Energies, transition rates, and electron electric-dipole-moment enhancement factors for Ce IV and Pr V

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Energies, transition rates, and electron electric-dipole-moment (EDM) enhancement factors are calculated for low-lying states of Ce IV and Pr V using relativistic many-body perturbation theory. This study is related to recent investigations of the more complicated Gd IV ion, which is promising for electron EDM experiments. The ions Ce IV and Pr V both have a single valence electron, permitting one to carry out reliable *ab initio* calculations of energy levels, transition rates, and other atomic properties using well-developed computational methods.

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I. INTRODUCTION

Recently, searches for an electron electric-dipole-moment (EDM) in atoms and molecules have gained considerable interest. Since an electron EDM violates time-reversal symmetry and parity, the discovery of an EDM would have many implications for modern fundamental theories (a general overview is given by Khriplovich and Lamoreaux [1]). The best limit on the value of the electron EDM was obtained by Regan *et al.* [2] in Tl, $d_e < 1.6\times 10^{-27}$ e cm. Although there is a large enhancement ($\sim$600) of the electron EDM in Tl, the density of atoms in a beam is much lower than in a solid-state system. To utilize the advantage of high densities, it has been proposed to use gadolinium gallium garnet $Gd_3Ga_5O_{12}$ or gadolinium iron garnet $Gd_3Fe_5O_{12}$ (densities $\sim 10^{22}/\mathrm{cm}^3$) in EDM experiments [3,4]. There are various features of these materials that make them particularly useful for such experiments. For example, magnetoelectric effects are forbidden owing to the face centered cubic symmetry of the crystals, simplifying the exclusion of systematics; the crystal $Gd_3Fe_5O_{12}$ has a very high resistivity ($\geqslant 10^{16}$ Ω cm); and spin alignment is relatively easy. The electron EDM enhancement for the Gd^{3+} ion ($\sim 2-3$) is much smaller than for Tl; nevertheless, there is a substantial gain in the number of atoms.

Motivated by proposed EDM measurements, calculations of EDM enhancement have been performed recently [5,6]. Core-polarization effects in Gd IV were discussed by Dzuba *et al.* [7] and found to decrease the size of the EDM enhancement factor from -3.3 to -2.2. Thus, there is a strong sensitivity of the EDM enhancement to many-body effects and further investigation is necessary.

The ion Gd^{+3}, which has a $4f^7$ ground-state configuration is extremely complicated and difficult for atomic theory, though some understanding was gained by Dzuba *et al.* [7] using a relativistic configuration-interaction (RCI) method and the widely used Cowan [8] code. As mentioned above, core polarization was found to be substantial. For example, to match the experimental $4f \rightarrow 5d$ transition energies, scaling factors of 0.8 and 0.85 for Coulomb integrals were used in the RCI and Cowan codes, respectively. In addition, a polarization potential was introduced in the RCI code to match experimental energies and a systematic energy shift of $\sim$18 000 cm^{-1} was made in the Cowan code. This shift can be attributed to core polarization by a single valence electron. An *ab initio* investigation of correlation should help to understand these empirical adjustments. The simplest ions (those having a single $4f$ valence electron) which exhibit core-polarization effects similar to Gd IV are Ce IV and Pr V. To gain a clearer understanding of the role of core polarization and other many-body effects in Ce IV and Pr V, we calculate energies, dipole transition matrix elements, and EDM enhancement factors for low-lying states using relativistic many-body perturbation theory (MBPT).

The present calculations of energies are carried out to third order in MBPT using the methods developed earlier to study the Li, Na, and Cu isoelectronic sequences [9–11]. The calculations of transition matrix elements are also carried out to third order in MBPT using the methods developed in Ref. [12] to treat the alkali-metal atoms and alkalilike ions. Here, we use the gauge-independent version of the third-order MBPT code described in Ref. [13]. The calculations of electron EDM enhancement factors, which involve a sum over intermediate states, are carried out in the random-phase approximation (RPA) following a procedure similar to that described in Ref. [14].

It should be mentioned that Ce^{+3}, which has a $4f_{5/2}$ ground state and an observed magnetic moment (2.3–2.5) μ_B can be embedded into garnet crystals and used in EDM experiments of the type proposed in Ref. [3]. In those experiments, a strong electric field polarizes ions which in turn produce a small magnetic field that is measured in a sensitive SQUID detector. The magnetic field at

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TABLE I. First-order (DHF) energies $E^{(1)}$, second- and third-order Coulomb energies $E^{(2)}$ and $E^{(3)}$, first- and second-order Breit corrections $B^{(1)}$ and $B^{(2)}$, and totals $E_{\rm tot}$ for Ce IV and Pr V are compared with energies $E_{\rm NIST}$ given by Martin *et al.* [15]. Units, cm^{-1}.

nlj	$E^{(1)}$	$B^{(1)}$	$E^{(2)}$	$B^{(2)}$	$E^{(3)}$	$E_{\rm tot}$	$E_{\rm NIST}$	δE
				Ce IV				
$4f_{5/2}$	−261361	616	−46747	−2552	15672	−294372	−296470	2098
$4f_{7/2}$	−259378	423	−46091	−2511	15398	−292158	−294217	2059
$5d_{3/2}$	−236793	292	−13516	−545	3753	−246809	−246733	−76
$5d_{5/2}$	−234637	220	−12957	−528	3675	−244226	−244244	18
$6s_{1/2}$	−203245	168	−10201	−200	3680	−209794	−209868	70
$6p_{1/2}$	−168978	167	−7283	−127	2329	−173891	−173885	−6
$6p_{3/2}$	−164703	120	−6648	−122	2118	−169236	−169178	−58
$6d_{3/2}$	−116268	67	−3989	−106	997	−119300	−119272	−28
$6d_{5/2}$	−115581	51	−3922	−106	977	−118580	−117557	−1024
$7s_{1/2}$	−110878	65	−3601	−74	1293	−113196	−112968	−226
				Pr V				
$4f_{5/2}$	−431686	798	−48799	−3008	16527	−466167	−464000	−2167
$4f_{7/2}$	−428863	551	−48175	−2965	16270	−463182	−460973	−2209
$5d_{3/2}$	−341470	395	−14968	−669	4088	−352624	−348948	−3676
$5d_{5/2}$	−338314	298	−14386	−651	3827	−349225	−345486	−3739
$6s_{1/2}$	−281133	225	−11649	−247	4241	−288563	−285029	−3535
$6p_{1/2}$	−239154	239	−9136	−169	2451	−245769	−240522	−5247
$6p_{3/2}$	−233035	171	−8489	−163	2040	−239477	−233961	−5516
$6d_{3/2}$	−171610	98	−5746	−141	792	−176576		
$6d_{5/2}$	−170572	75	−5647	−141	771	−175481		
$7s_{1/2}$	−156266	92	−4489	−97	1329	−161431	−159489	−1942

low temperatures is proportional to the product of the electric-dipole moment of the ion and its magnetic moment. The estimated EDM of Gd^{3+} is a factor of about 3 larger than for Ce^{3+} and the magnetic moment of Gd^{3+} [(7.9–8.0) μ_B] is also about three times larger; therefore, there is an overall advantage of nine in Gd^{3+} compared to Ce^{3+}. Nevertheless, the Ce^{3+} ion could still compete in setting experimental limits on the electron EDM owing to the fact that its ionic EDM has a significantly smaller theoretical uncertainty.

II. CALCULATION OF ENERGIES

First-, second-, and third-order Coulomb energies $E^{(n)}$, $n=1,\ 2,$ and 3, and first- and second-order Breit energies $B^{(n)}$, $n=1,2$, calculated using methods described in Refs. [9–11], are presented in Table I along with the resultant theoretical energies $E_{\rm tot}$ and values from the National Institute of Standards and Technology (NIST) $E_{\rm NIST}$ given by Martin *et al.* [15]. We see that second-order corrections are large and improve the accuracy of the first-order Dirac-Hartree-Fock (DHF) energies. Third-order MBPT further improves the ground-state energy. However, the third-order correction is relatively large (roughly one-third of the second order) and overshoots the experimental value, which indicates that oscillations in higher orders are likely. Using a geometric progression with $q=-1/3$ we can extrapolate the second- and third-order values to give a limiting ground-state energy $-296\,420$ cm^{-1} for Ce^{3+}, in close agreement with the value from [15]. The corresponding extrapolation for Pr^{4+} gives $-468\,290$ cm^{-1} differing from the ground-state energy given in [15] by about 4000 cm^{-1}. This rather large difference casts doubt on the threshold energy of Pr V predicted in Ref. [15] and explains the large differences with the NIST energies seen in lower half of Table I.

In Refs. [9–11], where the ionic ground-states were $2s$, $3s$, and $4s$, respectively, the third-order correction was uniformly much smaller than the second-order correction. The relatively large size of the third-order corrections in Ce IV and Pr V arises because of the double-well feature of the $4f$ Coulomb potential discussed, for example, by Cheng and Froese-Fischer [16].

III. CALCULATION OF TRANSITION MATRIX ELEMENTS AND TRANSITION RATES

Transition matrix elements provide another test of quality of atomic-structure calculations and another measure of the size of correlation corrections. Third-order MBPT reduced matrix elements for transitions between low-lying states of Ce^{3+} and Pr^{4+} are presented in Table II. The first-order reduced matrix elements $Z^{(1)}$ are obtained from length-form DHF calculations. Length-form and velocity-form matrix elements differ typically by 10%. Second-order matrix elements in the table, $Z^{(2)}$, which include $Z^{(1)}$, are extended to

TABLE II. Reduced matrix elements of the dipole operator in first-, second-, and third-order perturbation theory for transitions in Ce IV and Pr V.

	Ce IV			Pr V		
Transition	$Z^{(1)}$	$Z^{(2)}$	$Z^{(3)}$	$Z^{(1)}$	$Z^{(2)}$	$Z^{(3)}$
$4f_{5/2}\rightarrow 5d_{3/2}$	1.498	0.972	1.172	1.146	0.678	0.706
$4f_{5/2}\rightarrow 5d_{5/2}$	0.396	0.264	0.308	0.302	0.186	0.189
$4f_{7/2}\rightarrow 5d_{5/2}$	1.799	1.193	1.413	1.370	0.828	0.852
$5d_{3/2}\rightarrow 6p_{1/2}$	1.976	1.768	1.682	1.648	1.471	1.396
$5d_{3/2}\rightarrow 6p_{3/2}$	8.363	0.756	0.719	0.690	0.625	0.592
$5d_{5/2}\rightarrow 6p_{3/2}$	2.585	2.352	2.229	2.140	1.950	1.837
$6s_{1/2}\rightarrow 6p_{1/2}$	2.847	2.482	2.402	2.560	2.207	2.136
$6s_{1/2}\rightarrow 6p_{3/2}$	4.012	3.512	3.401	3.609	3.125	3.020

include all higher-order corrections associated with the random-phase approximation. These second-order calculations are practically gauge independent. In the present calculations, length- and velocity-form matrix elements in the RPA agree to six or more digits. The third-order matrix elements $Z^{(3)}$ include $Z^{(2)}$ plus Brueckner-orbital (BO), structural radiation, and normalization corrections described, for example, in Ref. [12]. These calculations are carried out in a gauge-independent manner, including appropriate derivative terms, as described in Ref. [13]. We truncated our basis set to include only those partial waves with $l\leqslant 8$, and found that length- and velocity-form third-order reduced matrix elements agreed to four digits.

As can be seen in Table II, RPA corrections are very large, 10–40 %, being largest for $4f\rightarrow 5d$ transitions, and must be taken into account. Such behavior can be attributed to core shielding which is substantial, because valence electrons penetrate deeply into the core. Third-order corrections are smaller, 2–4 % scaling as $1/Z_{\rm ion}$. If such scaling holds in higher orders, we can estimate the accuracy of our calculations to be 0.4–0.8%. The dominant contribution in third order comes from the BO correction which is approximately equal to the sum of the other third-order corrections.

Transition rates A (s^{-1}), oscillator strengths f, and wavelengths λ (nm) for electric-dipole transitions between low-lying states of Ce IV and Pr V are given in Table III. These data are calculated using the dipole matrix elements $Z^{(3)}$ from Table II and NIST transition energies [15]. In the two final columns of Table III, we compare our MBPT wavelengths with the wavelengths from Ref. [15]. We also compare our MBPT oscillator strengths with theoretical oscillator strengths obtained by Migdalek and Wyrozumska [17]. The data in Ref. [17] were obtained using a relativistic model potential (RMP) approach together with a core-polarization (CP) model potential. Our data and that from Ref. [17] agree well for the $5d$-$6p$ and $6s$-$6p$ transitions but differ for the $4f$-$5d$ transition, where f values are very small.

TABLE III. MBPT transition rates A (s^{-1}), oscillator strengths f, and wavelengths λ (nm) for transitions in Ce IV and Pr V. MBPT oscillator strengths are compared with theoretical calculations performed in Ref. [17]. MBPT wavelengths are compared with wavelengths from NIST [15]. Numbers in square brackets represent powers of 10.

Transitions	A [a]	f [a]	f [b]	λ [a]	λ [c]
			Ce IV		
$4f_{5/2}\rightarrow 5d_{3/2}$	8.56[7]	0.0346	0.0159	210.2	201.1
$4f_{5/2}\rightarrow 5d_{5/2}$	4.56[6]	0.0025	0.0013	199.4	191.5
$4f_{7/2}\rightarrow 5d_{5/2}$	8.41[7]	0.0379	0.0186	208.6	200.1
$5d_{3/2}\rightarrow 6p_{1/2}$	1.11[9]	0.157	0.158	137.1	137.3
$5d_{3/2}\rightarrow 6p_{3/2}$	1.22[8]	0.0304	0.0206	128.9	128.9
$5d_{5/2}\rightarrow 6p_{3/2}$	1.06[9]	0.189	0.189	133.4	133.2
$6s_{1/2}\rightarrow 6p_{1/2}$	2.72[8]	0.315	0.327	278.5	277.9
$6s_{1/2}\rightarrow 6p_{3/2}$	3.95[8]	0.715	0.745	246.5	245.8
			Pr V		
$4f_{5/2}\rightarrow 5d_{3/2}$	3.85[8]	0.0290	0.0318	88.1	86.9
$4f_{5/2}\rightarrow 5d_{5/2}$	2.01[7]	0.0021	0.0019	86.3	84.4
$4f_{7/2}\rightarrow 5d_{5/2}$	3.78[8]	0.0318	0.0285	87.8	86.6
$5d_{3/2}\rightarrow 6p_{1/2}$	2.52[9]	0.161	0.165	93.6	92.2
$5d_{3/2}\rightarrow 6p_{3/2}$	2.70[8]	0.0306	0.0311	88.4	87.0
$5d_{5/2}\rightarrow 6p_{3/2}$	2.37[9]	0.191	0.193	91.1	89.7
$6s_{1/2}\rightarrow 6p_{1/2}$	4.07[8]	0.308	0.321	233.7	224.7
$6s_{1/2}\rightarrow 6p_{3/2}$	6.15[9]	0.707	0.746	203.7	195.8

[a]Present MBPT calculations.
[b]Theoretical calculations performed in Ref. [17].
[c]NIST database [15].

IV. EDM ENHANCEMENT

A. Basic equations

According to Schiff's theorem [18], the electric-dipole moment of an atom induced by an intrinsic electron EDM vanishes in the nonrelativistic limit; however, as shown by Sandars [19], the atomic EDM is nonvanishing relativistically and can be a large multiple of the intrinsic electron moment for heavy atoms. If we assume that the electron has an intrinsic EDM d_e, then the EDM of a many-electron atom D may be written [14] as

$$D=2\sum_n \frac{\langle v j_v|eZ|n\rangle\langle n|H_{\rm EDM}|v j_v\rangle}{E_v-E_n}, \tag{1}$$

where eZ is the electric-dipole operator

$$eZ=\sum_i ez_i ,$$

and $H_{\rm EDM}$ is an equivalent EDM interaction [14] given by

$$H_{\rm edm}=-2i\frac{d_e}{e}c\sum_j p_j^2\beta_j(\gamma_5)_j=H^{\dagger}_{\rm EDM}.$$

This equivalent interaction, which automatically accounts for Schiff's theorem, is rotationally invariant and therefore conserves angular momentum; it violates both parity and time-reversal symmetry.

For an atom or ion with one valence electron, one-electron matrix elements of $H_{\rm EDM}$ may be written in lowest order as

$$\langle nj_n|H_{\rm EDM}|vj_v\rangle = \delta_{\kappa_n-\kappa_v}\delta_{j_nj_v}\langle n\|H_{\rm EDM}\|v\rangle, \qquad (2)$$

where the (somewhat unconventional) reduced matrix element is

$$\langle n\|H_{\rm EDM}\|v\rangle = 2c\frac{d_e}{e}\int_0^\infty dr\left[G_n(r)\frac{d^2F_v}{dr^2} - \frac{\kappa_v(\kappa_v-1)}{r^2}G_n(r)F_v(r) + F_n(r)\frac{d^2G_v}{dr^2} - \frac{\kappa_v(\kappa_v+1)}{r^2}F_n(r)G_v(r)\right].$$

In the above equation, $G_k(r)$ and $F_k(r)$ are the large and small components, respectively, of radial Dirac wave functions. Similarly, we may write

$$\langle vj_v|eZ|nj_v\rangle = \sqrt{\frac{j_v}{(2j_v+1)(j_v+1)}}\langle v\|eZ\|n\rangle \qquad (3)$$

with

$$\langle v\|eZ\|n\rangle = e\langle\kappa_v\|C_1\|-\kappa_v\rangle\times\int_0^\infty r\,dr[G_v(r)G_n(r) + F_v(r)F_n(r)],$$

$C_{1q}(\hat{r})$ being a normalized spherical harmonic. The expression for the atomic dipole moment in lowest-order MBPT then reduces to

$$D^{(1)} = 2\sqrt{\frac{j_v}{(2j_v+1)(j_v+1)}}\sum_i \frac{\langle v\|eZ\|i\rangle\langle i\|H_{\rm EDM}\|v\rangle}{\epsilon_v-\epsilon_i}, \qquad (4)$$

where ϵ_k are eigenvalues of the valence-electron Dirac equation.

B. RPA correlation corrections

Lowest-order calculations of the induced atomic EDM are carried out in a frozen-core V^{N-1} DHF potential. Such calculations were shown in Ref. [14] to be very sensitive to correlation corrections. For that reason, the lowest-order "bare" matrix elements in Eq. (4) are replaced by "dressed" RPA matrix elements.

1. Z-RPA

Thus, we replace the lowest-order dipole matrix element $\langle w||Z||v\rangle$ in Eq. (4) by

$$\langle w||Z^{\rm RPA}||v\rangle = \langle w||Z||v\rangle + \sum_{an}(-1)^{j_a-j_n+1}\frac{1}{3}\frac{\langle a||Z^{\rm RPA}||n\rangle Z_1(wnva)}{\epsilon_a-\epsilon_n} + \sum_{an}(-1)^{j_a-j_n+1}\frac{1}{3}\frac{Z_1(wavn)\langle n||Z^{\rm RPA}||a\rangle}{\epsilon_a-\epsilon_n}, \qquad (5)$$

where the index a extends over all core orbitals and the index n extends over all virtual orbitals permitted by angular-momentum selection rules. The quantities $Z_J(ijkl)$ are Coulomb integrals

$$Z_J(ijkl) = X_J(ijkl) + [J]\sum_L \begin{Bmatrix} i & k & J \\ j & l & L \end{Bmatrix} X_L(ijlk), \qquad (6)$$

where $X_J(ijkl)$ are defined by

$$X_J(ijkl) = (-1)^J\langle i\|C_J\|k\rangle\langle j\|C_J\|l\rangle R_J(ijkl),$$

$R_J(ijkl)$ being a Slater integral

$$R_J(ijkl) = \int_0^\infty\int_0^\infty dr\,dr'\frac{r_<^J}{r_>^{J+1}}[G_i(r)G_k(r)+F_i(r)F_k(r)] \times[G_j(r')G_l(r')+F_j(r')F_l(r')].$$

We designate the corresponding approximation to the atomic EDM by $D_Z^{\rm RPA}$. Note that if we replace $\langle n||Z^{\rm RPA}||a\rangle$ by $\langle n||Z||a\rangle$ on the right-hand side of Eq. (5), then we obtain the second-order correlation correction to the valence-excited dipole matrix element. The atomic EDM calculated in this approximation is designated by $D_Z^{(2)}$.

2. H-RPA

Similarly, we replace the bare matrix element of the EDM interaction $\langle w\|H_{\rm EDM}\|v\rangle$ by its dressed counterpart

$$\langle w||H_{\rm EDM}^{\rm RPA}||v\rangle = \langle w||H_{\rm EDM}||v\rangle + \sum_{an}\sqrt{\frac{[j_a]}{[j_v]}}\frac{\langle a||H_{\rm EDM}^{\rm RPA}||n\rangle Z_0(wnva)}{\epsilon_a-\epsilon_n} + \sum_{an}\sqrt{\frac{[j_a]}{[j_v]}}\frac{Z_0(wavn)\langle n||H_{\rm EDM}^{\rm RPA}||a\rangle}{\epsilon_a-\epsilon_n}. \qquad (7)$$

We designate the approximation to D obtained using the dressed matrix element from Eq. (7) by $D_H^{\rm RPA}$. Again, if we replace dressed matrix elements by bare matrix elements on the right hand side of Eq. (7), we obtain a second-order approximation to $\langle w||H_{\rm EDM}||v\rangle$. The resulting correction to the atomic EDM is designated by $D_H^{(2)}$.

Core-excited matrix elements $\langle n||Z^{\rm RPA}||a\rangle$ and $\langle n||H_{\rm EDM}^{\rm RPA}||a\rangle$ in Eqs. (5) and (7) satisfy sets of coupled equations given explicitly in Ref. [12].

TABLE IV. Comparison of first-order, second-order, and RPA calculations of the atomic EDM enhancement factor D/d_e for $4f$ states of Ce IV.

State	$D^{(1)}$	$\Delta D_H^{(2)}$	$\Delta D_Z^{(2)}$	$D^{(2)}$	$\Delta D_H^{\mathrm{RPA}}$	$\Delta D_Z^{\mathrm{RPA}}$	D^{RPA}
$4f_{5/2}$	-0.382	-0.388	0.332	-0.438	-0.785	0.387	-0.780
$4f_{7/2}$	-0.002	-0.033	0.022	-0.013	-0.045	0.015	-0.032

C. Calculations of EDM enhancement factors

The sums over intermediate states in Eqs. (4)–(7) are carried out using basis functions obtained as linear combinations of B splines as described in Ref. [20]. We use 40 splines of order 7 and constrain the ions to lie in a cavity of radius $R=35$ a.u. for Ce^{3+} and 30 a.u. for Pr^{4+}.

A detailed breakdown of the contributions to D for $4f$ states of Ce IV is given in Table IV, where we list the DHF approximation $D^{(1)}$, the second-order correction $D^{(2)}$, the RPA approximation D^{RPA}, and the individual contributions to the second-order and RPA corrections from the dipole and weak-interaction matrix elements. One can see from the table that the correlation corrections to the weak-interaction matrix element are comparable to or larger than the lowest-order matrix element. Moreover, there are significant changes in these correlation corrections going from second-order MBPT to full RPA calculations.

Finally, in Table V, we present DHF and RPA values of the EDM enhancement factors D/d_e for the low-lying $4f$, $5d$, $6s$, and $6p$ states of Ce IV and Pr V.

V. CONCLUSION

We have studied energies, transition probabilities, and EDM enhancement factors for Ce^{3+} and Pr^{4+}. We found that perturbation theory converges quite slowly and that RPA corrections are the dominant correlation corrections for transitions. We use our third-order MBPT with ‘‘dressed’’ matrix elements to obtain accurate transition rates. The most interesting discovery is that RPA corrections modify lowest-order values of the EDM enhancement factor significantly.

TABLE V. EDM enhancement factors D/d_e for low-lying states of Ce IV and Pr V.

State	$D^{(1)}$	$\Delta D_H^{\mathrm{RPA}}$	$\Delta D_Z^{\mathrm{RPA}}$	D^{RPA}
		Ce IV		
$4f_{5/2}$	-0.382	-0.785	0.387	-0.780
$4f_{7/2}$	-0.00225	-0.0451	0.0151	-0.0323
$5d_{3/2}$	-1.95	-3.38	0.779	-4.55
$5d_{5/2}$	0.425	-0.347	-0.136	-0.0628
$6s_{1/2}$	120	27.5	-19.8	128
$6p_{1/2}$	-158	-30.9	19.8	-169
$6p_{3/2}$	2.89	7.24	-1.07	9.06
		Pr V		
$4f_{5/2}$	-0.142	-0.0806	0.0926	-0.130
$4f_{7/2}$	-0.00266	-0.00444	-0.000912	-0.00802
$5d_{3/2}$	-1.80	-2.91	0.655	-4.05
$5d_{5/2}$	0.174	-0.827	0.125	-0.528
$6s_{1/2}$	127	27.3	-22.2	132
$6p_{1/2}$	-157	-30.0	21.7	-166
$6p_{3/2}$	2.78	6.06	-1.01	7.83

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