Excitation energies, polarizabilities, multipole transition rates, and lifetimes in Th IV

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, 223 Sharp Lab, University of Delaware, Newark, Delaware 19716, USA
(Received 17 August 2006; published 24 October 2006)

Excitation energies of the $ns_{1/2}$ (n=7–10), np_j (n=7–9), nd_j (n=6–8), nf_j (n=5–7), and ng_j (n=5,6) states in Th IV are evaluated. First-, second-, third-, and all-order Coulomb energies and first- and second-order Coulomb-Breit energies are calculated. Reduced matrix elements, oscillator strengths, transition rates, and lifetimes are determined for the 96 possible nl_j-$n'l'_{j'}$ electric-dipole transitions. 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 lifetimes of the $5f_{7/2}$ and $7s_{1/2}$ states. Matrix elements are calculated using both relativistic many-body perturbation theory, complete through third order, and a relativistic all-order method restricted to single and double excitations. Scalar and tensor polarizabilities for the $5f_{5/2}$ ground state in Th^{3+} are calculated using relativistic third-order and all-order methods. These calculations provide a theoretical benchmark for comparison with experiment and theory.

DOI: 10.1103/PhysRevA.74.042511 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 ($E1$) transitions in Fr-like ions with Z =89–92 was presented recently by Biémont *et al.* [1], where relativistic Hartree-Fock and Dirac-Fock atomic structure codes were used to calculate transition rates and oscillator strengths for a limited number of transitions using experimental energies given by Blaise and Wyart [2]. In the compilation [2], experimental energies are given for 56 levels of neutral Fr, 24 levels of Fr-like Th, and seven levels of Fr-like Ac and U. Experimental energies for 13 levels of Fr-like Ra were reported in the NIST compilation [3].

Lifetime measurements for the $7p_j$, $6d_j$, $9s_{1/2}$, and $8s_{1/2}$ levels of neutral francium were presented in Refs. [4–8]. In those papers, experimental measurements were compared with *ab initio* calculations performed by Johnson *et al.* [9], by Dzuba *et al.* [10,11], by Safronova *et al.* [12], and by Safronova and Johnson [13]. Third-order many-body perturbation theory was used in Ref. [9] to obtain $E1$ transition amplitudes for neutral alkali-metal atoms. The correlation potential method and the Feynman diagram technique were used in Refs. [10,11] to calculate $E1$ dipole matrix elements in neutral francium and in Fr-like radium. Calculations of atomic properties of alkali-metal atoms in Refs. [12,13] were based on the relativistic single-double (SD) approximation in which single and double excitations of Dirac-Fock wave functions were included in all orders in perturbation theory.

In the present paper, relativistic many-body perturbation theory (RMBPT) is used to determine energies, matrix elements, oscillator strengths, and transition rates for multipole transitions in Fr-like thorium. These calculations start from a radonlike closed-shell Dirac-Fock (DF) potential. It should be noted that Th IV is the first ion in the francium isoelectronic sequence with a [Rn]$5f_{5/2}$ ground state instead of a [Rn]$7s_{1/2}$ ground state, as for Fr I, Ra II, and Ac III. Correlation corrections become very important for such systems as was recently demonstrated by Savukov *et al.* [14], where it was shown that the ratio of the second-order to lowest-order removal energy for the [Xe]$4f_{5/2}$ ground state in Ce IV and Pr V is 18% and 11%, respectively.

We calculate excitation energies of $ns_{1/2}$ (n=7–10), np_j (n=7–9), nd_j (n=6–8), nf_j (n=5–7), and ng_j (n=5,6) states in Fr-like thorium. Reduced matrix elements, oscillator strengths, transition rates, and lifetimes are determined for the 96 possible nl_j-$n'l'_{j'}$ electric-dipole transitions. 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 lifetimes of $5f_{7/2}$ and $7s_{1/2}$ states. Scalar and tensor polarizabilities of the $5f_{5/2}$ ground state of Th^{3+} are also calculated. 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 excitations. Such calculations permit one to investigate the convergence of perturbation theory and estimate the error in theoretical data.

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

As mentioned in the Introduction, we carry out all of the calculations in this work using two methods, third-order MBPT, described in [9], and the relativistic all-order SD method, described in [15,16] and references therein. The SD method includes correlation corrections in a more complete

*Email address: usafrono@nd.edu
†URL: www.nd.edu/~johnson. Email address: johnson@nd.edu
‡Email address: msafrono@udel.edu

 ©2006 The American Physical Society

TABLE I. Zeroth- (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 Th IV. The total energies ($E^{(3)}_{\mathrm{tot}}=E^{(0)}+E^{(2)}+E^{(3)}+B^{(1)}+B^{(2)}+E_{\mathrm{LS}}$, $E^{\mathrm{SD}}_{\mathrm{tot}}=E^{(0)}+E^{\mathrm{SD}}+E^{(3)}_{\mathrm{extra}}+B^{(1)}+B^{(2)}+E_{\mathrm{LS}}$) for Th IV are compared with experimental energies E_{expt} [2], $\delta E=E_{\mathrm{tot}}-E_{\mathrm{expt}}$. Units: cm^{-1}.

nlj	$E^{(0)}$	$E^{(2)}$	$E^{(3)}$	$B^{(1)}$	$B^{(2)}$	E_{LS}	$E^{(3)}_{\mathrm{tot}}$	E^{SD}	$E^{(3)}_{\mathrm{extra}}$	$E^{\mathrm{SD}}_{\mathrm{tot}}$	E_{expt}	$\delta E^{(3)}$	δE^{SD}
$5f_{5/2}$	−206606	−32100	11739	704	−2747	0	−229010	−26327	4672	−230304	−231065	2055	761
$5f_{7/2}$	−203182	−30549	10954	521	−2616	0	−224872	−25252	4361	−226168	−226740	1868	571
$6d_{3/2}$	−211799	−13258	4129	438	−880	0	−221370	−11422	1663	−222000	−221872	502	−128
$6d_{5/2}$	−207574	−11608	3300	326	−807	0	−216364	−10208	1337	−216927	−216579	214	−348
$7s_{1/2}$	−200273	−11204	4402	325	−458	89	−207119	−9455	1697	−208075	−207934	815	−140
$7p_{1/2}$	−165095	−7991	2782	298	−272	0	−170278	−7147	1125	−171091	−170826	548	−265
$7p_{3/2}$	−153572	−6213	2124	184	−226	1	−157703	−5619	861	−158372	−158009	306	−363
$8s_{1/2}$	−109201	−3840	1462	122	−163	25	−111594	−3255	575	−111896	−111443	−151	−453
$7d_{3/2}$	−108639	−3815	1110	113	−199	0	−111429	−3559	496	−111787	−111380	−49	−406
$7d_{5/2}$	−107032	−3592	1011	86	−188	0	−109715	−3401	452	−110083	−109638	−77	−445
$6f_{5/2}$	−99921	−5078	1615	77	−270	0	−103577	−4763	710	−104167	−103796	219	−371
$6f_{7/2}$	−99481	−4998	1590	61	−276	0	−103103	−4644	696	−103644	−103250	146	−394
$8p_{1/2}$	−94597	−3199	1112	129	−116	0	−96670	−2861	460	−96984	−96549	−122	−436
$8p_{3/2}$	−89595	−2628	898	83	−101	0	−91342	−2397	371	−91638	−91194	−148	−444
$5g_{7/2}$	−70583	−1506	421	0	−4	0	−71672	−1592	207	−71971	−71694	22	−296
$5g_{9/2}$	−70602	−1491	422	0	−4	0	−71675	−1548	205	−71949	−71675	0	−255
$9s_{1/2}$	−69455	−1849	684	61	−80	11	−70628	−1620	275	−70810	−70337	−291	−473
$8d_{3/2}$	−68677	−1846	522	54	−93	0	−70040	−1821	244	−70292	−69111	−929	−1181
$8d_{5/2}$	−67864	−1767	488	42	−89	0	−69190	−1780	228	−69463	−68537	−653	−926
$7f_{5/2}$	−64674	−2576	798	40	−137	0	−66549	−2504	362	−66912	−66510	−39	−402
$7f_{7/2}$	−64454	−2517	782	31	−139	0	−66296	−2409	352	−66619	−66006	−290	−613
$9p_{1/2}$	−61858	−1663	566	68	−61	0	−62948	−1548	241	−63158			
$9p_{3/2}$	−59200	−1400	468	45	−54	0	−60141	−1352	199	−60362			
$6g_{7/2}$	−49121	−1042	281	0	−4	0	−49884	−1242	145	−50221	−49391	−493	−831
$6g_{9/2}$	−49138	−1022	285	0	−4	0	−49879	−1166	142	−50166	−49390	−489	−775
$10s_{1/2}$	−48177	−1046	376	35	−46	5	−48853	−990	154	−49018	−48624	−229	−394

way and is expected to yield more accurate results, especially when correlation corrections are significant. While the SD method includes fourth- and higher-order terms, it omits some third-order terms. These omitted terms are identified and added to our SD data (see [16] for details).

We use the B-spline method [17] to generate a complete set of basis DF orbitals for use in the evaluation of RMBPT expressions. For Th IV, we use 50 splines of order $k=8$ for each angular momentum. The basis orbitals are constrained to a spherical cavity of radius $R=45$ a.u. 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 only 40 out of 50 basis orbitals for each partial wave in our third-order and all-order energy calculations since contributions from higher-energy orbitals are negligible.

Results of our energy calculations for the 28 states of Th IV 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 corrections $B^{(2)}$, and Lamb shift E_{LS}. The sum of these six contributions is our final third-order RMBPT result $E^{(3)}_{\mathrm{tot}}$ listed in the eighth column of Table I. The all-order SD energies are listed in the column E^{SD}, and that part of the third-order energy omitted in the SD calculation is given in column $E^{(3)}_{\mathrm{extra}}$. We note that E^{SD} includes $E^{(2)}$ completely. We take the sum of the six terms $E^{(0)}$, E^{SD}, $E^{(3)}_{\mathrm{extra}}$, $B^{(1)}$, $B^{(2)}$, and E_{LS} to be our final all-order result $E^{\mathrm{SD}}_{\mathrm{tot}}$, listed in the 11th column of Table I. Experimental energies from Blaise and Wyart [2] are given in the column labeled E_{expt}. Differences between third-order and experimental energies $\delta E^{(3)}=E^{(3)}_{\mathrm{tot}}-E_{\mathrm{expt}}$, and between SD and experimental energies $\delta E^{\mathrm{SD}}=E^{\mathrm{SD}}_{\mathrm{tot}}-E_{\mathrm{expt}}$, are given in the last two columns of Table I, respectively.

As expected, the largest correlation contribution to the valence energy comes from the second-order term $E^{(2)}$. This term is relatively simple to calculate; thus, we calculate $E^{(2)}$ with better numerical accuracy than $E^{(3)}$ and E^{SD}. The second-order energy $E^{(2)}$ includes partial waves up to $l_{\mathrm{max}}=8$ and is extrapolated to account for contributions from higher partial waves (see, for example, [18,19]). As an example of the convergence of $E^{(2)}$ with the number of partial waves l, consider the $5f_{5/2}$ state in Th IV. Calculations of $E^{(2)}$ with $l_{\mathrm{max}}=6$ and 8 yield $E^{(2)}(5f_{5/2})=-30\,810$ and

$-31\,771\ \mathrm{cm}^{-1}$, respectively. Extrapolation of these calculations yields $-32\,100$ and $-32\,154\ \mathrm{cm}^{-1}$, respectively. Therefore, we estimate the numerical uncertainty of $E^{(2)}(5f_{5/2})$ to be approximately $54\ \mathrm{cm}^{-1}$. It should be noted that this is the largest contribution from the higher partial waves, since we obtain a numerical uncertainty of $26\ \mathrm{cm}^{-1}$ for $E^{(2)}(6d_j)$ and the numerical uncertainty of $1\ \mathrm{cm}^{-1}$ for $E^{(2)}(7s_j)$. Similar convergence patterns are found for all other states considered.

We use $l_{\max}=6$ in our all-order calculations owing to the numerical complexity of the E^{SD} calculation. As we noted above, the second-order $E^{(2)}$ is contained in the E^{SD} value. Therefore, we use our high-precision calculation of $E^{(2)}$ described above to account for the contributions of the higher partial waves. We simply replace $E^{(2)}[l_{\max}=6]$ value with the final high-precision second-order value $E^{(2)}_{\mathrm{final}}$. The same number of partial waves, $l_{\max}=6$, is used in the third-order calculation. Since the asymptotic l-dependence of the second- and third-order energies are similar (both fall off as l^{-4}), we use the second-order remainder as a guide to estimate the numerical errors in the third-order contribution. The contribution $E^{(3)}_{\mathrm{extra}}$ given in Table I accounts for that part of the third-order RMBPT correction not included in the SD energy. The values of $E^{(3)}_{\mathrm{extra}}$ are smaller than the values of $E^{(3)}$ by approximately a factor of 3.

The 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. The total $E^{(3)}_{\mathrm{tot}}$ in Table I is the sum of six terms, $E^{(0)}$, $E^{(2)}$, $E^{(3)}$, $B^{(1)}$, $B^{(2)}$, and E_{LS}. We find that the correlation corrections to energies are large, especially for the $5f_j$ states. For example, $E^{(2)}$ is about 15% of $E^{(0)}$ and $E^{(3)}$ is about 36% of $E^{(2)}$ for the $5f_j$ states. Despite the evident slow convergence of the perturbation theory expansion, the $5f_j$ energy from the third-order RMBPT calculation is within 0.9% of the measured energy. It should be noted that 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 $6d_j$, $7s_{1/2}$, and $10s_{1/2}$ states, respectively. An important consequence of the large size of correlation corrections for $5f_j$ states is a different ordering of uncorrelated and correlated energies. As can be seen from Table I, $-E^{(0)}$ values for $6d_j$ states are larger than $-E^{(0)}$ values for $5f_j$ states; however, $-(E^{(0)}+E^{(2)})$ values for $6d_j$ states are smaller than $-(E^{(0)}+E^{(2)})$ values for $5f_j$ states; thus, although DF calculations predict the ground state of Th IV to be $6d_{3/2}$, correlated calculations correctly predict the ground state to be $5f_{5/2}$.

The quantity $E^{\mathrm{SD}}_{\mathrm{tot}}$ in Table I is the sum of six terms; $E^{(0)}$, E^{SD}, $E^{(3)}_{\mathrm{extra}}$, $B^{(1)}$, $B^{(2)}$, and E_{LS}. The column labeled δE^{SD} in Table I gives differences between our *ab initio* results and the experimental values [2]. The SD results agree better with the experimental values than the third-order RMBPT results for low-lying states where the correlation correction is larger. Comparison of the results given in two last columns of Table I shows that the ratio of $\delta E^{(3)}$ and δE^{SD} is about 3 for the $5f_j$ states. As expected, including correlation to all orders led to significant improvement of the results. Better agreement of the all-order values with experiment demonstrates the importance of the higher-order correlation contributions.

III. ELECTRIC-DIPOLE MATRIX ELEMENTS, OSCILLATOR STRENGTHS, TRANSITION RATES, AND LIFETIMES IN Th IV

A. Electric-dipole matrix elements

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 Th IV calculated in third order RMBPT and in the SD approximation are presented in Table II.

Third-order matrix elements $Z^{(\mathrm{DF+2+3})}$ include DF contributions together with second-order $Z^{(2)}$ and third-order $Z^{(3)}$ correlation corrections. Second- and third-order random-phase-approximation $Z^{(\mathrm{RPA})}$ terms are iterated to all orders in the present calculation. Third-order corrections include Brueckner orbital $Z^{(\mathrm{BO})}$, structural radiation $Z^{(\mathrm{SR})}$, and normalization $Z^{(\mathrm{norm})}$ corrections, in addition to the third-order RPA terms (see [9]). The terms $Z^{(\mathrm{RPA})}$ and $Z^{(\mathrm{BO})}$ give the largest contributions to the total. The sum of terms $Z^{(\mathrm{RPA})}$ and $Z^{(\mathrm{BO})}$ is about 15–25 % of $Z^{(\mathrm{DF})}$ and has a different sign. Structural radiation and normalization corrections are small. We find correlation corrections $Z^{(2+3)}$ to be very large, 10–25 %, for many cases. All results given in Table II are obtained using length-form matrix elements. Length-form and velocity-form matrix elements differ typically by 5–20 % for 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 $Z^{(\mathrm{SD})}$ of Table II. The SD matrix elements $Z^{(\mathrm{SD})}$ 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 [20]. The SD matrix elements $Z^{(\mathrm{SD})}$ are smaller than $Z^{(\mathrm{DF+2})}$ but larger than $Z^{(\mathrm{DF+2+3})}$ for all of the transitions listed in Table II.

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. [21]. The precision of this method has been demonstrated previously 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. As in the case of the third-order energy calculation, a limited number of partial waves with $l_{\max}<7$ is included, giving rise to some loss of gauge invariance. Comparison of length- and velocity-form matrix elements serves as a measure of the numerical accuracy of the resulting calculations.

Length- and velocity-form matrix elements from DF, second-order, and third-order calculations are given in Table III for the limited number transitions in Th IV. Following the procedure discussed in Ref. [21], the DF and RPA matrix elements in the table were obtained by dividing the corresponding amplitude by the lowest-order transition energies while the third-order matrix elements were obtained by di-

TABLE II. Reduced electric-dipole matrix elements calculated to first, second, third, and all orders of RMBPT in Th IV.

Transition		$Z^{(DF)}$	$Z^{(DF+2+3)}$	$Z^{(SD)}$	Transition		$Z^{(DF)}$	$Z^{(DF+2+3)}$	$Z^{(SD)}$
$5g_{7/2}$	$5f_{5/2}$	1.1236	0.6400	0.7118	$6d_{5/2}$	$6f_{7/2}$	3.3539	3.1272	3.0192
$5g_{7/2}$	$5f_{7/2}$	0.2298	0.1344	0.1511	$6d_{5/2}$	$7f_{5/2}$	0.3586	0.2561	0.2398
$5g_{7/2}$	$6f_{5/2}$	9.9381	8.8278	8.8815	$6d_{5/2}$	$7f_{7/2}$	1.5854	1.1995	1.1083
$5g_{7/2}$	$6f_{7/2}$	1.9244	1.7141	1.7252	$6d_{5/2}$	$7p_{3/2}$	3.1975	2.7006	2.7549
$5g_{7/2}$	$7f_{5/2}$	8.5105	8.6350	8.4527	$6d_{5/2}$	$8p_{3/2}$	0.6529	0.4291	0.4288
$5g_{7/2}$	$7f_{7/2}$	1.6217	1.6446	1.6082	$6d_{5/2}$	$9p_{3/2}$	0.3496	0.1743	0.1438
$6g_{7/2}$	$5f_{5/2}$	0.8677	0.4157	0.4134	$7d_{5/2}$	$5f_{5/2}$	0.0048	0.0360	0.0521
$6g_{7/2}$	$5f_{7/2}$	0.1757	0.0766	0.0918	$7d_{5/2}$	$5f_{7/2}$	0.0703	0.2298	0.2961
$6g_{7/2}$	$6f_{5/2}$	1.3517	1.2696	1.1321	$7d_{5/2}$	$6f_{5/2}$	2.0852	1.8440	1.8605
$6g_{7/2}$	$6f_{7/2}$	0.2464	0.2319	0.2042	$7d_{5/2}$	$6f_{7/2}$	9.3944	8.3249	8.4004
$6g_{7/2}$	$7f_{5/2}$	14.6139	13.4006	13.5178	$7d_{5/2}$	$7f_{5/2}$	1.0359	1.1377	1.1176
$6g_{7/2}$	$7f_{7/2}$	2.8402	2.6137	2.6402	$7d_{5/2}$	$7f_{7/2}$	4.5090	4.9585	4.8615
					$7d_{5/2}$	$7p_{3/2}$	5.9481	5.3934	5.4192
$5g_{9/2}$	$5f_{7/2}$	1.3635	0.8187	0.9054	$7d_{5/2}$	$8p_{3/2}$	6.8642	6.5224	6.5180
$5g_{9/2}$	$6f_{7/2}$	11.3858	10.1422	10.2068	$7d_{5/2}$	$9p_{3/2}$	0.8580	0.7746	0.7645
$5g_{9/2}$	$7f_{7/2}$	9.5778	9.7291	9.5435					
$6g_{9/2}$	$5f_{7/2}$	1.0425	0.5803	0.5682	$8d_{5/2}$	$5f_{5/2}$	0.0062	0.0307	0.0461
$6g_{9/2}$	$6f_{7/2}$	1.4474	1.3738	1.2252	$8d_{5/2}$	$5f_{7/2}$	0.0082	0.2138	0.2520
$6g_{9/2}$	$7f_{7/2}$	16.8152	15.4636	15.5953	$8d_{5/2}$	$6f_{5/2}$	0.3783	0.3187	0.3357
					$8d_{5/2}$	$6f_{7/2}$	1.7787	1.5158	1.6020
$6d_{3/2}$	$5f_{5/2}$	2.4281	1.3367	1.5295	$8d_{5/2}$	$7f_{5/2}$	3.5961	3.3715	3.3634
$6d_{3/2}$	$6f_{5/2}$	2.6761	2.4407	2.3610	$8d_{5/2}$	$7f_{7/2}$	16.1550	15.1766	15.1464
$6d_{3/2}$	$7f_{5/2}$	1.2888	0.9082	0.8469	$8d_{5/2}$	$7p_{3/2}$	1.1741	0.8883	0.8651
$6d_{3/2}$	$7p_{1/2}$	2.5465	2.0723	2.1220	$8d_{5/2}$	$8p_{3/2}$	9.3341	8.9653	8.9992
$6d_{3/2}$	$7p_{3/2}$	0.9963	0.8270	0.8488	$8d_{5/2}$	$9p_{3/2}$	11.4942	11.1245	11.0183
$6d_{3/2}$	$8p_{1/2}$	0.4074	0.1809	0.1906					
$6d_{3/2}$	$8p_{3/2}$	0.2173	0.1410	0.1422	$7s_{1/2}$	$7p_{1/2}$	2.8994	2.3669	2.4196
$6d_{3/2}$	$9p_{1/2}$	0.2148	0.0314	0.0221	$7s_{1/2}$	$7p_{3/2}$	3.9933	3.2930	3.3677
$6d_{3/2}$	$9p_{3/2}$	0.1172	0.0568	0.0475	$7s_{1/2}$	$8p_{1/2}$	0.0565	0.2438	0.2346
					$7s_{1/2}$	$8p_{3/2}$	0.3273	0.0639	0.0679
$7d_{3/2}$	$5f_{5/2}$	0.0654	0.2134	0.2587	$7s_{1/2}$	$9p_{1/2}$	0.0550	0.1958	0.1849
$7d_{3/2}$	$6f_{5/2}$	7.8264	6.9261	6.9826	$7s_{1/2}$	$9p_{3/2}$	0.1326	0.0706	0.0674
$7d_{3/2}$	$7f_{5/2}$	3.5114	3.8940	3.8365					
$7d_{3/2}$	$7p_{1/2}$	3.8261	3.4234	3.4490	$8s_{1/2}$	$7p_{1/2}$	1.5874	1.5601	1.5492
$7d_{3/2}$	$7p_{3/2}$	2.0308	1.8374	1.8444	$8s_{1/2}$	$7p_{3/2}$	3.0768	3.0010	2.9756
$7d_{3/2}$	$8p_{1/2}$	5.4788	5.1788	5.1791	$8s_{1/2}$	$8p_{1/2}$	5.0325	4.6912	4.7280
$7d_{3/2}$	$8p_{3/2}$	2.1716	2.0607	2.0630	$8s_{1/2}$	$8p_{3/2}$	6.7737	6.3299	6.3880
$7d_{3/2}$	$9p_{1/2}$	0.4173	0.3208	0.3214	$8s_{1/2}$	$9p_{1/2}$	0.0758	0.1951	0.2099
$7d_{3/2}$	$9p_{3/2}$	0.3057	0.2822	0.2790	$8s_{1/2}$	$9p_{3/2}$	0.5353	0.4009	0.3719
$8d_{3/2}$	$5f_{5/2}$	0.0029	0.1874	0.2098	$9s_{1/2}$	$7p_{1/2}$	0.4722	0.4773	0.4657
$8d_{3/2}$	$6f_{5/2}$	1.6194	1.3910	1.4493	$9s_{1/2}$	$7p_{3/2}$	0.7567	0.7254	0.7123
$8d_{3/2}$	$7f_{5/2}$	13.4659	12.6494	12.6151	$9s_{1/2}$	$8p_{1/2}$	2.8858	2.8094	2.8070
$8d_{3/2}$	$7p_{1/2}$	0.9598	0.7550	0.7418	$9s_{1/2}$	$8p_{3/2}$	5.4176	5.3126	5.2854
$8d_{3/2}$	$7p_{3/2}$	0.3604	0.2581	0.2523	$9s_{1/2}$	$9p_{1/2}$	7.6975	7.4191	7.4316
$8d_{3/2}$	$8p_{1/2}$	5.9596	5.6802	5.7284	$9s_{1/2}$	$9p_{3/2}$	10.2453	9.8671	9.8961
$8d_{3/2}$	$8p_{3/2}$	3.2096	3.0818	3.0900					

TABLE II. (*Continued.*)

Transition		$Z^{(DF)}$	$Z^{(DF+2+3)}$	$Z^{(SD)}$	Transition		$Z^{(DF)}$	$Z^{(DF+2+3)}$	$Z^{(SD)}$
$8d_{3/2}$	$9p_{1/2}$	9.1563	8.8665	8.8044	$10s_{1/2}$	$7p_{1/2}$	0.2605	0.2651	0.2489
$8d_{3/2}$	$9p_{3/2}$	3.6602	3.5363	3.5120	$10s_{1/2}$	$7p_{3/2}$	0.4011	0.3784	0.3596
					$10s_{1/2}$	$8p_{1/2}$	0.7932	0.7936	0.7873
$6d_{5/2}$	$5f_{5/2}$	0.6391	0.3624	0.4116	$10s_{1/2}$	$8p_{3/2}$	1.2032	1.1808	1.1676
$6d_{5/2}$	$5f_{7/2}$	2.9557	1.7032	1.9190	$10s_{1/2}$	$9p_{1/2}$	4.5019	4.3611	4.3523
$6d_{5/2}$	$6f_{5/2}$	0.7669	0.7085	0.6847	$10s_{1/2}$	$9p_{3/2}$	8.3091	8.1560	8.0743

viding the third-order amplitude by the second-order transition energies. Values of $Z^{(DF)}$ differ in L and V forms by 2–15 % for the p-s transitions. Huge L-V differences in $Z^{(DF)}$ for d-f transitions can be seen in Table III. Third-order calculations essentially remove such differences; the residual differences (0.002–0.2 %) being explained by the limited number of partial waves used in the evaluation of third-order matrix elements.

C. Oscillator strengths, transition rates, and lifetimes

We calculate oscillator strengths and transition probabilities for 96 possible nl_j-$n'l'_{j'}$ electric-dipole transitions including the $ns_{1/2}$ (n=7–10), np_j (n=7–9), nd_j (n=6–8), nf_j (n=5–7), and ng_j (n=5,6) states in Fr-like thorium. Our results are presented in Tables IV and V. Wavelengths λ (Å), weighted transition rates gA (s^{-1}), and oscillator strengths gf in Th IV are given in Table IV. Our SD data, $gA^{(SD)}$ and $gf^{(SD)}$, are compared with theoretical calculations, $gA^{(HFR)}$ and $gf^{(HFR)}$, from Ref. [1]. It should be noted that experimental energies are used to calculate $gA^{(SD)}$ and $gf^{(SD)}$ as well as $gA^{(HFR)}$ and $gf^{(HFR)}$. Therefore, we really compare the dipole matrix elements (see Table II). The SD and HFR results for s-p and p-d transitions disagree by 6–25 %, except for the $7p_{1/2}$-$8s_{1/2}$ transition with 60% disagreement. There are also substantial disagreements (factors of 2–5) between SD and HFR results for the f-g and f-d transitions. Correlation corrections are very important for those transitions as discussed above (see Table II). The RPA and BO contributions have the same sign, opposite to that of the DF contributions, and the total values are half of the DF values. We see from Table IV that for the f-g and f-d transitions the values of $gA^{(HFR)}$ and $gf^{(HFR)}$ are larger by a factor of 2–5 than the $gA^{(SD)}$ and $gf^{(SD)}$ values, respectively. On the basis of these comparisons, it appears that correlation corrections were not included in Ref. [1] for transitions involving the $5f_j$ states. Our conclusion is confirmed by comparison of $gA^{(HFR)}$ and $gf^{(HFR)}$ with our $gA^{(DF)}$ and $gf^{(DF)}$ results (compare the $Z^{(DF)}$ and $Z^{(SD)}$ columns in Table II). The disagreement between HFR and DF values for transitions rates and oscillator strengths is significantly smaller (about 10–20 %) than the disagreement between HFR and SD (by a factor of 2–5).

TABLE III. Comparison of length (L) and velocity (V) results for reduced electric-dipole matrix elements in lowest and third orders of perturbation theory in Th IV.

Transition		$Z^{(DF)}$		$Z^{(DF+2+3)}$	
		L	V	L	V
$5g_{7/2}$	$5f_{5/2}$	−1.1236	−1.0851	−0.7094	−0.7080
$5g_{7/2}$	$5f_{7/2}$	0.2298	0.2211	0.1479	0.1476
$5g_{7/2}$	$6f_{5/2}$	9.9381	9.9552	8.9038	8.8996
$6d_{3/2}$	$5f_{5/2}$	−2.4281	−0.7698	−2.8562	−2.9000
$7d_{3/2}$	$5f_{5/2}$	−0.0654	−0.0403	−0.1829	−0.1810
$7d_{3/2}$	$9p_{3/2}$	0.3057	0.2702	0.2831	0.2830
$8d_{3/2}$	$5f_{5/2}$	0.0029	0.0123	−0.1588	−0.1579
$6d_{5/2}$	$5f_{5/2}$	0.6391	−2.2929	0.6529	0.6615
$6d_{5/2}$	$5f_{7/2}$	2.9557	0.5609	3.3454	3.3138
$7d_{5/2}$	$5f_{5/2}$	−0.0048	0.0017	−0.0309	−0.0303
$7d_{5/2}$	$5f_{7/2}$	−0.0703	−0.0425	−0.2007	−0.2025
$7d_{5/2}$	$6f_{5/2}$	2.0852	2.3007	1.7790	1.7779
$8d_{5/2}$	$5f_{7/2}$	−0.0082	−0.0178	0.1823	0.1833
$8d_{5/2}$	$6f_{5/2}$	0.3783	0.4084	0.3258	0.3256
$7s_{1/2}$	$7p_{1/2}$	2.8994	2.6904	2.3943	2.3936
$7s_{1/2}$	$7p_{3/2}$	−3.9933	−3.7030	−3.3434	−3.3432
$7s_{1/2}$	$8p_{1/2}$	−0.0565	−0.0910	−0.2334	−0.2335
$8s_{1/2}$	$9p_{1/2}$	−0.0758	−0.1060	−0.1931	−0.1932
$8s_{1/2}$	$9p_{3/2}$	0.5353	0.4761	0.4031	0.4030
$9s_{1/2}$	$7p_{1/2}$	−0.4722	−0.4420	−0.4737	−0.4736
$9s_{1/2}$	$7p_{3/2}$	0.7567	0.6966	0.7181	0.7180
$9s_{1/2}$	$8p_{1/2}$	−2.8858	−2.8249	−2.8139	−2.8137

We calculate lifetimes of $ns_{1/2}$ (n=8–10), np_j (n=7–9), nd_j (n=6–8), nf_j (n=6,7), and ng_j (n=5,6) states in Fr-like thorium using the SD results for dipole matrix elements and experimental energies [2]. We list lifetimes $\tau^{(SD)}$ in Table V. Unfortunately, there are no experimental measurements to compare with our results; however, we hope that our calculations provide a theoretical benchmark and lifetime measurements will be carried out.

Lifetimes for two excited levels $7s_{1/2}$ and $5f_{7/2}$ were not included in Table V since there are no electric-dipole transitions from these levels. Contributions of the electric- and magnetic-multipole transitions to the lifetime of the $7s_{1/2}$ and $5f_{7/2}$ levels are considered below.

IV. MULTIPOLE MATRIX ELEMENTS, TRANSITION RATES, AND LIFETIMES IN Th IV

Reduced matrix elements of the electric-quadrupole ($E2$), electric-octupole ($E3$), and magnetic-multipole ($M1$,$M2$,

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

Lower	Upper	$\lambda^{(expt)}$	$gA^{(SD)}$	$gA^{(HFR)}$	$gf^{(SD)}$	$gf^{(HFR)}$
$7s_{1/2}$	$7p_{3/2}$	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]
$7p_{1/2}$	$8s_{1/2}$	1684.00	1.02[+9]	1.62[+9]	4.33[−1]	6.9[−1]
$7p_{3/2}$	$8s_{1/2}$	2147.50	1.81[+9]	1.56[+9]	1.25[+0]	1.1[+0]
$8s_{1/2}$	$8p_{3/2}$	4938.44	6.87[+8]	7.06[+8]	2.51[+0]	2.6[+0]
$8s_{1/2}$	$8p_{1/2}$	6713.71	1.50[+8]	1.40[+8]	1.01[+0]	9.5[−1]
$6d_{3/2}$	$7p_{3/2}$	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]
$7p_{1/2}$	$7d_{3/2}$	1682.21	5.06[+9]	6.36[+9]	2.15[+0]	2.7[+0]
$7p_{3/2}$	$7d_{5/2}$	2067.35	6.73[+9]	6.16[+9]	4.32[+0]	4.0[+0]
$7p_{3/2}$	$7d_{3/2}$	2144.60	6.99[+8]	6.13[+8]	4.82[−1]	4.3[−1]
$7d_{3/2}$	$8p_{3/2}$	4953.85	7.09[+7]	8.03[+7]	2.61[−1]	3.0[−1]
$7d_{5/2}$	$8p_{3/2}$	5421.88	5.40[+8]	5.51[+8]	2.38[+0]	2.5[+0]
$7d_{3/2}$	$8p_{1/2}$	6742.22	1.77[+8]	1.59[+8]	1.21[+0]	1.1[+0]
$5f_{5/2}$	$6g_{7/2}$	550.433	2.08[+9]	7.40[+9]	9.43[−2]	3.4[−1]
$5f_{7/2}$	$6g_{7/2}$	563.858	9.51[+7]	2.55[+8]	4.54[−3]	1.2[−2]
$5f_{7/2}$	$6g_{9/2}$	563.861	3.65[+9]	8.93[+9]	1.74[−1]	4.3[−1]
$5f_{5/2}$	$5g_{7/2}$	627.392	4.16[+9]	8.14[+9]	2.45[−1]	4.8[−1]
$5f_{7/2}$	$5g_{7/2}$	644.892	1.72[+8]	2.78[+8]	1.08[−2]	1.7[−2]
$5f_{7/2}$	$5g_{9/2}$	644.971	6.19[+9]	9.72[+9]	3.86[−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]
$5f_{5/2}$	$6d_{3/2}$	10877.6	3.68[+6]	7.93[+6]	6.53[−2]	1.4[−1]

and $M3$) operators in lowest, second, third, and all orders of perturbation theory are given in Table VI for Th IV. Detailed descriptions of the calculations of the multipole matrix elements in lowest and second orders of perturbation theory were given in Refs. [22–24]. Third-order and all-order calculations are done in the same way as the calculations of the $E1$ matrix elements. In Table VI, we present $E2$, $E3$, $M1$, $M2$, and $M3$ matrix elements in the $Z^{(DF)}$, $Z^{(DF+2)}$, $Z^{(DF+2+3)}$, and $Z^{(SD)}$ approximations for the $5f_{5/2}$-$5f_{7/2}$, $5f_j$-$7s_{1/2}$, and $6d_j$-$7s_{1/2}$ transitions in Th IV.

TABLE V. Lifetimes τ (ns) for the nl levels in Fr-like Th IV.

Level	$\tau^{(SD)}$	Level	$\tau^{(SD)}$
$6d_{3/2}$	1090.0	$7p_{1/2}$	1.099
$6d_{5/2}$	676.0	$7p_{3/2}$	0.632
$7d_{3/2}$	0.667	$8p_{1/2}$	3.194
$7d_{5/2}$	0.854	$8p_{3/2}$	1.871
$8d_{3/2}$	1.176	$9p_{1/2}$	5.893
$8d_{5/2}$	1.600	$9p_{3/2}$	4.933
$5g_{7/2}$	0.815	$6f_{5/2}$	0.300
$5g_{9/2}$	0.780	$6f_{7/2}$	0.297
$6g_{7/2}$	1.768	$7f_{5/2}$	0.684
$6g_{9/2}$	1.567	$7f_{7/2}$	0.639
$8s_{1/2}$	0.707		
$9s_{1/2}$	1.031		
$10s_{1/2}$	1.634		

The second-order contribution is about 1–3 % for all transitions involving the $7s_{1/2}$ states, but it is different for the $5f_{5/2}$-$5f_{7/2}$ transition. It is very small (0.1%) for the $M1$ matrix elements and rather large (20%) for the $E2$ matrix elements. The large difference between $Z^{(DF)}$ and $Z^{(DF+2+3)}$ or $Z^{(SD)}$ for $E2$ and $E3$ operators could be explained by the large size of the Brueckner orbital correction; the ratios of $Z^{(BO)}$ and $Z^{(DF)}$ are equal to 0.06 and 0.3 for the $6d_j$-$7s_{1/2}$ and $5f_j$-$7s_{1/2}$ transitions, respectively.

Wavelengths and transition rates $A^{(SD)}$ for the electric-multipole ($E2$ and $E3$) and magnetic-multipole ($M1$, $M2$, and $M3$) transitions in Th IV calculated in the SD approximation are presented in Table VII. The largest contribution to the lifetime of the $5f_{7/2}$ state comes from the $M1$ transition. The largest contribution to the lifetime of the $7s_{1/2}$ state comes from $E2$ transitions. Our SD result for $M1$ matrix elements are in perfect agreement (0.5%) with HFR results obtained by Biémont *et al.* in Ref. [1]. The disagreement is much larger between HFR and SD results for $E2$ transitions; 6% and 18% for the $6d_{5/2}$-$7s_{1/2}$ and $6d_{5/2}$-$7s_{1/2}$ matrix ele-

TABLE VI. Reduced matrix elements of the electric-multipole ($E2, E3$) and magnetic-multipole ($M1$, $M2$, and $M3$) operators in first, second, third, and all orders of perturbation theory in Th IV.

	Transition		$Z^{(DF)}$	$Z^{(DF+2)}$	$Z^{(DF+2+3)}$	$Z^{(SD)}$
$M1$	$5f_{5/2}$	$5f_{7/2}$	1.8506	1.8525	1.8390	1.8514
$E2$	$5f_{5/2}$	$5f_{7/2}$	1.5669	1.2339	0.9724	1.0834
$E2$	$6d_{3/2}$	$7s_{1/2}$	7.7806	7.5518	6.9232	7.0631
$E2$	$6d_{5/2}$	$7s_{1/2}$	10.0084	9.7894	8.9992	9.1526
$E3$	$5f_{5/2}$	$7s_{1/2}$	12.9552	13.1718	9.3847	10.6349
$E3$	$5f_{7/2}$	$7s_{1/2}$	15.7681	16.0030	11.5616	13.0648
$M3$	$6d_{5/2}$	$7s_{1/2}$	59.2100	60.9891	59.7136	57.3087

ments, respectively. This is expected because the correlation correction to the $M1$ matrix elements is very small, but the correlation correction to $E2$ matrix element is large, as discussed above. Since the SD all-order method includes the correlation corrections in a rather complete way, we expect to see disagreements with HFR calculations in the cases where correlation corrections are significant.

Finally, we find that the lifetime of the $5f_{7/2}$ state is 1.07 s and the lifetime of the $7s_{1/2}$ state is 0.590 s. An estimate of the $7s_{1/2}$ state lifetime (about 1 s) was given by Peik and Tamm in Ref. [25], but no measurements have as yet been performed.

V. SCALAR AND TENSOR POLARIZABILITIES IN THE $5f_{5/2}$ GROUND STATE OF Th^{3+}

We calculate the tensor polarizability α_2 of Th^{3+} in a state v using a sum-over-states approach [26]

$$\alpha_2(v) = \sum_n I(v-n). \tag{1}$$

Here

$$I(v-n) = A(vn)\frac{Z_{vn}^2}{E_n - E_v}, \tag{2}$$

where

$$A(vn) = -4\sqrt{\frac{5j_v(2j_v-1)}{6(j_v+1)(2j_v+1)(2j_v+3)}} \times (-1)^{j_v+j_n+1}\begin{Bmatrix} j_v & 1 & j_n \\ 1 & j_v & 2 \end{Bmatrix}$$

and Z_{vn} is a reduced electric-dipole matrix element.

The calculation of the $\alpha_2(5f_{5/2})$ is divided into three parts:

$$\alpha_2^{\text{main}}(5f_{5/2}) = \sum_{n=6}^{8} I(5f_{5/2} - nd_j) + \sum_{n=5}^{6} I(5f_{5/2} - ng_{7/2});$$

$$\delta\alpha_2^{\text{core}}(5f_{5/2}) = \sum_{n=3}^{5} I(5f_{5/2} - nd_j);$$

$$\alpha_2^{\text{tail}}(5f_{5/2}) = \sum_{n=9}^{50} I(5f_{5/2} - nd_j) + \sum_{n=7}^{50} I(5f_{5/2} - ng_{7/2}). \tag{3}$$

We present the details of our calculations of tensor polarizabilities α_2 for the ground state $5f_{5/2}$ in Table VIII. We use experimental energies from [2]. Electric-dipole matrix elements evaluated in the third-order and all-order SD approximations are given in the columns labeled $Z^{(DF+2+3)}$ and $Z^{(SD)}$. The corresponding contributions to the tensor polarizability are given in the columns labeled $\alpha_2^{(DF+2+3)}$ and $\alpha_2^{(SD)}$. The contributions α_2^{tail} and $\delta\alpha_2^{\text{core}}$ are found to be very small and are calculated in the DF approximation. Our final result obtained in SD approximation is $\alpha_2(5f_{5/2}) = -6.2a_0^3$.

We calculate the scalar dipole polarizability α_0 of Th^{3+} in the $5f_{5/2}$ ground state using the expression (Ref. [26])

$$\alpha_0(5f_{5/2}) = \sum_n [I_S(nd_{3/2}) + I_S(nd_{5/2}) + I_S(ng_{7/2})], \tag{4}$$

where

$$I_S(nlj) = \frac{1}{9}\frac{Z^2_{5f_{5/2},nlj}}{E_{nlj} - E_{5f_{5/2}}}. \tag{5}$$

The breakdown of the contributions to the scalar dipole polarizability together with the final result for the ground state

TABLE VII. Wavelengths λ (Å) and transition rates $A^{(SD)}$ (s^{-1}) of the electric-multipole ($E2, E3$) and magnetic-multipole ($M1, M2$, and $M3$) transitions in Th IV calculated in the SD approximation. Numbers in brackets represent powers of 10.

	Transition		λ	$A^{(SD)}$
$M1$	$5f_{5/2}$	$5f_{7/2}$	23119.6	9.352[−1]
$E2$	$5f_{5/2}$	$5f_{7/2}$	23119.6	2.487[−5]
$E2$	$6d_{3/2}$	$7s_{1/2}$	7174.88	1.469[−0]
$E2$	$6d_{5/2}$	$7s_{1/2}$	11568.2	2.264[−1]
$M1$	$6d_{3/2}$	$7s_{1/2}$	7174.88	5.429[−5]
$E3$	$5f_{5/2}$	$7s_{1/2}$	4323.25	6.299[−7]
$E3$	$5f_{7/2}$	$7s_{1/2}$	5317.62	2.232[−7]
$M2$	$5f_{5/2}$	$7s_{1/2}$	4323.25	5.154[−9]
$M3$	$6d_{5/2}$	$7s_{1/2}$	11568.2	1.863[−8]

TABLE VIII. Contributions to the tensor polarizability of Th IV in the ground state $5f_{5/2}$ calculated using third-order MBPT $\alpha_2^{(\mathrm{DF+2+3})}$ and the all-order SD method $\alpha_2^{(\mathrm{SD})}$. The third-order and SD dipole matrix elements and corresponding experimental transition energies are also given. All values are in a.u.

Contribution	v	n	E_n-E_v	$Z_{vn}^{(\mathrm{DF+2+3})}$	$Z_{vn}^{(\mathrm{SD})}$	$\alpha_2^{(\mathrm{DF+2+3})}$	$\alpha_2^{(\mathrm{SD})}$
α_2^{main}	$5f_{5/2}$	$6d_{3/2}$	0.041888	1.337	−1.530	−4.740	−6.206
	$5f_{5/2}$	$7d_{3/2}$	0.545323	0.213	−0.259	−0.009	−0.014
	$5f_{5/2}$	$8d_{3/2}$	0.737917	0.187	−0.210	−0.005	−0.007
	$5f_{5/2}$	$6d_{5/2}$	0.066005	0.362	0.412	0.253	0.326
	$5f_{5/2}$	$7d_{5/2}$	0.553263	−0.036	−0.052	0.000	0.001
	$5f_{5/2}$	$8d_{5/2}$	0.740531	0.031	0.046	0.000	0.000
	$5f_{5/2}$	$5g_{7/2}$	0.726234	0.640	−0.712	−0.022	−0.028
	$5f_{5/2}$	$6g_{7/2}$	0.827772	−0.416	0.413	−0.008	−0.008
$\delta\alpha_2^{\mathrm{core}}$(DF)						0.042	0.042
α_2^{tail}(DF)						−0.273	−0.273
Total						−4.763	−6.166

$5f_{5/2}$ in Th^{3+} are presented in Table IX. Again, both third order and all-order results are listed. We use the same designations as in Table VIII. We also calculate the polarizability α_{core} of the radonlike ionic core in Th^{3+}. A detailed discussion of the α_{core} in Na, K, Rb, Cs, and Fr atomic systems was presented by Safronova *et al.* in Ref. [12]. We evaluate α_{core} using the random-phase approximation. We find $\alpha_{\mathrm{core}}(\mathrm{RPA})$ to be equal to $7.750a_0^3$ in a.u. This value was used to obtain our final result for the scalar ground state polarizability, $\alpha_0(5f_{5/2})=15.1a_0^3$. We note that, unlike in the case of neutral Fr, the core contribution is very large, 50%. The calculation of the ground-state polarizabilities for Fr-like Th provides another test of the quality of atomic-structure calculations. There are no experimental results for the Th IV polarizabilities at this time. An accurate measurement of the Th IV polarizability, combined with these calculations, may be used to derive the values of the $5f_{5/2}-6d_{3/2}$ $E1$ matrix elements and to evaluate the accuracy of the RPA core value.

VI. CONCLUSION

In summary, a systematic relativistic MBPT study of energies of $ns_{1/2}$ $(n=7-10)$, np_j $(n=7-9)$, nd_j $(n=6-8)$, nf_j $(n=5-7)$, and ng_j $(n=5,6)$ states in Fr-like thorium is presented. The energies are in good agreement with existing experimental energy data and provide a theoretical reference database for line identification. A systematic all-order SD study of reduced $E1$ matrix elements and transition rates for the 96 electric-dipole transitions in Th^{3+} is conducted. Lifetimes are calculated in the SD approximation for nl_j levels. 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 lifetimes of the $5f_{7/2}$ and $7s_{1/2}$ states. Scalar and tensor polarizabilities for the Th^{3+} ground state are calculated using relativistic third-order and all-order methods. We believe that our energy, lifetime, and polarizability results will be useful in analyzing existing experimental data and in planning future measurements.

TABLE IX. Contributions to the scalar polarizability of Th IV in the ground state $5f_{5/2}$ calculated using third-order MBPT $\alpha_0^{(\mathrm{DF+2+3})}$ and the all-order SD method $\alpha_0^{(\mathrm{SD})}$. The third-order and SD dipole matrix elements and corresponding experimental transition energies are also given. All values are in a.u.

Contribution	v	n	E_n-E_v	$Z_{vn}^{(\mathrm{DF+2+3})}$	$Z_{vn}^{(\mathrm{SD})}$	$\alpha_0^{(\mathrm{DF+2+3})}$	$\alpha_0^{(\mathrm{SD})}$
α_0^{main}	$5f_{5/2}$	$6d_{3/2}$	0.041888	1.337	−1.530	4.740	6.206
	$5f_{5/2}$	$6d_{5/2}$	0.066005	0.362	0.412	0.221	0.285
	$5f_{5/2}$	$5g_{7/2}$	0.726234	0.640	−0.712	0.063	0.078
	$5f_{5/2}$	$6g_{7/2}$	0.827772	−0.416	0.413	0.023	0.023
	$5f_{5/2}$	$7d_{3/2}$	0.545323	0.213	−0.259	0.009	0.014
	$5f_{5/2}$	$8d_{3/2}$	0.737917	0.187	−0.210	0.005	0.007
	$5f_{5/2}$	$7d_{5/2}$	0.553263	−0.036	−0.052	0.000	0.001
	$5f_{5/2}$	$8d_{5/2}$	0.740531	0.031	0.046	0.000	0.000
α_0^{tail}(DF)						0.762	0.762
α^{core}(RPA)						7.750	7.750
$\delta\alpha_0^{\mathrm{core}}$(RPA)						−0.050	−0.050
Total						13.523	15.073

ACKNOWLEDGMENTS

The work of W.R.J. 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. The work of U.I.S. was supported in part by DOE-NNSA/NV Cooperative Agreement No. DE-FC52-01NV14050.

[1] E. Biémont, V. Fivet, and P. Quinet, J. Phys. B **37**, 4193 (2004).
[2] J. Blaise and J. Wyart, http://www.lac.u-psud.fr/Database/Contents.html
[3] http://physics.nist.gov/PhysRefData/Handbook /Tables/radiumtable6.htm
[4] W. Z. Zhao, J. E. Simsarian, L. A. Orozco, W. Shi, and G. D. Sprouse, Phys. Rev. Lett. **78**, 4169 (1997).
[5] J. E. Simsarian, L. A. Orozco, G. D. Sprouse, and W. Z. Zhao, Phys. Rev. A **57**, 2448 (1998).
[6] J. M. Grossman, R. P. Fliller III, L. A. Orozco, M. R. Pearson, and G. D. Sprouse, Phys. Rev. A **62**, 062502 (2000).
[7] S. Aubin, E. Gomez, L. A. Orozco, and G. D. Sprouse, Opt. Lett. **28**, 2055 (2003).
[8] E. Gomez, L. A. Orozco, A. Perez Galvan, and G. D. Sprouse, Phys. Rev. A **71**, 062504 (2005).
[9] W. R. Johnson, Z. W. Liu, and J. Sapirstein, At. Data Nucl. Data Tables **64**, 279 (1996).
[10] V. A. Dzuba, V. V. Flambaum, and O. P. Sushkov, Phys. Rev. A **51**, 3454 (1995).
[11] V. A. Dzuba, V. V. Flambaum, and J. S. M. Ginges, Phys. Rev. A **63**, 062101 (2001).
[12] M. S. Safronova, W. R. Johnson, and A. Derevianko, Phys. Rev. A **60**, 4476 (1999).
[13] M. S. Safronova and W. R. Johnson, Phys. Rev. A **62**, 022112 (2000).
[14] I. M. Savukov, W. R. Johnson, U. I. Safronova, and M. S. Safronova, Phys. Rev. A **67**, 042504 (2003).
[15] S. A. Blundell, W. R. Johnson, and J. Sapirstein, Phys. Rev. A **43**, 3407 (1991).
[16] M. S. Safronova, W. R. Johnson, and A. Derevianko, Phys. Rev. A **60**, 4476 (1999).
[17] W. R. Johnson, S. A. Blundell, and J. Sapirstein, Phys. Rev. A **37**, 307 (1988).
[18] M. S. Safronova, W. R. Johnson, and U. I. Safronova, Phys. Rev. A **53**, 4036 (1996).
[19] M. S. Safronova, W. R. Johnson, and U. I. Safronova, J. Phys. B **30**, 2375 (1997).
[20] A. Derevianko and E. D. Emmons, Phys. Rev. A **66**, 012503 (2002).
[21] I. M. Savukov and W. R. Johnson, Phys. Rev. A **62**, 052512 (2000).
[22] W. R. Johnson, D. R. Plante, and J. Sapirstein, Adv. At., Mol., Opt. Phys. **35**, 255 (1995).
[23] U. I. Safronova, W. R. Johnson, D. Kato, and S. Ohtani, Phys. Rev. A **63**, 032518 (2001).
[24] S. M. Hamasha, A. S. Shlyaptseva, and U. I. Safronova, Can. J. Phys. **82**, 331 (2004).
[25] P. Peik and C. Tamm, Europhys. Lett. **61**, 181 (2003).
[26] M. S. Safronova and C. W. Clark, Phys. Rev. A **69**, 040501(R) (2004).