energies of Fr-like systems. The total energies are $E^{(3)}_{\mathrm{tot}}=E^{(0)}+E^{(2)}+E^{(3)}+B^{(1)}+B^{(2)}+E_{LS}$, $E^{\mathrm{SD}}_{\mathrm{tot}}=E^{(0)}+E^{\mathrm{SD}}+E^{(3)}_{\mathrm{extra}}+B^{(1)}+B^{(2)}+E_{LS}$ (units: cm^{-1}).

nlj	$E^{(0)}$	$E^{(2)}$	$E^{(3)}$	$B^{(1)}$	$B^{(2)}$	E_{LS}	$E^{(3)}_{\mathrm{tot}}$	E^{SD}	$E^{(3)}_{\mathrm{extra}}$	$E^{\mathrm{SD}}_{\mathrm{tot}}$
					Fr I, $Z=87$					
$7s_{1/2}$	−28767	−4763	1737	67	−131	13	−31845	−4658	724	−32753
$7p_{1/2}$	−18855	−1847	546	30	−35	0	−20162	−1991	255	−20597
$7p_{3/2}$	−17655	−1346	391	19	−30	0	−18621	−1433	184	−18915
$6d_{3/2}$	−13807	−2424	711	19	−62	0	−15563	−3180	326	−16990
$6d_{5/2}$	−13924	−2240	616	15	−61	0	−15594	−2854	288	−16744
$8s_{1/2}$	−12282	−1053	396	17	−32	2	−12952	−925	162	−13058
$8p_{1/2}$	−9240	−554	171	10	−13	0	−9625	−551	77	−9716
$8p_{3/2}$	−8811	−421	128	7	−11	0	−9108	−421	58	−9178
$7d_{3/2}$	−7724	−981	298	10	−30	0	−8427	−991	132	−8604
$7d_{5/2}$	−7747	−860	244	7	−28	0	−8384	−856	109	−8515
					Ra II, $Z=88$					
$7s_{1/2}$	−75898	−7529	2896	147	−250	33	−80634	−6692	1152	−81508
$6d_{3/2}$	−62356	−8727	2764	155	−398	0	−68562	−8042	1152	−69488
$6d_{5/2}$	−61592	−7537	2202	114	−360	0	−67174	−7034	926	−67947
$7p_{1/2}$	−56878	−4182	1370	102	−109	0	−59698	−4027	587	−60326
$7p_{3/2}$	−52906	−3130	1011	63	−90	0	−55053	−3020	433	−55519
$5f_{5/2}$	−28660	−2563	824	11	−63	0	−30452	−4438	371	−32780
$5f_{7/2}$	−28705	−2491	784	8	−61	0	−30466	−4159	353	−32564
					Ac III, $Z=89$					
$7s_{1/2}$	−133640	−9552	3739	233	−357	58	−139519	−8192	1456	−140442
$6d_{3/2}$	−130697	−11506	3639	296	−659	0	−138927	−10036	1479	−139617
$6d_{5/2}$	−128322	−10002	2902	218	−600	0	−135804	−8884	1186	−136401
$5f_{5/2}$	−95668	−26451	9684	403	−1785	0	−113818	−23325	3952	−116424
$5f_{7/2}$	−94161	−24695	8837	289	−1658	0	−111387	−22100	3607	−114022
$7p_{1/2}$	−106328	−6202	2118	193	−189	0	−110409	−5688	874	−111139
$7p_{3/2}$	−98868	−4745	1597	119	−157	0	−102054	−4380	659	−102626
					Th IV, $Z=90$					
$5f_{5/2}$	−206606	−32100	11739	704	−2747	0	−229010	−26327	4672	−230304
$5f_{7/2}$	−203182	−30549	10954	521	−2616	0	−224872	−25252	4361	−226168
$6d_{3/2}$	−211799	−13258	4129	438	−880	0	−221370	−11422	1663	−222000
$6d_{5/2}$	−207574	−11608	3300	326	−807	0	−216364	−10208	1337	−216927
$7s_{1/2}$	−200273	−11204	4402	325	−458	89	−207119	−9455	1697	−208075
$7p_{1/2}$	−165095	−7991	2782	298	−272	0	−170278	−7147	1125	−171091
$7p_{3/2}$	−153572	−6213	2124	184	−226	1	−157703	−5619	861	−158372
					Pa V, $Z=91$					
$5f_{5/2}$	−336671	−34071	12323	953	−3390	0	−360855	−27589	4831	−361865
$5f_{7/2}$	−331505	−32627	11592	713	−3255	0	−355081	−26571	4544	−356073
$6d_{3/2}$	−303549	−14627	4452	586	−1082	0	−314221	−12604	1795	−314854
$6d_{5/2}$	−297300	−12880	3556	438	−999	0	−307185	−11354	1446	−307768
$7s_{1/2}$	−274949	−12646	3359	425	−557	126	−284242	−10606	1348	−284212
$7p_{1/2}$	−232148	−9630	2566	417	−356	0	−239151	−8533	1040	−239580
$7p_{3/2}$	−216015	−7600	4939	258	−297	1	−218715	−6925	1900	−221079

TABLE I. (*Continued.*)

nlj	$E^{(0)}$	$E^{(2)}$	$E^{(3)}$	$B^{(1)}$	$B^{(2)}$	E_{LS}	$E^{(3)}_{\rm tot}$	$E^{\rm SD}$	$E^{(3)}_{\rm extra}$	$E^{\rm SD}_{\rm tot}$
					U VI, $Z=92$					
$5f_{5/2}$	−481613	−35163	12554	1194	−3929	0	−506958	−28393	4876	−507866
$5f_{7/2}$	−474700	−33781	11863	898	−3789	0	−499509	−27398	4604	−500385
$6d_{3/2}$	−404911	−15830	4675	742	−1275	0	−416599	−13737	1908	−417273
$6d_{5/2}$	−396467	−14000	3718	557	−1181	0	−407374	−12472	1538	−408025
$7s_{1/2}$	−357141	−13966	5366	533	−655	173	−365690	−11752	2079	−366763
$7p_{1/2}$	−306870	−11224	3742	548	−442	0	−314245	−10135	1541	−315358
$7p_{3/2}$	−285578	−9134	2452	338	−369	2	−292289	−10236	1173	−294669

that part of the third-order MBPT correction not included in the SD energy. The values of $E^{(3)}_{\rm extra}$ are quite large and including this term is important.

We find that the correlation corrections to energies are especially large for $5f$ states. For example, $E^{(2)}$ is about 15% of $E^{(0)}$ and $E^{(3)}$ is about 36% of $E^{(2)}$ for $5f$ states. Despite the evident slow convergence of the perturbation theory expansion, the $5f$ energy from the third-order MBPT calculation is within 0.9% of the measured energy. The correlation corrections are so large for the $5f$ states that inclusion of correlation leads to different ordering of states using the DF and $E^{(3)}_{\rm tot}$ energies. If we consider only DF energies the $6d_{3/2}$ state appears to be the ground state for Th IV, but the full correlation calculation shows that the $5f_{5/2}$ state is the ground state. The correlation corrections are much smaller for all other states; the ratios of $E^{(0)}$ and $E^{(2)}$ are equal to 6%, 5%, and 2% for the $6d$, $7s$, and $7p$ states, respectively.

The third-order and all-order results are compared with experimental values in Table II. The energies are given relative to the ground state to facilitate comparison with experiment. Experimental energies for Fr I, Ac III, Th IV, and U VI are taken from [2] and energies of Fr-like Ra are taken from the NIST compilation [6]. Differences of our third-order and all-order calculations with experimental data $\delta E^{(3)}=E^{(3)}_{\rm tot}-E_{\rm expt}$ and $\delta E^{\rm SD}=E^{\rm SD}_{\rm tot}-E_{\rm expt}$, respectively, are given in the two final columns of Table II. In general, the SD results agree better with the experimental values than the third-order MBPT values. Exceptions are the cases where the third-order fortuitously gives results that are close to experimental values. Comparison of results from the two last columns of Table II shows that the ratio of $\delta E^{(3)}$ and $\delta E^{\rm SD}$ is about three for the $5f$ states. As expected, including correlation to all orders led to significant improvement of the results. Better agreement of all-order energies with experiment demonstrates the importance of the higher-order correlation contributions.

Below, we describe a few numerical details of the calculation. We use the B-spline method described in [27] to generate a complete set of basis DF wave functions for use in the evaluation of the MBPT expressions. We use 50 splines of order $k=8$ for each angular momentum. The basis orbitals are constrained to a spherical cavity of radius $R=90-30$ a.u. for Fr I-U VI. The cavity radius is chosen large enough to accommodate all nl_j orbitals considered here and small enough that 50 splines can approximate inner-shell DF wave functions with good precision. We use 40 out of 50 basis orbitals for each partial wave in our third-order and all-order energy calculations, since contributions from the highest-energy orbitals are negligible.

A. Z dependence of energies in Fr-like ions

In Fig. 2, we illustrate the Z dependence of the second- and third-order energy corrections $E^{(n)}$ for the valence $7s$, $7p$, $6d$, and $5f$ states of Fr-like ions. The second-order energy $E^{(2)}$ is a smooth function of Z for the $7p_{1/2}$ and $5f_{7/2}$ states, but exhibits irregularities for the $7s_{1/2}$ state at $Z=96$ and for the $6d_{5/2}$ state at $Z=99$. These irregularities are caused by exceptionally small energy denominators in the expression for the second-order correlation energy. A typical second-order energy denominator is

$$\epsilon_v+\epsilon_a-\epsilon_m-\epsilon_n,$$

where ϵ_k is the DF eigenvalue for orbital k. In the sum, a designates a core orbital, v designates the valence orbital, and m,n designate virtual orbitals. For the ground state, the above expression is negative definite; however, for excited states, the denominator can be either negative or positive, and can change sign as Z increases along an isoelectronic sequence. Near a sign change, the energy denominator becomes anomalously small, leading to a sharp change in the second-order energy. Physically, the sharp feature corresponds to a near degeneracy between the single-particle valence state and a two-particle, one-hole state having the same angular momentum and parity. The perturbation expansion clearly fails for such cases and the correlation energy must be treated differently. As a specific example, consider the second-order energy of the $7s_{1/2}$ state. For $Z=95$, 96, 97, the denominator evaluates to −0.27, −0.015, +0.26 for the case where $a=6p_{3/2}$ and $m,n=4f_{5/2},5d_{3/2}$. At $Z=96$ this denominator is smaller than for neighboring values by a factor of about 20 leading to the sharp increase in correlation energy seen in Fig. 2 and signaling a failure of perturbation theory at $Z=96$. Similar irregularities show up in the perturbation expressions for transition matrix elements, as seen, for example, in Figs. 5 and 6. Again, these features can be traced to anomalously small energy denominators associated with level crossings. At the point of these irregularities, perturba-

TABLE II. The total third-order $E_{\mathrm{tot}}^{(3)}$ and all-order $E_{\mathrm{tot}}^{\mathrm{SD}}$ results for Fr-like ions are compared with experimental energies E_{expt} [2], $\delta E = E_{\mathrm{tot}} - E_{\mathrm{expt}}$. The energies are given relative to the ground state to facilitate comparison with experiment (units: cm^{-1}).

nlj	$E_{\mathrm{tot}}^{(3)}$	$E_{\mathrm{tot}}^{\mathrm{SD}}$	E_{expt}	$\delta E^{(3)}$	δE^{SD}
			Fr I, $Z=87$		
$7s_{1/2}$	0	0	0	0	0
$7p_{1/2}$	11683	12156	12237	−554	−81
$7p_{3/2}$	13224	13838	13924	−700	−86
$6d_{3/2}$	16282	16048	16230	52	−192
$6d_{5/2}$	16251	16217	16430	−179	−213
$8s_{1/2}$	18893	19695	19733	−840	−38
$8p_{1/2}$	22220	23037	23113	−893	−76
$8p_{3/2}$	22737	23575	23658	−921	−83
$7d_{3/2}$	23418	24149	24245	−827	−96
$7d_{5/2}$	23461	24238	24333	−872	−95
			Ra II, $Z=88$		
$7s_{1/2}$	0	0	0	0	0
$6d_{3/2}$	12072	12020	12084	−12	−64
$6d_{5/2}$	13460	13561	13743	−283	−182
$7p_{1/2}$	20936	21182	21351	−415	−169
$7p_{3/2}$	25581	25989	26209	−628	−220
$5f_{5/2}$	50182	48728	48988	1194	−260
$5f_{7/2}$	50168	48944	49272	896	−328
			Ac III, $Z=89$		
$7s_{1/2}$	0	0	0	0	0
$6d_{3/2}$	592	825	801	−209	24
$6d_{5/2}$	3715	4041	4204	−488	−163
$5f_{5/2}$	25701	24018	23454	2247	564
$5f_{7/2}$	28132	26420	26080	2052	340
$7p_{1/2}$	29110	29303	29466	−356	−163
$7p_{3/2}$	37465	37816	38063	−598	−247
			Th IV, $Z=90$		
$5f_{5/2}$	0	0	0	0	0
$5f_{7/2}$	4138	4136	4325	−187	−190
$6d_{3/2}$	7640	8304	9193	−1553	−889
$6d_{5/2}$	12646	13377	14486	−1841	−1109
$7s_{1/2}$	21891	22229	23131	−1240	−901
$7p_{1/2}$	58732	59213	60239	−1507	−1026
$7p_{3/2}$	71307	71932	73056	−1749	−1124
			U VI, $Z=92$		
$5f_{5/2}$	0	0	0	0	0
$5f_{7/2}$	7449	7481	7609	−160	−128
$6d_{3/2}$	90359	90593	91000	−641	−407
$6d_{5/2}$	99584	99841	100510	−926	−669
$7s_{1/2}$	141268	141103	141447	−179	−344
$7p_{1/2}$	192713	191989	193340	−627	−832
$7p_{3/2}$	214669	211747	215886	−1217	−2689

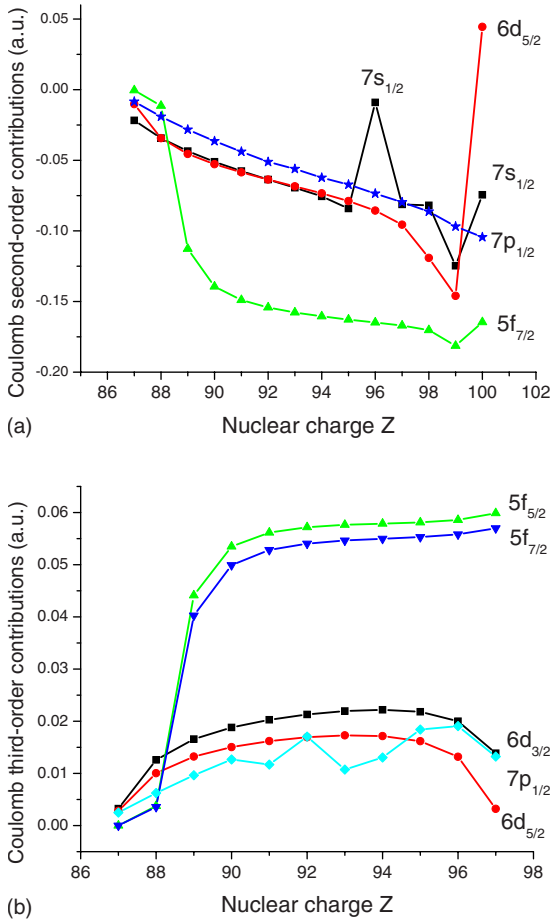

FIG. 2. (Color online) Coulomb second- and third-order energies as functions of Z for the $5f_j$, $6d_j$, $7s_{1/2}$, and $7p_{1/2}$ states in Fr-like ions.

tion theory clearly fails and other approaches must be employed.

The third-order energy $E^{(3)}$ is a smooth function of Z for the $6d$ and $5f$ states, but exhibits a similar sharp feature for the $7p_{1/2}$ state. Most of the sharp features for the $6d_j$ and $7p_j$ states occur at very high values of Z, $Z>97$. Comparison of the $E^{(2)}$ and $E^{(3)}$ corrections for the $6d$ and $5f$ states is illustrated by Fig. 3. This figure shows also the smooth dependence of second- and third-order corrections to the $6d_{5/2}$-$6d_{3/2}$ and $5f_{7/2}$-$5f_{5/2}$ fine-structure intervals. The total $E^{(3)}_{\rm tot}$ energies divided by $(Z-84)^2$ in Fr-like ions are shown in Fig. 4, where we plot the five energy levels for the $7s_{1/2}$, $6d_j$, and $5f_j$ states.

III. ELECTRIC-DIPOLE MATRIX ELEMENTS, OSCILLATOR STRENGTHS, TRANSITION RATES, AND LIFETIMES IN Fr-LIKE IONS

A. Electric-dipole matrix elements

The matrix element of a one-particle operator Z is given by [20]

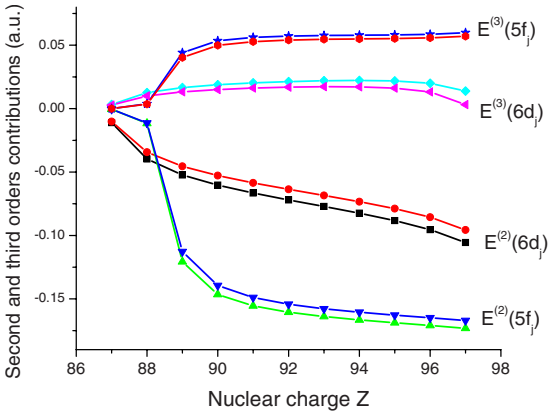

FIG. 3. (Color online) Coulomb second- and third-order energies as functions of Z for the $5f_j$ and $6d_j$ states in Fr-like ions.

$$Z_{wv} = \frac{\langle \Psi_w | Z | \Psi_v \rangle}{\sqrt{\langle \Psi_v | \Psi_v \rangle \langle \Psi_w | \Psi_w \rangle}}, \tag{5}$$

where Ψ_v is the exact wave function for the many-body "no-pair" Hamiltonian H. In MBPT, we expand the many-electron wave function Ψ_v in powers of V_I as

$$|\Psi_v\rangle = |\Psi_v^{(0)}\rangle + |\Psi_v^{(1)}\rangle + |\Psi_v^{(2)}\rangle + |\Psi_v^{(3)}\rangle + \cdots. \tag{6}$$

The denominator in Eq. (5) arises from the normalization condition that contributes starting from third order [28]. In the lowest order, we find

$$Z_{wv}^{(1)} = \langle \Psi_w^{(0)} | Z | \Psi_v^{(0)} \rangle = z_{wv}, \tag{7}$$

where z_{wv} is the corresponding one-particle matrix element [29]. Since $\Psi_w^{(0)}$ is a DF function we designate $Z^{(1)}$ by $Z^{(\rm DF)}$ below.

The second-order Coulomb correction to the transition matrix element in the DF case with V^{N-1} potential is given by [12]

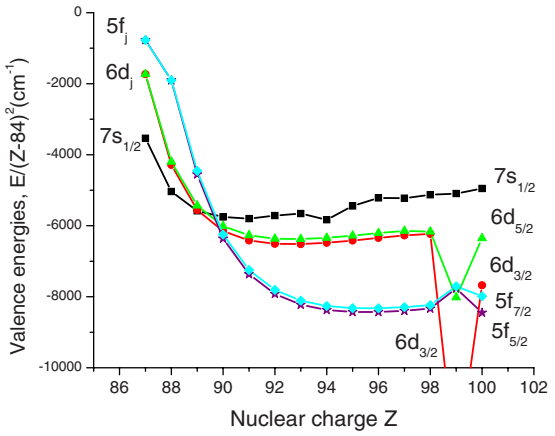

FIG. 4. (Color online) Valence removal energies $[E/(Z-84)^2$ in $\mathrm{cm}^{-1}]$ as functions of Z for the $5f_j$, $6d_j$, and $7s_{1/2}$ states in Fr-like ions.

TABLE III. Reduced electric-dipole matrix elements in Fr-like ions calculated to first, second, third, and all orders of MBPT.

Transition		$Z^{(DF)}$	$Z^{(DF+2)}$	$Z^{(DF+2+3)}$	$Z^{(SD)}$	Transition		$Z^{(DF)}$	$Z^{(DF+2)}$	$Z^{(DF+2+3)}$	$Z^{(SD)}$
		Fr I, $Z=87$						Th IV, $Z=90$			
$7s_{1/2}$	$7p_{1/2}$	5.1438	4.7412	4.1362	4.2641	$7s_{1/2}$	$7p_{1/2}$	2.8994	2.3748	2.3669	2.4196
$7s_{1/2}$	$7p_{3/2}$	7.0903	6.6001	5.6451	5.8619	$7s_{1/2}$	$7p_{3/2}$	3.9933	3.3399	3.2930	3.3677
$6d_{3/2}$	$7p_{1/2}$	9.2216	8.7781	7.1945	7.0276	$6d_{3/2}$	$7p_{1/2}$	2.5465	2.1374	2.0723	2.1220
$6d_{3/2}$	$7p_{3/2}$	4.2832	4.1100	3.3108	3.2217	$6d_{3/2}$	$7p_{3/2}$	0.9963	0.8784	0.8270	0.8488
$6d_{5/2}$	$7p_{3/2}$	12.8041	12.2858	10.1204	9.9456	$6d_{5/2}$	$7p_{3/2}$	3.1975	2.8348	2.7006	2.7549
$6d_{3/2}$	$5f_{5/2}$	11.4529	11.3002	6.7352	6.9611	$6d_{3/2}$	$5f_{5/2}$	2.4281	1.4501	1.3367	1.5295
$6d_{5/2}$	$5f_{5/2}$	3.0143	2.9714	1.9006	1.9515	$6d_{5/2}$	$5f_{5/2}$	0.6391	0.4070	0.3624	0.4116
$6d_{5/2}$	$5f_{7/2}$	13.4863	13.2942	8.5062	8.7332	$6d_{5/2}$	$5f_{7/2}$	2.9557	1.8844	1.7032	1.9190
		Ra II, $Z=88$						Pa V, $Z=91$			
$7s_{1/2}$	$7p_{1/2}$	3.8766	3.3758	3.1793	3.2545	$7s_{1/2}$	$7p_{1/2}$	2.6267	2.1111	2.1365	2.1822
$7s_{1/2}$	$7p_{3/2}$	5.3395	4.7241	4.3881	4.5106	$7s_{1/2}$	$7p_{3/2}$	3.6173	2.9720	2.9750	3.0327
$6d_{3/2}$	$7p_{1/2}$	4.4462	3.9314	3.3975	3.5659	$6d_{3/2}$	$7p_{1/2}$	2.1785	1.8079	1.7817	1.8152
$6d_{3/2}$	$7p_{3/2}$	1.8815	1.7070	1.4262	1.5117	$6d_{3/2}$	$7p_{3/2}$	0.8319	0.7327	0.7004	0.7119
$6d_{5/2}$	$7p_{3/2}$	5.8616	5.3340	4.6240	4.8232	$6d_{5/2}$	$7p_{3/2}$	2.6895	2.3817	2.2936	2.3185
$6d_{3/2}$	$5f_{5/2}$	5.3548	4.6786	4.5967	4.4491	$6d_{3/2}$	$5f_{5/2}$	1.9275	1.0904	1.0864	1.2092
$6d_{5/2}$	$5f_{5/2}$	1.4797	1.3062	1.3088	1.2465	$6d_{5/2}$	$5f_{5/2}$	0.5023	0.3061	0.2947	0.3241
$6d_{5/2}$	$5f_{7/2}$	6.6382	5.8609	5.8347	5.6357	$6d_{5/2}$	$5f_{7/2}$	2.3242	1.4102	1.3673	1.5020
		Ac III, $Z=89$						U VI, $Z=92$			
$7s_{1/2}$	$7p_{1/2}$	3.2787	2.7544	2.6859	2.7463	$7s_{1/2}$	$7p_{1/2}$	2.4165	1.9138	1.9562	1.9599
$7s_{1/2}$	$7p_{3/2}$	4.5157	3.8665	3.7271	3.8176	$7s_{1/2}$	$7p_{3/2}$	3.3271	2.6952	2.7168	2.2449
$6d_{3/2}$	$7p_{1/2}$	3.1529	2.6942	2.5241	2.6048	$6d_{3/2}$	$7p_{1/2}$	1.9249	1.5837	1.5688	1.5613
$6d_{3/2}$	$7p_{3/2}$	1.2726	1.1300	1.0275	1.0662	$6d_{3/2}$	$7p_{3/2}$	0.7202	0.6353	0.6054	0.4963
$6d_{5/2}$	$7p_{3/2}$	4.0423	3.6067	3.3438	3.4383	$6d_{5/2}$	$7p_{3/2}$	2.3417	2.0760	1.9887	1.6018
$6d_{3/2}$	$5f_{5/2}$	3.5764	2.3879	1.7460	2.1624	$6d_{3/2}$	$5f_{5/2}$	1.6274	0.8798	0.9034	0.9974
$6d_{5/2}$	$5f_{5/2}$	0.9577	0.6708	0.4760	0.5877	$6d_{5/2}$	$5f_{5/2}$	0.4209	0.2479	0.2470	0.2674
$6d_{5/2}$	$5f_{7/2}$	4.4148	3.1076	2.2956	2.7539	$6d_{5/2}$	$5f_{7/2}$	1.9492	1.1353	1.1293	1.2293

$$Z_{wv}^{(2)} = \sum_{na} \frac{z_{an}(g_{wnva} - g_{wnav})}{\varepsilon_a + \varepsilon_v - \varepsilon_n - \varepsilon_w} + \sum_{na} \frac{(g_{wavn} - g_{wanv})z_{na}}{\varepsilon_a + \varepsilon_w - \varepsilon_n - \varepsilon_v}. \quad (8)$$

Second-order Breit corrections are obtained from Eq. (8) by changing g_{ijkl} to b_{ijkl}, where b_{ijkl} is the matrix element of the Breit operator given in [30], but are not very important for the ions considered here.

In the all-order SD calculation, we substitute the all-order SD wave function Ψ_v^{SD} into the matrix element expression given by Eq. (5) and obtain the expression [20]

$$Z_{wv}^{(SD)} = \frac{z_{wv} + Z^{(a)} + \cdots + Z^{(t)}}{\sqrt{(1+N_w)(1+N_v)}}, \quad (9)$$

where z_{wv} is the lowest-order (DF) matrix element given by Eq. (7), and the terms $Z^{(k)}$, $k=a\cdots t$ are linear or quadratic functions of the excitation coefficients introduced in Eq. (4). The normalization terms N_w are quadratic functions of the excitation coefficients. As a result, certain sets of many-body perturbation theory terms are summed to all orders. In contrast to the energy, all-order SD matrix elements contain the entire third-order MBPT contribution.

The calculation of the transition matrix elements provides another test of the quality of atomic-structure calculations and another measure of the size of correlation corrections. Reduced electric-dipole matrix elements between low-lying states of Fr-like systems with $Z=87-92$ calculated in various approximations are presented in Table III.

Our calculations of the reduced matrix elements in the lowest, second, and third orders are carried out following the method described above. The lowest-order DF value is obtained from Eq. (7). The values $Z^{(DF+2)}$ are obtained as the sum of the second-order correlation correction $Z^{(2)}$ given by Eq. (8) and the DF matrix elements $Z^{(DF)}$. The second-order Breit corrections $B^{(2)}$ are rather small in comparison with the second-order Coulomb correction $Z^{(2)}$ (the ratio of $B^{(2)}$ to $Z^{(2)}$ is about 0.2– 2%).

The third-order matrix elements $Z^{(DF+2+3)}$ include the DF values, the second-order $Z^{(2)}$ results, and the third-order $Z^{(3)}$ correlation correction. $Z^{(3)}$ includes random-phase-approximation terms (RPA) iterated to all orders [12].

We find correlation corrections $Z^{(2+3)}$ to be very large, 10–25 %, for many cases. All results given in Table III are obtained using length form of the matrix elements. Length-form and velocity-form matrix elements differ typically by

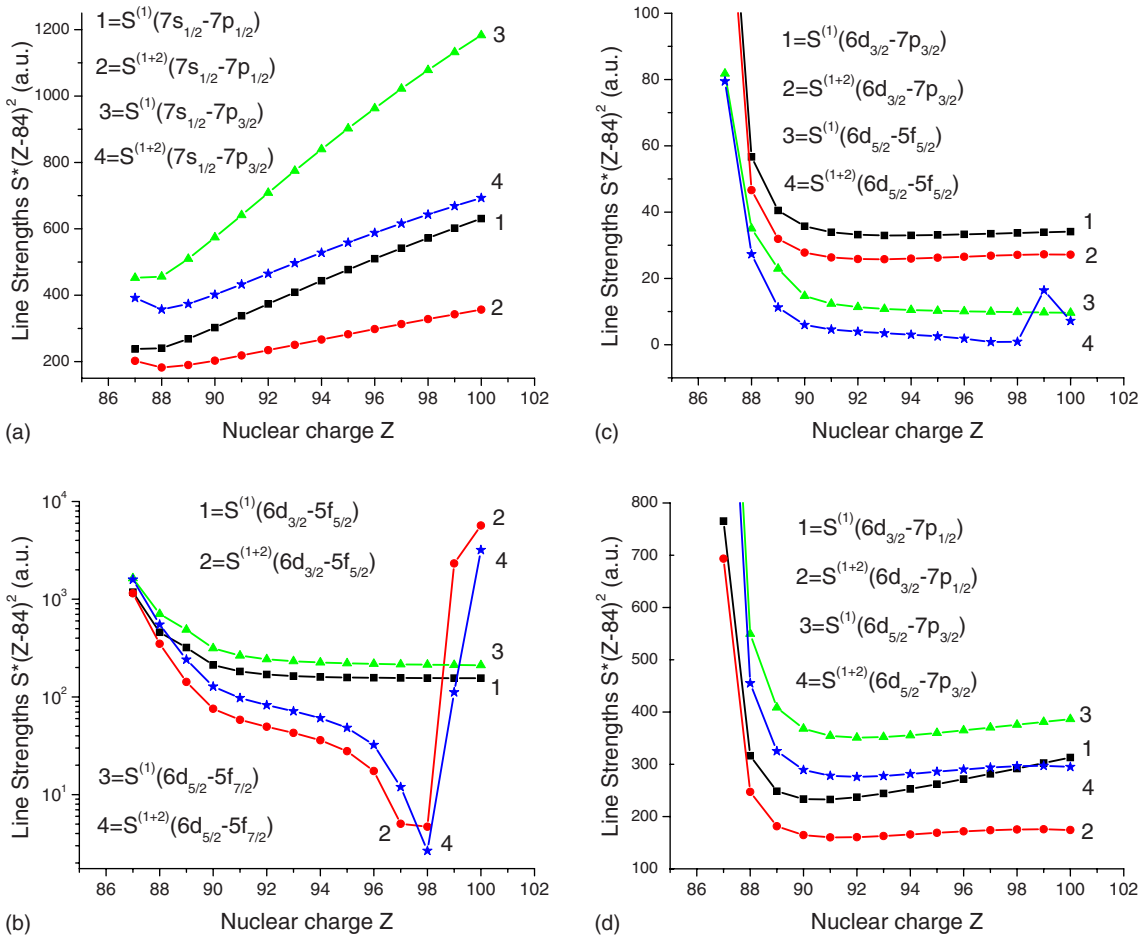

FIG. 5. (Color online) Line strengths $[S\times(Z-84)^2$ in a.u.] as functions of Z in Fr-like ions.

TABLE IV. Comparison of length (L) and velocity (V) results for reduced electric-dipole matrix elements in first, second, and third orders of perturbation theory in Fr-like systems with $Z=87-92$.

	$Z^{(\mathrm{DF})}$		$Z^{(\mathrm{DF+2})}$		$Z^{(\mathrm{DF+2+3})}$		$Z^{(\mathrm{DF})}$		$Z^{(\mathrm{DF+2})}$		$Z^{(\mathrm{DF+2+3})}$	
Ion	L	V	L	V	L	V	L	V	L	V	L	V
	$6d_{3/2}$-$5f_{5/2}$						$6d_{5/2}$-$5f_{7/2}$					
87	11.4529	11.4002	11.2693	11.2693	7.8982	7.8972	13.4863	13.4022	13.2703	13.2703	9.6464	9.6455
88	5.3549	5.1362	4.7603	4.7603	4.4885	4.4839	6.6382	6.3283	5.9720	5.9720	5.7071	5.7056
89	3.5764	3.1632	2.6134	2.6134	0.5254	0.4982	4.4148	3.8730	3.3832	3.3831	0.8484	0.8576
90	2.4281	0.7698	1.6597	1.6595	2.8562	2.9000	2.9557	0.5609	2.1257	2.1255	3.3454	3.3138
91	1.9275	2.0349	1.2702	1.2702	1.4017	1.4122	2.3242	2.4373	1.6097	1.6097	1.7219	1.7100
92	1.6274	1.6199	1.0312	1.0312	1.0559	1.0613	1.9492	1.9305	1.2978	1.2978	1.3024	1.2943
	$6d_{3/2}$-$7p_{1/2}$						$7s_{1/2}$-$7p_{3/2}$					
87	9.2216	9.9449	8.7906	8.7906	6.8407	6.8365	7.0903	6.6425	6.6268	6.6268	5.9488	5.9486
88	4.4462	2.0213	3.9815	3.9816	3.8547	3.8589	5.3395	4.9435	4.7968	4.7969	4.5150	4.5148
89	3.1529	2.3683	2.7533	2.7533	2.6221	2.6238	4.5158	4.1785	3.9641	3.9641	3.8018	3.8016
90	2.5465	2.0531	2.1960	2.1961	2.1074	2.1084	3.9933	3.7030	3.4515	3.4516	3.3434	3.3432
91	2.1785	1.8158	1.8631	1.8631	1.7957	1.7964	3.6173	3.3638	3.0915	3.0915	3.0121	3.0119
92	1.9249	1.6384	1.6343	1.6344	1.5743	1.5748	3.3271	3.1029	2.8190	2.8190	2.7460	2.7458

TABLE V. Wavelengths λ (Å), weighted transition rates gA (s^{-1}), and oscillator strengths gf in Ac III, Th IV, and U VI. The SD data ($gA^{(SD)}$ and $gf^{(SD)}$) are compared with theoretical ($gA^{(HFR)}$ and $gf^{(HFR)}$) values given in Ref. [1]. The numbers in brackets represent powers of 10.

Lower	Upper	$\lambda^{(expt)}$	$gA^{(SD)}$	$gA^{(HFR)}$	$gf^{(SD)}$	$gf^{(HFR)}$
			Ac III, $Z=89$			
$7s_{1/2}$	$7p_{1/2}$	2626.44	1.63[9]	1.55[9]	1.69[+0]	1.6[+0]
$6d_{3/2}$	$7p_{3/2}$	2682.90	1.19[8]	1.23[8]	1.29[−1]	1.3[−1]
$6d_{5/2}$	$7p_{3/2}$	2952.55	9.30[8]	8.23[8]	1.22[+0]	1.1[+0]
$7s_{1/2}$	$7p_{1/2}$	3392.78	3.91[8]	3.59[8]	6.75[−1]	6.2[−1]
$6d_{3/2}$	$7p_{1/2}$	3487.59	3.24[8]	2.75[8]	5.91[−1]	5.0[−1]
$6d_{3/2}$	$5f_{5/2}$	4413.09	1.10[8]	2.34[8]	3.22[−1]	6.9[−1]
$6d_{5/2}$	$5f_{7/2}$	4569.97	1.61[8]	3.02[8]	5.04[−1]	9.5[−1]
$6d_{5/2}$	$5f_{5/2}$	5193.21	4.99[6]	1.03[6]	2.02[−2]	4.2[−2]
			Th IV, $Z=90$			
$6d_{3/2}$	$7p_{3/2}$	1565.86	3.80[8]	4.08[8]	1.40[−1]	1.5[−1]
$6d_{5/2}$	$7p_{3/2}$	1707.37	3.09[9]	2.83[9]	1.35[+0]	1.2[+0]
$6d_{3/2}$	$7p_{1/2}$	1959.02	1.21[9]	1.04[9]	6.98[−1]	6.0[−1]
$7s_{1/2}$	$7p_{3/2}$	2003.00	2.86[9]	2.70[9]	1.72[+0]	1.6[+0]
$7s_{1/2}$	$7p_{1/2}$	2694.81	6.06[8]	5.55[8]	6.60[−1]	6.0[−1]
$5f_{5/2}$	$6d_{5/2}$	6903.05	1.04[6]	2.22[6]	7.45[−3]	1.6[−2]
$5f_{7/2}$	$6d_{5/2}$	9841.54	7.83[6]	1.53[7]	1.14[−1]	2.2[−1]
$5f_{5/2}$	$6d_{3/2}$	10877.55	3.68[6]	7.93[6]	6.53[−2]	1.4[−1]
			U VI, $Z=92$			
$6d_{3/2}$	$7p_{3/2}$	800.729	9.72[8]	1.72[9]	9.34[−2]	1.7[−1]
$6d_{5/2}$	$7p_{3/2}$	866.737	7.98[9]	1.26[10]	8.99[−1]	1.4[+0]
$6d_{3/2}$	$7p_{1/2}$	977.129	5.29[9]	4.87[9]	7.58[−1]	6.9[−1]
$5f_{5/2}$	$6d_{5/2}$	994.921	1.47[8]	3.51[8]	2.18[−2]	5.2[−2]
$5f_{7/2}$	$6d_{5/2}$	1076.40	2.46[9]	5.55[9]	4.26[−1]	9.5[−1]
$5f_{5/2}$	$6d_{3/2}$	1098.91	1.52[9]	3.64[9]	2.75[−1]	6.6[−1]
$7s_{1/2}$	$7p_{3/2}$	1343.39	4.21[9]	6.08[9]	1.14[+0]	1.7[+0]
$7s_{1/2}$	$7p_{1/2}$	1927.05	1.09[9]	1.03[9]	6.05[−1]	5.8[−1]

5–20 % for the DF matrix elements and 2–5 % for the second-order matrix elements in these calculations.

Electric-dipole matrix elements evaluated in the all-order SD approximation are given in columns labeled $Z^{(SD)}$ [Eq. (9)] of Table III. The SD matrix elements $Z^{(SD)}$ include $Z^{(3)}$ completely, along with important fourth- and higher-order corrections. The fourth-order corrections omitted from the SD matrix elements were discussed recently by Derevianko and Emmons [31]. The $Z^{(SD)}$ values are smaller than the $Z^{(DF+2)}$ values and larger than the $Z^{(DF+2+3)}$ values for all transitions given in Table III.

In Fig. 5, we illustrate the Z dependences of the line strengths for the $7s_{1/2}$-$7p_j$, $6d_j$-$7p_{j'}$, and $6d_j$-$5f_{j'}$ transitions. Two sets of line strengths values $S^{(1)}$ and $S^{(1+2)}$ are presented for each transition. The values of $S^{(1)}$ and $S^{(1+2)}$ are obtained as $(Z^{(DF)})^2$ and $(Z^{(DF+2)})^2$, respectively. It should be noted that the values are scaled by $(Z-84)^2$ to provide a better presentation of the line strengths. The difference between $S^{(1)}$ and $S^{(1+2)}$ curves increases with increasing Z; for the $7s_{1/2}$-$7p_{1/2}$ transition, the ratio of the second-order $(S^{(1+2)}$-$S^{(1)})$ and the first-order $(S^{(1)})$ contributions is equal to 15% and 37% for $Z=87$ and 92, respectively.

B. Form-independent third-order transition amplitudes

We calculate electric-dipole reduced matrix elements using the form-independent third-order perturbation theory developed by Savukov and Johnson in Ref. [32], where the precision of this method has been demonstrated for alkali-metal atoms. In this method, form-dependent "bare" amplitudes are replaced with form-independent random-phase-approximation ("dressed") amplitudes to obtain form-independent third-order amplitudes to some degree of accuracy. As in the case of the third-order energy calculation, a limited number of partial waves with $l_{max}<7$ is included. This restriction is not very important for ions considered here because the third-order correction is quite small, but it gives rise to some loss of gauge invariance. The gauge independence serves as a check that no numerical problems occurred.

TABLE VI. Wavelengths λ (Å), weighted transition rates gA (s^{-1}), and oscillator strengths gf in Fr I and Ra II. The SD data ($gA^{(SD)}$ and $gf^{(SD)}$) are compared with theoretical ($gA^{(HFR)}$, $gf^{(HFR)}$) values given in Refs. [1,3] and theoretical ($gA^{(MBPT)}$, $gf^{(MBPT)}$) values given in Ref. [14]. The numbers in brackets represent powers of 10.

Lower	Upper	$\lambda^{(expt)}$	$gA^{(SD)}$	$gA^{(MBPT)}$	$gA^{(HFR)}$	$gf^{(SD)}$	$gf^{(MBPT)}$	$gf^{(HFR)}$
				Fr I, $Z=87$				
$7s_{1/2}$	$7p_{3/2}$	7181.84	1.88[8]			1.45[+0]	1.46[+0]	1.5[+0]
$7s_{1/2}$	$7p_{1/2}$	8171.66	6.75[7]			6.76[−1]	6.84[−1]	6.5[−1]
$7p_{1/2}$	$7d_{3/2}$	8328.18	4.39[7]			4.57[−1]	4.40[−1]	6.9[−1]
$7p_{3/2}$	$7d_{5/2}$	9606.79	8.83[7]			1.22[+0]	1.18[+0]	1.1[+0]
$7p_{3/2}$	$7d_{3/2}$	9689.14	1.08[7]			1.52[−1]	1.49[−1]	1.2[−1]
$7p_{1/2}$	$8s_{1/2}$	13342.0	1.49[7]			3.99[−1]		
$7p_{3/2}$	$8s_{1/2}$	17216.1	2.18[7]			9.70[−1]		
				Ra II, $Z=88$				
$6d_{3/2}$	$5f_{5/2}$	2708.96	2.02[9]		1.59[9]	2.22[+0]		1.7[+0]
$6d_{5/2}$	$5f_{7/2}$	2813.76	2.89[9]		2.01[9]	3.43[+0]		2.4[+0]
$6d_{5/2}$	$5f_{5/2}$	2836.46	1.38[8]		9.80[7]	1.66[−1]		1.2[−1]
$7s_{1/2}$	$7p_{3/2}$	3814.42	7.42[8]	7.30[8]	7.14[8]	1.62[+0]	1.59[+0]	1.5[+0]
$7s_{1/2}$	$7p_{1/2}$	4682.28	2.09[8]	2.05[8]	1.93[8]	6.87[−1]	6.73[−1]	6.3[−1]
$6d_{3/2}$	$7p_{3/2}$	7077.95	1.30[7]	1.29[7]	1.27[7]	9.80[−2]	9.70[−2]	9.5[−2]
$6d_{5/2}$	$7p_{3/2}$	8019.70	9.13[7]	9.10[7]	7.85[7]	8.81[−1]	8.78[−1]	7.6[−1]
$6d_{3/2}$	$7p_{1/2}$	10788.2	2.05[7]	2.03[7]	1.79[7]	3.58[−1]	3.54[−1]	3.1[−1]

Length- and velocity-form matrix elements from DF, second-order (RPA), and third-order calculations are given in Table IV for the limited number of transitions in Fr-like systems with $Z=87-100$. The $Z^{(DF)}$ values differ in L and V forms by 2–15 % for the p-s transitions. The very large $L-V$ difference (by a factor of 2–3) is observed in the $Z^{(DF)}$ values for d-f transitions as illustrated in Table IV. The second-order RPA contribution removes this difference in $L-V$ values, and the L and V columns with the $Z^{(DF+2)}$ headings are almost identical. There are, however, small $L-V$ differences (0.002–0.2 %) in the third-order matrix elements. These remaining small differences can be explained by limitation in the number of partial waves taken into account in the third-order matrix element evaluations as already discussed in the previous section describing the energy calculations.

TABLE VII. Lifetimes τ in ns for the nl levels for neutral francium. Our SD results are compared with experimental measurements presented in Ref. [8] for the $7p_j$ levels, in Ref. [9] for the $7d_j$ levels, and in Ref. [11] for the $8s_{1/2}$ level.

Level	$\tau^{(SD)}$	$\tau^{(expt)}$
$7p_{1/2}$	29.62	29.45±0.11
$7p_{3/2}$	21.28	21.02±0.11
$7d_{3/2}$	73.08	73.6±0.3
$7d_{5/2}$	67.93	67.7±2.9
$8s_{1/2}$	54.36	53.30±0.44

C. Oscillator strengths, transition rates, and lifetimes

We calculate oscillator strengths and transition probabilities for the eight $7s$-$7p$, $7p$-$6d$, and $6d$-$5f$ electric-dipole transitions in Ra II, Ac III, Th IV, U VI, and for the seven $7s$-$7p$, $7p$-$7d$, and $7p$-$8s$ electric-dipole transitions in Fr I. Wavelengths λ (Å), weighted transition rates gA (s^{-1}), and oscillator strengths gf for Ac III, Th IV, and U VI ions are given in Table V and for Ra II and Fr I are given in Table VI.

The SD data ($gA^{(SD)}$ and $gf^{(SD)}$) are compared with theoretical ($gA^{(HFR)}$ and $gf^{(HFR)}$) results from Ref. [1]. The experimental energies were used to calculate the $gA^{(SD)}$, $gf^{(SD)}$, $gA^{(HFR)}$, and $gf^{(HFR)}$. Therefore, we really compare the values of the electric-dipole matrix elements. The SD and HFR results for s-p and p-d transitions disagree by about 6–25 % with the exception of the $6d_j$-$7p_{3/2}$ transitions where disagreement is 60%. The largest disagreement (by a factor of 2–5) is observed between the SD and HFR results for the f-d transitions. The correlation corrections are especially large for these transitions as illustrated in Table III. Therefore, we expect that our values, which include correlation correction in a rather complete way, will disagree with HFR calculations, which appear not to include any correlation effects for transitions which involve $5f$ states. Our conclusion is confirmed by comparison of the $gA^{(HFR)}$ and $gf^{(HFR)}$ and our $gA^{(DF)}$ and $gf^{(DF)}$ results (see also Ref [17]). Our values for transition rates and oscillator strengths are in reasonable agreement (10–20 %) with HFR data.

The SD data $gA^{(SD)}$ and $gf^{(SD)}$ for Fr I and Ra II given in Table VI are compared with theoretical data ($gA^{(HFR)}$, $gf^{(HFR)}$) given in Refs. [1,3] and theoretical

($gA^{(\mathrm{MBPT})}$ and $gf^{(\mathrm{MBPT})}$) values from Ref. [14]. The wavelengths $\lambda^{(\mathrm{expt})}$ given in Table VI are taken from NIST compilation [6] for Ra II and from Ref. [2] [$E(7p_{1/2})=12\,237.409\ \mathrm{cm}^{-1}$, $E(7p_{3/2})=13\,923.998\ \mathrm{cm}^{-1}$], Ref. [4] [$E(8s_{1/2})=19\,732.523\ \mathrm{cm}^{-1}$], and Ref. [5] [$E(7d_{3/2})=24\,244.831\ \mathrm{cm}^{-1}$ and $E(7d_{5/2})=24\,333.298\ \mathrm{cm}^{-1}$] for Fr I. Comparison of the gf and gA results obtained by three different approximations shows better agreement between our SD and MBPT [14] results than between our results and HFR results obtained by Biémont *et al.* in Refs. [1,3], owing to a more complete treatment of correlation in our calculation and in Ref. [14].

Our SD lifetime results are compared in Table VII with experimental measurements presented in Refs. [8,9,11] for the $7p_j$, $7d_j$, $8s_{1/2}$ levels in neutral francium. We find that our SD lifetimes are in excellent agreement with precise measurements provided in Refs. [8,9,11].

IV. MULTIPOLE MATRIX ELEMENTS, TRANSITION RATES, AND LIFETIMES IN Fr-LIKE IONS

Reduced matrix elements of the electric-quadrupole ($E2$) and magnetic-multipole ($M1$, $M2$, and $M3$) operators in lowest, second, third, and all orders of perturbation theory are given in Table VIII for Fr-like ions with $Z=88-92$. Detailed descriptions of the calculations of the multipole matrix elements in lowest and second orders of perturbation theory were given in Refs. [29,33,34]. Third-order and all-order calculations are carried out using the same method as the calculations of $E1$ matrix elements. In Table VIII, we present $E2$, $M1$, and $M3$ matrix elements in the $Z^{(\mathrm{DF})}$, $Z^{(\mathrm{DF+2})}$, $Z^{(\mathrm{DF+2+3})}$, and $Z^{(\mathrm{SD})}$ approximations for the $6d_j$-$7s_{1/2}$ transitions in Ra II and Ac III and the $M1$, $E2$ $5f_{5/2}$-$5f_{7/2}$ transition in Th IV, Pa V, and U VI. We already mentioned that the ground state in Ra II and Ac III is the $7s_{1/2}$ state with the $6d_{3/2}$ state being the next lowest states; however, the ground state in Th IV, Pa V, and U VI is the $5f_{5/2}$ state with the $5f_{7/2}$ being the next lowest state. The second-order contribution is about 1–3 % for all transitions involving the $7s_{1/2}$ states. For the $5f_{5/2}$-$5f_{7/2}$ transition, the second-order contribution (Coulomb and Breit) is very small (0.1%) for the $M1$ transition and is rather large (20%) for the $E2$ transition.

In Fig. 6, we illustrate the Z dependences of the line strengths for the $5f_{5/2}$-$5f_{7/2}$, $6dj$-$7s_{1/2}$, and $5f_j$-$7s_{1/2}$ transitions. Two sets of line strengths calculated in first- and second-order approximations are presented for each transition. The values of $S^{(1)}$ and $S^{(1+2)}$ are obtained as $(Z^{(\mathrm{DF})})^2$ and $(Z^{(\mathrm{DF+2})})^2$, respectively. The difference between $S^{(1)}$ and $S^{(1+2)}$ curves increases with increasing Z. For the $5f_{5/2}$-$5f_{7/2}$ transition, the ratio of the second-order $(S^{(1+2)}$-$S^{(1)})$ and the first-order $(S^{(1)})$ contributions is equal to 18% and 67% for $Z=89$ and 95, respectively.

Strong irregularities occur in the curves describing the second-order contributions [see, for example, $S^{(1+2)}(5f_j-7s_{1/2})$ for $Z=96$ and $S^{(1+2)}(6d_{3/2}-7s_{1/2})$ for $Z=95$, 99]. Those sharp features are explained by accidentally small energy denominators in MBPT expressions for correlation corrections as discussed above.

TABLE VIII. Reduced matrix elements of the electric-quadrupole ($E2$) and magnetic-multipole ($M1$ and $M3$) operators in first, second, third, and all orders of perturbation theory in Fr-like ions.

	Transition		$Z^{(\mathrm{DF})}$	$Z^{(\mathrm{DF+2})}$	$Z^{(\mathrm{DF+2+3})}$	$Z^{(\mathrm{SD})}$
			Ra II, $Z=88$			
$M3$	$6d_{5/2}$	$7s_{1/2}$	128.8000	131.1100	128.7695	120.0000
$E2$	$6d_{3/2}$	$7s_{1/2}$	17.2630	17.0350	13.7518	14.5885
$E2$	$6d_{5/2}$	$7s_{1/2}$	21.7710	21.5580	17.8089	18.6906
$M1$	$6d_{3/2}$	$7s_{1/2}$	0.0000	0.0008	0.0189	0.0014
			Ac III, $Z=89$			
$M3$	$6d_{5/2}$	$7s_{1/2}$	80.7820	82.9520	81.2050	76.2511
$E2$	$6d_{3/2}$	$7s_{1/2}$	10.6820	10.4410	9.2237	9.5149
$E2$	$6d_{5/2}$	$7s_{1/2}$	13.6550	13.4270	11.9668	12.2808
$M1$	$6d_{3/2}$	$7s_{1/2}$	0.0000	0.0015	0.0203	0.0013
			Th IV, $Z=90$			
$M1$	$5f_{5/2}$	$5f_{7/2}$	1.8506	1.8525	1.8390	1.8514
$E2$	$5f_{5/2}$	$5f_{7/2}$	1.5669	1.2339	0.9724	1.0834
			Pa V, $Z=91$			
$M1$	$5f_{5/2}$	$5f_{7/2}$	1.8505	1.8520	1.8421	1.8513
$E2$	$5f_{5/2}$	$5f_{7/2}$	1.1348	0.8203	0.7033	0.7613
			U VI, $Z=92$			
$M1$	$5f_{5/2}$	$5f_{7/2}$	1.8505	1.8518	1.8443	1.8512
$E2$	$5f_{5/2}$	$5f_{7/2}$	0.9153	0.6205	0.5413	0.5864

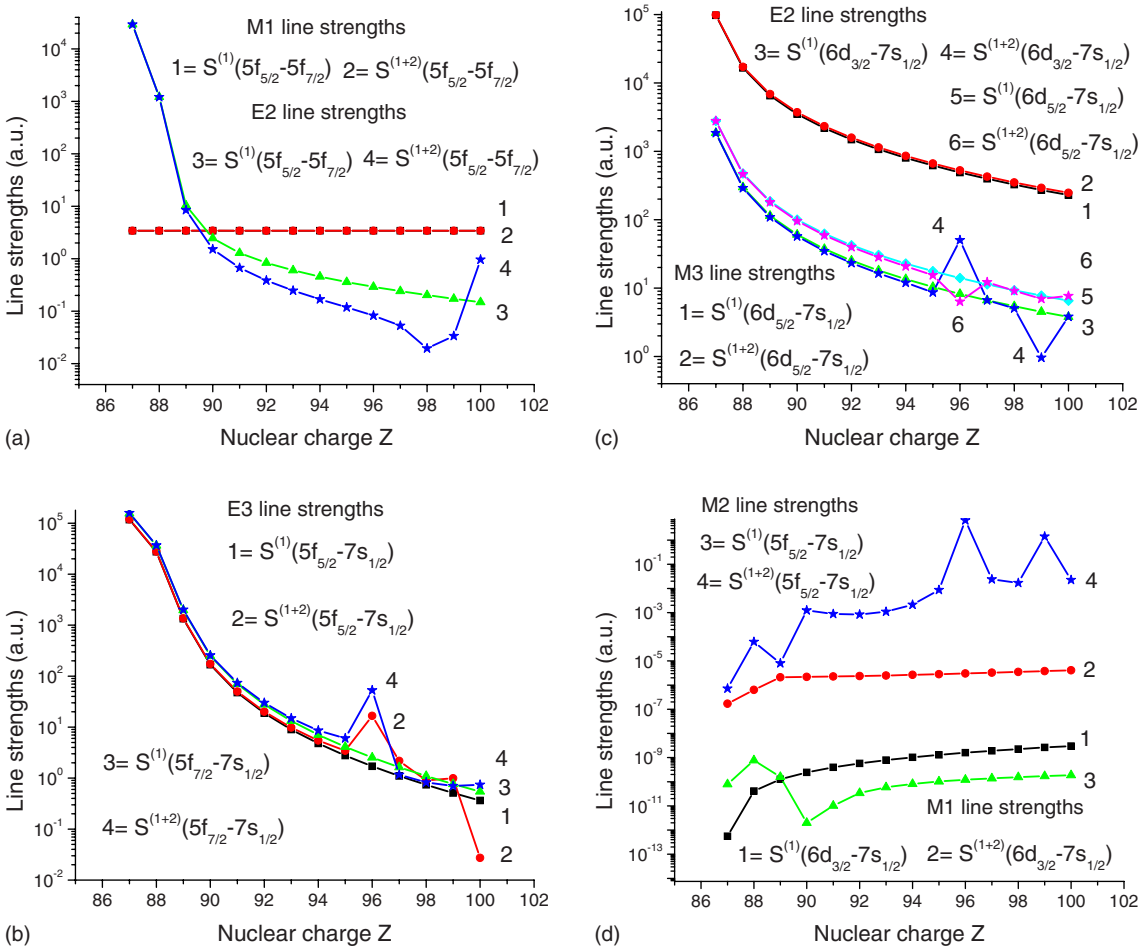

FIG. 6. (Color online) Multipole line strengths (S in a.u.) as functions of Z in Fr-like ions.

Wavelengths and transition rates $A^{(SD)}$ for the electric quadrupole ($E2$) and magnetic-multipole ($M1$ and $M3$) transitions in Ra II, Ac III, Th IV, and U VI calculated in the SD approximation are presented in Table IX. The largest contribution to the lifetime of the $6d_j$ state in Ra II and Ac III ions comes from the $E2$ transition, but the largest contribution to the lifetime of the $5f_{7/2}$ state in Th IV [17] and U VI ions comes the from the $M1$ transition. Our SD result for the $M1$ matrix element in the Th IV [17] ion agrees to 0.5% with HFR results obtained by Biémont *et al.* in Ref. [1] since the correlation is small for $M1$ transition.

Finally, we find that the lifetime of the $6d_{3/2}$ state is equal to 0.651 s in Ra II and 9.50×10^5 s in Ac III; the lifetime of the $6d_{3/2}$ state is equal to 0.313 s in Ra II and 271 s in Ac III. The lifetime of the $5f_{7/2}$ state is equal to 1.07 s in Th IV and 0.196 s in U VI.

TABLE IX. Wavelengths λ (Å) and transition rates $A^{(SD)}$ (s^{-1}) of the electric-quadrupole ($E2$) and magnetic-multipole ($M1$ and $M3$) transitions in Ra II, Ac III, Th IV, and U VI calculated in the SD approximation. The numbers in brackets represent powers of 10.

	Transition		λ	$A^{(SD)}$	λ	$A^{(SD)}$
			Ra II, $Z=88$		Ac III, $Z=89$	
$E2$	$7s_{1/2}$	$6d_{3/2}$	8275.145	1.536[+00]	124844.	1.053[−06]
$E2$	$7s_{1/2}$	$6d_{5/2}$	7276.373	3.197[+00]	23787.4	3.696[−03]
$M3$	$7s_{1/2}$	$6d_{5/2}$	7276.373	6.988[−07]	23787.4	7.070[−11]
$M1$	$7s_{1/2}$	$6d_{3/2}$	8275.145	2.281[−05]	124844.	4.354[−13]
			Th IV, $Z=90$		U VI, $Z=90$	
$M1$	$5f_{5/2}$	$5f_{7/2}$	23119.6	9.352[−01]	13143.0	5.089[+00]
$E2$	$5f_{5/2}$	$5f_{7/2}$	23119.6	2.487[−05]	13143.0	1.227[−04]

TABLE X. Contributions to the $7s_{1/2}$ static polarizabilities (a.u.) of Fr I, Ra II, and Ac III.

$v=7s_{1/2}$	Fr I	Ra II	Ac III
$\alpha_v^{\text{main}}(7p)$	289.24	93.08	46.74
$\alpha_v^{\text{main}}(8p)$	3.02	0.23	0.06
$\alpha_v^{\text{main}}(9p)$	0.54	0.03	
$\alpha_v^{\text{main}}(10p)$	0.19		
α_v^{main}	292.99	93.34	46.80
α_v^{tail}	1.20	0.11	0.04
α_c	20.40	13.79	11.42
α_{vc}	−0.95	−0.74	−0.54
α_v^{SD}	313.7	106.5	57.71

V. GROUND STATE STATIC POLARIZABILITIES FOR Fr-LIKE IONS

The static polarizability of Fr-like ions can be calculated as the sum of the polarizability of the ionic core α_c, a counterterm α_{vc} compensating for excitations from the core to the valence shell, which violates the Pauli principle, and a valence electron contribution α_v as follows:

$$\alpha = \alpha_c + \alpha_v + \alpha_{vc}. \tag{10}$$

These contributions are given by formulas listed, for example, in Refs. [35,36]. We calculate α_c in the relativistic RPA approximation (see Ref. [37]).

The $7s_{1/2}$ state is the ground state in the cases of Fr I, Ra II, and Ac III, and the corresponding polarizability terms are given by

$$\alpha_v = \sum_{n=7}^{N} [I_v(np_{1/2}) + I_v(np_{3/2})],$$

$$\alpha_{vc} = \sum_{n=2}^{6} [I_v(np_{1/2}) + I_v(np_{3/2})], \tag{11}$$

where

$$I_v(nlj) = \frac{2}{3(2j+1)} \frac{(Z_{v,nlj})^2}{E_{nlj} - E_v}, \tag{12}$$

and N is the size of the B-spline basis set ($N=50$ in this calculation). The calculation of the α_v is divided into two parts as follows:

$$\alpha_v^{\text{main}} = \sum_{n=7}^{k} [I_v(np_{1/2}) + I_v(np_{3/2})],$$

$$\alpha_v^{\text{tail}} = \sum_{n=k+1}^{N} [I_v(np_{1/2}) + I_v(np_{3/2})]. \tag{13}$$

Here, k is equal to 10, 9, and 8 for Fr I, Ra II, and Ac III. The values of α_v^{main} are calculated using SD values of dipole matrix elements $Z_{v,nlj}$ and experimental energies where they are available. We used SD energies when we did not find experimental data. The α_v^{tail} and α_c contributions are small and are calculated in the DF approximation.

TABLE XI. Contributions to the $5f_{5/2}$ static polarizabilities (a.u.) of Th IV calculated in the third-order—(a) and all-order—(b) approximations.

$v=5f_{5/2}$	$\alpha^{(a)}$	$\alpha^{(b)}$
$\alpha_v^{\text{main}}(6d)$	4.961	6.491
$\alpha_v^{\text{main}}(7d)$	0.009	0.015
$\alpha_v^{\text{main}}(8d)$	0.005	0.007
$\alpha_v^{\text{main}}(5g_{7/2})$	0.063	0.078
$\alpha_v^{\text{main}}(6g_{7/2})$	0.023	0.023
α_v^{main}	5.062	6.612
α_v^{tail}	0.762	0.762
α_c	7.750	7.750
α_{vc}	−0.050	−0.050
α_v	13.52	15.07

Our numerical results are given in Table X. The sum over n in the main polarizability term given by Eq. (13) converges faster for Ac III than for Fr I. The ratios of the second and first terms in the sum over n are equal to 1% for Fr I and only 0.1% for Ac III. Therefore, fast convergence allows us to limit the number of n in Eq. (13) to $n=8$ in Ac III, since we have no experimental energy values for high n for this ion.

Our SD results for α_{7s}^{SD} given in the last line of Table X are in good agreement with the recommended value (317.7±2.4) for Fr given by Derevianko *et al.* in Ref. [38] and the recommended value (104.0) for Ra II given recently by Lim and P. Schwerdtfeger in Ref. [39]. We did not find any data for α_{7s}^{SD} in Ac III. Our ionic core polarizabilities α_c given in Table X are in an excellent agreement with recommended values (20.4 in Fr I and 13.7 in Ra II) presented in Refs. [38,39].

The valence polarizability for the $5f_{5/2}$ state, which is the ground state in the case of Fr-like ions with $Z \geq 90$, is given by [17]

$$\alpha_v = \sum_{n=n_0}^{N} [I_v(nd_{3/2}) + I_v(nd_{5/2}) + I_v(ng_{7/2})]. \tag{14}$$

Here, n_0 equal to 6 for the nd states and 5 for the ng states.

We use the same designations as we used for the $7s_{1/2}$ polarizability given by Eqs. (10)–(13). Our results are listed in Table XI. The third-order (DF+2+3) and SD dipole matrix elements (a.u.) are calculated with 50 splines and cavity radius $R=45$ for Th IV. We use experimental energies [2] to calculate α_v^{main} in Table XI. Both third-order and all-order results for the dipole polarizability of Th IV in the ground state $5f_{5/2}$ are presented in Table XI (see also Ref. [17]). We see from this table that the largest contribution to the α_v^{main} term comes from $6d$ states [$\alpha_v^{\text{main}}(6d)$]. The core contribution ($\alpha_c=7.750\ a_0^3$) is larger than the main term, limiting the accuracy of our calculations. The α_v^{tail} and α_{vc} terms calculated in the DF approximation contribute only 5% to the final re-

TABLE XII. Contributions to the $5f_{5/2}$ static polarizabilities (a.u.) in Fr-like ions with $Z=91-100$ calculated in the DF—(*a*), second-order—(*b*), and RPA—(*c*) approximations.

	$Z=91$	$Z=92$	$Z=93$	$Z=94$	$Z=95$	$Z=96$	$Z=97$	$Z=98$	$Z=99$	$Z=100$
$\alpha_v^{\text{main}}(a)$	3.072	1.035	0.548	0.356	0.258	0.199	0.158	0.129	0.106	0.089
$\alpha_v^{\text{main}}(b)$	2.050	0.415	5.935	0.187	0.128	0.083	0.076	0.237	0.120	0.089
$\alpha_v^{\text{tail}}(a)$	0.367	0.206	0.119	0.067	0.036	0.018	0.009	0.005	0.003	0.010
$\alpha_{vc}(a)$	−0.048	−0.044	−0.040	−0.037	−0.033	−0.030	−0.028	−0.025	−0.023	−0.021
$\alpha_c(a)$	7.236	5.977	5.023	4.279	3.687	3.207	2.813	2.484	2.207	1.971
$\alpha_c(c)$	6.166	5.029	4.182	3.534	3.024	2.615	2.281	2.006	1.776	1.582
$\alpha_v^{(\text{DF})}$	10.627	7.174	5.649	4.665	3.948	3.394	2.952	2.593	2.293	2.049
$\alpha_v^{(\text{DF+2})}$	8.535	5.606	10.197	3.751	3.155	2.686	2.338	2.223	1.876	1.660

sults. No experimental data are available for the Th IV polarizability.

The $5f_{5/2}$ ground state polarizabilities for Fr-like ions with $Z=91-100$ are given in Table XII. Results are obtained in DF and second-order MBPT approximations. The contribution of the $5g_{7/2}$ state into the $\alpha_{5f_{5/2}}$ polarizability increases with increasing Z; 1% for the ion with $Z=90$ (Th IV), 19% for the ion with $Z=92$ (U VI), and 30% for the ion with $Z=95$ (Am IX). The main contributions are smaller than the core contributions. The calculations are conducted only in second-order approximation for these ions, owing to problems with accidentally very small denominators in the corresponding calculations of the properties involving $5g$ state. We mentioned previously that the core values $\alpha_c(c)$ are calculated in the relativistic RPA approximation, following the method described by Johnson *et al.* in Ref. [37]. Values of the core-polarizability $\alpha_c(c)$ from the present calculation disagree with results for Ra II-U VI given by Biémont *et al.* in Table I of Ref. [1], however, for Ra II, the present value agrees with the result given in Ref. [39].

VI. CONCLUSION

In summary, a systematic relativistic MBPT study of the atomic properties of the $7s_{1/2}$, $7p_j$, $6d_j$, and $5f_j$ states in Fr-like ions with nuclear charges $Z=87-100$ is presented. The energy values are in good agreement with available experimental energy data and provide a theoretical reference database for the line identification. A systematic all-order SD study of the reduced matrix elements and transition rates for eight $7s$-$7p$, $7p$-$6d$, and $6d$-$5f$ electric-dipole transitions is conducted. Multipole matrix elements ($7s_{1/2}$-$6d_j$, $7s_{1/2}$-$5f_j$, and $5f_{5/2}$-$5f_{7/2}$) are evaluated to obtain the lifetime data for the $6d_{3/2}$ and the $5f_{7/2}$ excited states. The scalar polarizabilities for the $7s_{1/2}$ ground state in Fr I, Ra II, and Ac III and the $5f_{5/2}$ ground state in Th IV are calculated using relativistic third-order and all-order methods. The scalar polarizabilities for Fr-like ions with nuclear charge $Z=90-100$ in the $5f_{5/2}$ ground state are calculated using relativistic second-order MBPT. These calculations provide a theoretical benchmark for comparison with experiment and theory.

ACKNOWLEDGMENTS

The work of W.R.J. and U.I.S. was supported in part by National Science Foundation Grant No. PHY-04-56828. The work of M.S.S. was supported in part by National Science Foundation Grant No. PHY-04-57078.

[1] E. Biémont, V. Fivet, and P. Quinet, J. Phys. B **37**, 4193 (2004).
[2] J. Blaise and J. Wyart, *Selected Constants: Energy Levels and Atomic Spectra of Actinides*, http://www.lac.u-psud.fr/Database/Contents.html
[3] E. Biémont, P. Quinet, and V. Van Renterghem, J. Phys. B **31**, 5301 (1998).
[4] J. E. Simsarian, W. Z. Zhao, L. A. Orozco, and G. D. Sprouse, Phys. Rev. A **59**, 195 (1999).
[5] J. M. Grossman, R. P. Fliller III, T. E. Mehlstäubler, L. A. Orozco, M. R. Pearson, G. D. Sprouse, and W. Z. Zhao, Phys. Rev. A **62**, 052507 (2000).
[6] http://physics.nist.gov/PhysRefData/Handbook/Tables/radiumtable6.htm
[7] W. Z. Zhao, J. E. Simsarian, L. A. Orozco, W. Shi, and G. D. Sprouse, Phys. Rev. Lett. **78**, 4169 (1997).
[8] J. E. Simsarian, L. A. Orozco, G. D. Sprouse, and W. Z. Zhao, Phys. Rev. A **57**, 2448 (1998).
[9] J. M. Grossman, R. P. Fliller III, L. A. Orozco, M. R. Pearson, and G. D. Sprouse, Phys. Rev. A **62**, 062502 (2000).
[10] S. Aubin, E. Gomez, L. A. Orozco, and G. D. Sprouse, Opt. Lett. **28**, 2055 (2003).
[11] E. Gomez, L. A. Orozco, A. Perez Galvan, and G. D. Sprouse, Phys. Rev. A **71**, 062504 (2005).
[12] W. R. Johnson, Z. W. Liu, and J. Sapirstein, At. Data Nucl. Data Tables **64**, 279 (1996).
[13] V. A. Dzuba, V. V. Flambaum, and O. P. Sushkov, Phys. Rev. A **51**, 3454 (1995).
[14] V. A. Dzuba, V. V. Flambaum, and J. S. M. Ginges, Phys. Rev. A **63**, 062101 (2001).
[15] M. S. Safronova, W. R. Johnson, and A. Derevianko, Phys. Rev. A **60**, 4476 (1999).

[16] M. S. Safronova and W. R. Johnson, Phys. Rev. A **62**, 022112 (2000).
[17] U. I. Safronova, W. R. Johnson, and M. S. Safronova, Phys. Rev. A **74**, 042511 (2006).
[18] I. M. Savukov, W. R. Johnson, U. I. Safronova, and M. S. Safronova, Phys. Rev. A **67**, 042504 (2003).
[19] J. Sucher, Phys. Rev. A **22**, 348 (1980).
[20] S. A. Blundell, W. R. Johnson, Z. W. Liu, and J. Sapirstein, Phys. Rev. A **40**, 2233 (1989).
[21] Z. W. Liu, Ph.D. thesis, Notre Dame University, 1989 (unpublished).
[22] S. A. Blundell, W. R. Johnson, and J. Sapirstein, Phys. Rev. A **43**, 3407 (1991).
[23] M. S. Safronova, A. Derevianko, and W. R. Johnson, Phys. Rev. A **58**, 1016 (1998).
[24] U. I. Safronova and W. R. Johnson, Phys. Rev. A **69**, 052511 (2004).
[25] M. S. Safronova, W. R. Johnson, and U. I. Safronova, Phys. Rev. A **53**, 4036 (1996).
[26] M. S. Safronova, W. R. Johnson, and U. I. Safronova, J. Phys. B **30**, 2375 (1997).
[27] W. R. Johnson, S. A. Blundell, and J. Sapirstein, Phys. Rev. A **37**, 307 (1988).
[28] S. A. Blundell, D. S. Guo, W. R. Johnson, and J. Sapirstein, At. Data Nucl. Data Tables **37**, 103 (1987).
[29] W. R. Johnson, D. R. Plante, and J. Sapirstein, Adv. At., Mol., Opt. Phys. **35**, 255 (1995).
[30] W. R. Johnson, S. A. Blundell, and J. Sapirstein, Phys. Rev. A **37**, 2764 (1988).
[31] A. Derevianko and E. D. Emmons, Phys. Rev. A **66**, 012503 (2002).
[32] I. M. Savukov and W. R. Johnson, Phys. Rev. A **62**, 052512 (2000).
[33] U. I. Safronova, W. R. Johnson, D. Kato, and S. Ohtani, Phys. Rev. A **63**, 032518 (2001).
[34] S. M. Hamasha, A. S. Shlyaptseva, and U. I. Safronova, Can. J. Phys. **82**, 331 (2004).
[35] T. R. Fowler and J. Yellin, Phys. Rev. A **1**, 1006 (1970).
[36] M. S. Safronova and C. W. Clark, Phys. Rev. A **69**, 040501(R) (2004).
[37] W. R. Johnson, D. Kolb, and K.-N. Huang, At. Data Nucl. Data Tables **28**, 333 (1983).
[38] A. Derevianko, W. R. Johnson, M. S. Safronova, and J. F. Babb, Phys. Rev. Lett. **82**, 3589 (1999).
[39] I. S. Lim and P. Schwerdtfeger, Phys. Rev. A **70**, 062501 (2004).