Alkaline earthlike spectra in highly ionized members of the Sm isoelectronic sequence

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Energies and radiative transition probabilities have been computed for the $5s^2$ 1S_0 –5s5p $^{1.3}P_J$ intervals in highly ionized members of the 62 electron samarium isoelectronic sequence by using ab initio multiconfiguration Dirac–Fock methods. For Z > 74 these become the lowest-lying levels, and the ion assumes an alkaline earthlike structure. Excitation energies and E1, M1, E2, and M2 transition probabilities for the 5s5p levels are reported for the ions Re⁺¹³ through U⁺³⁰. Isoelectronic trends in the relative spacings of the 5s5p levels were also investigated by using semiempirical screening parameterizations of the intermediate coupling equations for the spin–orbit and exchange energies. These trends are compared with systematic regularities noted earlier in the homologous Be, Mg, Zn, and Cd sequences, and possibilities for precise extrapolative predictions are examined.

INTRODUCTION

Highly ionized atomic systems consisting of one or two valence electrons outside a tightly bound core have been the object of much recent study because of their applications to controlled fusion devices containing heavy-metal contaminants. The low-excitation potentials and high oscillator strengths of intrashell transitions in these systems can lead to high radiative energy losses; atomic data are necessary for both diagnostic interpretation and dynamical modeling. For the two-valence electron systems, the resonance and spin intercombination ns^2 -nsnp transitions and the intraterm M1 and E2 transitions within the nsnp configuration can be useful as diagnostic probes. These transitions become stronger at high ionicity and are often identifiably isolated in a conveniently detectable wavelength region.

For sufficiently high stages of ionization, the 62 electron Sm isoelectronic sequence acquires an alkaline earthlike structure characterized by two electrons outside a core that is filled to the n=4 shell. In this limit the system becomes shell homologous to the Be, Mg, and Zn sequences, with ground and first-excited configurations ns^2 and nsnp. The system is also an isoelectronic converse to the Cd sequence, which, in contrast to the Sm sequence, loses its n=5 shell alkaline earthlike character for sufficiently high stages of ionization.

Theoretical studies of the corresponding alkalilike 61 electron systems in highly ionized members of the Pm isoelectronic sequence have been done. La Experimental searches for the strong resonance lines predicted have been made 50 by using fast ion beam-foil excitation, and a tentative identification of the promethiumlike resonance doublet in Au⁺¹⁸ has been reported. Alkaline earthlike transitions in corresponding members of the Sm sequence should appear in the same spectral region and could be studied simultaneously in the same experiments. This paper presents the first known theoretical calculations of energy levels and transition probabilities of alkaline earthlike systems in highly ionized members of the Sm isoelectronic sequence.

In studies of the Li,⁶ Na,⁷ and Cu (Ref. 8) alkalilike systems and the Be,⁹ Mg,¹⁰ Zn,¹¹ and Cd (Ref. 12) alkaline earthlike systems, it has been found that semiempirical regularities permit extrapolative and interpolative predictions of accuracy greatly superior to those attainable with current available *ab initio* methods. In order to investigate the applicability of these methods to the Sm sequence, the theoretical calculations reported herein were treated as simulated data and were subjected to the same screening parameter systematizations as were used for experimental results in the lower homologous sequences. These expositions provide criteria useful in selecting among theoretical options and suggest methods for incorporating *ab initio* calculations into extrapolative semiempirical predictions.

THEORETICAL CALCULATIONS

The *ab initio* multiconfiguration Dirac–Fock calculations were carried out through network on the National Magnetic Fusion Center CRAY X-MP E computer and on the University of Toledo NAS 6650 and VAX 785 computers. Several theoretical codes were used, including the program of Desclaux, ¹³ version 2¹⁴ of the program developed by Grant and co-workers, ¹⁵ and a Hartree–Slater utility code. ¹⁶ The results quoted were obtained primarily by using the program of Grant, ^{14,15} and the other codes were used to test for consistency.

Calculations were performed by using both single-configuration (SCDF) and multiconfiguration (MCDF) Dirac–Fock methods. The multiconfiguration calculations were carried out by using the MCDF-AL (average level), the MCDF-EAL (extended average level), and the MCDF-OL (optimal level) options. These various calculations were compared and selected for presentation with the aid of the screening parameter systematizations. To obtain convergence, the calculations were begun at an unphysically high value of the nuclear charge (Z=99) and successively stepped to lower Z by using the preceding wave functions as starting values.

The MCDF calculations assumed a closed 46-electron Pd core (filled to 4d), with the configurations $4f^{14}5s^2$, $4f^{14}5s^5p$, $4f^{13}5s^25p$, and $4f^{13}5s^5p^2$ included in the calculation. Perturbative corrections were included to account for the finite size of the nucleus and the Breit interaction as well as vacuum polarization, electron self-energy, and other quantum electrodynamic effects.

The angular momentum coupling for the 5s5p levels is intermediate to the LS and the jj coupling limits. Therefore a spin-neutral notation iP_J will be adopted here for identifying the four levels in the 5s5p configuration, which traces them from the LS to the jj limit:

$${}^{T}P_{1} \equiv {}^{1}P_{1} \rightarrow \left(\frac{1}{2}, \frac{3}{2}\right)_{1},$$
 (1)

$${}^{T}P_{2} \equiv {}^{3}P_{2} \rightarrow \left(\frac{1}{2}, \frac{3}{2}\right)_{2},$$
 (2)

$${}^{B}P_{1} \equiv {}^{3}P_{1} \rightarrow \left(\frac{1}{2}, \frac{1}{2}\right)_{1},$$
 (3)

$${}^{B}P_{0} \equiv {}^{3}P_{0} \rightarrow \left(\frac{1}{2}, \frac{1}{2}\right)_{0}.$$
 (4)

Here the spin designation of the LS notation has been replaced by i = T or i = B, denoting the higher or lower (top or bottom) doublet in the jj notation.

The TP_1 and BP_1 levels decay dominantly through spinmixed E1 transitions to the 1S_0 ground state (known in alkaline earthlike spectroscopy as the resonance and intercombination lines). The BP_0 level cannot (in the absence of hyperfine quenching) decay radiatively, since the only energetically accessible transition would be to the ground level, which is absolutely forbidden by the $J=0 \not\rightarrow J=0$ selection rule. The TP_2 level has no E1 decay channels and decays through intraconfiguration M1 and E2 transitions and M2 transitions to the ground state. MCDF calculations were made for these processes. E1 transition probabilities were computed by using both the Coulomb and the Babushkin gauges. Armstrong et al. 18 have suggested that the Babushkin gauge is less suitable for nonrealitivistic comparisons, and the Coulomb gauge results were selected for tabulation.

SCREENING PARAMETER FORMULATION

Earlier studies $^{10-12}$ in alkaline earthlike systems have shown that the relative spacing of energy levels within an nsnp configuration can be described accurately by a screening parameterization of the intermediate coupling equations (Ref. 19, p. 111). Specification of the relative positions of the four levels in Eqs. (1)-(4) requires three independent parameters, but the intermediate coupling equations involve only two quantities, the spin-orbit energy 5 and the Slater exchange energy G_1 . To provide a complete specification by removing the constraint of exact validity of the intermediate coupling equations, two independent exchange energies G_{1T} and G_{1B} were defined, corresponding to the T and B indices on the levels. Thus, the three independent relative spacings of the levels can be mapped into corresponding values for the three quantities ξ , G_{1T} and G_{1B} through the inversion of the equations¹⁹:

$${}^{T}P_{1} = E_{0} + [(G_{1T} + \zeta/4)^{2} + \zeta^{2}/2]^{1/2},$$
 (5)

$${}^{T}P_{2} = E_{0} - G_{1T} + 3\zeta/4, \tag{6}$$

$${}^{B}P_{1} = E_{0} - [(G_{1B} + \zeta/4)^{2} + \zeta^{2}/2]^{1/2},$$
 (7)

$${}^{B}P_{0} = E_{0} - G_{1B} - 3\zeta/4. \tag{8}$$

The quantity E_0 (the centroid of the J=1 levels in the limit $G_{1T}=G_{1B}$) is eliminated when relative spacings are considered but is useful in characterizing the degree of the intermediate coupling.

In terms of the quantities in Eqs. (5)–(8), the spacing of the levels can be described graphically by an intermediate coupling diagram (Ref. 19, p. 113), in which an ordinate and an abscissa are defined:

$$y = ({}^{i}P_{J} - E_{0})/(G_{1i} + 3\zeta/4),$$
 (9)

$$x = (3\zeta/4)/(G_{1i} + 3\zeta/4). \tag{10}$$

A plot of y versus x is given in Fig. 1 and traces the general locus of nsnp levels as the coupling scheme moves from the pure LS limit (x=0) to the pure jj limit (x=1). This formulation is a slight extension of that in Ref. 19, since separate values for G_1 are defined for the upper and lower pairs of levels. When data for a given ion are reduced, these definitions produce a slight offset in the value of x determined through the various pairs of levels. A reduction of the theoretical calculations reported here is indicated by the vertical lines in Fig. 1 and illustrates this offset. This exposition will be discussed further in the section entitled Results.

In previous experimental studies of alkaline earthlike systems, it has been found that the spin-orbit and exchange energies can be described by screened hydrogenic expressions for the corresponding quantities. As in earlier studies, $^{10-12}$ a screened Sommerfeld-Dirac expansion is used to parameterize ζ :

$$\zeta = R\alpha^2 (Z - S_c)^4 / 3n^2 + \text{higher order.}$$
 (11)

Here R is the reduced-mass-corrected Rydberg constant, α is

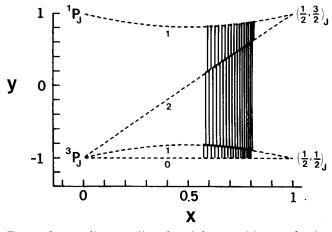


Fig. 1. Intermediate coupling plot of the quantities y and x (as defined in Eqs. (9) and (10) for the 5s5p levels. The dashed lines trace the locus of the general nsnp levels from pure LS (x=0) to pure jj (x=1) coupling. The vertical lines represent the calculations reported here and have a horizontal offset at each locus because of the extended definition of G_1 .

the fine-structure constant, Z is the nuclear charge, and S_{ζ} denotes the empirical screening parameter that Eq. (11) serves to define. The higher-order terms in Eq. (11) include additional contributions to the Dirac energy²⁰ and radiative corrections.²¹

The exchange Slater energy can be parameterized by using the expression for the corresponding quantity calculated by using screened hydrogenlike wave functions. It can be shown¹² that, assuming the same screening parameter S_{Gi} for the s and p electrons, the hydrogenic expression is given by

$$G_{1i} = C(nsnp)R(Z - S_{Gi}), \tag{12}$$

where C(nsnp) is a known¹² rational fraction. To within seven-figure accuracy, C(5s5p) = 0.010568848.

The three independent energy intervals, already reexpressed as the three intermediate coupling parameters, can now be further reexpressed as the three screening parameters S_{\S} , S_{GT} , and S_{GB} . The measured data are reduced to these three effective screening parameters, denoted generically as S_k , and their isoelectronic behavior is studied as a function of the reciprocal screened charge $1/(Z-S_k)$.

When displayed in this manner, experimental data and MCDF calculations in the homologous Mg, Zn, and Cd sequences show interesting trends. ^{10–12} Both are slowly varying and regular in this exposition, but the experimental measurements form straight lines, whereas the MCDF calculations exhibit curvatures. Although the origin of these empirical linearities is unclear, they provide a predictive empirical systematization, and the failure of MCDF calculations to reproduce them is clearly indicative of inadequacies in the theoretical representation.

RESULTS

MCDF calculations were performed for all members of the Sm isoelectronic sequence from Z = 92 to Z = 67. A subset of ions was selected from this group for which the alkaline earthlike criteria ($5s^2$ is the ground configuration and 5s5p is the lowest excited configuration) are satisfied.

The calculations indicated that $4f^{14}5s^2$ 1S_0 becomes the ground state at Z=70 where it plunges through the $4f^{13}5s^25p$ 3G term. Although $4f^{13}5s^25p$ is the lowest excited core configuration, it contains no S or P terms and perturbs neither the $5s^2$ nor the 5s5p configuration. Strong perturbations to the $4f^{14}5s5p$ terms occur in the region from Z=68 to Z=74, where they plunge through the $4f^{13}5s5p^2$ terms. For example, in W^{+12} some of the $4f^{14}5s5p$ and $4f^{13}5s5p^2$ levels are so strongly mixed that it is difficult to assign a dominant configuration. For $Z \geq 75$ the mixing is small and the levels can be easily traced isoelectronically.

Various types of calculations were performed, and the results selected for presentation here use a slightly different approach for the determination of the energy levels than for the transition probabilities. For the energy-level determinations, MCDF-OL calculations were selected, in which each of the four 5s5p-level wave functions was individually optimized in the presence of members of its own complex (levels of the same spin and parity). These arrays were unwieldy for transition probability calculations, and for these quantities MCDF-EAL calculations were selected, in which all levels connected by the appropriate transition mo-

ment were jointly optimized with members of their respective complexes.

The differences between the MCDF-EAL and the MCDF-OL energy levels were generally much less than 1%. This is negligible at the level of accuracy of transition probability measurements but is significant for spectroscopic classification work. Screening parameter studies of these results indicated that the inclusion of levels from different complexes in the energy-level determination could sometimes shift the MCDF relative to the SCDF in a direction contrary

Table 1. Individually Optimized MCDF-OL Calculations for the Lowest Five Energy Levels in Highly Ionized Members of the Sm Isoelectronic Sequence (in cm⁻¹)

Z Ion	$5s^2{}^1S_0$	$5s5p ^B\!P_0$	$5s5p ^B\!P_1$	$5s5p\ ^TP_2$	5s5p ^T P ₁
75 Re + 13	0	231 277	251 016	353 526	421 054
$76 \mathrm{Os} + 14$	0	244 730	265 806	381 986	451 812
77 Ir + 15	0	$258\ 270$	$280\ 672$	411 554	483 150
78 Pt + 16	0	271 914	295 636	442 411	515 656
79 Au + 17	0	285 669	310 705	474 659	549 501
80 Hg + 18	0	299 558	325 902	508 401	584 808
81 Tl + 19	0	313571	341 216	543701	621 651
82 Pb + 20	0	327 716	356 655	580 651	660 126
83 Bi + 21	0	342002	$372\ 229$	619 335	$700\ 322$
84 Po + 22	0	356 437	387 946	659 847	$742\ 332$
85 At + 23	0	371 011	403 795	$702\ 267$	786 238
$86 \mathrm{Rn} + 24$	0	385677	419 730	746 634	832 080
$87 \mathrm{Fr} + 25$	0	400 605	435923	793 230	880 141
88 Ra + 26	0	$415\ 545$	$452\ 122$	841 886	930 251
89 Ac + 27	0	430716	468 547	892 946	982 754
$90 \mathrm{Th} + 28$	0	$446\ 012$	485 091	946 407	1 037 645
91 Pa + 29	0	461 509	501 836	$1\ 002\ 476$	1 095 134
92 U + 30	0	477 080	$518\ 649$	1061133	$1\ 155\ 199$

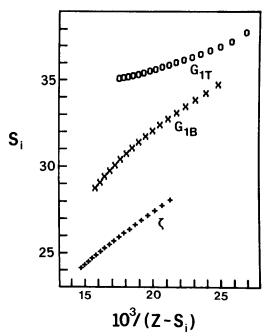


Fig. 2. Screening parameters versus reciprocal screened charge for the MCDF calculations. The symbols indicate screening parameters determined by Eqs. (5)–(8), (11), and (12) from (0) G_{1T} , (\times) G_{1B} , and (+) ζ .

Table 2. Transition Probabilities for U^{+30} Computed by the MCDF-EAL Method Applied Simultaneously to All Levels with the Configurations $5s^2$, 5s5p, and $5s5p^2$

Transition	Туре	Transition Probability $(\sec^{-1})^a$
${}^{1}S_{0} - {}^{T}P_{1}$	E1	5.46(11)
$^{B}P_{0}$ -	M 1	1.24(6)
$^{B}P_{1}^{\circ}$ -	M 1	5.86(5)
TP_2 –	M1	4.63(3)
$^{B}P_{1}^{-}$	$\mathbf{E}2$	4.14(5)
TP_2 –	E 2	1.50(1)
${}^{1}S_{0} - {}^{B}P_{1}$	$\mathbf{E}1$	1.27(10)
$^{B}P_{0}$ -	M1	1.00(3)
$^BP_1 - ^TP_2$	M1	1.52(6)
$^{B}P_{0}$ -	$\mathbf{E}2$	1.28(5)
$^{B}P_{1}$ $-$	$\mathbf{E}2$	1.51(5)
${}^{1}S_{0}$ -	M2	3.06(3)

^a The notation a(b) indicates $a \times 10^b$.

Table 3. Predicted Wavelengths and Lifetimes of E1
Transitions within the n = 5 Shell for Highly Ionized
Members of the Sm and Pm Sequences

	$\frac{\text{Samarium Sequence}}{{}^{(1}S_0 - {}^{T}P_1)} \qquad {}^{(1}S_0 - {}^{B}P_1)$				$\frac{\text{Promethiun}}{(^2S_{1/2}-^2P_{3/2})}$	$\frac{1}{(^2S_{1/2}-^2P_{1/2})}$
Z Ion			$\lambda(\mathring{A}) \tau(\text{psec})$			$\lambda(\mathring{A}) \tau(psec)$
75 Re	237.5	17.4	398.4	608	-	
76 Os	221.3	12.8	376.2	502		
77 Ir	207.0	11.1	356.3	421	226 [212] 20	325 [319] 63
78 Pt	193.9	9.7	338.3	357	. ,	
79 Au	182.0	8.6	321.8	307	199 [186] 16	297 [290] 56
80 Hg	171.0	7.5	306.8	266	. ,	
81 Tl	160.9	6.7	293.1	232		
82 Pb	151.5	5.9	280.4	205	166[155] 11	263 [256] 47
83 Bi	142.8	5.2	268.7	182		
84 Po	134.7	4.6	257.8	162		
85 At	127.2	4.1	247.7	146		
86 Rn	120.2	3.7	238.2	132		
87 Fr	113.6	3.3	229.4	119		
88 Ra	107.5	2.9	221.2	109		
89 Ac	101.8	2.6	213.4	100		
90 Th	96.4	2.3	206.1	92		
91 Pa	91.3	2.1	199.3	84		
92 U	86.6	1.8	192.8	78	96 [87] 4	186 [180] 31

^a MCHF calculations with relativistic corrections are reprinted from Ref. 1. Bracketed wavelengths are MCDF recalculations reprinted from Ref. 3.

to homologous trends, which motivated the separate approaches. Because of the lack of low-lying S states in configurations with a single hole in the 4f shell, the $5s^2$ 1S_0 was relatively free of perturbations, and its energy could be determined by SCDF calculations.

Energy Levels

The results of the MCDF-OL calculation of the excitation energies of the $5s5p\,^iP_J$ levels relative to the $5s^2\,^1S_1$ level are given for the ions Re⁺¹³ to U⁺³⁰ in Table 1.

An intermediate coupling plot of the quantities y and x [as defined by Eqs. (9) and (10)] is given in Fig. 1. The vertical lines indicate the individual ions in the sequence (Z=75-92 from left to right). The slight offset at each level locus

demonstrates that the difference between G_{1T} and G_{1B} is small compared with the level spacings, although its influence on the highly sensitive screening parameters is much greater. The plot shows that the coupling is closer to the jj limit than to the LS limit but is not accurately described by either limiting case.

Plots of screening parameter reductions for the three quantities G_{1T} , G_{1B} , and ζ [obtained by inversion of Eqs. (5)– (8), (11), and (12)] versus reciprocal screened charge are displayed in Fig. 2. These plots are consistent with the homologous theoretical trends noted earlier and exhibit smooth curvatures. However, previous experimental studies9-12 suggest that these curvatures may be an artifact of the theoretical calculations and that the true behavior may follow straight lines on this plot. It should be noted that these MCDF codes treat the Breit interaction perturbatively rather than self-consistently, which could be a source of these discrepancies. The comparison of experimental results with similar calculations in the homologous Cd sequence¹² indicated that this theoretical approach tends to overestimate the spin-orbit screening and underestimate the exchange screening. A few well-chosen experimental measurements could test the homologous persistence of the linear behavior to this sequence and perhaps permit precise quantitative corrections in these theoretical curves.

Transition Probabilities

The three configurations $4f^{14}5s^2$, $4f^{14}5s^5p$, and $4f^{13}5s^5p^2$ contain 65 different levels. MCDF-EAL calculations for all E1, M1, E2, and M2 transitions involving these levels are very demanding in computational time and were performed completely only for U⁺³⁰. The results of this calculation for transitions connecting the lowest five levels are presented in Table 2. Through comparisons with these results, accurate but less demanding calculations were made for the sequence.

It can be seen from Table 2 that the E1 channel is the overwhelmingly dominant (more than 10^5 times greater) contribution to the decay of both the $^T\!P_1$ and $^B\!P_1$ levels. MCDF-EAL calculations of these E1 transitions that included only the J=0 even-parity levels and the J=1 odd-parity levels yielded results that differed by less than 1% from the general results for the $\rm U^{+30}$ example in Table 2. By using this approach throughout the sequence and neglecting the higher-order moments, Table 3 presents the predicted lifetimes τ of the $^T\!P_1$ and $^B\!P_1$ levels together with their corresponding predicted transition wavelengths λ .

As the coupling moves away from the LS limit and toward the jj limit, the alkaline earthlike singlet resonance line and singlet—triplet intercombination line become increasingly similar to the alkalilike resonance doublet that occurs in the next stage of ionization. For comparison and for convenience in spectroscopic identification, previously reported predictions 1,3 for the lifetimes and wavelengths of the alkalilike resonance transitions in the Pm sequence are also reproduced in Table 3. [The first calculations 1 were by multiconfiguration Hartree–Fock (MCHF) methods with relativistic corrections. MCDF recalculations 3 of these wavelengths are given in brackets.]

Various methods of calculation for the M1, E2, and M2 decays were used and compared. It was found that exclusion of the $4f^{13}5s5p^2$ configuration for these higher moments

Table 4. Transition Probabilities^a (in \sec^{-1}) for Decay Channels of the ${}^{T}P_{2}$ Level

			<u> </u>	
Z Ion	$_{(^BP_{1}-^TP_{2})}^{A(\mathbf{M}1)}$	$A(E2) \ (^BP_1-^TP_2)$	$A(E2)$ $({}^{B}P_{0}-{}^{T}P_{2})$	A(M2) $({}^{1}S_{0}{}^{-T}P_{2})$
75 Re	1.31(4)	2.87(2)	3.48(2)	3.26(1)
76 Os	1.87(4)	4.55(2)	5.32(2)	4.46(1)
77 Ir	2.63(4)	7.10(2)	8.04(2)	6.06(1)
78 Pt	3.66(4)	1.09(3)	1.20(3)	8.16(1)
79 Au	5.04(4)	1.66(3)	1.77(3)	1.09(2)
80 Hg	6.87(4)	2.48(3)	2.58(3)	1.45(2)
81 Tl	9.27(4)	3.67(3)	3.73(3)	1.92(2)
82 Pb	1.24(5)	5.38(3)	5.33(3)	2.52(2)
83 Bi	1.65(5)	7.79(3)	7.56(3)	3.30(2)
84 Po	2.17(5)	1.12(4)	1.06(4)	4.29(2)
85 At	2.84(5)	1.59(4)	1.49(4)	5.57(2)
86 Rn	3.69(5)	2.25(4)	2.06(4)	7.19(2)
87 Fr	4.77(5)	3.15(4)	2.84(4)	9.27(2)
88 Ra	6.13(5)	4.39(4)	3.90(4)	1.19(3)
89 Ac	7.83(5)	6.07(4)	5.31(4)	1.52(3)
90 Th	9.96(5)	8.33(4)	7.19(4)	1.95(3)
91 Pa	1.26(6)	1.14(5)	9.69(4)	2.48(3)
92 U	1.59(6)	1.54(5)	1.30(5)	3.15(3)

^a The notation a(b) indicates $a \times 10^b$.

produced insignificant differences (less than 5%) from the values listed in Table 2. Table 4 presents MCDF-EAL calculations of the decay channels for the TP_2 level that included the lowest five levels.

CONCLUSIONS

Although ab initio theoretical methods are known to be capable of predicting certain atomic energy levels to within a few percent in alkali and alkaline earth systems with as many as 30 electrons, experimental tests of these methods for more complex electronic systems are lacking. One- and two-valence electron transitions in highly ionized members of the Pm and Sm sequences provide such a test. As recent measurements⁵ have shown in the Pm sequence, these transitions can be intense in fast ion beam-foil spectra, since they are heavily repopulated by cascade transitions along the alkali and alkaline earth yrast chains. The predictions presented here can serve as a guide to the identification of lines of this type in the Sm sequence. Observation and classification of these lines would provide a stringent test of ab initio MCDF calculations and produce a data base for their semiempirical systematization.

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