Correlation and relativistic effects for the 4*f*-*nl* multipole transitions in Yb III ions

U. I. Safronova[1,2] and M. S. Safronova[3]
[1]*Physics Department, University of Nevada, Reno, Nevada 89557, USA*
[2]*Institute of Spectroscopy, Russian Academy of Science, Troitsk, Moscow, Russia*
[3]*Department of Physics and Astronomy, 217 Sharp Lab, University of Delaware, Newark, Delaware 19716, USA*

(Received 21 December 2008; published 19 March 2009)

Wavelengths, transition rates, and line strengths are calculated for the multipole (E1, M1, E2, M2, and E3) transitions between the excited $[\mathrm{Xe}]4f^{13}ns$, $[\mathrm{Xe}]4f^{13}nd$, and $[\mathrm{Xe}]4f^{13}np$ and the ground $[\mathrm{Xe}]4f^{14}$ state in Yb III ion with the nuclear charge $Z=70$ ($[\mathrm{Xe}]=[\mathrm{Ni}]4s^2 4p^6 4d^{10} 5s^2 5p^6$). Relativistic many-body perturbation theory (RMBPT), including the Breit interaction, is used to evaluate energies and transition rates for multipole transitions in this hole-particle system. This method is based on the relativistic many-body perturbation theory that agrees with multiconfiguration Dirac-Fock calculations in lowest-order, includes all second-order correlation corrections, and includes corrections from negative energy states. The calculations start from a $[\mathrm{Xe}]4d^{14}$ Dirac-Fock potential. First-order perturbation theory is used to obtain intermediate-coupling coefficients, and second-order RMBPT is used to determine the matrix elements. Evaluated multipole matrix elements for transitions from excited states into the ground states and transitions between excited states are used to determine the lifetime of the 20 $[\mathrm{Xe}]4f^{13}5d(J)$ levels, four $[\mathrm{Xe}]4f^{13}6s(J)$ levels, 12 $[\mathrm{Xe}]4f^{13}6p(J)$ levels, and four $[\mathrm{Xe}]4f^{13}7s(J)$ levels.

DOI: 10.1103/PhysRevA.79.032511 PACS number(s): 31.15.ac, 31.15.ag, 31.15.aj

I. INTRODUCTION

This work further develops the application of the relativistic many-body perturbation theory (RMBPT) to the studies of atomic characteristics of hole-particle excitations of closed-shell ions. Recently, RMBPT calculations of energies, multipole transition rates, and lifetimes in Ne-like [1,2], Ni-like [3–8], and Pd-like [9,10] ions have been performed. The present paper focuses on the RMBPT calculations of energies, multipole transition rates, and lifetimes in Er-like Yb III ion. The difference between Pd-like and Er-like ions is in additional filled 4*f*, 5*s*, and 5*p* shells ($[\mathrm{Pd}]4f^{14}5s^2 5p^6 = [\mathrm{Xe}]4f^{14}$). The Yb III ion has very interesting level structure. All states up to $E=53\,736$ cm^{-1} (counting from the ground state) belong to either $[\mathrm{Xe}]4f^{13}5d$ or $[\mathrm{Xe}]4f^{13}6s$ odd configurations [11]. The gap between these levels and next (even) configurations is over $18\,775$ cm^{-1}. Only three of these $[\mathrm{Xe}]4f^{13}5d$ levels have total angular momentum $J=1$ and, therefore, can decay to the ground state via strong electric-dipole transitions. As a result, all remaining 21 $[\mathrm{Xe}]4f^{13}5d$ and $[\mathrm{Xe}]4f^{13}6s$ levels with $J=0,2-6$ are metastable.

The second-order RMBPT calculations for Er-like Yb III ion start from a $[\mathrm{Xe}]4f^{14}$ Dirac-Fock potential. We consider the 4*f* hole and n_1s, n_1p, and n_2d ($n_1=6,7$ and $n_2=5,6$) particles leading to the 48 odd-parity $4f^{13}n_1s(J)$ and $4f^{13}n_2d(J)$ excited states and the 24 even-parity $4f^{13}n_1p(J)$ excited states.

This work is motivated in part by recent experiments by Öberg and Lundberg [12] that provided measurements of transition probabilities and improved data of energies levels. Radiative lifetimes of nine out of the twelve $4f^{13}6p$ levels in Yb III were measured [12]. A Penning discharge lamp was introduced as a continuous plasma source, in which the lifetimes were determined with the time-resolved laser-induced fluorescence technique by pumping from metastable 5*d* and 6*s* levels [12].

Some years previously, experimental and theoretical energy levels, transition probabilities, and radiative lifetimes in Yb III were reported by Biémont *et al.* [13]. Radiative lifetimes of two excited $4f^{13}6p$ states of Yb III have been measured for the first time using time-resolved laser induced fluorescence following two-photon excitation. The theoretical approach considered in Ref. [13] was the relativistic Hartree-Fock method of Cowan [14] including the core-polarization effects. The configuration sets retained for the calculations were $4f^{14}$, $4f^{13}6p$, $4f^{13}7p$, $4f^{13}5f$, $4f^{13}6f$, and $4f^{13}7f$ for even parity and $4f^{13}5d$, $4f^{13}6d$, $4f^{13}7d$, $4f^{13}6s$, and $4f^{13}7s$ for odd parity states [13]. Lifetimes of three levels belonging to the configuration $4f^{13}5d$ with $J=1$ in Yb III were measured for the first time using the time-resolved laser-induced fluorescence method in [15]. Experimental transition probabilities were deduced for the transitions between the levels studied and the ground state. The comparison of the experimental lifetimes with theoretical data, deduced within the relativistic Hartree-Fock (HFR) approach, underlines the dramatic importance of an adequate consideration of core polarization effects in the theoretical model and the sensitivity of one of the lifetime values to small correlation effects [15]. It was underlined by Biémont *et al.* [13] that doubly-ionized ytterbium has been considered much less in the literature than the neutral or singly-ionized species.

Another motivation of this work is a study of correlation effects in heavy systems. Yb ions represent excellent example for such study, as the correlation effects are very large, in part due to the 4*f* shell. Both neutral Yb and Yb II ions are of interest to many applications, ranging from study of fundamental interaction (parity violation) [16] to the development of next generation frequency standards [17]. Yb is also of interest to study of the long-range interactions [18]. However, both neutral Yb and Yb II ion present major difficulties to high-precision studies owing to large correction contribution from the 4*f* shell. For example, relativistic all-order method [19] fails to converge for both Yb and Yb II calcula-

TABLE I. Possible hole-particle states in the $4f_jnl_{j'}(J)$ complexes; jj coupling schemes.

Odd-parity states		Odd-parity states		Even-parity states	
$4f_{5/2}5d_{5/2}(0)$	$4f_{7/2}6s_{1/2}(3)$	$4f_{7/2}5d_{5/2}(1)$	$4f_{7/2}6s_{1/2}(4)$	$4f_{5/2}6p_{3/2}(1)$	$4f_{7/2}6p_{3/2}(2)$
$4f_{5/2}6d_{5/2}(0)$	$4f_{7/2}5d_{3/2}(3)$	$4f_{5/2}5d_{5/2}(1)$	$4f_{7/2}5d_{3/2}(4)$	$4f_{5/2}7p_{3/2}(1)$	$4f_{5/2}6p_{1/2}(2)$
	$4f_{7/2}5d_{5/2}(3)$	$4f_{5/2}5d_{3/2}(1)$	$4f_{7/2}5d_{5/2}(4)$		$4f_{5/2}6p_{3/2}(2)$
$4f_{7/2}5d_{3/2}(2)$	$4f_{5/2}6s_{1/2}(3)$	$4f_{7/2}6d_{5/2}(1)$	$4f_{5/2}5d_{3/2}(4)$	$4f_{7/2}6p_{1/2}(3)$	$4f_{7/2}7p_{3/2}(2)$
$4f_{7/2}5d_{5/2}(2)$	$4f_{5/2}5d_{3/2}(3)$	$4f_{5/2}6d_{5/2}(1)$	$4f_{5/2}5d_{5/2}(4)$	$4f_{7/2}6p_{3/2}(3)$	$4f_{5/2}7p_{1/2}(2)$
$4f_{5/2}6s_{1/2}(2)$	$4f_{5/2}5d_{5/2}(3)$	$4f_{5/2}6d_{3/2}(1)$	$4f_{7/2}7s_{1/2}(4)$	$4f_{5/2}6p_{1/2}(3)$	$4f_{5/2}7p_{3/2}(2)$
$4f_{5/2}5d_{3/2}(2)$	$4f_{7/2}7s_{1/2}(3)$		$4f_{7/2}6d_{3/2}(4)$	$4f_{5/2}6p_{3/2}(3)$	
$4f_{5/2}5d_{5/2}(2)$	$4f_{7/2}6d_{3/2}(3)$	$4f_{7/2}5d_{3/2}(5)$	$4f_{7/2}6d_{5/2}(4)$	$4f_{7/2}7p_{1/2}(3)$	$4f_{7/2}6p_{1/2}(4)$
$4f_{7/2}6d_{3/2}(2)$	$4f_{7/2}6d_{5/2}(3)$	$4f_{7/2}5d_{5/2}(5)$	$4f_{5/2}6d_{3/2}(4)$	$4f_{7/2}7p_{3/2}(3)$	$4f_{7/2}6p_{3/2}(4)$
$4f_{7/2}6d_{5/2}(2)$	$4f_{5/2}7s_{1/2}(3)$	$4f_{5/2}5d_{5/2}(5)$	$4f_{5/2}6d_{5/2}(4)$	$4f_{5/2}7p_{1/2}(3)$	$4f_{5/2}6p_{3/2}(4)$
$4f_{5/2}7s_{1/2}(2)$	$4f_{5/2}6d_{3/2}(3)$	$4f_{7/2}6d_{3/2}(5)$		$4f_{5/2}7p_{3/2}(3)$	$4f_{7/2}7p_{1/2}(4)$
$4f_{5/2}6d_{3/2}(2)$	$4f_{5/2}6d_{5/2}(3)$	$4f_{7/2}6d_{5/2}(5)$	$4f_{7/2}5d_{5/2}(6)$	$4f_{7/2}6p_{3/2}(5)$	$4f_{7/2}7p_{3/2}(4)$
$4f_{5/2}6d_{5/2}(2)$		$4f_{5/2}6d_{5/2}(5)$	$4f_{7/2}6d_{5/2}(6)$	$4f_{7/2}7p_{3/2}(5)$	$4f_{5/2}7p_{3/2}(4)$

tions. Therefore, it is essential to study the $4f$ shell excitation in detail on the example of Yb III for better understanding of the convergence problem in neutral Yb and Yb II ion.

In the present paper, RMBPT is used for systematic study of atomic transitions in Er-like Yb III ion. Specifically, we determine energies of $4f^{13}ns$, $4f^{13}np$, and $4f^{13}nd$ excited states. The calculations are carried out to second order in perturbation theory. RMBPT is also used to determine line strengths, oscillator strengths, and transition rates for all allowed and forbidden electric-multipole and magnetic-multipole (E1, E2, E3, M1, M2) transitions from the $4f^{13}ns$, $4f^{13}np$, and $4f^{13}nd$ excited states into the ground state. Additionally, we calculate dipole transitions between odd-parity $4f^{13}ns$ and $4f^{13}nd$ states and even-parity $4f^{13}np$ states to determine the lifetime values for $4f^{13}6p$ and $4f^{13}7s$ states. The M1 and E2 transitions between levels of even-parity $4f^{13}ns$ and $4f^{13}nd$ states are evaluated to calculate the lifetime values for $4f^{13}5d$ and $4f^{13}6s$ levels.

II. METHOD

Details of the RMBPT method for hole-particle states were presented in Ref. [3] for calculation of energies, in Refs. [1,3–6,9,10] for calculation of multipole matrix elements for transitions from excited states into the ground state, and in Refs. [2,7,8] for calculation of multipole matrix

TABLE II. Second-order contributions to the energy matrices (a.u.) for odd-parity states with $J=4$ in the case of Yb III. One-body and two-body second-order Coulomb and Breit-Coulomb contributions are given in columns labeled $E_1^{(2)}$, $E_2^{(2)}$, $B_1^{(2)}$, and $B_2^{(2)}$, respectively.

$4l_1j_1\ nl_2j_2, 4l_3j_3\ nl_4j_4$		Coulomb Interaction $E_1^{(2)}$	$E_2^{(2)}$	Breit-Coulomb Correction $B_1^{(2)}$	$B_2^{(2)}$
$4f_{7/2}6s_{1/2}$	$4f_{7/2}6s_{1/2}$	−0.162 189	0.006 938	0.041 882	0.000 509
$4f_{7/2}5d_{3/2}$	$4f_{7/2}5d_{3/2}$	−0.173 885	−0.020 808	0.040 577	0.001 327
$4f_{7/2}5d_{5/2}$	$4f_{7/2}5d_{5/2}$	−0.168 912	−0.023 587	0.040 788	0.000 990
$4f_{5/2}5d_{3/2}$	$4f_{5/2}5d_{3/2}$	−0.191 570	−0.030 581	0.041 469	0.001 359
$4f_{5/2}5d_{5/2}$	$4f_{5/2}5d_{5/2}$	−0.186 597	−0.019 993	0.041 680	0.000 994
$4f_{7/2}7s_{1/2}$	$4f_{7/2}7s_{1/2}$	−0.132 052	−0.011 573	0.042 723	0.000 162
$4f_{7/2}6d_{3/2}$	$4f_{7/2}6d_{3/2}$	−0.133 195	−0.005 471	0.042 449	0.000 159
$4f_{7/2}6d_{5/2}$	$4f_{7/2}6d_{5/2}$	−0.132 237	−0.007 111	0.042 496	0.000 129
$4f_{5/2}6d_{3/2}$	$4f_{5/2}6d_{3/2}$	−0.150 880	−0.005 163	0.043 341	0.000 157
$4f_{5/2}6d_{5/2}$	$4f_{5/2}6d_{5/2}$	−0.149 923	−0.006 567	0.043 388	0.000 132
$4f_{7/2}6s_{1/2}$	$4f_{7/2}5d_{3/2}$	0.000 000	−0.001 284	0.000 000	−0.000 071
$4f_{7/2}5d_{3/2}$	$4f_{7/2}6s_{1/2}$	0.000 000	0.004 521	0.000 000	0.000 042
$4f_{7/2}6s_{1/2}$	$4f_{7/2}5d_{5/2}$	0.000 000	−0.003 008	0.000 000	−0.000 119
$4f_{7/2}5d_{5/2}$	$4f_{7/2}6s_{1/2}$	0.000 000	0.007 588	0.000 000	0.000 094
$4f_{7/2}6s_{1/2}$	$4f_{5/2}5d_{3/2}$	0.000 000	−0.000 054	0.000 000	−0.000 018
$4f_{5/2}5d_{3/2}$	$4f_{7/2}6s_{1/2}$	0.000 000	0.000 750	0.000 000	0.000 008

TABLE III. Contributions to the energy matrix $E[4fj_1\ nl_2j_2, 4fj_3\ nl_4j_4]=E^{(0)}+E^{(1)}+E^{(2)}+B^{(1)}+B^{(2)}$ before diagonalization. These contributions are given for Yb III ion with a $[\mathrm{Xe}]4f^{14}$ core, in the case of odd-parity states with $J=4$.

$4fj_1\ nl_2j_2$	$4fj_3\ nl_4j_4$	$E^{(0)}$	$E^{(1)}$	$B^{(1)}$	$E^{(2)}$	$B^{(2)}$
$4f_{7/2}6s_{1/2}$	$4f_{7/2}6s_{1/2}$	0.592 472	−0.309 483	−0.007 363	−0.155 252	0.042 391
$4f_{7/2}5d_{3/2}$	$4f_{7/2}5d_{3/2}$	0.703 066	−0.383 615	−0.007 235	−0.194 692	0.041 904
$4f_{7/2}5d_{5/2}$	$4f_{7/2}5d_{5/2}$	0.705 251	−0.377 557	−0.007 428	−0.192 499	0.041 778
$4f_{5/2}5d_{3/2}$	$4f_{5/2}5d_{3/2}$	0.761 508	−0.396 183	−0.009 833	−0.222 152	0.042 828
$4f_{5/2}5d_{5/2}$	$4f_{5/2}5d_{5/2}$	0.763 694	−0.376 420	−0.010 005	−0.206 590	0.042 674
$4f_{7/2}7s_{1/2}$	$4f_{7/2}7s_{1/2}$	0.814 736	−0.157 036	−0.007 772	−0.143 625	0.042 885
$4f_{7/2}6d_{3/2}$	$4f_{7/2}6d_{3/2}$	0.850 232	−0.166 783	−0.007 756	−0.138 666	0.042 608
$4f_{7/2}6d_{5/2}$	$4f_{7/2}6d_{5/2}$	0.851 407	−0.164 892	−0.007 807	−0.139 348	0.042 624
$4f_{5/2}6d_{3/2}$	$4f_{5/2}6d_{3/2}$	0.908 674	−0.169 822	−0.010 335	−0.156 043	0.043 498
$4f_{5/2}6d_{5/2}$	$4f_{5/2}6d_{5/2}$	0.909 849	−0.164 618	−0.010 380	−0.156 490	0.043 519
$4f_{7/2}6s_{1/2}$	$4f_{7/2}5d_{5/2}$	0.000 000	−0.001 712	0.000 002	−0.003 008	−0.000 119
$4f_{7/2}5d_{5/2}$	$4f_{7/2}6s_{1/2}$	0.000 000	−0.001 712	0.000 002	0.007 588	0.000 094
$4f_{7/2}6s_{1/2}$	$4f_{7/2}7s_{1/2}$	0.000 000	0.064 004	0.000 002	0.040 515	0.001 781
$4f_{7/2}7s_{1/2}$	$4f_{7/2}6s_{1/2}$	0.000 000	0.064 004	0.000 002	−0.070 868	−0.002 181
$4f_{7/2}5d_{3/2}$	$4f_{7/2}5d_{5/2}$	0.000 000	0.001 976	0.000 000	−0.001 963	0.000 009
$4f_{7/2}5d_{5/2}$	$4f_{7/2}5d_{3/2}$	0.000 000	0.001 976	0.000 000	−0.001 990	0.000 010

elements for transitions between excited states. The calculations are carried out using sets of basis Dirac-Fock (DF) orbitals. The orbitals used in the present calculation are obtained as linear combinations of B splines. These B-spline basis orbitals are determined using the method described in Ref. [20]. We use 50 B splines of order 10 for each single-particle angular momentum state, and we include all orbitals with orbital angular momentum $l \leq 9$ in our basis set.

For atoms with one hole in the closed shells and one electron above the closed shells, the model space is formed from hole-particle states of the type $a_v^{+}a_a|0\rangle$, where $|0\rangle$ is the closed-shell $[\mathrm{Xe}]4f_{5/2}^{6}4f_{7/2}^{8}$ ground state, and a_i^{+} and a_j are creation and annihilation operators, respectively. The single-particle indices v and a designate the valence and core states, respectively. For our study of low-lying states $4f^{-1}nl'$ states of Er-like ion, the values of a are $4f_{5/2}$ and $4f_{7/2}$ while the values of v are $6s_{1/2}$, $6p_{1/2}$, $6p_{3/2}$, $5d_{3/2}$, $5d_{5/2}$, $7s_{1/2}$, $7p_{1/2}$, $7p_{3/2}$, $6d_{3/2}$, and $6d_{5/2}$.

To obtain orthonormal model states, we consider the coupled states $\Phi_{JM}(av)$ defined by

$$\Phi_{JM}(av) = \sqrt{(2J+1)}\sum_{m_a m_v}(-1)^{j_v-m_v}\begin{pmatrix} j_v & J & j_a \\ -m_v & M & m_a \end{pmatrix} \times a^{\dagger}_{vm_v}a_{am_a}|0\rangle. \tag{1}$$

Combining the $4f_j$ hole orbitals and the $6s_{1/2}$, $6p_{1/2}$, $6p_{3/2}$, $5d_{3/2}$, $5d_{5/2}$, $7s_{5/2}$, $7p_{1/2}$, $7p_{3/2}$, $6d_{3/2}$, and $6d_{5/2}$ particle orbitals, we obtain 48 odd-parity states consisting of two $J=0$ states, six $J=1$ states, ten $J=2$ states, 12 $J=3$ states, ten $J=4$ states, six $J=5$ states, and two $J=6$ states. Additionally, there are 24 even-parity states consisting of two $J=1$ states, six $J=2$ states, eight $J=3$ states, six $J=4$ states, and two $J=5$ states. The distribution of the 72 states in the model space is summarized in Table I. Instead of using the $4f_j^{-1}nl'_{j'}$,

TABLE IV. Energies of Yb III for odd-parity states with $J=4$ relative to the ground state. $E^{(0+1)} \equiv E^{(0)}+E^{(1)}+B^{(1)}$.

jj coupling	$E^{(0+1)}$	$E^{(2)}$	$B^{(2)}$	E_{LS}	E_{tot}
$4f_{7/2}6s_{1/2}$	58 128	−31 173	9298	82	36 336
$4f_{7/2}5d_{3/2}$	63 467	−26 416	9177	−105	46 122
$4f_{7/2}5d_{5/2}$	65 566	−27 319	9190	−10	47 427
$4f_{5/2}5d_{3/2}$	72 574	−30 508	9354	18	51 438
$4f_{5/2}5d_{5/2}$	78 314	−29 882	9351	138	57 921
$4f_{7/2}7s_{1/2}$	144 978	−32 667	9395	90	121 796
$4f_{7/2}6d_{3/2}$	153 177	−35 227	9310	77	127 338
$4f_{7/2}6d_{5/2}$	153 751	−34 980	9319	84	128 174
$4f_{5/2}6d_{3/2}$	165 212	−39 371	9503	−83	135 261
$4f_{5/2}6d_{5/2}$	166 034	−38 806	9515	−77	136 666

TABLE V. Energies (10^3 cm^{-1}) of odd- and even-parity states relative to the ground state in Yb III calculated in the first-order and second-order RMBPT. RMBPT values are compared with recommended NIST data [11].

Level	RMBPT1	RMBPT	NIST	Level	RMBPT1	RMBPT	NIST
$4f_{7/2}6s_{1/2}(4)$	58 128	36 336	34 656	$4f_{7/2}7s_{1/2}(4)$	144 978	121 796	120 247
$4f_{7/2}6s_{1/2}(3)$	62 358	44 429	39 141	$4f_{7/2}7s_{1/2}(3)$	145 019	121 872	120 365
$4f_{5/2}6s_{1/2}(2)$	70 326	45 194	44 854	$4f_{5/2}7s_{1/2}(2)$	157 231	130 196	130 457
$4f_{5/2}6s_{1/2}(3)$	70 575	47 959	45 208	$4f_{5/2}7s_{1/2}(3)$	157 261	130 254	130 551
$4f_{5/2}5d_{5/2}(0)$	71 917	49 469	45 277	$4f_{5/2}6d_{5/2}(0)$	165 609	135 693	
$4f_{7/2}5d_{5/2}(1)$	74 895	39 762	39 721	$4f_{7/2}6d_{5/2}(1)$	153 820	128 129	
$4f_{5/2}5d_{5/2}(1)$	64 736	47 664	50 029	$4f_{5/2}6d_{5/2}(1)$	165 415	135 609	133 997
$4f_{5/2}5d_{3/2}(1)$	80 273	55 144	53 365	$4f_{5/2}6d_{3/2}(1)$	165 760	135 667	
$4f_{7/2}5d_{3/2}(2)$	58 121	39 755	33 386	$4f_{7/2}6d_{3/2}(2)$	152 843	126 620	125 987
$4f_{7/2}5d_{5/2}(2)$	63 643	44 488	40 288	$4f_{7/2}6d_{5/2}(2)$	153 570	127 769	133 997
$4f_{5/2}5d_{3/2}(2)$	73 940	52 632	48 415	$4f_{5/2}6d_{3/2}(2)$	165 306	135 450	135 355
$4f_{5/2}5d_{5/2}(2)$	76 401	55 361	51 463	$4f_{5/2}6d_{5/2}(2)$	165 891	136 313	136 351
$4f_{7/2}5d_{3/2}(3)$	58 452	36 764	34 991	$4f_{7/2}6d_{3/2}(3)$	153 096	127 175	126 559
$4f_{7/2}5d_{5/2}(3)$	65 799	45 862	43 019	$4f_{7/2}6d_{5/2}(3)$	153 736	128 190	132 864
$4f_{5/2}5d_{3/2}(3)$	76 328	55 978	51 582	$4f_{5/2}6d_{3/2}(3)$	165 460	135 836	135 355
$4f_{5/2}5d_{5/2}(3)$	77 804	56 856	53 123	$4f_{5/2}6d_{5/2}(3)$	166 001	136 566	136 700
$4f_{7/2}5d_{3/2}(4)$	63 467	46 122	40 160	$4f_{7/2}6d_{3/2}(4)$	153 177	127 338	125 810
$4f_{7/2}5d_{5/2}(4)$	65 565	47 427	42 425	$4f_{7/2}6d_{5/2}(4)$	153 751	128 174	126 456
$4f_{5/2}5d_{3/2}(4)$	72 574	51 438	47 057	$4f_{5/2}6d_{3/2}(4)$	165 212	135 261	132 864
$4f_{5/2}5d_{5/2}(4)$	78 314	57 921	53 736	$4f_{5/2}6d_{5/2}(4)$	166 034	136 666	136 849
$4f_{7/2}5d_{3/2}(5)$	60 641	42 569	37 020	$4f_{7/2}6d_{3/2}(5)$	152 969	126 890	
$4f_{7/2}5d_{5/2}(5)$	66 152	48 991	43 623	$4f_{7/2}6d_{5/2}(5)$	153 781	128 270	
$4f_{5/2}5d_{5/2}(5)$	75 391	54 313	50 357	$4f_{5/2}6d_{5/2}(5)$	165 824	136 206	
$4f_{7/2}5d_{5/2}(6)$	62 449	44 360	39 085	$4f_{7/2}6d_{5/2}(6)$	153 525	127 697	
$4f_{5/2}6p_{3/2}(1)$	115 842	86 729	87 613	$4f_{5/2}7p_{3/2}(1)$	172 777	146 519	
$4f_{7/2}6p_{3/2}(2)$	104 061	79 043	78 183	$4f_{7/2}7p_{3/2}(2)$	160 592	138 275	
$4f_{5/2}6p_{1/2}(2)$	111 318	82 129	82 907	$4f_{5/2}7p_{1/2}(2)$	170 964	144 547	
$4f_{5/2}6p_{3/2}(2)$	116 727	87 925	88 977	$4f_{5/2}7p_{3/2}(2)$	172 921	146 824	
$4f_{7/2}6p_{1/2}(3)$	98 803	73 274	72 140	$4f_{7/2}7p_{1/2}(3)$	158 667	136 064	
$4f_{7/2}6p_{3/2}(3)$	104 540	79 512	78 779	$4f_{7/2}7p_{3/2}(3)$	160 674	138 394	
$4f_{5/2}6p_{1/2}(3)$	111 101	81 757	82 546	$4f_{5/2}7p_{1/2}(3)$	170 927	144 461	
$4f_{5/2}6p_{3/2}(3)$	117 037	88 432	89 397	$4f_{5/2}7p_{3/2}(3)$	172 980	146 906	
$4f_{7/2}6p_{1/2}(4)$	98 959	73 457	72 487	$4f_{7/2}7p_{1/2}(4)$	158 685	136 098	
$4f_{7/2}6p_{3/2}(4)$	104 867	80 103	79 283	$4f_{7/2}7p_{3/2}(4)$	160 733	138 528	
$4f_{5/2}6p_{3/2}(4)$	116 368	87 546	88 498	$4f_{5/2}7p_{3/2}(4)$	172 865	146 703	
$4f_{7/2}6p_{3/2}(5)$	103 979	78 889	78 020	$4f_{7/2}7p_{3/2}(5)$	160 583	138 252	

designations, we use simpler designations $4f_jnl'_{j'}$ in this table and in all following tables and the text below.

III. EXCITATION ENERGIES

In Table II, we give various contributions to the second-order energies for Yb III ion. In this table, we show the one-body and two-body second-order Coulomb contributions to the energy matrix labeled $E_1^{(2)}$ and $E_2^{(2)}$, respectively. The corresponding Breit-Coulomb contributions are given in columns headed $B_1^{(2)}$ and $B_2^{(2)}$ of Table II. The one-body second-order energy is obtained as a sum of the valence $E_v^{(2)}$ and hole $E_a^{(2)}$ energies with the later being the dominant contribution.

The values of $E_1^{(2)}$ and $B_1^{(2)}$ are nonzero only for diagonal matrix elements. Although there are 72 diagonal and 496 nondiagonal matrix elements for the $4f_jnl_{j'}(J)$ hole-particle states, we list only the part of odd-parity subset with $J=4$ in Table II to provide an example of such calculations. The second-order Breit-Coulomb corrections are relatively large and, therefore, must be included in accurate calculations. The values of nondiagonal matrix elements given in columns

TABLE VI. E1, M2, and E3 uncoupled reduced matrix elements in length form for transitions from $av(J)$ states with $J=1$, 2, and 3 into the ground state in Yb III.

$av(J)$	$Z^{(1)}$	$Z^{(2)}$	$B^{(2)}$	$P^{(\mathrm{derv})}$
		E1 uncoupled reduced matrix elements		
$4f_{7/2}5d_{5/2}(1)$	−0.9404	0.1945	−0.0037	−0.9404
$4f_{5/2}5d_{5/2}(1)$	−0.1951	0.0565	−0.0011	−0.1951
$4f_{5/2}5d_{3/2}(1)$	0.7510	−0.2299	0.0034	0.7510
		M2 uncoupled reduced matrix elements		
$4f_{7/2}5d_{3/2}(2)$	1.9942	1.1268	0.0061	3.9884
$4f_{7/2}5d_{5/2}(2)$	−5.0987	−1.9805	−0.0202	10.1972
$4f_{5/2}6s_{1/2}(2)$	−0.0000	0.0090	0.0000	−0.0000
$4f_{5/2}5d_{3/2}(2)$	1.4193	0.2942	0.0067	2.8386
$4f_{5/2}5d_{5/2}(2)$	0.0000	0.1950	0.0000	0.0000
		E3 uncoupled reduced matrix elements		
$4f_{7/2}6s_{1/2}(3)$	−2.9168	−0.1845	−0.0328	−8.8052
$4f_{7/2}5d_{3/2}(3)$	1.9037	−0.0280	0.0186	5.7710
$4f_{7/2}5d_{5/2}(3)$	3.3194	0.0020	0.0326	9.9924
$4f_{5/2}6s_{1/2}(3)$	−2.2001	−0.1591	−0.0314	−6.5934
$4f_{5/2}5d_{3/2}(3)$	−2.2944	0.0049	−0.0276	−6.8880
$4f_{5/2}5d_{5/2}(3)$	1.8833	0.0079	0.0228	5.6145

TABLE VII. Energies (E in cm^{-1}) and radiative rates (A_r in s^{-1}) for E1, M2, and E3 transitions from $4f5d$ and $4f6s$ states to the ground state in Yb III. Numbers in brackets represent powers of 10.

	E (cm^{-1})	Transition rate A_r (s^{-1})	
$av(J)$	NIST [11]	RMBPT1	RMBPT
		E1 transitions	
$4f_{7/2}5d_{5/2}(1)$	39 721	1.015[+7]	5.524[+6]
$4f_{5/2}5d_{5/2}(1)$	50 029	1.338[+6]	6.215[+5]
$4f_{5/2}5d_{3/2}(1)$	53 365	1.263[+8]	2.985[+7]
		M2 transitions	
$4f_{7/2}5d_{3/2}(2)$	33 386	1.956[−4]	1.662[−4]
$4f_{7/2}5d_{5/2}(2)$	40 288	5.340[−4]	2.298[−4]
$4f_{5/2}6s_{1/2}(2)$	44 854	1.581[−6]	4.465[−7]
$4f_{5/2}5d_{3/2}(2)$	48 415	2.592[−4]	3.058[−5]
$4f_{5/2}5d_{5/2}(2)$	51 463	3.562[−7]	3.547[−5]
		E3 transitions	
$4f_{7/2}6s_{1/2}(3)$	34 991	2.785[−7]	2.276[−7]
$4f_{7/2}5d_{3/2}(3)$	39 141	3.639[−7]	4.043[−7]
$4f_{7/2}5d_{5/2}(3)$	43 019	1.231[−6]	1.207[−6]
$4f_{5/2}6s_{1/2}(3)$	45 208	9.164[−7]	6.657[−7]
$4f_{5/2}5d_{3/2}(3)$	51 582	2.513[−6]	2.517[−6]
$4f_{5/2}5d_{5/2}(3)$	53 123	2.825[−7]	2.425[−7]

headed $E_2^{(2)}$ and $B_2^{(2)}$ are comparable with values of diagonal two-body matrix elements. However, the values of one-body contributions, $E_1^{(2)}$ and $B_1^{(2)}$, are larger than the values of two-body contributions, $E_2^{(2)}$ and $B_2^{(2)}$, respectively. As a result, total second-order diagonal matrix elements are much larger than the nondiagonal matrix elements, which are shown in Table II.

In Table III, we present results for the zeroth-, first-, and second-order Coulomb contributions, $E^{(0)}$, $E^{(1)}$, and $E^{(2)}$, and the first- and second-order Breit-Coulomb corrections, $B_{(1)}$ and $B^{(2)}$. Importance of correlation contribution is evident from this table; the ratio of the first and zeroth orders ($E^{(1)}/E^{(0)}$) is about 20–50%, and the ratio of the second and first ($E^{(2)}/E^{(1)}$) orders is even larger, 50–90%. It should be noted that corrections for the frequency-dependent Breit interaction [21] are included in the first order only. The difference between the first-order Breit corrections calculated with and without frequency dependence is 1–3%, however, the ratio of the first-order Breit and Coulomb corrections is also 2–5%. As one can see from Table III, the ratio of nondiagonal and diagonal matrix elements is larger for the second-order contributions than for the first-order contributions. Another difference in the first- and second-order contributions is the symmetry properties: the first-order nondiagonal matrix elements are symmetric, but the second-order nondiagonal matrix elements are not symmetric. The values of $E^{(2)}[a'v'(J),av(J)]$ and $E^{(2)}[av(J),a'v'(J)]$ matrix elements differ in some cases by a factor 2–3 and occasionally have opposite signs.

We now discuss how the final energy levels are obtained from the above contributions. To determine the first-order energies of the states under consideration, we diagonalize the symmetric first-order effective Hamiltonian, including both Coulomb and Breit interactions. The first-order expansion coefficient $C^N[av(J)]$ (often called a mixing coefficient) is the Nth eigenvector of the first-order effective Hamiltonian, and $E^{(1)}[N]$ is the corresponding eigenvalue. The resulting eigenvectors are used to determine the second-order Coulomb correction $E^{(2)}[N]$, the second-order Breit-Coulomb correction $B^{(2)}[N]$, and the quantum electrodynamics (QED) correction $E_{\mathrm{LS}}[N]$.

In Table IV, we list the following contributions to the energies of 13 excited states in Yb^{2+}: the sum of the zeroth- and first-order energies $E^{(0+1)}=E^{(0)}+E^{(1)}+B^{(1)}$, the second-order Coulomb energy $E^{(2)}$, the second-order Breit-Coulomb correction $B^{(2)}$, the QED correction E_{LS}, and the sum of the above contributions E_{tot}. The Lamb shift E_{LS} is approximated as the sum of the one-electron self-energy and the first-order vacuum-polarization energy. The vacuum-polarization contribution is calculated from the Uehling potential using the results of Fullerton and Rinker [22]. The self-energy contribution is estimated for s, $p_{1/2}$, and $p_{3/2}$ orbitals by interpolating among the values obtained by [23–25] using Coulomb wave functions. For this purpose, an effective nuclear charge Z_{eff} is obtained by finding the value of Z_{eff} required to give a Coulomb orbital with the same average $\langle r\rangle$ as the Dirac-Hartree-Fock (DHF) orbital.

When starting calculations from relativistic DF wave functions, it is natural to use jj designations for uncoupled energy matrix elements; however, neither jj nor LS coupling describes the *physical* states properly. We find out that the mixing coefficients are equal to 0.5–0.7. Therefore, we still

TABLE VIII. Energies (E in cm^{-1}), radiative rates (Λr in s^{-1}), and sum of radiative rates (ΣA_r in s^{-1}) for M1 and E2 transitions between the levels of $4f5d$ and $4f6s$ configurations in Yb III. Numbers in brackets represent powers of 10.

Transitions		E_{NIST} (cm^{-1})		Transition rates Λr		ΣA_r (s^{-1})	
$av(J)$	$a'v'(J')$	Lower	Upper	RMBPT1	RMBPT	RMBPT1	RMBPT
			Magnetic-dipole transitions				
$4f_{7/2}5d_{3/2}(2)$	$4f_{5/2}6s_{1/2}(2)$	33 386	44 854	1.748[−3]	1.725[−3]	1.748[−3]	1.725[−3]
$4f_{7/2}6s_{1/2}(3)$	$4f_{5/2}6s_{1/2}(2)$	34 991	44 854	1.549[1]	1.549[1]	1.549[1]	1.549[1]
$4f_{7/2}5d_{3/2}(3)$	$4f_{5/2}6s_{1/2}(2)$	39 141	44 854	1.819[−3]	1.818[−3]	1.549[1]	1.549[1]
$4f_{7/2}5d_{5/2}(2)$	$4f_{5/2}6s_{1/2}(2)$	40 288	44 854	3.581[−3]	3.583[−3]	1.550[1]	1.550[1]
$4f_{7/2}5d_{5/2}(1)$	$4f_{5/2}6s_{1/2}(2)$	39 721	44 854	1.806[−4]	1.647[−4]	1.550[1]	1.550[1]
$4f_{7/2}5d_{5/2}(3)$	$4f_{5/2}6s_{1/2}(3)$	43 019	44 854	5.711[−4]	5.714[−4]	1.550[1]	1.550[1]
			Electric-quadrupole transitions				
$4f_{7/2}5d_{3/2}(2)$	$4f_{5/2}6s_{1/2}(2)$	33 386	44 854	3.136[−3]	2.184[−3]	3.136[−3]	2.184[−3]
$4f_{7/2}6s_{1/2}(4)$	$4f_{5/2}6s_{1/2}(2)$	34 656	44 854	2.052[−4]	2.849[−4]	3.341[−3]	2.469[−3]
$4f_{7/2}6s_{1/2}(3)$	$4f_{5/2}6s_{1/2}(2)$	34 991	44 854	4.768[−4]	4.033[−3]	3.818[−3]	6.502[−3]
$4f_{7/2}5d_{3/2}(3)$	$4f_{5/2}6s_{1/2}(2)$	39 141	44 854	9.840[−6]	7.165[−6]	3.828[−3]	6.509[−3]
$4f_{7/2}5d_{5/2}(1)$	$4f_{5/2}6s_{1/2}(2)$	39 721	44 854	9.515[−4]	7.936[−4]	4.779[−3]	7.303[−3]
$4f_{7/2}5d_{3/2}(4)$	$4f_{5/2}6s_{1/2}(2)$	40 160	44 854	3.270[−4]	3.647[−4]	5.106[−3]	7.667[−3]
$4f_{7/2}5d_{5/2}(2)$	$4f_{5/2}6s_{1/2}(2)$	40 288	44 854	9.559[−6]	2.946[−5]	5.116[−3]	7.697[−3]
$4f_{7/2}5d_{5/2}(4)$	$4f_{5/2}6s_{1/2}(2)$	42 425	44 854	1.405[−5]	1.887[−5]	5.130[−3]	7.716[−3]
$4f_{7/2}5d_{5/2}(3)$	$4f_{5/2}6s_{1/2}(2)$	43 019	44 854	2.533[−7]	5.179[−7]	5.130[−3]	7.716[−3]

use the jj designations in Table IV. We already mentioned the importance of including the correlation contribution in order to obtain accurate energy values for Er-like Yb III ion. The second-order Coulomb contribution $E^{(2)}$ gives 30% to the total values of the $4f_j6s$ energies and almost 90% in the case of the $4f_j5d_{j'}$ energies. Therefore, we expect energies to be accurate to few 1000 cm^{-1} for the $4f_j6s$ and $4f_j5d_{j'}$ states. Better accuracy is expected for higher states.

In Table V, we compare our RMBPT results for the $4f6s$, $4f7s$, $4f6p$, $4f7p$, $4f5d$, and $4f6d$ excitation energies in Yb III with recommended National Institute of Standards and Technology (NIST) data [11]. The largest difference between our RMBPT values and NIST data is found to be about 10% for the first $4f6s$ and $4f5d$ states. It is expected, as already underlined previously since the contribution of the second-order Coulomb contribution $E^{(2)}$ to the total energies for the $4f6s$ and $4f5d$ states with $J=4$ is very large (compare columns with headings "$E^{(2)}$" and "E_{tot}" in Table IV). The difference between the RMBPT and NIST data (about 1%) is much smaller for the $4f6p$ and $4f7s$ states. The difference between the RMBPT and NIST data for the $4f6d$ states is equal to 1%-3%. We did not find any experimental data for the $4f7p$ states.

To show size of the correlation contribution, we added in Table V the data evaluated in the first-order approximation in columns labelled "RMBPT1." These data are obtained as a sum of the $E^{(0)}$, $E^{(1)}$, and $B^{(1)}$ values (see explanation of Table IV). It should be noted that these RMBPT1 values are often referred to as the multiconfiguration Dirac-Fock (MCDF) values [26]. The ratios of values in the RMBPT1 and RMBPT columns range from 1.2 to 1.6. We note how poorly the first-order values agree with the NIST recommended data in comparison with our final second-order RMBPT results. We would like to mention that our RMBPT values presented in Table V are first *ab initio* values for the energy levels in Yb III.

IV. MULTIPOLE MATRIX ELEMENTS, TRANSITION RATES, AND LIFETIMES FOR THE 4*f*5*d* AND 4*f*6*s* STATES

We already mentioned that all states up to $E=53\,736$ cm^{-1} (counting from the ground state) belong to either [Xe]$4f^{13}5d$ or [Xe]$4f^{13}6s$ odd configurations [11]. Only three of these [Xe]$4f^{13}5d$ levels have total angular momentum $J=1$ and, therefore, can decay to the ground state via strong electric-dipole transitions. As a result, all remaining 21 [Xe]$4f^{13}5d$ and [Xe]$4f^{13}6s$ levels with $J=0,2-6$, are metastable. Below, we consider all possible multipole (E1, M2, and E3) transitions from the [Xe]$4f^{13}5d$ and [Xe]$4f^{13}6s$ excited states to the ground state [Xe]$4f^{14}\,{}^1S_0$. Additionally, we consider the M1 and E2 transitions between levels of even-parity [Xe]$4f^{13}ns$ and [Xe]$4f^{13}nd$ states to calculate the lifetimes of [Xe]$4f^{13}5d$ and [Xe]$4f^{13}6s$ levels.

A. Multipole transitions from excited states into the ground state

We calculate electric-dipole (E1) matrix elements for the transitions between the six odd-parity $4f_j5d_{j'}(1)$ and $4f_j6d_{j'}(1)$ excited states and the ground state, magnetic-quadrupole (M2) matrix elements between the ten odd-parity $4f_j5d_{j'}(2)$, $4f_j6d_{j'}(2)$, $4f_j6s_{j'}(2)$, and $4f_j7s_{j'}(2)$ excited

TABLE IX. Energies (E in cm^{-1}) and radiative rates (A_r in s^{-1}) in Yb III. The sum of radiative rates from all possible E1, M2, and M3 transitions from $4f5d$ and $4f6s$ states to the ground state are listed in columns labeled "E1, M2, M3 ." The M1 and E2 transitions inside of the $4f5d$ and $4f6s$ configuration sets are listed in the respective columns labeled "M1 transitions" and "E2 transitions." Sum of radiative rates from multipole transitions (A_r in s^{-1}) and lifetime values (τ in seconds) of $4f5d$ and $4f6s$ states are listed in four last columns. Numbers in brackets represent powers of 10.

	E	E1, M2, E3		M1 transitions		E2 transitions		ΣA_r in s^{-1}		τ in seconds	
$av(J)$	NIST	RMBPT1	RMBPT	RMBPT1	RMBPT	RMBPT1	RMBPT	RMBPT1	RMBPT	RMBPT1	RMBPT
$4f_{7/2}5d_{3/2}(2)$	33 386	1.956[−4]	1.662[−4]	0.000[0]	0.000[0]	0.000[0]	0.000[0]	1.956[−4]	1.662[−4]	5.112[3]	6.017[3]
$4f_{7/2}6s_{1/2}(4)$	34 656	0.000[0]	0.000[0]	0.000[0]	0.000[0]	5.483[−5]	1.661[−5]	5.483[−5]	1.661[−5]	1.824[4]	6.020[4]
$4f_{7/2}6s_{1/2}(3)$	34 991	2.785[−7]	2.276[−7]	4.512[−4]	4.877[−4]	2.691[−6]	9.372[−7]	4.542[−4]	4.889[−4]	2.202[3]	2.046[3]
$4f_{7/2}5d_{3/2}(5)$	37 020	0.000[0]	0.000[0]	4.144[−6]	9.894[−7]	1.405[−3]	4.232[−4]	1.409[−3]	4.242[−4]	7.097[2]	2.357[3]
$4f_{7/2}5d_{5/2}(6)$	39 085	0.000[0]	0.000[0]	3.745[−1]	3.806[−1]	7.390[−2]	2.363[−2]	4.484[−1]	4.042[−1]	2.230[0]	2.474[0]
$4f_{7/2}5d_{3/2}(3)$	39 141	3.639[−7]	4.043[−7]	1.053[−1]	1.100[−1]	8.283[−2]	2.879[−2]	1.881[−1]	1.388[−1]	5.315[0]	7.205[0]
$4f_{7/2}5d_{5/2}(1)$	39 721	1.015[7]	5.524[6]	5.575[0]	5.702[0]	2.036[−2]	3.516[−2]	1.015[7]	5.524[6]	9.852[−8]	1.810[−7]
$4f_{7/2}5d_{3/2}(4)$	40 160	0.000[0]	0.000[0]	7.848[−2]	7.920[−2]	2.109[−1]	7.672[−2]	2.894[−1]	1.559[−1]	3.456[0]	6.414[0]
$4f_{7/2}5d_{5/2}(2)$	40 288	5.340[−4]	2.298[−4]	3.791[−1]	3.938[−1]	6.943[−2]	6.557[−2]	4.491[−1]	4.596[−1]	2.227[0]	2.176[0]
$4f_{7/2}5d_{5/2}(4)$	42 425	0.000[0]	0.000[0]	4.378[−1]	4.466[−1]	8.273[−1]	5.703[−1]	1.265[0]	1.017[0]	7.905[−1]	9.834[−1]
$4f_{7/2}5d_{5/2}(3)$	43 019	1.231[−6]	1.207[−6]	8.036[−1]	8.217[−1]	7.222[−1]	8.391[−1]	1.526[0]	1.661[0]	6.554[−1]	6.021[−1]
$4f_{7/2}5d_{5/2}(5)$	43 623	0.000[0]	0.000[0]	6.070[−1]	6.237[−1]	1.894[0]	1.588[0]	2.501[0]	2.212[0]	3.998[−1]	4.521[−1]
$4f_{5/2}6s_{1/2}(2)$	44 854	1.581[−6]	4.465[−7]	1.550[1]	1.550[1]	5.130[−3]	7.716[−3]	1.551[1]	1.551[1]	6.449[−2]	6.448[−2]
$4f_{5/2}6s_{1/2}(3)$	45 208	9.164[−7]	6.657[−7]	1.724[1]	1.724[1]	3.814[−2]	2.885[−2]	1.728[1]	1.727[1]	5.788[−2]	5.791[−2]
$4f_{5/2}5d_{5/2}(0)$	45 277	0.000[0]	0.000[0]	6.718[0]	6.706[0]	2.116[−3]	5.209[−3]	6.720[0]	6.711[0]	1.488[−1]	1.490[−1]
$4f_{5/2}5d_{3/2}(4)$	47 057	0.000[0]	0.000[0]	1.458[1]	1.459[1]	8.983[−2]	5.719[−2]	1.467[1]	1.465[1]	6.817[−2]	6.827[−2]
$4f_{5/2}5d_{3/2}(2)$	48 415	2.592[−4]	3.058[−5]	1.564[1]	1.565[1]	2.027[−1]	5.500[−1]	1.584[1]	1.620[1]	6.312[−2]	6.173[−2]
$4f_{5/2}5d_{5/2}(1)$	50 029	1.338[6]	6.215[5]	1.974[1]	1.970[1]	2.976[−1]	2.378[0]	1.338[6]	6.215[5]	7.474[−7]	1.609[−6]
$4f_{5/2}5d_{5/2}(5)$	50 357	0.000[0]	0.000[0]	1.886[1]	1.880[1]	4.064[−1]	3.353[0]	1.927[1]	2.215[1]	5.190[−2]	4.514[−2]
$4f_{5/2}5d_{5/2}(2)$	51 463	3.562[−7]	3.547[−5]	1.533[1]	1.532[1]	3.376[−1]	4.261[1]	1.567[1]	5.793[1]	6.383[−2]	1.726[−2]
$4f_{5/2}5d_{3/2}(3)$	51 582	2.513[−6]	2.517[−6]	2.025[1]	2.027[1]	4.337[−1]	2.356[0]	2.068[1]	2.263[1]	4.835[−2]	4.420[−2]
$4f_{5/2}5d_{5/2}(3)$	53 123	2.825[−7]	2.425[−7]	1.858[1]	1.857[1]	1.332[0]	4.106[1]	1.991[1]	5.963[1]	5.022[−2]	1.677[−2]
$4f_{5/2}5d_{3/2}(1)$	53 365	1.263[8]	2.985[7]	2.326[1]	2.357[1]	6.068[0]	2.882[1]	1.263[8]	2.985[7]	7.918[−9]	3.350[−8]
$4f_{5/2}5d_{5/2}(4)$	53 736	0.000[0]	0.000[0]	1.684[1]	1.686[1]	1.558[0]	6.044[0]	1.840[1]	2.290[1]	5.435[−2]	4.366[−2]

states and the ground state, and electric-octupole (E3) matrix elements between the 12 odd-parity $4f_j5d_{j'}(3)$, $4f_j6d_{j'}(3)$, $4f_j6s_{j'}(3)$, and $4f_j7s_{j'}(3)$ excited states and the ground state. Analytical expressions in the first- and the second-order RMBPT are given by Eqs. (2.12)–(2.17) of Ref. [3] for the E1 matrix elements and in Refs. [4–6] for the M2 and E3 matrix elements.

The first- and second-order Coulomb corrections and second-order Breit-Coulomb corrections to reduced E1, M2, and E3 matrix elements will be referred to as $Z^{(1)}$, $Z^{(2)}$, and $B^{(2)}$, respectively, throughout the text. In Table VI, we list values of *uncoupled* first- and second-order E1, M2, and E3 matrix elements $Z^{(1)}$, $Z^{(2)}$, and $B^{(2)}$, together with derivative terms $P^{(\mathrm{derv})}$, for Yb III (see, for detail, Refs. [4–6]). We include in this table transitions from the $4f_j5d_{j'}(J)$ and $4f_j6s_{1/2}(J)$ states since their transitions are important to evaluate lifetimes of $4f_j5d_{j'}(J)$ and $4f_j6s_{1/2}(J)$ states. Importance of correlation contribution is evident from this table; the ratio of the second and first $(Z^{(2)}/Z^{(1)})$ orders is very large for E1 transitions (40–50%) and M2 transitions (20–60%). However, the ratio of the second and first $(Z^{(2)}/Z^{(1)})$ orders much for E3 transitions is about 1–6%.

The E1, M2, and E3 transition probabilities A_r (s^{-1}) for the transitions between the ground state and the $4f_jnd_{j'}(J)$ and $4f_jns_{j'}(2)$ states are obtained in terms of line strengths S (a.u.) and energies E (a.u.) as

$$A(E1) = \frac{2.142\,00 \times 10^{10}}{(2J+1)}[E]^3 S(E1),$$

$$A(M2) = \frac{0.759\,26}{(2J+1)}[E]^5 S(M2),$$

$$A(E3) = \frac{1.026\,83 \times 10^{-6}}{(2J+1)}[E]^7 S(E3). \qquad (2)$$

It should be noted that the line strengths $S(E1)$, $S(M2)$, and $S(E3)$ are obtained as a square of *coupled* E1, M2, and E3 matrix elements. The E1, M2, and E3 *coupled* matrix elements are evaluated using an intermediate-coupling scheme (see [3] for detail). Results of our calculation are given in Table VII. In columns with headings RMBPT1 and RMBPT of this table, we list radiative transitions rates [Eq. (2)] evalu-

TABLE X. Energies (E in cm^{-1}) and lifetime values (τ in ns) of the $4f_j5d_{j'}(1)$ states of Yb III. These are the only levels that decay to the ground state via electric-dipole transitions. Experimental measurements (Expt.) and theoretical values (Theory) are from Ref. [15]

Level $av(J)$	E (cm^{-1}) NIST[11]	RMBPT1	Lifetimes τ (ns) RMBPT	Theory(A)	Theory(B)	Expt.
$4f_{7/2}5d_{5/2}(1)$	39 721	98.5	181	166	270	230(20)
$4f_{5/2}5d_{5/2}(1)$	50 029	748	1609	272	476	280(30)
$4f_{5/2}5d_{3/2}(1)$	53 365	7.9	33.5	6.3	10.3	11.4(7)

ated with NIST energies. The values A_r^{RMBPT1} are the first-order RMBPT values. In the column with headings RMBPT of this table, we list transition rates using line strengths $S(E1)$, $S(M2)$, and $S(E3)$ evaluated in the second-order RMBPT. We can see substantial differences between those results. The differences give the value of the second-order contribution. The ratios of multipole transition rates A_r^{E1}/A_r^{M2} and A_r^{M2}/A_r^{E3} are equal to 10^9-10^{12} and $10-10^3$, respectively.

B. Multipole transitions between excited hole-particle states

To evaluate lifetime values for the $4f_j5d_{j'}(J)$ and $4f_j6s_{1/2}(J)$ levels, we need to consider transitions between levels of the same parity: $4f_jnd_{j'}(J)$ and $4f_jns_{1/2}(J)$ states. We consider all possible magnetic-dipole (M1), electric-quadrupole (E2), and magnetic-octupole (M3) transitions between levels of the $4f_j5d_{j'}(J)$ and $4f_j6s_{1/2}(J)$ configurations. Analytical expressions for the multipole matrix elements in the first-and the second-order RMBPT for those transitions are given by Eqs. (1) and (2)–(8) of Ref. [8]. The number of such transitions increases dramatically in comparison with transitions from excited states to the ground state considered above. We calculated the line strengths and transition rates for numerous transitions between the $4f_j5d_{j'}(J)$ and $4f_j6s_{1/2}(J)$ set of states. Final results of our calculations are given in Table VIII.

Energies, radiative rates, and sum of radiative rates A_r for the M1 and E2 transitions between levels of the $4f_j5d_{j'}(J)$ and $4f_j6s_{1/2}(J)$ configurations in Yb III are listed in Table VIII. We do not include M3 transitions since A_r for these transitions is smaller by two to three orders of magnitude than for E2 transitions. As a result, it gives very small contribution to the lifetimes of the $4f_j5d_{j'}(J)$ and $4f_j6s_{1/2}(J)$ states. We can see from Table VIII that the E2 transition rates are smaller by one to three orders magnitude than the M1 transitions. In this table, we include transitions from the $4f_j6s_{1/2}(J=2)$ level into all levels with energies less than the energy of the $4f_j6s_{1/2}(J=2)$ level. Those energies are given in two columns of Table VIII with E_{NIST} headings. Those NIST energies [11] are used to evaluate transition rates A_r listed in the next two columns of Table VIII. We can see from this table that the largest A_r values come from the M1 $[4f_j6s_{1/2}(J=3)$-$4f_j6s_{1/2}(J=2)]$ transition. The values A_r^{RMBPT1} and A_r^{RMBPT1} are obtained as the first-order and second-order RMBPT values, respectively. The second-order RMBPT contribution is more important for E2 transitions than for M1 transitions. In two last columns of Table VIII, we list sum of A_r values that is used for the evaluation of the lifetime of the $4f_j6s_{1/2}(J=2)$ level.

C. Lifetime data

The lifetimes are obtained by taking into account multipole transition rates from each upper level to all possible lower levels. Radiative rates (A_r in s^{-1}) for E1, M2, and E3 transitions from the $4f5d$ and $4f6s$ states to the ground state are listed in Table VII. Short list of radiative rates (A_r in s^{-1}) for M1 and E2 transitions between levels of the $4f5d$ and $4f6s$ configurations is given in Table VIII. In Table IX, we summarize all those results. We use jj designations to label levels given in the first column of Table IX. NIST energies [11] are listed in the second column. The RMBPT1 and RMBPT columns give results evaluated in the first- and second-orders of RMBPT. The sum of radiative rates from all possible E1, M2, and M3 transitions from $4f5d$ and $4f6s$ states to the ground state are listed in columns labeled "E1, M2, M3." The M1 and E2 transitions inside of the $4f5d$

TABLE XI. E1 uncoupled reduced matrix elements in length L and velocity V forms for transitions between excited $av(J)-a'v'(J')$ states in Yb III.

$av(J)$	$a'v'(J')$	$Z_L^{(1)}$	$Z_V^{(1)}$	$Z_L^{(2)}$	$Z_V^{(2)}$	$B_L^{(2)}$	$B_V^{(2)}$	$P_L^{(\mathrm{derv})}$	$P_V^{(\mathrm{derv})}$
$4f_{7/2}6s_{1/2}(4)$	$4f_{7/2}6p_{1/2}(4)$	−4.439 560	−4.242 370	1.698 445	−1.090 692	−0.005 850	0.002 115	−4.439 560	−0.000 013
$4f_{7/2}6s_{1/2}(4)$	$4f_{7/2}6p_{3/2}(4)$	5.204 210	4.951 410	−2.004351	1.609 249	0.007 062	−0.006 251	5.204 180	−0.000 036
$4f_{7/2}5d_{3/2}(4)$	$4f_{7/2}6p_{1/2}(4)$	4.423 380	−27.215 700	−4.155 636	302.890 100	0.014 878	−0.831 895	4.423 380	0.000 000
$4f_{7/2}5d_{3/2}(4)$	$4f_{7/2}6p_{3/2}(4)$	−1.175 670	−0.007 543	1.156 960	−11.998 654	−0.004 291	0.033 923	−1.175 670	0.000 001
$4f_{7/2}5d_{5/2}(4)$	$4f_{7/2}6p_{3/2}(4)$	4.480 850	−1.006 250	−4.237 799	47.252 730	0.011 286	−0.094 497	4.480 850	0.000 003

TABLE XII. Coupled reduced matrix elements $av(J)-a'v'(J')$ calculated in length L and velocity V forms for Yb III.

		First order		RMBPT	
$av(J)$	$a'v'(J')$	L	V	L	V
$4f_{7/2}6s_{1/2}(4)$	$4f_{7/2}6p_{1/2}(4)$	3.957	4.598	2.975	3.007
$4f_{7/2}6s_{1/2}(4)$	$4f_{7/2}6p_{3/2}(4)$	−5.279	−5.319	−3.993	−4.112
$4f_{7/2}5d_{3/2}(4)$	$4f_{7/2}6p_{1/2}(4)$	4.301	−26.353	4.218	3.780
$4f_{7/2}5d_{3/2}(4)$	$4f_{7/2}6p_{3/2}(4)$	−2.546	1.876	−2.324	−2.144
$4f_{7/2}5d_{5/2}(4)$	$4f_{7/2}6p_{3/2}(4)$	4.247	−0.424	3.885	3.512

and $4f6s$ configuration sets are listed in the respective columns labeled "M1 transitions" and "E2 transitions." We evaluate the 131 M1 transition rates and the 196 E2 transition rates. Then, we sum those transition rates as was illustrated in Table VIII. Next columns of Table IX (labeled ΣA_r) summarize results given in columns with E1, M2, E3, M1 transitions, and E2 transitions labels. The lifetime values (in seconds) are obtained as $1/\Sigma A_{r,}$. The four low-lying metastable levels have the longest lifetime values (10^3-10^4 s). The lifetime values of other 17 metastable levels range from 10^{-2} s up to 10 s. Three levels that can decay via electric-dipole transitions have much shorter lifetime values $10^{-6}-10^{-8}$ s, as expected.

Our RMBPT1 and RMBPT lifetime data for the $4f_j5d_{j'}(1)$ levels are compared with theoretical values "Theory(A)" and "Theory(B)" and experimental measurements "Expt." of Zhang *et al.* [15] in Table X. These are the only levels that decay to the ground state via electric-dipole transitions. The calculations in [15] were carried out using the relativistic Hartree-Fock method of Cowan [14] with including the core-polarization (CP) effects. More extensive calculations [Theory(B)] in which CP was considered by including explicitly in the physical model some configurations with excitation from the $5s$, $5p$, and $4f$ core orbitals were also performed [15]. Theory(B) values are larger than Theory(A) values by 60–70%. We note that our RMBPT values are larger than RMBPT1 by a factor of 2–3, indicating that the second-order contribution is very large (see Table X).

Disagreement between our theoretical values with experimental values may be explained by the slow convergence of the perturbation theory method for Yb III. It should be noted that our RMBPT values presented in this table are the only *ab initio* calculations of lifetime values in Yb III.

TABLE XIII. Energies (E in cm^{-1}) and radiative rates (A_r in s^{-1}) for E1 $[4f5d+4f6s]-4f6p$ transitions in Yb III. Numbers in brackets represent powers of 10.

Transitions		$E_{\rm NIST}$ (cm^{-1})		Transition rates A_r	
$av(J)$	$a'v'$ (J')	Lower	Upper	RMBPT1	RMBPT
$4f_{7/2}6s_{1/2}(4)$	$4f_{7/2}6p_{1/2}(3)$	34 656	72 140	4.322[8]	2.821[8]
$4f_{7/2}5d_{3/2}(2)$	$4f_{7/2}6p_{1/2}(3)$	33 386	72 140	2.097[8]	2.057[8]
$4f_{7/2}6s_{1/2}(3)$	$4f_{7/2}6p_{1/2}(4)$	34 991	72 487	3.332[8]	2.187[8]
$4f_{7/2}5d_{3/2}(5)$	$4f_{7/2}6p_{1/2}(4)$	37 020	72 487	2.904[8]	2.839[8]
$4f_{7/2}6s_{1/2}(4)$	$4f_{7/2}6p_{3/2}(5)$	34 656	78 020	7.302[8]	4.980[8]
$4f_{7/2}5d_{5/2}(6)$	$4f_{7/2}6p_{3/2}(5)$	39 085	78 020	4.228[8]	3.730[8]
$4f_{7/2}6s_{1/2}(3)$	$4f_{7/2}6p_{3/2}(2)$	34 991	78 183	7.587[8]	5.214[8]
$4f_{7/2}6s_{1/2}(3)$	$4f_{7/2}6p_{3/2}(3)$	34 991	78 779	5.726[8]	3.823[8]
$4f_{7/2}6s_{1/2}(4)$	$4f_{7/2}6p_{3/2}(4)$	34 656	79 283	4.592[8]	3.050[8]
$4f_{5/2}6s_{1/2}(2)$	$4f_{5/2}6p_{1/2}(3)$	44 854	82 546	3.208[8]	2.091[8]
$4f_{5/2}5d_{3/2}(4)$	$4f_{5/2}6p_{1/2}(3)$	47 057	82 546	3.021[8]	2.924[8]
$4f_{5/2}6s_{1/2}(3)$	$4f_{5/2}6p_{1/2}(2)$	45 208	82 907	4.536[8]	2.979[8]
$4f_{5/2}6s_{1/2}(2)$	$4f_{5/2}6p_{3/2}(1)$	44 854	87 613	7.283[8]	4.974[8]
$4f_{5/2}5d_{5/2}(1)$	$4f_{5/2}6p_{3/2}(1)$	50 029	87 613	2.344[8]	2.046[8]
$4f_{5/2}6s_{1/2}(3)$	$4f_{5/2}6p_{3/2}(4)$	45 208	88 498	7.270[8]	4.956[8]
$4f_{5/2}5d_{5/2}(5)$	$4f_{5/2}6p_{3/2}(4)$	50 357	88 498	4.094[8]	3.609[8]
$4f_{5/2}6s_{1/2}(2)$	$4f_{5/2}6p_{3/2}(2)$	44 854	88 977	6.153[8]	4.115[8]
$4f_{5/2}6s_{1/2}(3)$	$4f_{5/2}6p_{3/2}(3)$	45 208	89 397	4.163[8]	2.759[8]
$4f_{5/2}5d_{5/2}(4)$	$4f_{5/2}6p_{3/2}(3)$	53 736	89 397	2.403[8]	2.137[8]

TABLE XIV. Energies (E in cm^{-1}), sum of radiative rates from dipole transitions (A_r in s^{-1}), and lifetime values (τ in ns) of the $4f6p$ and $4f7s$ states in Yb III. Results are obtained by including $[4f5d+4f6s+4f6d+4f7s]-[4f6p+4f7p]$ transitions in Yb III. Experimental measurements (Expt.) are from Ref. [12]. Numbers in brackets represent powers of 10.

	E	ΣA_r in s^{-1}		Lifetime τ in ns		
$av(J)$	NIST	RMBPT1	RMBPT	RMBPT1	RMBPT	Expt.
$4f_{7/2}6p_{1/2}(3)$	72 140	9.225[8]	7.422[8]	1.084	1.347	2.28
$4f_{7/2}6p_{1/2}(4)$	72 487	9.075[8]	7.269[8]	1.102	1.376	2.22
$4f_{7/2}6p_{3/2}(5)$	78 020	1.274[9]	9.777[8]	0.785	1.023	1.53
$4f_{7/2}6p_{3/2}(2)$	78 183	1.231[9]	9.802[9]	0.813	1.020	1.48
$4f_{7/2}6p_{3/2}(3)$	78 779	1.234[9]	9.449[8]	0.810	1.058	1.41
$4f_{7/2}6p_{3/2}(4)$	79 283	1.266[9]	9.630[8]	0.790	1.038	1.40
$4f_{5/2}6p_{1/2}(3)$	82 546	8.983[8]	7.145[8]	1.113	1.399	2.11
$4f_{5/2}6p_{1/2}(2)$	82 907	8.811[8]	6.921[8]	1.135	1.445	2.35
$4f_{5/2}6p_{3/2}(1)$	87 613	1.268[9]	9.727[8]	0.789	1.028	1.40
$4f_{5/2}6p_{3/2}(4)$	88 498	1.254[9]	9.594[8]	0.797	1.042	1.67
$4f_{5/2}6p_{3/2}(2)$	88 977	1.256[9]	9.525[8]	0.796	1.050	1.43
$4f_{5/2}6p_{3/2}(3)$	89 397	1.245[9]	9.448[8]	0.803	1.058	1.32
$4f_{5/2}7s_{1/2}(4)$	120 247	7.731[8]	4.615[8]	1.293	1.030	1.24
$4f_{5/2}7s_{1/2}(3)$	120 365	7.693[8]	9.711[8]	1.300	1.035	1.36
$4f_{7/2}7s_{1/2}(2)$	130 457	7.723[8]	9.658[8]	1.295	1.030	1.08
$4f_{7/2}7s_{1/2}(3)$	130 551	7.686[8]	9.708[8]	1.301	1.036	1.66

V. DIPOLE MATRIX ELEMENTS, TRANSITION RATES, AND LIFETIMES FOR THE 4*f*6*p* AND 4*f*7*s* STATES

In order to evaluate the lifetimes of the $4f6p$ and $4f7s$ states, we consider all possible transitions from these configurations into the lower-energy states. In this calculation, we need to consider the transitions between the following mixed configurations: $[4f5d+4f6s]$-$[4f6p]$ and $[4f5d+4f6s+4f6d+4f7s]$-$[4f6p+4f7p]$.

A. Matrix elements

We calculate electric-dipole (E1) matrix elements for the transitions between $[4f5d+4f6s+4f6d+4f7s]$ and $[4f6p+4f7p]$ states. That gives us the 664 E1 transitions. Analytical expressions for the multipole matrix elements in the first- and the second-order RMBPT for those transitions are given by Eqs. (2)–(8) of Ref. [2].

In Table XI, we list a few values of the first- and second-order contributions to electric-dipole matrix elements $Z^{(1)}, Z^{(2)}$, and the matrix element of the derivative term $P^{(\mathrm{derv})}$ for the odd-even $av(J)$-$a'v'(J')$ transitions with $J=4$ and $J'=4$ in Yb III. Both length and velocity forms of the matrix elements are given. We use the symbol B in Table XI to denote the Coulomb-Breit contributions to the second-order matrix elements. The first-order contributions $Z^{(1)}$ are different in length and velocity forms. One also observes that the second-order corrections $Z^{(2)}$ are also very different in length and velocity forms; the $Z_V^{(2)}$ values are even larger than the $Z_V^{(1)}$ values in some transitions.

Values of *coupled* reduced matrix elements in length and velocity forms are given in Table XII for the transitions considered in Table XI. The first two columns in Table XII show L and V values of *coupled* reduced matrix elements calculated without the second-order contribution. We can see very large L-V differences for some transitions. The second-order contribution dramatically decreases those L-V difference down to 1%–10%. These small L-V differences arise because we start our RMBPT calculations using a nonlocal Dirac-Fock (DF) potential.

B. Transition rates and lifetime data

We calculated line strengths and transition probabilities for 664 transitions between $[4f5d+4f6s+4f6d+4f7s]$ and $[4f6p+4f7p]$ states. The results were calculated in both length and velocity forms, but only length-form results are presented in the following tables since the L form is less sensitive to various contributions.

In Table XIII, we list the $[4f_{j_1}6s_{1/2}(J)$-$4f_{j_1}6p_{j'}(J')]$ and $[4f_{j_1}5d_j(J)$-$4f_{j_1}6p_{j'}(J')]$ transitions with largest values of transition rates A_r. It should be noted that all transitions shown in Table XIII are the allowed one-particle ($6s$-$6p$ and $5d$-$6p$) transitions. The transition rates A_r of two-particle transitions ($[4f_{j_1}6s_{1/2}(J)$-$4f_{j_2}6p_{j'}(J')]$ and $[4f_{j_1}5d_j(J)$-$4f_{j_2}6p_{j'}(J')]$ are smaller by two to four orders of magnitude in comparison with the transition rates A_r listed in Table XIII. It was already demonstrated previously (see Table XI) that the second-order matrix elements $Z^{(2)}$ are almost equal to the first-order matrix elements $Z^{(1)}$. We have observed unusually large ratios of the second-to first-order contributions in Er-like Yb III in comparison with the ratios in Ne-like [1,2], Ni-like [3–8], and Pd-like [9,10] systems calculated by RMBPT method. The large contribution of the second-order RMBPT is evident from comparison of values in columns labelled RMBPT1 and RMBPT. The differences between the RMBPT1 and RMBPT values directly give second-order contribution.

Energies, sums of radiative rates from dipole transitions (A_r in s^{-1}) and lifetime values (τ in ns) for $4f6p$ and $4f7s$ states in Yb III are presented in Table XIV. Results are obtained with including $[4f5d+4f6s+4f6d+4f7s]$-$[4f6p+4f7p]$ transitions in Yb III. First, we evaluate the 166 $[4f_{j_1}6s_{1/2}(J)$-$4f_{j_1}6p_{j'}(J')]$ and $[4f_{j_1}5d_j(J)$-$4f_{j_1}6p_{j'}(J')]$ transitions. Then, we sum those transition rates to obtain values for the $4f_j6p_{j'}(J)$ states listed in columns labelled ΣA_r. We also consider the $[4f_{j_1}7s_{1/2}(J)$-$4f_{j_1}6p_{j'}(J')]$ transitions to evaluate values of the ΣA_r for the $4f_j7s_{1/2}(J)$ states.

The lifetime values (s) are obtained as $1/\Sigma A_r$. Those results are presented in two columns of Table XIV with the RMBPT1 and RMBPT labels.

Our RMBPT1 and RMBPT lifetime data for the $4f_j6p_{j'}(J)$ and $4f_j7s_{1/2}(J)$ levels are compared with experimental measurements presented by Öberg and Lundberg in [12]. Our theoretical values are in reasonable agreement with experimental data taking into account the large size of the correlation corrections in Yb III.

VI. CONCLUSION

We have presented a systematic second-order relativistic MBPT study of excitation energies, reduced matrix elements, and transition rates for multipole transitions in Yb III. Our retarded $E1$ matrix elements include correlation corrections from Coulomb and Breit interactions. We determine energies of the $4f_j5d_{j'}(J)$, $4f_j6d_{j'}(J)$, $4f_j6s_{1/2}(J)$, $4f_j7s_{1/2}(J)$, $4f_j6p_{j'}(J)$, and $4f_j7p_{j'}(J)$ excited states. Numerous number of evaluated multipole matrix elements for transitions from excited states into ground states and transitions between excited states allow us to determine the lifetime of the 20 $4f_j5d_{j'}(J)$ levels, four $4f_j6s_{1/2}(J)$ levels, 12 $4f_j6p_{j'}(J)$ levels, and four $4f_j7s_{1/2}(J)$ levels. We would like to underline that our RMBPT results presented in this paper are the only *ab initio* calculations of energies, transition rates, and lifetime values in Yb III.

ACKNOWLEDGMENTS

The work of M.S.S. was supported in part by National Science Foundation under Grant No. PHY-07-58088. U.I.S. would like to thank Dr. V. Dzuba for the interesting and useful discussions.

[1] U. I. Safronova, C. Namba, I. Murakami, W. R. Johnson, and M. S. Safronova, Phys. Rev. A **64**, 012507 (2001).
[2] U. I. Safronova, T. E. Cowan, and A. S. Safronova, J. Phys. B **38**, 2741 (2005).
[3] U. I. Safronova, W. R. Johnson, and J. P. Albritton, Phys. Rev. A **62**, 052505 (2000).
[4] S. M. Hamasha, A. S. Shlyaptseva, and U. I. Safronova, Can. J. Phys. **82**, 331 (2004).
[5] U. I. Safronova, A. S. Safronova, S. M. Hamasha, and P. Beiersdorfer, At. Data Nucl. Data Tables **92**, 47 (2006).
[6] U. I. Safronova, A. S. Safronova, and P. Beiersdorfer, J. Phys. B **39**, 4491 (2006).
[7] U. I. Safronova, A. S. Safronova, and P. Beiersdorfer, J. Phys. B **40**, 955 (2007).
[8] U. I. Safronova, A. S. Safronova, and P. Beiersdorfer, Phys. Rev. A **77**, 032506 (2008).
[9] U. I. Safronova, T. E. Cowan, and W. R. Johnson, Can. J. Phys. **83**, 813 (2005).
[10] U. I. Safronova, R. Bista, R. Bruch, and H. Merabet, Can. J. Phys. **86**, 131 (2008).
[11] Yu. Ralchenko, F.-C. Jou, D. E. Kelleher, A. E. Kramida, A. Musgrove, J. Reader, W. L. Wiese, and K. Olsen, NIST Atomic Spectra Database, Version 3.0.2, National Institute of Standards and Technology, Gaithersburg, MD, 2005 (http://physics.nist.gov/asd3).
[12] K. J. Öberg and H. Lundberg, Eur. Phys. J. D **42**, 15 (2007).
[13] E. Biémont, H. P. Garnir, Z. S. Li, V. Lokhnygin, P. Palmeri, P. Quinet, S. Svanberg, J. F. Wyart, and Z. G. Zhang, J. Phys. B **34**, 1869 (2001).
[14] R. D. Cowan, *The Theory of Atomic Structure and Spectra* (University of California Press, Berkeley, 1981).
[15] Z. G. Zhang, Z. S. Li, S. Svanberg, P. Palmeri, P. Quinet, and E. Biémont, Eur. Phys. J. D **15**, 301 (2001).
[16] K. Tsigutkin, J. E. Stalnaker, D. Budker, S. J. Freedman, V. V. Yashchuk, e-print arXiv:physics/0608314.
[17] Z. W. Barber, J. E. Stalnaker, N. D. Lemke, N. Poli, C. W. Oates, T. M. Fortier, S. A. Diddams, L. Hollberg, C. W. Hoyt, A. V. Taichenachav, and V. I. Yudin, Phys. Rev. Lett. **100**, 103002 (2008).
[18] P. Julienne, R. Ciurylo, M. Kitagawa, K. Enomoto, K. Kasa, and Y. Takahashi, American Physical Society, Proceedings of the 38th Annual Meeting of the Division of Atomic, Molecular, and Optical Physics (2007).
[19] M. S. Safronova and W. R. Johnson, Adv. At., Mol., Opt. Phys. **55**, 191 (2008).
[20] W. R. Johnson, S. A. Blundell, and J. Sapirstein, Phys. Rev. A **37**, 2764 (1988).
[21] M. H. Chen, K. T. Cheng, and W. R. Johnson, Phys. Rev. A **47**, 3692 (1993).
[22] L. W. Fullerton and G. A. Rinker Jr., Phys. Rev. A **13**, 1283 (1976).
[23] P. J. Mohr, Ann. Phys. (N.Y.) **88**, 26 (1974).
[24] P. J. Mohr, Ann. Phys. (N.Y.) **88**, 52 (1974).
[25] P. J. Mohr, Phys. Rev. Lett. **34**, 1050 (1975).
[26] U. I. Safronova, W. R. Johnson, A. Shlyaptseva, and S. Hamasha, Phys. Rev. A **67**, 052507 (2003).