

Method for detecting the isomeric state $I = (3/2)^+$ in ^{229}Th with laser-induced fluorescenceJ. Dembczyński,^{1,*} M. Elantkowska,² and J. Ruczkowski¹¹*Institute of Control and Information Engineering, Faculty of Electrical Engineering, Poznan University of Technology, Piotrowo 3A, 60-965 Poznan, Poland*²*Laboratory of Quantum Engineering and Metrology, Faculty of Technical Physics, Poznan University of Technology, Piotrowo 3, 60-965 Poznan, Poland*

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There are different predictions regarding the position of the isomeric state of ^{229m}Th . There is some question as to whether it even exists. We propose simple experiments to provide the evidence of the existence of this isomeric state. If the metastable isomeric state exists, we should be able to observe the effects of mixing of the nuclear wave functions of the ground state $I = 5/2$ and the isomeric $I = 3/2$ state via electronic shells. It will be shown as the differences between the hyperfine A and B constants, which will be measured by means of the laser-induced fluorescence methods and those predicted by semiempirical calculations. The wave function for the atomic state $|\text{conf.}SLJIF\rangle$ contains contributions from both nuclear states $I = 5/2$ and $3/2$, thus its effects on the hyperfine-structure patterns of spectral lines should be observed, confirming the existence of this isomeric state.

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I. INTRODUCTION

The study of the structure of ^{229}Th isotope is interesting both from the point of view of nuclear physics as well as its application to the frequency standard. Gerstenkorn *et al.* [1] and Kälber *et al.* [2] showed that the investigations of the hyperfine structure (hfs) of spectral lines provide information on the ^{229}Th nucleus and its interaction with the electron shell.

The first-excited isomeric state of the ^{229}Th nucleus exhibits the lowest known nuclear excitation energy. At the same time, the exact value of the frequency for the transition from the isomeric state to the ground state remains unknown. This extraordinarily low value of the nuclear excitation energy triggered a multitude of investigations, both theoretical and experimental, to precisely determine the transition energy, and to specify other properties of the isomeric excited state, such as lifetime and magnetic moment [3–15]. The nuclear transition from the isomeric state to the ground state is of great interest since it makes it possible to construct a nuclear clock with the theoretical precision of $\Delta\lambda/\lambda \approx 10^{-19}$ [8,16,17], i.e., about two orders of magnitude more precise than current high-precision clocks. The long-term comparisons of this type of a clock to a conventional atomic one could detect possible frequency shifts induced by a variation of the electromagnetic coupling constant α with time [18] or the effect of quark mass variation [19]. Moreover, other proposals suggest the use of the isomer as a qubit for quantum computing [8], as a milestone to develop a unique γ -ray laser working on the magnetic dipole ($M1$) transition in the optical range [20], or for investigations on nuclear excitation by electron transition process (NEET) [21], which could help in pumping the isomeric state from the ground state.

Although the excitation energy was for a long time reported in the literature as 3.5 ± 1.0 eV [4], current experiments corrected this value to 7.6 ± 0.5 eV [10,12], which corresponds to the vacuum ultraviolet range (163 ± 11 nm). On

the other hand, in 2010, Sakharow questioned the existence of the isomeric state altogether [22]. The energy of the $^{229g}\text{Th} \rightarrow ^{229m}\text{Th}$ transition was inferred only indirectly by high-resolution gamma-ray spectroscopy. Therefore, the next necessary step was to observe the transition directly by optical spectroscopy, and to determine the transition energy with high precision. Inamura and Haba [11] searched for this state in the region of 3.5 eV using the hollow-cathode electric discharge. The verification of the existence of a low-lying isomeric state can be easily done by a systematic study of the hyperfine structure for the electronic levels of the ^{229}Th atom or ions by means of the laser-induced fluorescence (LIF) method in a Paul trap, in the hollow cathode, or on atomic beam.

Porsev and Flambaum [23] theoretically determined the positions of several high-lying even-parity levels and their g_J factors, which are not presented in experimental atomic spectra databases. Herrera-Sancho *et al.* [24,25] showed that it is possible to reach high-lying electronic levels of $^{232}\text{Th}^+$ by a two-photon laser excitation and observed 43 previously unknown energy levels within the energy range from 7.3 to 8.3 eV. In 2014, Redman *et al.* reported precise observations of the thorium-argon hollow-cathode lamp emission spectrum in the region between 350 and 1175 nm using a high-resolution Fourier transform spectrometer [26]. Their measurements are combined with results from seven previously published thorium line lists to reoptimize the energy levels of neutral, singly, and doubly ionized thorium. They also found nine new energy levels for Th II.

In 2012, Sonnenschein *et al.* reported a preparatory work aiming at the identification of the isomeric state and the measurements of the hyperfine structure of atomic thorium using the Ion Guide Isotope Separator OnLine (IGISOL) facility of the University of Jyväskylä [27,28]. Also, other experiments toward direct observation of the ^{229}Th isomer transition were reported by Hehlen *et al.* [29] and by Wense *et al.* [30]. Moreover, Zhao *et al.* [31] presented the study of the photon emission from recoil nuclei originating from the α decay of ^{233}U , implanted into MgF_2 plates, in the ultraviolet spectral range. The result was interpreted as the

*jerzy.dembczynski@put.poznan.pl

first direct observation of the deexcitation of the lowest-lying isomeric state in ^{229}Th . The isomer half-life of 6(1) h was also deduced. Finally, Peik and Zimmermann [32] pointed out that the radioluminescence resulting from the decay of other nuclei of the ^{233}U decay chain produces signals with similar time dependence, but unrelated to the isomeric state in ^{229}Th .

If the metastable state $I = 3/2$ exists, we should observe the effects of mixing of the nuclear wave functions of the ground state $I = 5/2$ and the isomeric $I = 3/2$ state via electronic shells, introducing small but observable shifts of the hyperfine sublevels [33].

Recently, Bely [34] proposed the search for the nuclear excitation energy by means of precision microwave spectroscopy of the $5F_{5/2,7/2}$ hyperfine manifolds in the ion $^{229}\text{gTh}^{3+}$. He demonstrated that the accurate atomic structure calculations may be combined with the measurement of the hyperfine intervals to quantify the effects of the mixing.

In this work, we suggest experiments that can be easily conducted to confirm the existence of the isomeric state. If this state exists, the effects of mixing it with the electron states should appear on the hyperfine structure. In the following, we predict the hyperfine-structure pattern for a spectral line in the case when the nuclear isomeric state is included.

II. PROCEDURE OF CALCULATIONS

Our thesis is as follows: If the metastable isomeric state exists, we should observe the effects of mixing of the nuclear wave functions of the ground state $I = 5/2$ and the isomeric $I = 3/2$ state via electronic shells. It will be shown as the differences between the hyperfine A and B constants which will be measured by means of the laser-induced fluorescence methods (LIF), in the hollow cathode [35,36] in the case of Th^+ or in the atomic beam [37,38] in the case of a neutral atom, and those predicted by semiempirical calculations given in Table I. Therefore, we consider it advisable to conduct a systematic study of the hyperfine structure of the electronic levels of the ^{229}Th atom or ions.

In order to precisely describe the atomic structure, we developed a method, which allows to analyze a complex electronic system composed of a configuration of up to four open shells, taking into account all electromagnetic interactions expected in an atom, in accordance with the second-order perturbation theory. Within this theory, all possible combinations following the excitation of one or two electrons from closed shells to particular open shells were considered. The appropriate formulas and computer codes have been developed for many years by our research group. The scheme of computational procedures was presented in Fig. 1 in our previous paper [39]. With the use of this code, both the electronic and atomic wave functions were produced on the basis of experimentally determined energy levels. The quality of these wave functions was proved by the comparison of the experimental g_J factors and experimental hfs A and B constants with those calculated with the use of the wave functions obtained by the application of our computer code. It should be pointed out that the wave functions were created for all the states of the considered system simultaneously, and all attributes of the free atom were predicted in the same way. More details about our procedure can be found in the recently published papers [39,40]. The

recently performed experiments [41] provided the opportunity to apply our procedure for the analysis of the electronic structure of a niobium atom [42].

III. APPLICATION FOR THE ^{229}Th ION AND COMPARISON WITH THEORETICAL CALCULATIONS

For the study of Th^+ , we considered the system of 70 even configurations:

$\sum_{n'=6}^{11} 5f^2 n' d + \sum_{n'=7}^{11} 5f^2 n' s + \sum_{n'=5}^9 5f^2 n' g + \sum_{n'=7}^{11} 5f 6d n' p + 5f 6d 6f + \sum_{n'=7}^{11} 5f 7s n' p + 5f 6f 7s + 6d^3 + \sum_{n'=7}^{11} 6d^2 n' s + \sum_{n'=7}^{11} 6d^2 n' d + \sum_{n'=5}^9 6d^2 n' g + 6d 7s^2 + \sum_{n'=8}^{11} 6d 7s n' s + \sum_{n'=7}^{11} 6d 7s n' d + \sum_{n'=5}^9 6d 7s n' g + 6d 7p^2 + 7s 7p^2 + \sum_{n'=8}^{11} 7s^2 n' s + \sum_{n'=7}^{11} 7s^2 n' d$. This system has 3804 energy eigenvalues, the same number for predicted A constant and 3486 B constant. In our procedure, we use all the experimental data known so far, i.e., the values of the 316 energy electronic levels, 11 A and 10 B hfs constants. In fine-structure analysis, we used 111 independent parameters. The mean difference between experimental and calculated energies amounts to 79 cm^{-1} . For the hyperfine-structure A and B constants, the corresponding values are 13 and 71 MHz.

The results of the semiempirical fine- and hyperfine-structure analysis for the Th ion, together with the predictions of the energy values and hfs constants for the levels up to approximately 68000 cm^{-1} , are shown in the Table I. The energy values were taken from [26]. Similar predictions can be performed for odd configurations system of the Th ion, and also for both systems of the Th atom, if the sufficient amount of the hfs data is available.

For the reason of scarcity of the experimental data, especially for the hfs, not all contributions from one- and two-electron excitation to the atomic structure can be determined. Therefore, with the increase of the experimental data, especially for the hfs constants, the accuracy of our predictions given in Table I could be essentially improved. Moreover, the calculated values of hfs A constants are a more sensitive test of an admixture of the $7s$ electron to the wave functions describing particular states than the g_J Lande factors. In this way, the confirmation of notation of the energy levels given in column 4 is possible. In Tables II and III, we give the comparison of our predictions with the theoretical calculations presented by Porsev and Flambaum [23] and Safronova *et al.* [15]. The structure of these tables is similar to those presented by Porsev and Flambaum. We added the columns showing the difference between the experimental and calculated energy values that can facilitate the comparison of the accuracy of the presented methods.

Each of the A or B hfs constants is the sum of many one- and two-body contributions. Their individual values can be quantitatively determined as shown for the configuration $(5d+6s)^3$ system of a lanthanum atom [40]. The two-body contributions, originating from the excitations of the type “closed shell–open shell” or the type “open shell–empty shell,” are SL dependent. Therefore, the measurements of the hyperfine-structure intervals for different SL terms are necessary. The above-mentioned paper explained the method of parametrization and quantitative determination of the effects of the breakdown of nl, J as a good quantum number. A similar

TABLE I. Comparison of the experimental and calculated energy values (cm^{-1}) and hfs A and B constants (MHz) for Th II.

$E_{\text{expt.}}$	$E_{\text{calc.}}$	%	Main comp.	%	Sec. comp.	$g_{J_{\text{calc.}}}$	$g_{J_{\text{expt.}}}$	$A_{\text{expt.}}$	$A_{\text{calc.}}$	$B_{\text{expt.}}$	$B_{\text{calc.}}$
$J = 1/2$											
6244.294	6228	66.97	$6d^2(^3P)7s^4P$	12.11	$6d^2(^3P)7s^2P$	2.190	2.112		3266		
7828.560	7927	36.87	$6d^3^2P$	34.67	$6d^2(^3P)7s^2P$	1.184	1.254		-624		
14349.388	14378	87.68	$6d^3^4P$	5.50	$6d^2(^3P)7s^2P$	2.545	2.555		-328		
19594.347	19599	63.39	$6d^2(^1S)7s^2S$	11.74	$6d^3^2P$	1.848			3145		
23346.890	23348	37.17	$6d^2(^3P)7s^2P$	34.95	$6d^3^2P$	0.908			1386		
34782.731	34745	24.72	$5f^2(^3P)7s^4P$	13.15	$5f\ 6d7p(^1D)^2P$	1.459	1.670		1699		
35425.627	35533	90.21	$5f\ 7s7p(^3P)^4D$	3.57	$5f\ 6d7p(^3D)^4D$	0.039	0.265		-1083		
36040.836	35998	31.77	$5f^2(^3P)7s^4P$	9.57	$5f\ 6d7p(^1D)^2P$	1.598	1.210		353		
36812.418	36751	42.47	$5f^2(^3P)7s^2P$	13.38	$5f^2(^3F)6d^2P$	0.809	0.737		-40		
38867.171	38918	43.93	$5f\ 6d7p(^3D)^4D$	14.09	$5f\ 6d7p(^3D)^2P$	0.618	0.947		139		
39948.392	39853	33.20	$5f^2(^3F)6d^4P$	12.28	$5f^2(^3P)6d^4P$	1.850	1.542		-60		
40523.728	40638	42.45	$5f\ 6d7p(^3F)^4D$	9.80	$5f\ 6d7p(^1D)^2P$	0.338	0.500		258		
42008.131	41946	31.45	$5f\ 6d7p(^3P)^4D$	16.21	$5f\ 6d7p(^3D)^4P$	0.946	0.800		136		
42246.014	42310	27.41	$5f^2(^3F)6d^2P$	15.05	$5f\ 6d7p(^3D)^4P$	1.107	0.800		246		
43965.624	43924	32.86	$5f\ 6d7p(^3D)^4P$	16.13	$5f^2(^3F)6d^4D$	1.332	1.555		102		
44789.289	44838	24.95	$5f^2(^1D)6d^2S$	14.14	$5f^2(^3P)6d^2P$	1.055	0.840		132		
	46094	18.22	$5f^2(^3F)6d^4D$	16.67	$5f^2(^1D)6d^2S$	0.927			130		
	46524	15.78	$5f^2(^1S)7s^2S$	15.54	$5f\ 6d7p(^3F)^2S$	1.625			1636		
47145.759	47136	30.04	$5f\ 6f7s(^3F)^4D$	11.74	$5f\ 6f7s(^3F)^2P$	0.386			-364		
	47841	13.62	$5f^2(^3P)6d^4D$	13.09	$5f\ 6d7p(^3F)^4D$	0.498			-54		
	48659	61.73	$7s\ 7p^2(^3P)^4P$	6.30	$5f\ 6f7s(^3F)^4D$	2.153			1880		
49485.517	49511	13.27	$5f\ 6f7s(^1F)^2S$	12.45	$5f^2(^1D)6d^2P$	1.591			694		
	49918	13.92	$5f^2(^3P)6d^2P$	11.12	$5f\ 6d7p(^3F)^4P$	1.448			-71		
	50197	24.14	$5f\ 6d7p(^3F)^4P$	10.25	$5f^2(^3P)6d^2P$	1.543			363		
	50336	95.79	$6d\ 7s8s(^3S)^4D$	1.29	$6d^2(^3F)7d^4D$	0.003			-1416		
51653.973	51675	20.40	$5f^2(^3P)6d^4P$	12.79	$5f^2(^1D)6d^2P$	1.705			-166		
	52234	25.16	$5f^2(^3P)6d^4D$	8.29	$5f\ 6f7s(^3F)^2P$	0.769			105		
	52518	20.88	$5f^2(^3P)6d^4D$	15.78	$5f\ 6f7s(^3F)^2P$	0.625			-84		
	53336	32.09	$5f^2(^3P)6d^4P$	11.42	$5f\ 6f7s(^1F)^2S$	2.123			-339		
	54100	22.38	$5f\ 6d7p(^3F)^2P$	9.14	$5f\ 6d7p(^3D)^2P$	1.127			719		
	54716	52.43	$6d^2(^3P)8s^4P$	11.91	$6d^2(^1S)8s^2S$	2.164			842		
	56270	25.19	$5f\ 6d7p(^1F)^2S$	7.99	$5f\ 6d7p(^3F)^2S$	1.632			-178		
	56715	20.90	$6d\ 7p^2(^3P)^2P$	18.30	$7s\ 7p^2(^3P)^2P$	0.776			-178		
	56925	26.18	$6d^2(^3F)7d^2P$	15.09	$6d^2(^3F)7d^4D$	0.786			65		
	57942	14.28	$5f\ 6d7p(^1F)^2P$	12.38	$6d\ 7p^2(^1D)^2P$	1.007			95		
	58217	27.45	$6d\ 7p^2(^3P)^4D$	15.41	$6d^2(^3P)8s^2P$	0.898			147		
	58852	19.40	$7s^2(^1S)8s^2S$	9.87	$6d^2(^3F)7d^4P$	1.575			369		
	59258	18.38	$7s^2(^1S)8s^2S$	13.61	$6d^2(^3F)7d^4P$	1.830			549		
	60285	44.27	$5f\ 6f7s(^3F)^4P$	13.76	$5f\ 6d6f(^3D)^4P$	2.395			1608		
	60886	38.03	$6d^2(^3P)8s^2P$	13.55	$7s\ 7p^2(^3P)^2P$	0.785			215		
	61358	23.11	$6d^2(^3F)7d^4D$	15.02	$6d^2(^3F)7d^2P$	0.739			-153		
	61968	19.19	$6d\ 7p^2(^3P)^4P$	14.10	$6d^2(^1D)7d^2S$	1.835			299		
	62421	18.07	$6d\ 7s7d(^3D)^4D$	8.86	$6d\ 7s7d(^3D)^2P$	0.557			-273		
	63041	11.89	$6d^2(^3P)7d^2P$	9.92	$5f\ 6d6f(^1G)^2P$	0.990			53		
	63235	8.68	$6d\ 7p^2(^3P)^4P$	7.98	$6d\ 7s7d(^3D)^4D$	1.180			189		
	63647	9.48	$5f\ 6d6f(^1D)^2P$	8.22	$6d^2(^1D)7d^2S$	1.199			420		
	64208	13.36	$6d\ 7s7d(^3D)^4D$	9.09	$6d\ 7p^2(^3P)^4P$	1.197			119		
	64701	11.73	$5f\ 6d6f(^3G)^2P$	8.21	$6d^2(^1D)7d^2S$	1.010			36		
	65220	11.23	$6d\ 7s7d(^3D)^2P$	10.04	$6d^2(^3P)7d^2P$	0.738			-57		
	65425	19.90	$5f\ 7s8p(^3P)^4D$	12.47	$5f\ 6f7s(^1F)^2P$	0.481			-191		
	65950	43.69	$5f\ 7s8p(^3P)^4D$	12.12	$6d\ 7s7d(^3D)^4D$	0.181			-582		
	66740	12.57	$6d^2(^3P)7d^2P$	9.09	$5f\ 6f7s(^1F)^2P$	0.961			342		
	67046	9.99	$5f\ 6d6f(^3D)^4P$	8.48	$5f\ 6f7s(^1F)^2P$	1.675			-29		
	67530	14.81	$5f\ 6d6f(^3D)^2P$	8.27	$5f\ 6d6f(^3P)^4D$	0.819			319		
	67773	15.20	$5f\ 6d6f(^3P)^4D$	13.64	$5f\ 6d6f(^3G)^4D$	0.763			473		
	68008	16.23	$5f\ 6d8p(^3D)^4D$	7.95	$5f\ 7s8p(^3P)^4D$	0.932			486		
	68156	13.27	$5f\ 6d8p(^3D)^4D$	12.76	$5f\ 6d6f(^1F)^2S$	0.830			65		
	68378	23.58	$6d^2(^3P)7d^4D$	8.29	$5f\ 6d6f(^3F)^4D$	0.624			565		

TABLE I. (Continued.)

$E_{\text{expt.}}$	$E_{\text{calc.}}$	%	Main comp.	%	Sec. comp.	$g_{J_{\text{calc.}}}$	$g_{J_{\text{expt.}}}$	$A_{\text{expt.}}$	$A_{\text{calc.}}$	$B_{\text{expt.}}$	$B_{\text{calc.}}$
$J = 3/2$											
0.000	-18	43.37	$6d^2(^3F)7s^4F$	26.38	$6d\ 7s^2\ ^2D$	0.628	0.639	-444.2	-443	303	354
1859.938	1868	49.87	$6d^2(^3F)7s^4F$	35.62	$6d\ 7s^2\ ^2D$	0.594	0.586	-285	-310	1140	743
7001.420	7059	48.09	$6d^3\ ^4F$	16.45	$6d\ 7s^2\ ^2D$	0.726	0.800		8		-652
8018.192	8051	85.18	$6d^2(^3P)7s^4P$	3.02	$5f^2(^3P)7s^4P$	1.657	1.608	1110	1101	1170	1187
8460.352	8463	33.44	$6d^3\ ^4F$	22.12	$6d^3\ ^2P$	0.982	0.968	-270	-273		-374
12219.976	12209	50.74	$6d^2(^1D)7s^2D$	10.13	$6d^3\ ^4P$	0.991	0.977		-352		-448
15236.637	15236	65.58	$6d^3\ ^4P$	19.22	$6d^2(^3P)7s^2P$	1.565	1.592		-419		-1158
18118.701	18095	38.34	$6d^3\ ^2D$	17.77	$6d^3\ ^2D$	0.902	0.930		-279		-1342
25381.923	25378	38.66	$6d^3\ ^2P$	30.03	$6d^2(^3P)7s^2P$	1.248	1.250		-482		-66
26762.273	26716	36.36	$5f^2(^3F)7s^4F$	19.99	$5f\ 7s7p(^3P)^4F$	0.497	0.400		-434		-462
27631.224	27561	46.68	$5f\ 7s7p(^3P)^4F$	26.43	$5f^2(^3F)7s^4F$	0.494	0.625		-627		149
28011.157	27934	41.63	$6d^3\ ^2D$	33.01	$6d^3\ ^2D$	0.838	0.717		234		1583
32959.477	33063	15.51	$5f^2(^3F)7s^4F$	14.49	$5f\ 6d7p(^3F)^2D$	0.868	0.874		-216		-602
34019.244	34080	18.19	$5f^2(^1D)7s^2D$	13.74	$5f\ 6d7p(^1D)^2D$	0.815	0.823		-193		-218
35021.373	35036	68.56	$5f\ 7s7p(^3P)^4D$	10.28	$5f\ 7s7p(^3P)^2D$	1.033	1.042		342		-799
36328.601	36397	46.99	$5f^2(^3P)7s^4P$	16.29	$5f\ 6d7p(^3F)^4P$	1.601	1.615		864		630
37542.160	37612	20.12	$5f^2(^3P)7s^2P$	10.41	$5f\ 6d7p(^3D)^2P$	1.174	1.003		-140		-597
37821.962	37831	13.37	$5f^2(^3F)6d^4P$	9.92	$5f\ 6d7p(^1D)^2P$	1.225	1.150		145		585
38372.016	38305	22.78	$5f\ 6d7p(^3D)^4F$	13.69	$5f\ 6d7p(^3F)^4F$	0.772	1.200		100		-247
38757.181	38672	36.01	$5f\ 7s7p(^1P)^2D$	9.90	$5f\ 6d7p(^3D)^2P$	0.982	0.935		171		948
38836.187	38763	16.05	$5f\ 6d7p(^3P)^4F$	11.90	$5f\ 6d7p(^3F)^4F$	0.864	1.013		82		-930
39150.678	39052	9.67	$5f\ 6d7p(^3D)^4F$	9.45	$5f^2(^1G)6d^2D$	0.926	0.739		-110		-225
40222.908	40176	38.36	$5f\ 7s7p(^3P)^2D$	10.70	$5f\ 6d7p(^3P)^4F$	0.837	0.738		-341		823
40278.125	40509	11.91	$5f\ 6d7p(^3P)^4F$	9.74	$5f\ 6d7p(^1D)^2P$	0.858	0.705		113		438
40991.565	40988	19.97	$5f\ 7s7p(^3P)^2D$	11.91	$5f^2(^3H)6d^4F$	0.863	1.036		-108		473
41676.853	41747	33.20	$5f^2(^3F)6d^4P$	7.87	$5f\ 6d7p(^1D)^2P$	1.390	1.220		22		411
41936.530	42003	19.05	$5f^2(^3F)6d^2D$	11.22	$5f\ 6d7p(^3P)^4D$	0.984	1.095		112		-637
43244.860	43257	20.99	$5f\ 6d7p(^3F)^4D$	14.21	$5f\ 6d7p(^3D)^4D$	1.163	1.080		92		623
43807.541	44063	14.09	$5f^2(^3F)6d^2P$	10.73	$5f\ 6d7p(^3D)^4P$	1.149	1.211		107		-216
44300.552	44396	38.63	$5f\ 6d7p(^3D)^4P$	10.91	$5f^2(^3F)6d^2P$	1.498	1.342		10		36
44889.804	44896	10.12	$5f\ 6d7p(^3D)^4D$	9.09	$5f\ 6d7p(^3D)^2P$	1.143	1.346		63		162
45306.158	45328	40.57	$5f^2(^3F)6d^4F$	13.12	$5f\ 6d7p(^3D)^4F$	0.528	0.600		195		-497
46264.242	46213	28.29	$5f^2(^3F)6d^4D$	9.68	$5f\ 6d7p(^3F)^2D$	1.024	0.891		22		-84
46395.972	46422	16.25	$5f\ 6f7s(^3F)^4S$	10.36	$5f\ 6d7p(^3F)^4S$	1.396			564		-401
46935.661	46803	21.06	$5f^2(^3P)6d^2P$	12.94	$5f^2(^1D)6d^2P$	1.249	0.956		145		84
47148.599	47133	20.77	$5f^2(^3F)6d^4F$	12.88	$5f^2(^3P)6d^4F$	0.793	1.090		145		-49
	47693	10.41	$5f^2(^3P)6d^4F$	7.03	$5f^2(^3H)6d^4F$	0.861			250		-8
47869.601	47883	26.05	$5f\ 6f7s(^3F)^4S$	9.03	$5f\ 6d6f(^3F)^4S$	1.347			492		-177
	48275	14.68	$5f\ 6f7s(^3F)^4D$	9.16	$5f\ 6f7s(^3F)^4S$	1.123			454		669
48689.945	48665	31.08	$5f^2(^3H)6d^4F$	27.37	$5f^2(^3P)6d^4F$	0.569	0.922		257		446
48817.970	48826	25.10	$5f\ 6f7s(^3F)^4D$	8.43	$5f\ 6d7p(^3F)^4D$	1.079	0.956		70		128
49414.651	49405	57.34	$6d^2(^3F)8s^4F$	12.00	$6d^2(^1D)8s^2D$	0.670	1.003		-53		296
	50095	38.51	$5f\ 6d7p(^3F)^4S$	9.89	$5f\ 6d7p(^1D)^2P$	1.421			91		379
	50380	13.34	$5f\ 6d7p(^3D)^2D$	9.14	$5f\ 6d7p(^3P)^2D$	1.019			267		450
50735.464	50700	50.99	$6d\ 7s8s(^3S)^4D$	5.31	$6d^2(^3F)8s^4F$	1.183	1.360		585		163
50907.79	50828	26.15	$6d\ 7s8s(^3S)^4D$	9.82	$5f\ 6d7p(^3F)^4P$	1.267	1.300		546		512
51024.821	51129	27.53	$7s\ 7p^2(^3P)^4P$	13.70	$5f\ 6d7p(^3F)^4P$	1.436	1.270		620		891
51676.063	51655	16.76	$5f^2(^3P)6d^4P$	8.09	$5f^2(^1D)6d^2P$	1.301			170		-442
	51846	15.28	$5f\ 6d7p(^1P)^2D$	14.11	$5f\ 6d7p(^3P)^2D$	1.014			394		947
52307.484	52266	39.00	$7s\ 7p^2(^3P)^4P$	19.30	$5f\ 6d7p(^3F)^4P$	1.555			639		918
52735.742	52685	33.40	$5f^2(^3P)6d^4D$	10.64	$5f\ 6d7p(^3P)^4D$	1.232			110		507
	53305	35.05	$6d\ 7s8s(^1S)^2D$	13.96	$6d^2(^1D)8s^2D$	0.970			-25		549
	53581	27.68	$5f\ 6f7s(^1F)^2D$	14.33	$5f\ 6d7p(^1F)^2D$	0.904			203		-429
	53835	18.75	$6d\ 7p^2(^3P)^4F$	11.67	$7s\ 7p^2(^1D)^2D$	0.883			-59		1219
	54506	9.14	$5f^2(^1G)6d^2D$	8.06	$6d\ 7p^2(^3P)^4F$	0.923			-21		-56
54922.092	54818	13.98	$6d\ 7s8s(^1S)^2D$	11.70	$5f^2(^3P)6d^4P$	1.178			-55		-718
	55366	12.74	$5f^2(^1D)6d^2D$	10.42	$5f^2(^3P)6d^4P$	1.018			-38		-666

TABLE I. (Continued.)

$E_{\text{expt.}}$	$E_{\text{calc.}}$	%	Main comp.	%	Sec. comp.	$g_{J_{\text{calc.}}}$	$g_{J_{\text{expt.}}}$	$A_{\text{expt.}}$	$A_{\text{calc.}}$	$B_{\text{expt.}}$	$B_{\text{calc.}}$
56235.197	56241	21.78	5f 6d7p (^3F) ^2P	9.33	$5f^2(^1\text{D})6d^2\text{D}$	1.158			155		-599
56717.633	56713	34.11	6d $7p^2$ (^3P) ^4F	14.78	6d $7p^2$ (^3P) ^2P	0.928			82		-219
57128.642	57104	26.73	5f 6f7s (^3F) ^4F	14.29	$6d^2(^3\text{P})8s^4\text{P}$	0.736			-91		-25
	57116	57.74	$6d^2(^3\text{P})8s^4\text{P}$	9.26	5f 6f7s (^3F) ^4F	1.345			118		675
	57391	10.70	5f 6d7p (^3P) ^2D	9.84	$5f^2(^1\text{S})6d^2\text{D}$	0.945			51		837
	58534	14.10	$5f^2(^3\text{P})6d^2\text{D}$	10.64	6d $7p^2$ (^1D) ^2D	0.959			119		892
	58933	21.84	7s $7p^2$ (^1D) ^2D	14.54	$6d^2(^3\text{F})7d^4\text{D}$	1.069			-59		652
	59379	9.11	5f 6d7p (^1F) ^2P	5.94	6d $7s7d$ (^1D) ^2D	1.046			-35		227
59477.400	59483	20.42	$6d^2(^3\text{F})7d^4\text{D}$	12.23	6d $7p^2$ (^3P) ^4D	1.167			9		-363
60380.100	60314	13.14	5f 6d7p (^1F) ^2P	8.39	$6d^2(^3\text{P})8s^2\text{P}$	1.194			-3		-795
60618.600	60553	14.59	$6d^2(^3\text{F})7d^4\text{P}$	11.53	$6d^2(^3\text{F})7d^2\text{P}$	1.291			154		190
61032.400	60974	18.55	5f 6f7s (^3F) ^4P	11.64	6d $7p^2$ (^3P) ^4D	1.394			306		168
	61053	27.48	5f 6f7s (^3F) ^4P	9.64	5f 6d6f (^3D) ^4P	1.427			241		144
61726.300	61705	10.64	5f 6d6f (^1D) ^2D	6.45	5f 6d6f (^3F) ^2D	1.091			44		-42
61963.600	61964	17.72	$6d^2(^3\text{P})8s^2\text{P}$	7.75	7s $7p^2$ (^1D) ^2D	1.115			-128		10
62373.800	62377	11.41	$6d^2(^3\text{F})7d^4\text{F}$	5.94	5f 7s8p (^3P) ^4F	0.893			2		-89
	62528	26.34	5f 7s8p (^3P) ^4F	4.49	5f 6f7s (^3F) ^2D	0.792			-245		216
62562.200	62584	10.14	5f 7s8p (^3P) ^4F	8.38	$6d^2(^3\text{P})7d^2\text{P}$	1.070			157		-40
	63077	13.23	$6d^2(^3\text{F})7d^2\text{D}$	9.21	5f 6f7s (^3F) ^2D	0.963			-43		-517
	63516	24.79	6d $7s7d$ (^3D) ^4D	6.42	5f 7s8p (^3P) ^4D	1.043			-193		-536
	63549	8.16	$6d^2(^3\text{P})7d^4\text{F}$	7.14	5f 6d6f (^1D) ^2D	0.801			-25		296
	63630	7.15	$6d^2(^3\text{P})7d^4\text{F}$	6.76	$6d^2(^3\text{F})7d^2\text{D}$	1.039			42		-54
	63943	12.85	$6d^2(^3\text{P})7d^4\text{F}$	5.38	5f 6d6f (^1G) ^2P	0.902			22		-154
	64037	23.72	$6d^2(^3\text{F})7d^4\text{F}$	4.44	5f 6d6f (^3P) ^4F	0.756			65		404
64150.300	64189	9.23	6d $7s8s$ (^3S) ^2D	7.37	$6d^2(^1\text{D})8s^2\text{D}$	0.903			-104		-204
64560.400	64571	8.83	6d $7s7d$ (^3D) ^4D	8.12	6d $7s7d$ (^3D) ^4F	0.986			2		-28
64920.100	64858	11.52	5f 6d6f (^3D) ^4D	8.12	5f 6d6f (^3D) ^2P	0.963			3		333
65037.700	65053	25.29	6d $7p^2$ (^3P) ^4P	14.28	$6d^2(^3\text{P})7d^4\text{P}$	1.417			-40		-213
	65405	13.76	5f 7s8p (^1P) ^2D	12.05	5f 7s8p (^3P) ^4F	0.883			39		107
65730.400	65681	23.95	5f 7s8p (^3P) ^4D	11.66	6d $7s7d$ (^3D) ^4F	1.011			143		-36
65799.600	65895	23.59	6d $7s7d$ (^3D) ^4F	17.01	5f 7s8p (^3P) ^4D	0.828			35		-17
	66052	9.19	5f 7s8p (^3P) ^4D	6.65	6d $7s7d$ (^3D) ^4D	1.045			230		-360
$J = 5/2$											
1521.896	1582	65.86	$6d^2(^3\text{F})7s^4\text{F}$	15.35	$6d^2(^1\text{D})7s^2\text{D}$	1.069	1.076	477	499	240	240
4113.359	4161	36.37	6d $7s^2$ ^2D	26.69	$6d^2(^3\text{F})7s^4\text{F}$	1.165	1.163	210	190	780	762
8605.841	8578	43.99	$6d^2(^3\text{F})7s^2\text{F}$	15.02	$6d^2(^3\text{P})7s^4\text{P}$	1.062	0.986		-4		548
9061.103	9078	56.62	$6d^2(^3\text{P})7s^4\text{P}$	20.39	$6d^2(^3\text{F})7s^2\text{F}$	1.348	1.419		535		-556
9400.964	9365	72.20	$6d^3$ ^4F	13.06	$6d^2(^3\text{F})7s^2\text{F}$	1.027	1.034		-156		-209
13250.509	13179	39.33	$6d^2(^1\text{D})7s^2\text{D}$	18.43	6d $7s^2$ ^2D	1.252	1.245		478		18
15786.985	15750	85.88	$6d^3$ ^4P	4.14	$6d^3$ ^2D	1.563	1.571		-331		1735
20158.739	20148	59.53	$6d^3$ ^3D	13.05	$6d^2(^1\text{D})7s^2\text{D}$	1.199	1.190		155		-1230
22106.433	22141	61.33	$6d^3$ ^2F	8.23	$6d^2(^3\text{F})7s^2\text{F}$	0.937	0.920		204		2456
26488.647	26475	35.86	5f 7s7p (^3P) ^4G	23.08	5f 7s7p (^3P) ^4F	0.825	0.776		84		824
27593.968	27609	33.94	$5f^2(^3\text{F})7s^4\text{F}$	26.23	$5f^2(^3\text{F})7s^2\text{F}$	0.968	0.963		741		-736
28026.349	28060	55.47	$6d^3$ ^2D	13.26	$6d^3$ ^2F	1.149	1.130		19		1381
28823.653	28826	27.53	5f 7s7p (^3P) ^4G	19.63	5f 7s7p (^3P) ^4F	0.929	0.987		207		1799
29345.896	29553	29.66	$5f^2(^3\text{F})7s^2\text{F}$	28.63	$5f^2(^3\text{F})7s^4\text{F}$	0.930	0.935		-223		-213
31259.296	31275	21.91	5f 6d7p (^3F) ^4G	13.84	$5f^2(^3\text{F})7s^2\text{F}$	0.775	0.781		212		176
31754.210	31828	40.49	5f 7s7p (^3P) ^2F	12.17	5f 7s7p (^3P) ^4F	0.942	0.948		-374		596
33730.934	33648	19.51	$5f^2(^1\text{D})7s^2\text{D}$	7.85	5f 6d7p (^3F) ^2D	1.054	1.031		445		-924
34174.542	34189	25.34	5f 7s7p (^3P) ^4D	19.81	5f 7s7p (^3P) ^4F	1.025	0.986		272		28
34543.556	34473	18.47	5f 6d7p (^3D) ^4G	8.17	$5f^2(^1\text{D})7s^2\text{D}$	0.937	1.003	366.1	366	-90	-1
35741.297	35702	19.75	5f 6d7p (^3F) ^4G	19.72	$5f^2(^3\text{F})6d^4\text{G}$	0.788	0.954		169		-255
36065.740	36252	16.48	$5f^2(^3\text{F})6d^4\text{G}$	10.11	$5f^2(^1\text{D})7s^2\text{D}$	1.041	0.887		296		-474
37465.458	37390	15.28	5f 6d7p (^3D) ^4D	6.58	5f 6d7p (^3F) ^4G	1.063	1.048		105		24
37945.109	37980	20.73	5f 7s7p (^1P) ^2F	11.47	$5f^2(^3\text{P})7s^4\text{P}$	1.036	0.893		181		-526
38105.072	38201	15.93	5f 7s7p (^1P) ^2F	13.29	$5f^2(^3\text{P})7s^4\text{P}$	1.135	1.172		179		-402
38728.682	38696	16.64	5f 6d7p (^3P) ^4G	9.48	$5f^2(^3\text{H})6d^2\text{F}$	0.946	1.255		154		538

TABLE I. (Continued.)

$E_{\text{expt.}}$	$E_{\text{calc.}}$	%	Main comp.	%	Sec. comp.	$g_{J_{\text{calc.}}}$	$g_{J_{\text{expt.}}}$	$A_{\text{expt.}}$	$A_{\text{calc.}}$	$B_{\text{expt.}}$	$B_{\text{calc.}}$
38863.845	38876	11.21	$5f^2(^3P)7s^4P$	10.61	$5f\ 6d7p(^3D)^2F$	1.112	0.967		325		-115
39366.906	39340	24.36	$5f\ 7s7p(^3P)^4D$	24.20	$5f\ 7s7p(^3P)^2D$	1.105	1.140		79		-81
39700.581	39604	13.60	$5f\ 6d7p(^3P)^4F$	10.23	$5f\ 6d7p(^3F)^4F$	1.098	1.090		236		-377
40216.116	40311	7.89	$5f\ 6d7p(^3D)^4G$	7.55	$5f\ 6d7p(^3F)^4F$	1.025	1.024		127		-583
40644.334	40551	16.45	$5f\ 6d7p(^3D)^4G$	12.25	$5f\ 6d7p(^3P)^4G$	0.909	0.856		192		938
40923.622	40944	28.28	$5f\ 6d7p(^3D)^4F$	9.74	$5f^2(^3F)6d^4F$	1.016	0.988		174		-199
41328.348	41240	19.88	$5f\ 7s7p(^1P)^2D$	10.45	$5f\ 6d7p(^3F)^4F$	1.113	1.101		210		992
42336.830	42167	14.04	$5f\ 6d7p(^3D)^4P$	11.15	$5f\ 6d7p(^3D)^4D$	1.254	1.150		44		947
42352.126	42516	10.69	$5f\ 6d7p(^3F)^2F$	10.21	$5f\ 6d7p(^3P)^4F$	1.053	1.126		75		548
43096.532	43192	11.17	$5f^2(^3F)6d^4D$	9.20	$5f\ 6d7p(^3F)^4D$	1.125	0.982		121		85
43227.861	43390	10.20	$5f\ 6d7p(^3D)^2F$	9.42	$5f\ 6d7p(^3F)^4D$	1.094	1.153		96		681
43772.470	43708	15.25	$5f\ 6d7p(^1D)^2F$	13.99	$5f\ 6d7p(^3D)^2F$	0.996	1.040		130		278
44388.766	44469	14.62	$5f\ 7s7p(^1P)^2D$	9.55	$5f\ 6d7p(^3P)^2F$	1.136	1.158		103		481
44552.676	44575	11.62	$5f\ 6d7p(^3P)^2F$	11.19	$5f\ 6d7p(^3D)^4P$	1.229	1.182		101		-584
45189.645	45081	37.97	$5f^2(^3H)6d^4G$	15.09	$5f^2(^3F)6d^4G$	0.692	0.674		170		169
45610.623	45523	18.68	$5f\ 6d7p(^3P)^4D$	17.57	$5f\ 6d7p(^3D)^4P$	1.291	1.075		91		1240
45800.263	45641	9.19	$5f\ 6d7p(^3P)^2F$	7.13	$5f\ 6d7p(^3F)^4D$	1.045	1.300		118		-82
46581.301	46522	18.25	$5f^2(^3F)6d^4F$	11.39	$5f^2(^3F)6d^4D$	1.136	1.018		105		175
46603.188	46597	23.85	$5f\ 6d7p(^1P)^2F$	14.46	$5f^2(^1G)6d^2F$	0.983	1.112		183		-1226
46902.535	46743	33.18	$5f^2(^3F)6d^4F$	10.48	$5f\ 6d7p(^3D)^4F$	1.090	1.143		142		-133
47324.386	47409	25.90	$5f^2(^3F)6d^4D$	13.50	$5f\ 6f7s(^3F)^4D$	1.268	1.189		85		-152
	47720	8.02	$5f\ 6f7s(^3F)^4G$	7.62	$5f\ 6f7s(^3F)^2F$	1.005			35		-561
48320.798	48277	38.48	$5f\ 6f7s(^3F)^4G$	7.26	$5f\ 6d7p(^3F)^2F$	0.831		-152			-180
48492.019	48627	16.38	$5f\ 6f7s(^3F)^4G$	9.00	$5f^2(^1D)6d^2F$	0.925			32		802
49068.808	48963	42.45	$5f^2(^3P)6d^4F$	6.86	$5f\ 6d7p(^1F)^2D$	1.051			61		571
	49298	11.80	$5f^2(^3H)6d^4F$	10.79	$5f\ 6d7p(^3P)^4F$	1.069			251		353
	49645	27.84	$5f\ 6f7s(^3F)^4D$	9.22	$5f\ 6d7p(^3F)^4D$	1.198			288		362
49873.129	49873	27.72	$6d^2(^3F)8s^4F$	13.71	$6d^2(^1D)8s^2D$	1.100			376		342
50663.614	50650	9.04	$5f\ 6d7p(^3F)^4D$	8.29	$5f\ 6f7s(^3F)^4D$	1.191			44		382
51362.879	51421	53.29	$6d\ 7s8s(^3S)^4D$	12.59	$6d^2(^3F)8s^4F$	1.242			857		901
51865.136	51858	16.36	$5f^2(^1G)6d^2F$	9.61	$5f^2(^3F)6d^2F$	1.021			75		-128
51935.685	51935	8.60	$5f\ 6d7p(^3F)^4P$	8.35	$5f\ 6f7s(^3F)^2F$	1.183			34		193
	52222	17.80	$5f\ 6f7s(^3F)^2F$	8.20	$5f\ 6d7p(^1F)^2D$	1.117			-60		-9
	52939	21.22	$5f^2(^3P)6d^4D$	9.80	$5f\ 6d7p(^3F)^4P$	1.257			110		-680
	53118	12.54	$6d^2(^3F)8s^2F$	11.15	$6d^2(^3F)8s^4F$	1.074			16		512
	53595	21.96	$6d\ 7s8s(^3S)^4D$	18.14	$6d^2(^3F)8s^4F$	1.208			129		375
53845.399	53832	17.55	$7s\ 7p^2(^3P)^4P$	10.82	$5f^2(^3P)6d^4P$	1.257			251		532
	53971	17.31	$5f\ 6d7p(^1P)^2D$	9.29	$5f\ 6d7p(^3F)^4P$	1.276			143		941
	54350	27.75	$7s\ 7p^2(^3P)^4P$	9.01	$5f\ 6f7s(^1F)^2D$	1.295			369		-608
54493.994	54546	37.53	$5f^2(^3P)6d^4P$	8.31	$5f^2(^3F)6d^4P$	1.438			36		475
	55612	6.94	$5f\ 6d7p(^3F)^2D$	6.48	$5f^2(^3H)6d^2F$	1.090			101		-168
	55713	23.55	$6d^2(^3F)8s^2F$	9.57	$5f^2(^1D)6d^2F$	1.008			66		692
56391.005	56346	23.93	$6d^2(^3F)7d^2F$	6.08	$6d^2(^3F)7d^4G$	1.042			136		-83
	56578	19.82	$6d^2(^3F)7d^2F$	14.22	$5f\ 6d7p(^1F)^2D$	1.042			89		52
	57037	18.74	$6d\ 7p^2(^3P)^4F$	15.07	$6d^2(^3F)7d^4G$	0.911			123		74
	57402	16.04	$5f^2(^1D)6d^2D$	12.60	$6d\ 7s8s(^1S)^2D$	1.216			322		-338
	57938	36.17	$5f\ 6f7s(^3F)^4F$	9.07	$5f\ 6d6f(^3F)^4F$	1.052			235		-122
	58218	32.19	$6d^2(^3P)8s^4P$	12.07	$6d\ 7p^2(^3P)^4F$	1.282			145		154
	58577	21.83	$6d^2(^3P)8s^4P$	18.67	$6d\ 7p^2(^3P)^4F$	1.107			189		265
	58760	19.66	$6d^2(^3F)7d^4G$	11.86	$6d\ 7p^2(^1D)^2F$	0.934			83		736
	59061	30.17	$6d\ 7s8s(^1S)^2D$	14.99	$6d^2(^3P)8s^4P$	1.259			93		1142
	60490	23.26	$6d^2(^3F)7d^4D$	6.81	$6d^2(^3F)7d^2F$	1.255			11		-695
	60795	23.02	$5f\ 6f7s(^3F)^4P$	11.69	$5f\ 6f7s(^1F)^2D$	1.307			423		-257
	60935	15.50	$5f^2(^3P)6d^2F$	7.04	$7s\ 7p^2(^1D)^2D$	1.143			241		1080
61428.600	61356	12.82	$6d\ 7s7d(^3D)^2F$	8.58	$6d\ 7p^2(^3P)^4D$	0.993			-118		74
	61378	18.66	$7s\ 7p^2(^1D)^2D$	7.18	$7s\ 7p^2(^3P)^4P$	1.153			399		1710
	61885	8.42	$5f\ 6d6f(^3H)^4G$	7.57	$5f\ 6d6f(^3F)^4G$	0.886			153		585
	62062	9.95	$5f^2(^3P)6d^2D$	7.67	$5f\ 6f7s(^3F)^4P$	1.208			162		1177
	62123	12.69	$5f\ 7s8p(^3P)^4G$	10.83	$6d^2(^3F)7d^4D$	1.082			56		577

TABLE I. (Continued.)

$E_{\text{expt.}}$	$E_{\text{calc.}}$	%	Main comp.	%	Sec. comp.	$g_{J_{\text{calc.}}}$	$g_{J_{\text{expt.}}}$	$A_{\text{expt.}}$	$A_{\text{calc.}}$	$B_{\text{expt.}}$	$B_{\text{calc.}}$
62307.200	62389	14.65	5f 7s8p (3P) 4G	6.84	6d 7p 2 (3P) 4D	1.059			-52		892
62560.100	62646	11.33	5f 6f7s (3F) 4P	8.91	5f 6d6f (1G) 2D	1.164			175		-388
	62948	10.21	6d 7p 2 (3P) 4P	6.76	5f 7s8p (3P) 4F	1.122			159		201
	62982	17.88	6d 7p 2 (3P) 4D	5.84	5f 6d6f (1G) 2D	1.095			174		161
63257.500	63222	32.74	5f 7s8p (3P) 4F	8.52	5f 7s8p (3P) 4G	1.025			316		946
	63499	7.09	6d 2 (1D)8s 2D	6.52	5f 7s8p (3P) 4G	1.118			96		445
	63913	15.96	6d 7s7d (3D) 4D	8.88	5f 7s8p (3P) 4D	1.215			322		-58
	63991	9.07	5f 6d6f (3D) 4G	7.80	6d 7s7d (3D) 4G	0.950			77		-43
	64208	12.46	5f 6d6f (3G) 4G	11.98	6d 7s7d (3D) 4G	0.862			41		342
	64479	6.06	6d 2 (1D)8s 2D	5.94	6d 7s7d (3D) 4D	1.067			191		-129
	64632	9.24	5f 6d6f (1D) 2D	8.37	5f 6d6f (3F) 2D	1.067			119		112
64813.700	64819	8.82	6d 7p 2 (3P) 4P	7.14	5f 7s8p (3P) 4D	1.175			135		271
	65081	15.34	6d 2 (3P)7d 4F	10.63	6d 7p 2 (3P) 4P	1.155			16		780
65144.400	65138	16.88	6d 2 (3F)7d 4F	8.36	6d 2 (3P)7d 4F	1.036			68		-181
	65234	10.75	6d 7s7d (3D) 4G	6.38	6d 2 (1D)8s 2D	1.031			147		357
	65516	7.81	6d 7s7d (3D) 4D	7.20	6d 7s7d (1D) 2D	1.109			84		-202
65738.100	65692	9.09	5f 6d6f (3G) 4G	8.05	5f 7s8p (3P) 4D	0.983			223		-97
65910.000	65863	19.72	6d 2 (3F)7d 4F	6.86	5f 6f7s (1F) 2F	0.991			138		313
65946.900	65922	17.59	5f 6d8p (3F) 4G	10.08	5f 6d8p (3F) 2F	0.850			69		99
	66152	8.18	6d 7s7d (3D) 4F	5.41	6d 7s7d (3D) 4D	1.031			218		255
	66541	13.59	5f 6d6f (3D) 4D	8.64	6d 2 (3P)7d 4D	1.140			52		-267
	66695	6.44	5f 6d8p (1D) 2F	6.24	6d 7s7d (3D) 4F	0.944			113		682
66855.600	66866	5.90	5f 6f7s (1F) 2F	4.86	5f 7s8p (1P) 2F	0.980			58		766
	66942	7.31	5f 7s8p (3P) 2F	6.12	6d 7s7d (3D) 4F	1.043			123		762
	67236	6.95	6d 2 (3P)7d 4F	5.99	6d 7s7d (3D) 4F	1.076			86		1109
	67288	10.94	6d 2 (3P)7d 2F	7.53	6d 7p 2 (3P) 2F	0.975			130		543
	67448	8.53	5f 6d8p (3P) 4G	7.91	5f 6d8p (3D) 4G	0.938			51		1220
	67643	11.24	5f 6d6f (3P) 4D	7.41	5f 2 (1S)6d 2D	1.163			62		107
	67826	16.06	5f 7s8p (1P) 2F	10.05	5f 6d8p (3P) 4G	0.881			189		661
	68265	7.40	5f 6d6f (3D) 4D	5.92	7s 2 (1S)7d 2D	1.104			145		-34
	68354	11.62	5f 6d8p (3F) 4G	9.66	5f 6d8p (3F) 4F	1.000			132		96
$J = 7/2$											
4146.576	4141	94.31	6d 2 (3F)7s 4F	2.30	6d 2 (3F)7s 2F	1.234	1.232	450	446	750	841
9711.962	9645	42.34	6d 2 (1G)7s 2G	30.51	6d 3 2G	0.963	0.953	-150	-128	2100	2105
10855.323	10832	48.71	6d 3 4F	27.94	6d 2 (3F)7s 2F	1.165	1.166		-268		475
12570.493	12560	38.41	6d 2 (3F)7s 2F	28.70	6d 3 4F	1.125	1.131		-258		904
16818.065	16930	48.27	6d 3 2G	31.65	6d 2 (1G)7s 2G	0.916	0.916		-184		1962
22834.134	22849	72.50	6d 3 2F	14.85	6d 2 (3F)7s 2F	1.137	1.120		-36		1034
24381.799	24336	68.46	5f 2 (3H)7s 4H	17.25	5f 6d7p (3F) 4H	0.694	0.700		-193		1732
27257.149	27372	27.56	5f 7s7p (3P) 2F	26.53	5f 7s7p (3P) 4G	1.046	1.032		660		327
29431.848	29283	26.01	5f 2 (3F)7s 4F	25.86	5f 2 (1G)7s 2G	1.034	1.100		-109		-31
29873.952	29892	38.14	5f 2 (3F)7s 4F	29.76	5f 2 (3F)7s 2F	1.153	1.100		467		-719
30879.419	30867	41.86	5f 7s7p (3P) 4F	20.34	5f 7s7p (3P) 4D	1.208	1.213		283		1169
32576.748	32513	20.63	5f 6d7p (3D) 4H	12.16	5f 7s7p (3P) 2F	0.957	1.024		104		749
32736.188	32734	18.33	5f 2 (3F)7s 2F	16.52	5f 6d7p (3D) 4H	0.965	0.904		-26		716
33209.396	33072	43.07	5f 7s7p (3P) 4G	11.18	5f 7s7p (3P) 4F	1.040	1.051		138		1947
33637.230	33755	21.04	5f 6d7p (3F) 4H	14.11	5f 6d7p (3F) 4G	0.831	0.830		123		1334
34279.328	34294	28.35	5f 7s7p (3P) 2G	15.85	5f 7s7p (3P) 4D	1.057	1.047		181		1938
34726.574	34739	18.88	5f 6d7p (3F) 4G	17.48	5f 2 (3F)6d 4G	0.939	0.950		130		290
35878.860	35873	13.00	5f 6d7p (1D) 2G	8.39	5f 6d7p (3D) 4H	0.993	0.983		152		1067
36809.280	36922	12.24	5f 6d7p (3P) 4G	11.07	5f 6d7p (3D) 4G	1.069	1.022		126		688
37277.369	37262	18.84	5f 7s7p (1P) 2G	16.61	5f 2 (3F)6d 4H	0.915	0.881		72		1508
37787.878	37792	15.36	5f 6d7p (3F) 4G	9.90	5f 2 (3F)6d 4G	1.007	1.062		105		309
38165.355	38107	23.32	5f 2 (3F)6d 4H	13.01	5f 7s7p (1P) 2G	0.906	0.981		144		1219
38291.795	38302	21.15	5f 7s7p (3P) 4D	14.49	5f 7s7p (3P) 2G	1.172	0.949		137		729
38389.374	38446	13.16	5f 2 (3H)6d 4G	13.15	5f 6d7p (3D) 4G	0.985	1.088		105		766
39068.688	39069	19.85	5f 2 (3F)6d 2F	8.09	5f 2 (1G)6d 2F	1.128	1.114		107		-147
39458.281	39560	15.07	5f 2 (3F)6d 4G	11.52	5f 6d7p (3F) 4H	0.947	0.979		125		759

TABLE I. (Continued.)

$E_{\text{expt.}}$	$E_{\text{calc.}}$	%	Main comp.	%	Sec. comp.	$g_{\text{calc.}}$	$g_{\text{expt.}}$	$A_{\text{expt.}}$	$A_{\text{calc.}}$	$B_{\text{expt.}}$	$B_{\text{calc.}}$
40411.472	40254	9.64	5f 6d7p (^3F) ^2F	8.84	5f 6d7p (^3P) ^4G	1.137	1.106		54		315
40570.629	40456	11.09	5f 6d7p (^3D) ^2G	9.44	5f 6d7p (^3P) ^4F	1.096	1.100		101		500
41488.137	41546	11.71	5f 6d7p (^3D) ^4G	9.95	5f 6d7p (^3D) ^4F	1.059	1.010		128		221
41688.435	41824	11.50	5f 7s7p (^1P) ^2F	9.34	5f 6d7p (^3P) ^4G	1.026	0.940		65		115
42222.301	42174	42.05	5f 2 (^3H)6d ^4H	11.67	5f 2 (^3F)6d ^4H	0.796	0.935		157		366
42518.912	42368	16.64	5f 6d7p (^3P) ^4F	14.71	5f 7s7p (^1P) ^2F	1.125	1.080		136		96
42751.327	42916	14.77	5f 6d7p (^3F) ^4F	7.05	5f 2 (^3H)6d ^4H	1.097	1.090		95		-196
43246.825	43324	12.93	5f 2 (^3H)6d ^4H	11.98	5f 6d7p (^3P) ^2F	1.001	1.033		101		-69
43803.979	43666	13.05	5f 6d7p (^3P) ^4G	12.70	5f 7s7p (^1P) ^2F	1.075	1.026		119		1310
44503.779	44407	16.72	5f 6d7p (^1F) ^2G	9.03	5f 2 (^3F)6d ^2G	1.001	1.058		138		139
44807.934	44802	17.70	5f 6d7p (^3F) ^4D	16.84	5f 2 (^1G)6d ^2G	1.085	1.078		111		-224
44898.770	44924	19.75	5f 6d7p (^3F) ^4F	11.38	5f 2 (^3P)6d ^4F	1.190	1.181		86		1262
45395.040	45358	13.36	5f 2 (^3F)6d ^4D	11.76	5f 6d7p (^3D) ^2F	1.164	1.216		101		672
46352.224	46346	15.40	5f 2 (^3F)6d ^4F	11.77	5f 2 (^1G)6d ^2G	1.065	1.100		107		-575
46385.411	46477	34.72	5f 2 (^3H)6d ^4G	17.69	5f 2 (^3F)6d ^4G	1.014	1.070		115		279
46706.254	46633	18.73	5f 6d7p (^1D) ^2F	11.55	5f 6d7p (^3D) ^2F	1.117	1.081		89		1347
	47778	11.51	5f 6d7p (^3F) ^2F	10.48	5f 2 (^3F)6d ^4D	1.098			79		668
47871.384	47966	19.07	5f 6d7p (^3P) ^4D	18.23	5f 2 (^3P)6d ^4D	1.258	1.194		61		1189
48298.492	48339	10.49	5f 6d7p (^3D) ^4D	8.42	5f 2 (^3P)6d ^4D	1.221	1.070		55		-514
48453.110	48553	21.48	5f 6f7s (^3F) ^4G	15.86	5f 6f7s (^3F) ^2F	1.174			363		-201
	48803	13.60	5f 6f7s (^3F) ^4D	12.62	5f 2 (^1G)6d ^2G	1.162			186		-883
49377.162	49303	35.92	5f 6f7s (^3F) ^4G	9.38	5f 2 (^3F)6d ^4D	1.133	1.200		240		-90
49960.573	50115	21.75	5f 2 (^3P)6d ^4F	11.38	5f 2 (^3H)6d ^2G	1.095	1.248		95		571
50407.274	50458	20.04	5f 6d7p (^3F) ^4D	10.74	5f 6f7s (^3F) ^4G	1.224			153		38
	50660	23.27	5f 2 (^3H)6d ^4F	10.59	5f 2 (^3F)6d ^4F	1.164			99		802
51268.114	51262	18.45	5f 2 (^3P)6d ^4F	11.33	5f 6d7p (^3P) ^4F	1.201			95		1505
51830.510	51581	18.96	5f 6d7p (^1F) ^2F	10.69	5f 2 (^3H)6d ^2G	1.108			92		705
52272.321	52065	10.43	5f 6f7s (^1F) ^2G	9.04	5f 6f7s (^3F) ^2F	1.071			105		430
52562.518	52554	21.45	5f 6f7s (^1F) ^2G	15.94	5f 6d7p (^1F) ^2G	0.997			64		323
	53077	77.72	6d 2 (^3F)8s ^4F	6.05	6d 2 (^3F)8s ^2F	1.205			120		958
	53653	24.63	5f 6f7s (^3F) ^2F	8.65	5f 6f7s (^1F) ^2G	1.095			361		-47
54010.169	54066	14.47	5f 2 (^1D)6d ^2G	12.48	5f 2 (^1I)6d ^2G	0.959			113		1783
54169.668	54200	95.14	6d 7s8s (^3S) ^4D	1.26	6d 2 (^3F)7d ^4D	1.428			882		2283
	54569	40.77	5f 2 (^3P)6d ^4D	18.60	5f 6d7p (^3P) ^4D	1.365			42		2721
	55203	16.90	5f 6d7p (^1F) ^2F	9.69	5f 2 (^1G)6d ^2F	1.081			77		-46
	55594	25.69	5f 6f7s (^3F) ^4H	16.66	5f 6d6f (^3F) ^4H	0.767			-35		734
	56191	14.59	6d 2 (^3F)8s ^2F	12.39	5f 2 (^3F)6d ^2G	0.966			12		1669
56639.993	56690	19.19	6d 2 (^3F)8s ^2F	10.33	5f 2 (^3F)6d ^2G	1.059			13		947
	57826	14.79	6d 2 (^3F)7d ^2F	14.68	6d 2 (^3F)7d ^4H	0.940			17		-31
	58195	11.58	6d 2 (^3F)7d ^4G	10.85	5f 2 (^1D)6d ^2F	1.034			108		1194
	58563	16.84	6d 2 (^3F)7d ^4G	14.68	6d 2 (^3F)8s ^2F	1.056			39		1266
58875.500	58945	39.49	5f 6f7s (^3F) ^4F	10.73	5f 6d6f (^3F) ^4F	1.206			216		-317
59387.317	59341	34.07	6d 2 (^3F)7d ^4G	6.60	6d 7s7d (^1D) ^2G	1.008			58		1131
59803.000	59945	29.21	6d 2 (^3F)7d ^4H	24.19	6d 2 (^3F)7d ^2F	0.959			43		593
60721.300	60715	12.53	5f 6f7s (^3F) ^2G	11.21	5f 6d6f (^3F) ^2G	0.950			-18		334
	61050	52.89	6d 2 (^1G)8s ^2G	8.51	6d 2 (^3F)8s ^2F	0.976			34		2986
61388.000	61338	22.87	5f 2 (^3P)6d ^2F	10.07	5f 2 (^1D)6d ^2F	1.115			75		862
	61532	14.73	5f 2 (^1D)6d ^2G	7.71	6d 7p 2 (^3P) ^4F	1.009			183		1753
	61781	14.13	6d 7p 2 (^3P) ^4F	11.58	6d 7s7d (^3D) ^2F	1.088			229		1621
	62289	21.95	5f 6d6f (^1G) ^2G	13.30	5f 6d6f (^3G) ^2G	0.903			77		23
62477.000	62487	7.98	6d 2 (^3F)7d ^4D	5.45	5f 7s8p (^3P) ^4G	1.090			140		1250
	62595	22.26	6d 2 (^3F)7d ^4D	10.48	6d 2 (^3F)7d ^2G	1.149			67		-16
62753.100	62815	13.77	6d 7s7d (^3D) ^2F	13.40	6d 7p 2 (^3P) ^4F	1.138			234		1731
63298.400	63237	22.62	5f 7s8p (^3P) ^4G	14.97	5f 7s8p (^3P) ^2F	1.079			455		1075
63557.683	63611	8.68	5f 6d6f (^3F) ^4G	8.28	5f 6d6f (^3H) ^4G	0.964			62		757
	63828	14.82	6d 2 (^3F)7d ^2G	8.27	6d 7p 2 (^3P) ^4D	1.041			42		1820
64122.000	64117	10.51	5f 6d6f (^3D) ^4H	7.89	5f 7s8p (^3P) ^4F	0.965			161		591
	64316	13.68	5f 6d8p (^3D) ^4H	6.83	5f 7s8p (^3P) ^4G	0.958			90		1280

TABLE I. (Continued.)

$E_{\text{expt.}}$	$E_{\text{calc.}}$	%	Main comp.	%	Sec. comp.	$g_{J_{\text{calc.}}}$	$g_{J_{\text{expt.}}}$	$A_{\text{expt.}}$	$A_{\text{calc.}}$	$B_{\text{expt.}}$	$B_{\text{calc.}}$
	64507	13.21	5f 7s8p (^3P) ^4F	8.90	5f 7s8p (^3P) ^2F	1.010			283		1017
	64719	14.12	5f 6d6f (^3D) ^4H	5.38	5f 6d6f (^3G) ^4G	0.941			107		1293
	64874	13.69	5f 6d8p (^3D) ^4H	7.19	6d 7p 2 (^3P) ^4D	1.031			135		1023
	65111	15.73	6d 7s7d (^3D) ^4G	5.32	5f 6d8p (^3D) ^4G	1.053			83		752
	65563	11.83	6d 7s7d (^3D) ^4G	6.87	6d 2 (^1D)7d ^2G	1.113			102		940
65753.783	65720	17.68	5f 6f7s (^1F) ^2F	8.31	5f 6d6f (^3G) ^2F	1.097			143		162
	65825	13.25	6d 2 (^3P)7d ^4F	12.63	6d 7s7d (^3D) ^4D	1.141			168		50
$J = 9/2$											
6213.490	6181	88.50	6d 2 (^3F)7s ^4F	7.58	6d 2 (^1G)7s ^2G	1.314	1.312	444	456	1440	1479
10379.122	10330	33.72	6d 2 (^1G)7s ^2G	32.13	6d 3 ^2G	1.156	1.153		160		2071
13248.708	13225	55.09	6d 3 ^4F	34.62	6d 2 (^1G)7s ^2G	1.242	1.242		129		1073
15305.264	15288	63.14	6d 3 ^2H	14.82	6d 3 ^4F	1.008	1.006	90	67	2700	2694
19880.079	19940	51.94	6d 3 ^2G	23.06	6d 3 ^2H	1.080	1.080		58		1426
25246.297	25101	36.30	5f 2 (^3H)7s ^2H	35.74	5f 2 (^3H)7s ^4H	0.953	0.960		520		1687
27526.950	27526	42.66	5f 2 (^3H)7s ^4H	31.95	5f 2 (^3H)7s ^2H	0.944	0.930		-173		1977
29515.134	29567	21.75	5f 2 (^1G)7s ^2G	21.72	5f 2 (^3F)7s ^4F	1.112	1.030		394		241
30452.725	30472	37.89	5f 6d7p (^3F) ^4I	15.50	5f 6d7p (^1D) ^2H	0.917	1.035		291		2653
31773.079	31710	39.85	5f 7s7p (^3P) ^4F	26.84	5f 7s7p (^3P) ^4G	1.224	1.222		505		288
33384.428	33203	46.98	5f 2 (^3F)7s ^4F	22.54	5f 2 (^1G)7s ^2G	1.211	1.140		437		-267
34270.239	34257	25.35	5f 2 (^3H)6d ^2H	14.29	5f 2 (^3H)6d ^4I	0.949	0.938		195		1107
34553.954	34587	19.03	5f 7s7p (^3P) ^4G	16.18	5f 7s7p (^3P) ^2G	1.101	1.069		349		2713
35456.183	35485	15.93	5f 6d7p (^3F) ^4I	13.11	5f 2 (^3H)6d ^2H	1.007	1.054		257		2081
35545.585	35634	63.91	5f 2 (^3H)6d ^4I	9.20	5f 2 (^1G)6d ^2H	0.812	0.826		189		1142
36125.341	36031	26.31	5f 6d7p (^3D) ^4H	15.50	5f 7s7p (^3P) ^4G	1.032	1.035		186		1759
37063.305	36958	26.06	5f 6d7p (^3F) ^4H	17.89	5f 2 (^3F)6d ^4H	0.979	0.999		127		2050
37840.843	37791	23.63	5f 2 (^3F)6d ^4G	16.43	5f 6d7p (^3F) ^4G	1.084	1.070		115		238
38179.944	38143	14.12	5f 7s7p (^3P) ^2G	13.86	5f 6d7p (^1D) ^2H	1.050	0.979		236		1831
38617.681	38636	37.54	5f 7s7p (^3P) ^2G	12.21	5f 7s7p (^3P) ^4G	1.106	1.160		206		2983
39552.230	39610	17.28	5f 6d7p (^3D) ^4G	6.74	5f 6d7p (^3P) ^4G	1.121	1.100		119		1003
39895.422	39978	15.43	5f 6d7p (^1D) ^2G	7.56	5f 2 (^3F)6d ^4H	1.061	1.024		135		949
40367.444	40303	11.09	5f 2 (^3F)6d ^4H	9.66	5f 6d7p (^3F) ^2G	1.102	1.176		118		354
41047.206	41154	14.12	5f 7s7p (^1P) ^2G	9.49	5f 6d7p (^3F) ^2H	1.094	1.112		75		2066
41398.510	41436	10.74	5f 2 (^3F)6d ^4H	10.13	5f 6d7p (^3F) ^4G	1.039	0.983		117		1370
41909.326	42048	11.59	5f 6d7p (^3D) ^4G	11.27	5f 6d7p (^3F) ^4G	1.089	1.097		55		1806
42200.211	42360	9.18	5f 6d7p (^3P) ^4G	8.88	5f 6d7p (^3F) ^4H	1.096	1.080		93		1076
42955.843	43026	15.06	5f 6d7p (^3D) ^2G	11.29	5f 6d7p (^1F) ^2G	1.156	1.141		101		1130
43809.258	43645	19.51	5f 6d7p (^3F) ^4G	11.01	5f 6d7p (^3F) ^4H	1.137	1.102		109		1750
44096.250	44011	12.90	5f 2 (^1D)6d ^2G	8.19	5f 2 (^3H)6d ^2G	1.141	1.140		86		1126
44450.274	44408	59.73	5f 2 (^3H)6d ^4H	13.99	5f 6d7p (^3D) ^4H	0.986	1.040		120		614
45126.228	45192	22.42	5f 2 (^3F)6d ^4F	18.85	5f 6d7p (^3P) ^4F	1.215	1.210		88		250
45904.397	45929	20.21	5f 6d7p (^3F) ^4F	12.72	5f 6d7p (^1F) ^2G	1.172	1.020		85		78
46253.326	46388	13.02	5f 2 (^1G)6d ^2G	10.41	5f 6d7p (^3D) ^4F	1.120	1.010		90		1396
	46764	65.08	5f 6f7s (^3F) ^4I	7.76	5f 6d6f (^3F) ^4I	0.775			-154		2276
47171.374	47119	14.70	5f 6d7p (^1D) ^2G	8.11	5f 2 (^1D)6d ^2G	1.078	1.150		55		1361
47731.500	47714	19.81	5f 2 (^3H)6d ^4G	16.80	5f 6d7p (^1F) ^2H	1.094	1.100		94		1487
48006.863	48006	12.28	5f 6d7p (^1D) ^2G	11.28	5f 2 (^1G)6d ^2G	1.092	1.130		79		1244
48844.959	48856	10.47	5f 6d7p (^3F) ^2G	10.41	5f 2 (^3H)6d ^4G	1.121	1.100		85		1354
49837.657	49738	14.08	5f 6d7p (^1F) ^2H	9.07	5f 6d7p (^3F) ^2G	1.089			115		1427
	50140	26.37	5f 6f7s (^3F) ^4G	10.57	5f 2 (^3F)6d ^4F	1.174			114		312
50470.032	50467	40.22	5f 6f7s (^3F) ^4G	10.06	5f 2 (^3F)6d ^4F	1.192	1.180		232		-53
51224.259	51215	20.94	5f 2 (^3F)6d ^2H	18.90	5f 2 (^1D)6d ^2H	1.007			91		1875
51681.984	51585	28.02	5f 6f7s (^3F) ^2H	10.45	5f 2 (^3P)6d ^4F	1.076			-50		1391
	52089	12.86	5f 2 (^3P)6d ^4F	10.50	5f 6f7s (^3F) ^2H	1.145			44		1851
	52239	35.32	5f 2 (^3H)6d ^4F	20.65	5f 2 (^3P)6d ^4F	1.287			35		1879
53520.903	53580	16.24	5f 2 (^3H)6d ^2G	11.00	5f 2 (^3F)6d ^2G	1.091			82		1000
	54226	22.66	5f 6d7p (^1P) ^2G	16.42	5f 2 (^1D)6d ^2G	1.099			24		2583
54845.313	54940	14.45	5f 6f7s (^1F) ^2G	12.78	5f 6f7s (^3F) ^2G	1.119			5		864
	55318	50.70	6d 2 (^3F)8s ^4F	8.42	5f 6f7s (^3F) ^2G	1.230			38		1429

TABLE I. (*Continued.*)

$E_{\text{expt.}}$	$E_{\text{calc.}}$	%	Main comp.	%	Sec. comp.	$g_{J_{\text{calc.}}}$	$g_{J_{\text{expt.}}}$	$A_{\text{expt.}}$	$A_{\text{calc.}}$	$B_{\text{expt.}}$	$B_{\text{calc.}}$
55496.806	55510	28.43	$6d^2(^3F)8s^4F$	17.28	$5f\ 6d7p(^1F)^2G$	1.156			63		993
	56684	16.67	$5f^2(^3F)6d^2G$	14.33	$5f\ 6d7p(^3D)^2H$	1.029			99		1302
57078.529	57010	33.63	$5f\ 6f7s(^3F)^4H$	20.97	$5f\ 6d6f(^3F)^4H$	0.980			106		777
	58155	14.72	$5f^2(^1D)6d^2H$	14.32	$5f^2(^3F)6d^2H$	1.023			113		1578
	59463	20.37	$6d^2(^3F)7d^4G$	19.39	$6d^2(^3F)7d^4H$	1.068			61		405
	59540	28.17	$5f\ 6f7s(^3F)^4F$	8.00	$5f\ 6d6f(^3G)^4F$	1.222			240		-217
	60504	21.40	$5f\ 6d6f(^3H)^4I$	15.77	$5f\ 6d6f(^3G)^4I$	0.884			156		1588
	60849	40.24	$6d^2(^1G)8s^2G$	20.01	$5f^2(^1D)6d^2G$	1.114			212		3445
	60986	20.02	$6d^2(^3F)7d^4G$	11.70	$6d^2(^1G)8s^2G$	1.120			88		1450
	61367	20.72	$6d^2(^1G)8s^2G$	18.01	$6d^2(^3F)7d^4G$	1.106			103		2085
	62009	11.41	$5f^2(^1D)6d^2G$	9.30	$5f\ 6f7s(^1F)^2G$	1.064			144		1420
	62396	19.11	$5f\ 6d6f(^1D)^2H$	18.00	$5f\ 6d6f(^3G)^4I$	0.905			98		1206
	62595	21.63	$6d^2(^3F)7d^4H$	12.20	$6d^2(^3F)7d^2H$	0.978			83		1100
	62778	20.65	$6d^2(^3F)7d^2H$	10.57	$5f\ 6d6f(^1G)^2G$	0.982			100		804
	63456	12.60	$6d^2(^1D)7d^2G$	7.89	$6d^2(^3F)7d^2H$	1.064			167		887
	63968	29.69	$6d\ 7p^2(^3P)^4F$	12.40	$6d^2(^3F)7d^4F$	1.197			90		1406
	63985	21.71	$5f\ 6f7s(^1F)^2H$	11.73	$5f\ 6d6f(^3G)^2H$	0.972			123		1120
	64252	20.89	$5f\ 6d8p(^3F)^4I$	12.14	$6d^2(^3F)7d^2G$	0.962			142		2033
	64435	10.01	$5f\ 6d8p(^3F)^4I$	6.78	$6d^2(^3F)7d^2G$	1.031			169		1867
	65057	16.74	$5f\ 7s8p(^3P)^4G$	6.86	$6d\ 7s7d(^3D)^4G$	1.088			227		1392
	65238	11.55	$6d^2(^3F)7d^2G$	9.67	$5f\ 6d6f(^1D)^2G$	1.035			66		876
	65465	16.26	$5f\ 7s8p(^3P)^4G$	6.11	$5f\ 7s8p(^3P)^2G$	1.089			172		1286
	65678	29.14	$5f\ 6d6f(^3D)^4H$	8.21	$5f\ 6d6f(^3G)^4H$	0.990			69		747
	66139	20.95	$5f\ 6d8p(^3F)^4I$	8.48	$5f\ 7s8p(^3P)^4F$	1.029			197		1551
	66389	20.14	$6d\ 7s7d(^3D)^4G$	11.80	$5f\ 7s8p(^3P)^2G$	1.112			233		1387
	66682	15.33	$5f\ 6d8p(^3D)^4H$	8.36	$5f\ 6d8p(^3D)^2H$	1.004			139		1580
	66859	15.90	$5f\ 6d6f(^3D)^4G$	13.82	$6d\ 7s7d(^3D)^4G$	1.094			174		1376
	67060	17.79	$5f\ 6d6f(^3F)^4I$	5.80	$5f\ 6d6f(^1D)^2H$	1.000			69		1268
	67294	15.43	$6d^2(^3P)7d^4F$	12.39	$5f\ 7s8p(^3P)^4F$	1.200			165		621
	67398	17.50	$5f\ 6d6f(^3G)^4G$	10.69	$6d^2(^3F)7d^4F$	1.154			90		915
	67703	12.45	$5f\ 6d6f(^3G)^4G$	11.29	$5f\ 6d6f(^3D)^4G$	1.115			122		1225
	67949	11.61	$5f\ 6d8p(^3F)^4I$	10.28	$5f\ 7s8p(^3P)^4F$	1.072			164		1589
	68208	18.28	$5f\ 6d8p(^3D)^4H$	9.60	$5f\ 6d8p(^3F)^4H$	1.060			176		2070
	68410	10.34	$5f\ 6d6f(^1F)^2H$	9.78	$5f\ 6d6f(^3D)^2H$	1.040			165		1294
	68519	13.25	$6d\ 7p^2(^3P)^4F$	8.07	$6d\ 7s7d(^3D)^4F$	1.137			165		705
	68802	11.06	$6d\ 7s7d(^3D)^4F$	6.67	$5f\ 6d6f(^3F)^4F$	1.174			147		1123
	69009	20.97	$5f\ 6d6f(^1H)^2H$	9.38	$6d\ 7p^2(^3P)^4F$	1.082			158		752
	69230	10.98	$5f\ 6d8p(^1D)^2H$	10.44	$5f\ 6d8p(^3D)^2G$	1.081			148		1354
	69433	18.78	$5f\ 7s8p(^3P)^2G$	10.40	$5f\ 7s8p(^3P)^4G$	1.093			196		2047
	69594	11.67	$5f\ 6d8p(^3F)^4H$	6.28	$5f\ 6d6f(^1F)^2H$	1.056			147		1463
	69838	8.90	$5f^2(^3H)8s^4H$	8.75	$5f^2(^3H)8s^2H$	1.046			147		1686
	70052	12.93	$5f\ 6d6f(^3F)^4H$	11.75	$6d^2(^3F)7d^4F$	1.082			76		1289
	70369	11.02	$5f\ 6d8p(^3P)^4G$	9.16	$6d\ 7s7d(^3D)^4F$	1.163			104		1676
	70546	14.84	$5f\ 6d8p(^3P)^4G$	10.52	$6d\ 7s7d(^3D)^4F$	1.156			109		1642
	70635	18.39	$5f\ 6d8p(^3D)^4G$	15.04	$5f\ 6d8p(^3F)^4G$	1.123			86		1269
	70719	10.35	$5f\ 6f7s(^3F)^2G$	9.32	$5f\ 6d6f(^1F)^2G$	1.093			180		388
	71079	19.40	$5f\ 6d8p(^3F)^4G$	8.42	$5f\ 6d8p(^1F)^2H$	1.103			87		1258
	71355	22.26	$5f\ 6d6f(^3P)^4G$	6.46	$5f\ 6d6f(^3F)^4H$	1.100			90		1104
$J = 11/2$											
17727.246	17714	92.40	$6d^3\ ^2H$	2.82	$5f^2(^1G)6d^2H$	1.091	1.090		-7		3552
27937.072	28029	67.74	$5f^2(^3H)7s^4H$	17.54	$5f^2(^3H)7s^2H$	1.123	1.120		434		1958
30484.711	30450	57.78	$5f^2(^3H)7s^2H$	16.40	$5f^2(^3H)7s^4H$	1.096	1.080		-161		2275
32620.857	32681	67.95	$5f^2(^3H)6d^4K$	12.90	$5f^2(^1G)6d^2I$	0.829	0.826		177		3301
34661.709	34592	39.21	$5f\ 6d7p(^3F)^4I$	12.34	$5f^2(^3H)6d^4I$	1.003	0.998		146		2790
35525.170	35431	16.13	$5f\ 6d7p(^3F)^4I$	16.08	$5f^2(^3H)6d^2H$	1.008	1.024		129		2177
37053.439	37047	57.93	$5f^2(^1I)7s^2I$	5.47	$5f\ 6d7p(^1F)^2I$	0.975			-89		3760
37562.261	37566	35.67	$5f^2(^3H)6d^4I$	10.61	$5f\ 7s7p(^3P)^4G$	1.077	1.008		141		1860
37679.696	37802	36.49	$5f^2(^3H)6d^4I$	12.74	$5f^2(^1I)7s^2I$	1.026	1.130		78		2347
38740.447	38654	56.16	$5f\ 7s7p(^3P)^4G$	9.18	$5f^2(^1G)6d^2I$	1.177	1.188		318		3476

TABLE I. (Continued.)

$E_{\text{expt.}}$	$E_{\text{calc.}}$	%	Main comp.	%	Sec. comp.	$g_{J_{\text{calc.}}}$	$g_{J_{\text{expt.}}}$	$A_{\text{expt.}}$	$A_{\text{calc.}}$	$B_{\text{expt.}}$	$B_{\text{calc.}}$
38862.815	38916	23.05	5f 6d7p (3D) 4H	11.83	5f 6d7p (3F) 2H	1.100	1.083		114		2036
39352.287	39243	17.72	5f 2 (3F)6d 4H	11.87	5f 6d7p (3F) 2H	1.069	1.050		129		2841
39939.113	39836	17.98	5f 2 (3F)6d 4G	17.63	5f 6d7p (3F) 4I	1.121	1.120		84		2482
40574.750	40416	13.86	5f 2 (3F)6d 4H	13.34	5f 2 (3H)6d 2H	1.163	1.140		123		1558
41223.556	41273	27.17	5f 6d7p (3F) 2H	19.52	5f 2 (3F)6d 4G	1.130	1.110		98		2504
42146.531	42037	19.38	5f 6d7p (3D) 4G	9.63	5f 6d7p (3F) 4G	1.151	1.158		76		1162
43127.211	43340	27.01	5f 6d7p (3F) 2I	16.45	5f 6d7p (1F) 2I	1.038	1.037		128		3682
44177.264	44169	28.94	5f 2 (3F)6d 4H	28.49	5f 6d7p (3F) 4H	1.129	1.120		97		2085
44727.235	44626	17.42	5f 6d7p (3P) 4G	16.13	5f 6d7p (3D) 4G	1.183	1.200		79		1442
45735.093	45600	31.07	5f 6d7p (3F) 4G	11.68	5f 2 (3H)6d 4H	1.139	1.141		111		1782
46216.578	46179	19.52	5f 6d7p (3D) 4G	16.36	5f 6d7p (3F) 4H	1.152	1.160		92		3086
46555.598	46585	29.85	5f 2 (3H)6d 4H	14.16	5f 6d7p (3D) 4H	1.158			87		1135
46861.585	46848	20.76	5f 2 (1G)6d 2H	20.24	5f 2 (1D)6d 2I	1.064	1.150		106		1878
47675.046	47737	64.56	5f 6f7s (3F) 4I	7.44	5f 6d6f (3F) 4I	0.974	1.150		211		2460
49124.553	49239	31.44	5f 2 (1I)6d 2H	13.44	5f 6d7p (3D) 2H	1.045			108		1530
49357.993	49475	26.24	5f 2 (3H)6d 4G	16.64	5f 6d7p (3P) 4G	1.191	1.150		73		1468
50631.124	50684	32.44	5f 6f7s (3F) 2H	23.44	5f 6f7s (3F) 4G	1.136			323		1264
	51220	28.27	5f 2 (3H)6d 2I	22.32	5f 2 (1G)6d 2I	0.965			112		2378
52170.204	52266	27.61	5f 6d7p (1F) 2H	10.60	5f 6d7p (3D) 4G	1.151	1.120		82		1698
	52517	29.05	5f 6f7s (3F) 4G	18.09	5f 6f7s (1F) 2I	1.098			206		1806
	53316	28.28	5f 6f7s (1F) 2I	10.21	5f 6f7s (3F) 2I	1.000			182		2148
	53974	14.73	5f 6d7p (1F) 2H	13.96	5f 6f7s (3F) 2H	1.082			192		1502
56945.138	56917	20.32	5f 6d7p (3F) 2I	15.79	5f 6d7p (1F) 2I	0.995	1.100		84		3982
	58158	23.49	5f 2 (1I)6d 2H	13.54	5f 6d7p (3D) 2H	1.075			101		1732
	58301	32.72	5f 6f7s (3F) 4H	20.26	5f 6d6f (3F) 4H	1.111			153		1034
	61071	30.98	5f 6d6f (1G) 2I	23.05	5f 6d6f (3H) 2I	0.945			76		1530
	61849	39.79	6d 2 (3F)7d 4G	18.07	6d 2 (3F)7d 4H	1.186			-5		980
	62195	58.18	5f 6d6f (3G) 4K	6.73	5f 6d6f (1F) 2I	0.843			107		2149
	62865	33.77	5f 6d6f (3H) 4I	27.94	5f 6d6f (3G) 4I	0.986			100		2004
	63317	58.35	6d 2 (3F)7d 4H	12.53	6d 2 (3F)7d 4G	1.154			-12		1411
	64345	19.75	5f 6d6f (3G) 4K	16.65	5f 6f7s (3F) 2I	0.931			-5		2153
	65018	22.34	5f 6d6f (1D) 2H	11.34	5f 6d6f (3F) 2H	1.068			84		1011
	65296	21.93	5f 6d6f (3G) 2H	12.09	5f 6d6f (3H) 2H	1.090			57		1373
	65484	24.76	6d 2 (3F)7d 2H	13.81	6d 2 (1G)7d 2H	1.096			50		1535
	65849	14.11	5f 6d6f (3D) 2H	13.17	5f 6d6f (3D) 4H	1.070			40		1212
	67004	17.19	5f 6f7s (1F) 2H	16.36	5f 6d8p (3F) 4I	1.061			60		1814
	67112	23.10	5f 6d8p (3F) 4I	10.48	5f 6f7s (1F) 2H	1.042			67		2696
	67485	22.81	6d 7s7d (3D) 4G	19.29	5f 7s8p (3P) 4G	1.170			238		2001
	67705	19.67	6d 7s7d (3D) 4G	13.82	5f 6d6f (3F) 4I	1.112			160		2130
	68086	12.58	5f 6d6f (3D) 4H	7.14	5f 6d6f (3H) 4G	1.153			104		1558
	68234	37.28	5f 6d6f (1F) 2I	9.88	5f 6f7s (3F) 2I	1.040			69		1466
$J = 13/2$											
30548.664	30746	86.40	5f 2 (3H)7s 4H	8.83	5f 6d7p (3F) 4H	1.227	1.230		378		2311
35400.772	35435	90.49	5f 2 (3H)6d 4K	4.41	5f 2 (1G)6d 2I	0.974	0.980		125		3791
37575.233	37520	74.64	5f 2 (1I)7s 2I	5.90	5f 6d7p (1F) 2I	1.085	1.088		356		4210
38517.974	38369	50.49	5f 2 (3H)6d 4I	21.99	5f 6d7p (3F) 4I	1.109	1.111		121		2638
39085.540	39240	29.29	5f 2 (1G)6d 2I	24.71	5f 2 (3H)6d 2I	1.105	1.100		78		2514
40724.732	40678	26.02	5f 2 (3H)6d 4I	25.37	5f 6d7p (3F) 4I	1.138	1.129		113		2497
41882.378	41880	41.44	5f 2 (3F)6d 4H	20.26	5f 2 (3H)6d 4H	1.187			68		1760
42644.884	42550	33.89	5f 6d7p (3F) 4I	22.62	5f 6d7p (3D) 4H	1.136	1.100		116		4321
43014.143	43015	46.61	5f 2 (1I)6d 2K	34.48	5f 2 (3H)6d 2K	0.963	0.976		127		3752
46378.852	46417	29.48	5f 2 (3F)6d 4H	28.51	5f 2 (3H)6d 4H	1.183	1.130		75		2744
46910.780	47002	25.27	5f 6d7p (3F) 4H	16.42	5f 6d7p (3F) 2I	1.156	1.180		85		3431
48612.223	48562	51.01	5f 2 (1I)6d 2I	12.11	5f 2 (1G)6d 2I	1.082	1.080		117		2774
	48952	35.14	5f 6d7p (3F) 4H	25.80	5f 6d7p (3D) 4H	1.219			95		2697
49527.314	49446	61.39	5f 6f7s (3F) 4I	7.51	5f 2 (1D)6d 2I	1.107	1.100		212		2789
52918.919	52936	30.11	5f 2 (3H)6d 2I	17.60	5f 2 (1G)6d 2I	1.042			103		2984
	55290	37.50	5f 6f7s (1F) 2I	26.66	5f 6f7s (3F) 2I	1.062			-56		3399
	56245	29.07	5f 2 (3H)6d 2K	22.62	5f 2 (1D)6d 2K	0.998			87		3138

TABLE I. (Continued.)

$E_{\text{expt.}}$	$E_{\text{calc.}}$	%	Main comp.	%	Sec. comp.	$g_{J_{\text{calc.}}}$	$g_{J_{\text{expt.}}}$	$A_{\text{expt.}}$	$A_{\text{calc.}}$	$B_{\text{expt.}}$	$B_{\text{calc.}}$
	58876	26.31	5f 6d7p (¹ F) ² I	23.88	5f 6d7p (³ F) ² I	1.082			141		4920
	59244	15.58	5f 6d6f (³ H) ⁴ L	12.50	5f 6f7s (³ F) ⁴ H	1.054			156		3075
	59765	35.22	5f 6d6f (³ H) ⁴ L	19.77	5f 6f7s (³ F) ⁴ H	1.023			163		2857
	61765	39.63	5f 6d6f (³ H) ⁴ L	14.94	5f 6d6f (¹ G) ² K	0.940			125		3393
	63793	17.11	5f 6f7s (¹ F) ² I	13.75	5f 6d6f (³ H) ² I	1.037			172		2500
	64210	49.84	5f 6d6f (³ G) ⁴ K	6.08	5f 6d6f (¹ G) ² K	0.987			105		2535
	64852	73.88	6d ² (³ F)7d ⁴ H	4.49	6d ² (¹ G)7d ² I	1.219			-32		1576
	64979	29.08	5f 6d6f (³ G) ⁴ I	28.80	5f 6d6f (³ H) ⁴ I	1.070			109		2495
	65593	16.92	5f 6f7s (¹ F) ² I	16.04	5f 6d6f (³ F) ² I	1.071			168		2491
	66348	49.18	5f 6d6f (¹ H) ² K	19.74	5f 6d6f (³ G) ² K	0.968			106		3167
	68401	39.95	5f 6d6f (³ F) ⁴ I	19.79	5f 6d6f (³ G) ⁴ I	1.119			74		1618
	68657	30.81	5f 6d6f (³ D) ⁴ H	12.46	5f 6d6f (³ G) ⁴ H	1.179			85		1319
	70517	22.60	6d ² (¹ G)7d ² I	21.73	5f 6d6f (¹ H) ² I	1.096			100		2493
	70649	72.17	5f 6d8p (³ F) ⁴ I	6.25	5f 6d6f (³ F) ⁴ I	1.109			100		4570
	71150	38.60	6d ² (¹ G)7d ² I	26.14	5f 6d6f (¹ F) ² I	1.088			104		2899
	71737	45.84	5f 6d8p (³ D) ⁴ H	21.56	5f 6d8p (³ F) ⁴ H	1.195			81		3048
	72154	35.24	5f 6d6f (¹ H) ² I	15.39	5f 6d6f (³ F) ⁴ H	1.124			104		1967
	72952	26.45	5f 6d6f (³ F) ⁴ H	19.19	5f 6f7s (³ F) ⁴ H	1.181			124		1456
	74219	41.50	5f 6d8p (¹ F) ² I	23.69	5f 6d8p (³ F) ² I	1.110			82		4654
	74791	31.15	5f 6d8p (³ F) ⁴ H	25.62	5f ² (³ H)8s ⁴ H	1.225			99		2277
	75152	59.01	5f ² (³ H)7d ⁴ K	21.29	5f 6d6f (³ H) ⁴ K	0.977			91		2391
	76077	49.75	5f 6d6f (³ H) ⁴ K	21.81	5f ² (³ H)7d ⁴ K	0.984			96		2685
	76891	24.42	5f 6d6f (¹ G) ² K	24.13	5f 6d6f (³ H) ² K	0.955			97		2489
	77316	27.39	5f ² (³ H)7d ⁴ I	15.89	5f ² (³ H)8s ⁴ H	1.152			87		1944
	77686	46.55	5f ² (³ H)7d ⁴ I	20.49	5f ² (³ H)8s ⁴ H	1.142			98		1889
	78113	27.44	5f 6d6f (¹ G) ² I	17.30	5f 6d6f (³ H) ² I	1.093			86		1980
	79013	35.06	5f 6d6f (³ H) ⁴ I	26.09	5f 6d6f (³ G) ⁴ I	1.096			76		1292
	79537	32.94	6d ² (³ F)5g ² K	20.76	6d ² (³ F)5g ⁴ K	1.013			23		570
	79967	37.06	6d ² (³ F)8d ⁴ H	10.41	5f 6d6f (³ G) ⁴ H	1.158			16		1680
$J = 15/2$											
38107.098	38052	98.11	5f ² (³ H)6d ⁴ K	0.83	5f ² (³ H)7d ⁴ K	1.090	1.080		90		4093
41099.065	41068	82.18	5f ² (³ H)6d ⁴ I	8.04	5f 6d7p (³ F) ⁴ I	1.189	1.170		66		2344
45095.234	45190	41.67	5f 6d7p (³ F) ⁴ I	31.73	5f ² (¹ D)6d ² K	1.123			94		5278
45994.361	45980	42.26	5f 6d7p (³ F) ⁴ I	20.95	5f ² (¹ D)6d ² K	1.148			90		4911
	50782	91.71	5f ² (¹ I)6d ² L	4.09	5f ² (¹ D)6d ² K	0.949			137		6411
	51493	71.08	5f 6f7s (³ F) ⁴ I	9.02	5f 6d6f (³ F) ⁴ I	1.200			266		3098
	56918	58.17	5f ² (³ H)6d ² K	35.05	5f ² (¹ D)6d ² K	1.067			98		4030
	62066	73.83	5f 6d6f (³ H) ⁴ L	10.88	5f 6d6f (³ H) ² K	0.991			103		4535
	64082	35.84	5f 6d6f (¹ G) ² K	32.31	5f 6d6f (³ H) ² K	1.049			84		3451
	66110	66.04	5f 6d6f (³ G) ⁴ K	6.45	5f 6d6f (³ H) ⁴ K	1.093			81		2773
	66953	31.95	5f 6d6f (³ G) ⁴ I	30.11	5f 6d6f (³ H) ⁴ I	1.158			68		2764
	68528	25.63	5f 6d6f (¹ H) ² K	19.46	5f 6d6f (¹ H) ² L	1.081			84		3792
	70206	36.51	5f 6d6f (¹ H) ² L	34.20	5f 6d6f (³ F) ⁴ I	1.098			100		3166
	71006	36.59	5f 6d6f (¹ H) ² L	16.87	5f 6d6f (¹ H) ² K	1.062			87		3531
$J = 17/2$											
	40631	97.90	5f ² (³ H)6d ⁴ K	0.85	5f ² (³ H)7d ⁴ K	1.176			63		4487
	52469	97.09	5f ² (¹ I)6d ² L	1.75	5f 6d6f (¹ H) ² L	1.060			78		6656
	64791	98.13	5f 6d6f (³ H) ⁴ L	0.88	5f 6d6f (³ G) ⁴ K	1.078			80		5207
	68457	83.67	5f 6d6f (³ G) ⁴ K	12.49	5f 6d6f (³ H) ⁴ K	1.174			60		2820
	73797	93.76	5f 6d6f (¹ H) ² L	2.01	5f 6d6f (³ G) ⁴ K	1.062			81		5558

TABLE II. Comparison of the experimental and calculated energy values and Lande g_J factors for Th II in the energy range up to 40644 cm^{-1} .

Conf.	J	E (expt.)	g_J (expt.)	This work			Porsev and Flambaum [23]			Safronova <i>et al.</i> [15]		
				E (calc.)	ΔE	g_J (calc.)	E (calc.)	ΔE	g_J (calc.)	E (calc.)	ΔE	g_J (calc.)
6d ² 7s	3/2	0	0.639	-18	18	0.628	0	0	0.712	0	0	0.662
6d ² 7s	5/2	1522	1.076	1582	-60	1.069				1722	-200	1.070
6d ² 7s	3/2	1859	0.586	1868	-9	0.594				1948	-89	0.554
6d 7s ²	5/2	4113	1.163	4161	-48	1.165				4185	-72	1.150
6d ² 7s	7/2	4147	1.232	4141	6	1.234				4374	-227	1.227
6d ² 7s	9/2	6213	1.312	6181	32	1.314				6528	-315	1.309
6d ² 7s	1/2	6244	2.112	6228	16	2.190				6972	-728	2.144
6d ³	3/2	7001	0.800	7059	-58	0.726				7779	-778	0.806
6d ² 7s	1/2	7828	1.254	7927	-99	1.184				8509	-681	1.201
6d ² 7s	3/2	8018	1.608	8051	-33	1.657				8622	-604	1.608
6d ³	3/2	8460	0.968	8463	-3	0.982				9209	-749	0.945
6d ² 7s	5/2	8606	0.986	8578	28	1.062				9198	-592	0.982
6d ² 7s	5/2	9061	1.419	9078	-17	1.348				9680	-619	1.408
6d ³	5/2	9401	1.034	9365	36	1.027				10145	-744	1.035
6d ² 7s	7/2	9712	0.953	9645	67	0.963				10502	-790	0.947
6d ² 7s	9/2	10379	1.153	10330	49	1.156				11158	-779	1.145
6d ³	7/2	10855	1.166	10832	23	1.165				11621	-766	1.171
6d ² 7s	3/2	12220	0.977	12209	11	0.991				13270	-1050	0.946
6d ³	7/2	12570	1.131	12560	10	1.125				13297	-727	1.122
6d ³	9/2	13249	1.242	13225	24	1.242				14217	-968	1.256
6d ² 7s	5/2	13251	1.245	13179	72	1.252				14220	-969	1.235
6d ³	1/2	14349	2.555	14378	-29	2.545				15632	-1283	2.564
6d ³	3/2	15237	1.592	15236	1	1.565				16503	-1266	1.612
6d ³	9/2	15305	1.006	15288	17	1.008				16585	-1280	0.983
6d ³	5/2	15787	1.571	15750	37	1.563				17100	-1313	1.566
6d ³	7/2	16818	0.916	16930	-112	0.916				18247	-1429	0.906
6d ³	11/2	17727	1.09	17714	13	1.091				19039	-1312	1.086
6d ³	3/2	18119	0.93	18095	24	0.902	21351	-3232	0.887	19973	-1854	0.862
6d ³	9/2	19880	1.08	19940	-60	1.080				21328	-1448	1.075
6d ³	5/2	20159	1.19	20148	11	1.199	23731	-3572	1.198	22144	-1985	1.189
6d ³	5/2	22106	0.92	22141	-35	0.937	26005	-3899	0.931			
6d ³	7/2	22834	1.12	22849	-15	1.137				25165	-2331	1.132
5f ² 7s	9/2	25246	0.96	25101	145	0.953				30481	-5235	0.939
6d ³	3/2	25382	1.25	25378	4	1.248	29632	-4250	1.242			
5f 7s7p	5/2	26489	0.776	26475	14	0.825	26971	-482	0.747			
5f ² 7s	3/2	26762	0.4	26716	46	0.497	27561	-799	0.480			
5f ² 7s	5/2	27594	0.963	27609	-15	0.968	28396	-802	0.975			
5f 7s7p	3/2	27631	0.625	27561	70	0.494	28082	-451	0.518			
5f ² 7s	11/2	27937	1.12	28029	-92	1.123				33216	-5279	1.118
6d ³	3/2	28011	0.717	27934	77	0.838	32348	-4337	0.841			
6d ³	5/2	28026	1.13	28060	-34	1.149	32764	-4738	0.975			
5f 7s7p	5/2	28824	0.987	28826	-2	0.929	29367	-543	0.993			
5f ² 7s	5/2	29346	0.935	29553	-207	0.930	30440	-1094	0.933			
5f ² 7s	11/2	30485	1.08	30450	35	1.096				35702	-5217	1.085
5f ² 7s	13/2	30549	1.23	30746	-197	1.227				35827	-5278	1.221
5f 6d7p	5/2	31259	0.781	31275	-16	0.775	31973	-714	0.903			
5f 7s7p	5/2	31754	0.948	31828	-74	0.942	32554	-800	0.997			
5f ² 7s	11/2	32621	0.826	32681	-60	0.829				37981	-5360	0.885
5f 6d7p	3/2	32959	0.874	33063	-104	0.868	34051	-1092	0.834			
5f ² 7s	5/2	33731	1.031	33648	83	1.054	34891	-1160	1.014			
5f ² 7s	3/2	34019	0.823	34080	-61	0.815	35306	-1287	0.910			
5f ² 7s	5/2	34175	0.986	34189	-14	1.025	35727	-1552	1.095			
5f 7s7p	5/2	34544	1.003	34473	71	0.937	34732	-188	0.965			
5f 7s7p	3/2	35021	1.042	35036	-15	1.033	35535	-514	1.001			
5f ² 6d	13/2	35401	0.98	35435	-34	0.974				41108	-5707	0.973

TABLE II. (Continued.)

Conf.	J	E (expt.)	g_J (expt.)	This work			Porsev and Flambaum [23]			Safronova <i>et al.</i> [15]		
				E (calc.)	ΔE	g_J (calc.)	E (calc.)	ΔE	g_J (calc.)	E (calc.)	ΔE	g_J (calc.)
5f 6d7p	5/2	35741	0.954	35702	39	0.788	37326	-1585	0.996			
5f ² 6d	5/2	36066	0.887	36252	-186	1.041	36864	-798	0.834			
5f ² 7s	3/2	36329	1.615	36397	-68	1.601	38069	-1740	1.636			
5f 6d7p	5/2	37465	1.048	37390	75	1.063	39615	-2150	0.958			
5f ² 7s	3/2	37542	1.003	37612	-70	1.174	38787	-1245	0.870			
5f ² 7s	13/2	37575	1.088	37520	55	1.085				42291	-4716	1.120
5f 7s7p	3/2	37822	1.15	37831	-9	1.225	39376	-1554	0.942			
5f 7s7p	5/2	37945	0.893	37980	-35	1.036	38975	-1030	0.987			
5f ² 7s	5/2	38105	1.172	38201	-96	1.135	38653	-548	0.918			
5f ² 6d	3/2	38372	1.200	38305	67	0.772	40194	-1822	1.295			
5f 6d7p	5/2	38729	1.255	38696	33	0.946	40305	-1576	1.177			
5f ² 7s	3/2	38757	0.935	38672	85	0.982	40937	-2180	0.903			
5f 6d7p	3/2	38836	1.013	38763	73	0.864	39919	-1083	1.046			
5f 6d7p	5/2	38864	0.967	38876	-12	1.112	40386	-1522	1.076			
5f 6d7p	3/2	39151	0.739	39052	99	0.926	40336	-1185	0.823			
5f 7s7p	5/2	39367	1.140	39340	27	1.105	40679	-1312	1.277			
5f 6d7p	5/2	39701	1.090	39604	97	1.098	41000	-1299	1.177			
5f 6d7p	5/2	40216	1.024	40311	-95	1.025	41967	-1751	0.941			
5f 7s7p	3/2	40223	0.738	40176	47	0.837	41738	-1515	0.887			
5f 7s7p	3/2	40278	0.705	40509	-231	0.858	41890	-1612	0.595			
5f ² 6d	5/2	40644	0.856	40551	93	0.909	42229	-1585	0.979			

procedure can be performed for the effects of the breakdown of I as a good quantum number. Some of the two-body contributions to the hyperfine-structure constants are expected in the range of a few MHz, hence, the hfs constants should be determined with this accuracy.

This study was conducted on the assumption that the isomeric state does not disturb atomic states $|\text{conf. } SLJIF\rangle$. If the differences between predicted and experimentally obtained A and B values appear, they will provide the evidence that the ground state $|g_I = 5/2\rangle$ and the isomeric state $|g_I = 3/2\rangle$ are mixed via electronic states.

For example, for the electronic state $J = 1/2$ the following possible atomic states are possible: $F = 3$, $F = 2$ for nuclear spin $I = 5/2$ and $F = 1$, $F = 2$ for isomeric nuclear spin $I = 3/2$. Therefore, the wave function for the atomic state $F = 2$ contains contributions from both nuclear states $I = 5/2$ and $3/2$. Thus, for weak mixing we should observe a broadening of the transition lines from $F = 2$ state. For stronger mixing, by using experimental methods with appropriate precision, we should resolve these lines into two components. Due to the fact that the lifetime of the isomeric state is many orders of magnitude greater than the lifetime

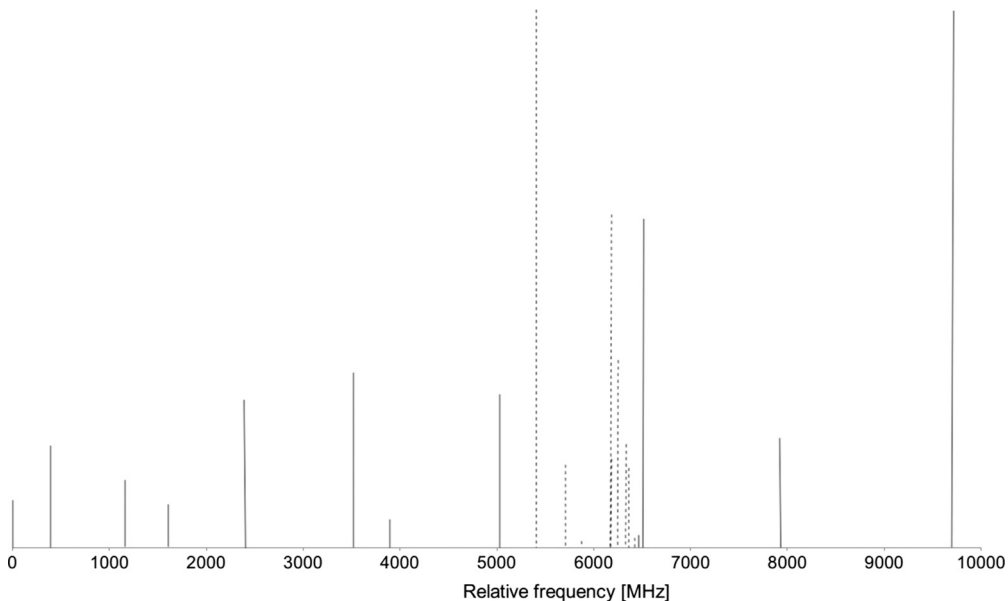


FIG. 1. Simulation of the line structure for the transition $34\,543.556\text{ cm}^{-1} \rightarrow 17\,121.620\text{ cm}^{-1}$.

TABLE III. Comparison of the experimental and calculated energy values and Lande g_J factors for Th II in the energy range from 40924 to 56391 cm^{-1} .

Conf.	J	E (expt.)	g_J (expt.)	This work			Porsev and Flambaum [23]		
				E (calc.)	ΔE	g_J (calc.)	E (calc.)	ΔE	g_J (calc.)
5f 6d7p	5/2	40924	0.988	40944	-20	1.016	42449	-1525	1.063
5f 6d7p	3/2	40992	1.036	40988	4	0.863	42501	-1509	1.037
5f 7s7p	5/2	41328	1.101	41240	88	1.113	42747	-1419	0.957
5f ² 6d	3/2	41677	1.220	41747	-70	1.390	43943	-2266	1.264
5f ² 6d	3/2	41937	1.095	42003	-66	0.984	43236	-1299	1.088
5f ² 6d + 5f 6d7p	5/2	42337	1.15	42167	170	1.254	44239	-1902	1.041
5f ² 6d + 5f 6d7p	5/2	42352	1.126	42516	-164	1.053	44305	-1953	1.237
5f ² 6d + 5f 6d7p	5/2	43097	0.982	43192	-95	1.125	44716	-1619	0.995
5f ² 6d + 5f 6d7p	5/2	43228	1.153	43390	-162	1.094	44876	-1648	1.135
5f ² 6d	3/2	43245	1.08	43257	-12	1.163	45161	-1916	1.107
5f ² 6d + 5f 6d7p	5/2	43772	1.04	43708	64	0.996	45900	-2128	0.985
5f 6d7p	3/2	43808	1.211	44063	-255	1.149	45544	-1736	1.271
5f ² 6d	3/2	44301	1.342	44396	-95	1.498	46287	-1986	1.357
5f ² 6d + 5f 6d7p	5/2	44389	1.158	44469	-80	1.136	46283	-1894	1.087
5f ² 6d + 5f 6d7p	5/2	44553	1.182	44575	-22	1.229	46775	-2222	1.224
5f ² 6d	3/2	44890	1.346	44896	-6	1.143	46742	-1852	0.960
5f ² 6d + 5f 6d7p	5/2	45190	0.674	45081	109	0.692	46928	-1738	0.729
5f 6d7p	3/2	45306	0.6	45328	-22	0.528	46994	-1688	0.910
5f ² 6d + 5f 6d7p	5/2	45611	1.075	45523	88	1.291	47310	-1699	1.076
5f ² 6d + 5f 6d7p	5/2	45800	1.3	45641	159	1.045	47877	-2077	1.249
5f 6d7p	3/2	46264	0.891	46213	51	1.024	47778	-1514	0.936
5f 6d7p	3/2	46396		46422	-26	1.396	48554	-2158	1.268
5f ² 6d + 5f 6d7p	5/2	46581	1.018	46522	59	1.136	48439	-1858	1.058
5f ² 6d + 5f 6d7p	5/2	46603	1.112	46597	6	0.983	48616	-2013	1.135
5f ² 6d + 5f 6d7p	5/2	46903	1.143	46743	160	1.090	48835	-1932	1.147
5f ² 6d	3/2	46936	0.956	46803	133	1.249	49401	-2465	0.567
5f 6d7p	3/2	47149	1.09	47133	16	0.793	49137	-1988	1.316
5f ² 6d + 5f 6d7p	5/2	47324	1.189	47409	-85	1.268	49355	-2031	1.231
5f ² 6d	3/2	47870		47883	-13	1.347	50324	-2454	0.849
5f ² 6d + 5f 6d7p	5/2	48321		48277	44	0.831	50553	-2232	1.155
5f ² 6d + 5f 6d7p	5/2	48492		48627	-135	0.925	50633	-2141	1.025
5f 6d7p	3/2	48690	0.922	48665	25	0.569	50924	-2234	1.079
5f ² 6d	3/2	48818	0.956	48826	-8	1.079	50749	-1931	0.727
5f ² 6d + 5f 6d7p	5/2	49069		48963	106	1.051	51463	-2394	1.061
5f 6d7p	3/2	49415	1.003	49405	10	0.670	51692	-2277	1.213
5f ² 6d + 5f 6d7p	5/2	49873		49873	0	1.100	51941	-2068	1.054
5f ² 6d + 5f 6d7p	5/2	50664		50650	14	1.191	52964	-2300	1.207
5f 6d7p	3/2	50735	1.36	50700	35	1.183	52761	-2026	1.585
5f 6d7p	3/2	50908	1.3	50828	80	1.267	53760	-2852	0.852
5f ² 6d + 5f 6d7p	3/2	51025	1.270	51129	-104	1.436	54511	-3486	1.286
5f ² 6d + 5f 6d7p	5/2	51363		51421	-58	1.242	54363	-3000	1.271
5f 6d7p	3/2	51676		51655	21	1.301	54796	-3120	1.069
5f ² 6d + 5f 6d7p	5/2	51865		51858	7	1.021	54851	-2986	1.031
5f ² 6d + 5f 6d7p	5/2	51936		51935	1	1.183	55511	-3575	1.279
5f 6d7p	3/2	52307		52266	41	1.555	55562	-3255	1.036
5f 6d7p	3/2	52736		52685	51	1.232	57665	-4929	1.246
5f ² 6d + 5f 6d7p	5/2	53845		53832	13	1.257	56279	-2434	1.253
5f ² 6d + 5f 6d7p	5/2	54494		54546	-52	1.438	57274	-2780	1.198
5f 6d7p	3/2	54922		54818	104	1.178	58868	-3946	1.102
5f 6d7p	3/2	56235		56241	-6	1.158	59107	-2872	0.884
5f ² 6d + 5f 6d7p	5/2	56391		56346	45	1.042	58037	-1646	1.446

TABLE IV. The values of the hyperfine-structure sublevels energy and relative positions of the line components for the transition $34\,543.556\text{ cm}^{-1} \rightarrow 17\,121.620\text{ cm}^{-1}$ (in MHz).

Energy level	F	ΔE_F	ΔE_F
34543.556 $J = 5/2$		Ground nuclear state $I = 5/2$	
	0	-3266.375	
	1	-2878.675	306.67
	2	-2111.375	216.51
	3	-980.675	43.77
	4	489.125	-256.55
17121.620 $J = 3/2$	5	2265.625	
	0		6.50
	1	2621.500	-155.90
	2	1393.500	-239.70
	3	-126.000	237.10
	4	-1550.000	
Transition	$F' - F$	Relative frequency	
		Ground nuclear state $I = 5/2$	Isomeric state $I = 3/2$
	1 - 0		6188.045
	0 - 1	0.0	
	1 - 1	387.7	6350.445
	2 - 1	1155.0	6260.285
	1 - 2	1615.7	6434.245
	2 - 2	2383.0	6344.085
	3 - 2	3513.7	6171.345
	2 - 3	3902.5	5867.285
	3 - 3	5033.2	5694.545
	3 - 4	6457.2	
	4 - 3	6503.0	5394.225
	4 - 4	7927.0	
	5 - 4	9703.5	

of the excited electronic state, being practically infinite from the perspective of the electron, the electron is affected by both values of nuclear magnetic moments $I = 5/2$ and $3/2$. The observed patterns should be similar in the case of two odd isotopes, without mass and charge distribution effects. In this case, we should construct the hyperfine-structure energy matrix both for the nuclear spin $I = 5/2$ and for $I = 3/2$ independently, on the basis of both nuclear states and all electronic states of the considered configuration system. As a result, we will obtain the predicted values of atomic energy levels, which will be eigenvalues obtained by means of those atomic wave functions.

In contrast to the method proposed by Beloy [34], we do not need to know the exact quantitative effect of the isomeric state on the hyperfine-structure intervals. What we need is to precisely specify the range of energy levels with the largest effect.

IV. SIMULATION OF THE HYPERFINE-STRUCTURE PATTERN

The effects of mixing of the wave functions for ground and isomeric nuclear states should be observed in the hyperfine-structure patterns of spectral lines. As an example, we present the simulation for the transition $34\,543.556\text{ cm}^{-1} \rightarrow 17\,121.620\text{ cm}^{-1}$ in Fig. 1. The values of the hyperfine constants were taken from the paper of Kälber *et al.* [2]. The

corresponding values for the isomeric state were calculated using the values of nuclear moments μ and Q equal to $0.45\mu_N$ [1], $3.11b$ [43] and $-0.08\mu_N$ [20], $1.74b$ [20] for the ground and the isomeric nuclear states, respectively. The same occupancy of the ground and the isomeric states was assumed.

The values of relative positions of hyperfine-structure sublevels and relative frequencies of the line components are presented in Table IV. The origin of the x axis is determined by the transitions between hyperfine-structure sublevels $F' = 0$ and $F = 1$ for the ground nuclear state. The solid lines show the intensities of the line components, for the ground nuclear state, for the transitions $F' = 0 \rightarrow F = 1$ at the beginning to $F' = 5 \rightarrow F = 4$ at the end of the x axis. For the isomeric state, the dashed lines illustrate the line components for transitions $F' = 0 \rightarrow F = 1$ and $F' = 3 \rightarrow F = 4$, respectively. Depending on the linewidth observed in the experiment, the existence of the isomeric state will be revealed in the middle of the hyperfine-structure pattern as broadening and distortion of the line components or as additional line components. Therefore, the hyperfine-structure constants derived from the observed spectral line shape will differ from those determined in the absence of nuclear isomeric state admixture.

Similar simulations can be easily performed for each $^{229}\text{Th}^+$ spectral line, which will be of interest. Additionally, in the case of precise laser rf double-resonance method in a Paul trap on the ground or metastable electronic levels, the effects

of the breakdown of I as a good quantum number should be observed as discrepancies between g_F values calculated and derived from Zeeman pattern. The possibility and accuracy of this method was demonstrated previously in the case of Eu^+ [44].

V. DETERMINATION OF THE NUCLEAR QUADRUPOLE MOMENT

The contributions from one-electron excitation to the observed hyperfine structure are commonly known as Sternheimer or pseudoquadrupole effects [33,45,46]. The way to determine these effects, on the basis of the experimental data and their precise definitions, for configuration system $(5d+6s)^3$ of the lanthanum atom, was presented in our work from 2010 [40]. The system of even configurations of Th^+ has a similar structure, however, there are only 10 known B electric quadrupole interaction constants, while in the lanthanum atom the constant values are known for all levels of $(6d+7s)^3$ configuration. For magnetic dipole interaction, there are known 11 A hyperfine-structure constants. These constants were measured for the levels belonging to six terms from the configuration system $(6d+7s)^N$. Thus, it was not sufficient to exclude all linear dependencies in both A and B equation systems of the many-body hyperfine-structure parametrization method. For this reason, additional assumptions from fine-structure analysis had to be included in our hfs-fitting procedure. Eigenvectors describing the states of the model space $(6d+7s)^N$ include contributions derived from the configuration with 7p and 5f electrons. Both the spin-orbit radial parameter ζ_{nl} and the one-body radial parameters describing the electric quadrupole interactions $b_{nl}^{\kappa k}$ are proportional to the radial integrals $\langle r^{-3} \rangle_{nl}^{\text{eff}}$, which are the relativistic radial integrals, as was shown by Lindgren [47], which can be calculated *ab initio* theoretically, and the radial parameters represented configuration interaction effects which reduced to one body [48], commonly named “core polarization effects” [33]. Therefore, the contribution from the 7p and 5f electrons to the B electric quadrupole constants were introduced by the relation $\zeta_{5f} : \zeta_{7p} : \zeta_{6d} = b_{5f}^{\text{O}2} : b_{7p}^{\text{O}2} : b_{6d}^{\text{O}2}$.

The values of the spin-orbit parameters can be precisely determined from the many-body fine-structure parametrization in the extended model space of 70 configurations. The effects of excitations of one electron from a closed shell to an open shell were taken into account by electrostatically correlated spin-orbit interaction (EL-SO). The operators of the electrostatically correlated spin-orbit interaction (EL-SO) and the electrostatically correlated hfs interaction (EL-HFS) have the same structure, hence, an analogy can be drawn between (EL-SO) and (EL-HFS). Due to the fact that they both contain one-electron operators $\mathbf{T}^{(\kappa k)K}$, (H_{SO}), exactly the same one-electron excitations are responsible for these second-order effects. Therefore, it is reasonable to parametrize the above effects analogously. As an important consequence of the described analogy, the following relations should be fulfilled:

$$\frac{D^t(n_0l_0nl, nlnl)\zeta_{n_0l_0, nl}}{\zeta_{nl}} \approx \frac{D^t(n_0l_0nl, nlnl)P^{\kappa k}(n_0l_0, nl)}{b_{nl}^{\kappa k}}, \quad (1)$$

where $t = 0, 2, 4$, $nl = 5f$ or $7p$ and $\kappa k = 01, 12$, and 02 . The radial parameters $D^t(n_0l_0nl, nlnl)\zeta_{n_0l_0, nl}$ and $D^t(n_0l_0nl, nlnl)P^{\kappa k}(n_0l_0, nl)$, corresponding to the electrostatically correlated spin-orbit interactions and electrostatically correlated hfs interactions, respectively, are detailed described in [39,40]. For $nl = 6d$, the above-mentioned effects were parametrized directly, without any preliminary assumptions.

In the fitting procedure $a_{nl}^{\kappa k}$ and $b_{nl}^{\kappa k}$ parameters are determined, the same for all aforesaid configurations. The respective one-body fs and hfs radial parameters include the contributions from one- and two-body interactions. The relations allowing elimination of those contributions and determination of the radial one-body parameters characteristic of the individual configurations $6d^3$, $6d^27s$, and $6d7s^2$, which form the model space $(6d+7s)^3$, for excitations “closed shell–open shell”(c–o), are as follows:

$$\begin{aligned} a_{6d}^{\text{O}1}(nd^N n' s^{N'}) &= a_{6d}^{\text{O}1}(c-o) + 2ND^0(n_0d6d, 6d6d)P^{\text{O}1}(n_0d, 6d) \\ &+ \frac{2}{7}D^2(n_0d6d, 6d6d)P^{\text{O}1}(n_0d, 6d) \\ &- \frac{8}{25}D^4(n_0d6d, 6d6d)P^{\text{O}1}(n_0d, 6d) \\ &- \frac{2}{5}E^2(n_0d7s, 7s6d)P^{\text{O}1}(n_0d, 6d)\delta(N', 2), \end{aligned} \quad (2)$$

$$\begin{aligned} b_{6d}^{\text{O}2}(nd^N n' s^{N'}) &= b_{6d}^{\text{O}2}(c-o) + 2ND^0(n_0d6d, 6d6d)P^{\text{O}2}(n_0d, 6d) \\ &- \frac{62}{49}D^2(n_0d6d, 6d6d)P^{\text{O}2}(n_0d, 6d) \\ &+ \frac{8}{49}D^4(n_0d6d, 6d6d)P^{\text{O}2}(n_0d, 6d) \\ &- \frac{2}{5}E^2(n_0d7s, 7s6d)P^{\text{O}2}(n_0d, 6d)\delta(N', 2). \end{aligned} \quad (3)$$

The method of quantitative determination of two-body contributions to the fine and the hyperfine structures, resulting from the excitations from electronic closed shells to open shells and from open shells to empty shells, which was presented in [40], can be used for the study of the thorium ion because it is different from the lanthanum atom only in the number of closed shells.

Applying the effective hfs parameters to Eqs. (2) and (3), one can calculate the values of $a_{6d}^{\text{O}1}$, $b_{6d}^{\text{O}2}$ for $6d^27s$ configuration and determine the nuclear quadrupole moment Q , which should be almost free from Sternheimer effects up to second order of perturbation theory:

$$Q = \frac{2\mu_B g_I}{e^2} \frac{b_{6d}^{\text{O}2}}{a_{6d}^{\text{O}1}} = (2.87 \pm 0.66)b, \quad (4)$$

where g_I is the nuclear g_I factor expressed in nuclear magnetons, for the ^{229}Th nucleus $g_I = +0.18$ [1]; the values of the parameter $a_{6d}^{\text{O}1} = 107(16)$ and $b_{6d}^{\text{O}2} = 4197(55)$ are given in MHz.

This value is consistent with the values reported by Bemis *et al.* (3.149 ± 0.032) [49] and Campbell *et al.* (3.11 ± 0.16) [43] and additionally should be consistent with the value obtained from measurements on the muonic atom, if they had been carried out.

VI. CONCLUSIONS

We hope to be able to carry out the experiments discussed above, perhaps in cooperation with other groups. Our procedures allow for effective interactions between the calculations and the experiment. All experimental data improve calculated predictions and this update can be achieved in the short period of time. Similar procedures can also be applied to the odd system Th^+ , as well as to both odd and even systems of neutral Th, if the sufficient amount of the experimental data is available.

The accuracy of hfs constants for Th II available so far is very poor [1,2]. Therefore, our hfs predictions contain the error of the same order of magnitude. New measurements carried out with better accuracy will enable a precise determination of all the one- and two-body contributions to the hyperfine-structure splittings and enhance our semiempirical predictions.

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