Argonne National Laboratory

THE ELECTRONIC ENERGY LEVELS OF THE HEAVY ACTINIDES
$Bk^{+3}(5f^8)$, $Cf^{+3}(5f^9)$, $Es^{+3}(5f^{10})$, AND $Fm^{+3}(5f^{11})$

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Extensive experimental data have been gathered and numerous theoretical treatments have been developed to explain lanthanide spectra, but much less is known about actinide spectra. Experimentally, one must normally contend with rather high levels of radioactivity in the 5f series of elements and with corresponding problems of handling, shielding, and radiation decomposition. These factors, together with the extremely small stocks of transcurium elements presently available, help to explain why more work involving the actinides has not appeared in the literature. From a theoretical standpoint, there has been some question as to the relative magnitude of spin-orbit and ligand field interactions in the actinides, whereas with the lanthanides, ligand field effects are considerably less than those associated with spin-orbit coupling.

The absorption spectrum of a given lanthanide or actinide ion in a crystalline matrix, rather than in solution, is of primary interest in terms of correlation with theoretical calculations since, in principle, one can identify individual transitions from polarization and Zeeman effect data taken with crystals at low temperatures. However, very few analyses of actinide spectra in crystals have been attempted. It is clear that the density and complexity of states are very great, so progress will necessarily be slow. Thus, at present, it is useful to employ solution spectra data, at least to establish the general characteristics of the energy level schemes.

A recent investigation[1] showed that a good correlation can be obtained between the calculated field-free energy levels of the light trivalent actinides and the solution absorption spectra of these species. Such a correlation emphasizes the fact that, although the trivalent actinides might have been expected to be more susceptible to ligand field effects than the lanthanides (because of the greater spatial extension of the 5f wave functions), one actually finds that ligand field effects are relatively small compared to Coulomb and spin-orbit interaction energies in both series. In the investigation referred to, the combined matrices of electrostatic and spin-orbit interaction were diagonalized, giving a complete intermediate coupling calculation. The electrostatic interaction was expressed in terms of linear

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combinations of the Slater radial integrals, F_2, F_4, and F_6; the spin-orbit matrices were calculated in terms of a spin-orbit coupling constant, ζ. In practice, these radial integrals are treated as empirical parameters to be varied to obtain the best fit to experimental data. To simplify the calculations, it is desirable to reduce the number of variables. If the nf-radial wave functions are assumed to be hydrogenic, values for the ratios of the Slater integrals F_4/F_2 and F_6/F_2 can be calculated, leaving only F_2 and ζ to be assigned values consistent with the experimental data. Experience has shown that these hydrogenic ratios are more realistic than might have been supposed. Attempts were made to fit the energy levels of the nf^6 configuration with several different Slater F_k ratios, including those based on Hartree-Fock calculations.[2] These attempts, along with preliminary results of a study in which a computer was programed to maximize the fit of all four parameters to the experimental results for $Am^{+3}(5f^6)$,[3] all indicate that the best correlation is obtained with Slater F_k ratios close to those of the hydrogenic approximation.

One result of the study of the light actinide spectra was that values of F_2 and ζ that gave a good fit to the experimental data, to a first approximation, increased linearly with atomic number Z (see Figs. 1 and 2). This suggested that it would be useful to extrapolate directly the parameters F_2 and ζ into the second half of the actinide series. Then the 5f-hydrogenic ratios of F_4/F_2 and F_6/F_2 could be used to carry out a complete intermediate coupling calculation for the configurations $5f^8$ to $5f^{13}$. It was not practical to use this type of approach previously, since patterns in the behavior of the light actinides had not been established. In addition, experimental data on the transcurium elements are not sufficient to establish clearly the parameters for such calculations. Only with Cf^{+3} have any absorption bands actually been observed.[4]

Fig. 1

Extrapolation of Values of ζ_{5f} Versus Z Based on Best Fits to Experimental Data for U^{+3} through Cm^{+3}

combinations of the Slater radial integrals, F_k, E_k, and F_k'; the spin-orbit matrices were calculated in terms of a spin-orbit coupling constant ζ. In practice, these radial integrals are treated as empirical parameters to be varied to obtain the best fit to experimental data. To simplify the calculations, it is desirable to reduce the number of variables. If the nf-radial wave functions are assumed to be hydrogenic, values for the ratios of the Slater integrals F_4/F_2 and F_6/F_2 can be calculated, leaving only F_2 and ζ to be assigned values consistent with the experimental data. Experience has shown that those hydrogenic ratios are more realistic than might have been supposed. Attempts were made to fit the energy levels of the nf configuration with several different Slater F_k ratios, including those based on Hartree-Fock calculations.[3] These attempts, along with preliminary results of a study in which a computer was programmed to maximize the fit of all four parameters to the experimental results for $Am^{+3}(5f^6)$,[3] all indicate that the best correlation is obtained with Slater F_k ratios close to those of the hydrogenic approximation.

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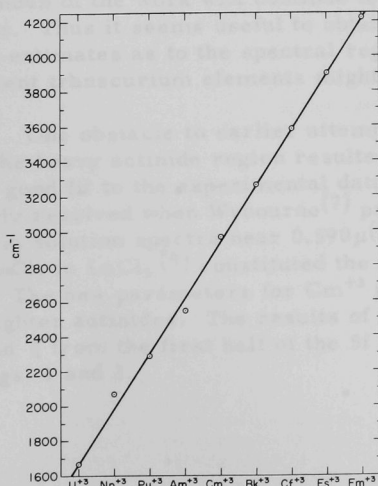
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Extrapolation of Values of
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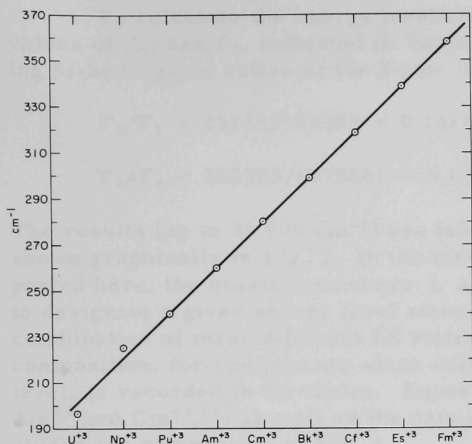Data for U^{+3} through Cm^{+3}

Fig. 2

Extrapolation of Values of F_2
Versus Z Based on Best Fits
to Experimental Data for U^{+3}
through Cm^{+3}

Experimental observation of the absorption spectra of elements be-
yond fermium will probably not be feasible since radioactive half-lives are
too short to make it practical to produce even microgram amounts of these
elements. It is expected, on the basis of projected transplutonium produc-
tion programs, that 100-mg quantities of berkelium and californium, 10-mg
quantities of Es^{253}, and 100-μgm quantities of Fm^{254} can eventually be made
from 300 gm of Pu^{242} during a 1.5-year irradiation.[5] The problem associ-
ated with radiation decomposition of the solvent in the presence of macro
amounts of short-lived isotopes was exemplified by early attempts to ob-
serve the spectrum of curium using Cm^{242}.[6] This type of problem, and
the necessity for remote handling of many of the isotopes in this region
due to the neutron hazard (short, spontaneous-fission half-lives), suggest
that much of the work will continue to be done with essentially micro tech-
niques. Thus it seems useful to obtain, on the basis of present information,
some estimates as to the spectral regions in which absorption bands of the
trivalent transcurium elements might be expected to occur.

One obstacle to earlier attempts to extrapolate values of F_2 and ζ
into the heavy actinide region resulted from apparent difficulties in achiev-
ing a good fit to the experimental data for Cm^{+3}. Such problems were
largely resolved when Wybourne[7] proposed that a weak absorption band,
seen in solution spectra near 0.590μ[8] but not in the fluorescence spectrum
of $CmCl_3$ in $LaCl_3$,[9] constituted the first excited multiplet level in the sys-
tem. The new parameters for Cm^{+3} proved to be consistent with those for
the lighter actinides. The results of the direct extrapolation of values of
F_2 and ζ from the first half of the 5f series into the second half are shown
in Figs. 1 and 2.

To calculate the energy levels for Bk^{+3} through Fm^{+3}, the extrapolated values of ζ_{5f} and F_2, collected in Table 1, were used, together with the following 5f-hydrogenic ratios of the Slater integrals:[10]

$$F_4/F_2 = 23255/163559 = 0.1422;$$

$$F_6/F_2 = 102725/6378801 = 0.0161.$$

The results (up to 30,000 cm^{-1}) are tabulated in Tables 2, 3, 4, and 5, and shown graphically in Fig. 3. In the intermediate coupling calculations reported here, the quantum numbers L and S cannot be employed usefully to designate a given energy level since each level is composed of a linear combination of many different LS states, all having the same J-value. This composition, for components which contribute $\geq 10\%$ of the character of the level, is recorded in the tables. Experimental and calculated results for Am^{+3} and Cm^{+3},[1] as well as the data of Conway et al.[4] for Cf^{+3}, are included for comparison in Fig. 3.

Table 1

EXTRAPOLATED VALUES OF ζ_{5f} AND F_2 FOR Bk^{+3} THROUGH Fm^{+3}

Ionic Species	F_2 (cm^{-1})	ζ_{5f} (cm^{-1})
Bk^{+3}	299	3260
Cf^{+3}	318	3580
Es^{+3}	338	3900
Fm^{+3}	358	4220

Table 2

ELECTRONIC ENERGY LEVELS OF Bk^{+3}
(0 to 30,000 cm^{-1})

J	Calculated Energy (cm^{-1})	% Composition of States[a]	J	Calculated Energy (cm^{-1})	% Composition of States[a]
6	0	74% ^7F; 21% ^5G	3	22,795	43% ^5G; 21% ^5H; 15% ^3F; 12% ^3G
4	4,588	52% ^7F; 25% ^5D	8	22,813	42% ^5L; 19% ^3K; 17% ^5I; 13% ^5K
5	4,946	82% ^7F; 11% ^5G	9	23,001	65% ^5L; 17% ^5K; 11% ^3M
3	7,775	71% ^7F; 17% ^5D	6	23,594	37% ^5L; 21% ^3K; 13% ^5H; 12% ^5G
2	8,367	63% ^7F; 21% ^5D	2	24,693	69% ^5G; 21% ^3F
1	9,939	73% ^7F; 21% ^5D	5	26,026	36% ^5F; 26% ^5G; 14% ^3G; 11% ^5H
0	10,241	71% ^7F; 23% ^5D	6	26,373	26% ^5I; 23% ^3H; 16% ^5H; 13% ^5G
6	15,936	20% ^3H; 13% ^3K; 13% ^3I; 13% ^7F	7	26,584	40% ^5L; 32% ^5H; 13% ^5I
4	16,032	40% ^7F; 34% ^5D; 15% ^3F	3	27,045	45% ^5D; 19% ^5F; 14% ^7F
10	19,981	67% ^5L; 25% ^3M	0	27,497	39% ^3P; 34% ^1S; 17% ^7F; 10% ^5D
4	20,071	22% ^5D; 21% ^5G; 19% ^5H; 13% ^3H; 11% ^3G	4	27,866	37% ^5F; 20% ^5G; 14% ^5D; 12% ^5H
7	20,938	26% ^5H; 21% ^5L; 17% ^3K; 16% ^3I; 11% ^5I	5	28,070	24% ^3H; 19% ^3G; 19% ^5G
5	21,451	33% ^5H; 25% ^5G; 13% ^3H; 12% ^5I	7	28,828	27% ^3I; 26% ^5I; 17% ^5H; 13% ^3K; 10% ^5K
2	22,117	38% ^3P; 25% ^7F; 12% ^3D	8	29,257	47% ^5I; 37% ^5L; 13% ^3K

a Only components amounting to 10% or greater are shown.

To calculate the energy levels for $Br^{+?}$ through $Fm^{+?}$, the extrapolated values of ζ_d and F_2, collected in Table 1, were used, together with the follow-ing Sl-hydrogenic ratios of the Slater integrals:[10]

$$F_4/F_2 = 23256/35569 = 0.1422.$$

$$F_6/F_2 = 18272/627860 = 0.0161.$$

The results (up to 30,000 cm^{-1}) are tabulated in Tables 2, 3, 4, and 5, and shown graphically in Fig. 3. In the intermediate coupling calculations re-ported here, the quantum numbers L and S cannot be employed usefully to designate a given energy level since each level is composed of a linear combination of many different LS states, all having the same J-value. This composition, for components which constitute a1% of the character of the level, is recorded in the tables. Experimental and calculated results for $Am^{+?}$ and $Cm^{+?}$,[1] as well as the data of Conway et al.[4] for $Cf^{+?}$, are in-cluded for comparison in Fig. 3.

Table 1

EXTRAPOLATED VALUES OF ζ_d AND F_2
FOR $Br^{+?}$ THROUGH $Fm^{+?}$

Ionic Species	$F_2 (cm^{-1})$	$\zeta_d (cm^{-1})$
$Br^{+?}$	293	3260
$Cr^{+?}$	318	3880
$Re^{+?}$	338	3900
$Fm^{+?}$	358	4220

6

Table 3

ELECTRONIC ENERGY LEVELS OF Cf^{+3}
(0 to 30,000 cm^{-1})

J	Calculated Energy (cm^{-1})	% Composition of States[a]	J	Calculated Energy (cm^{-1})	% Composition of States[a]
15/2	0	72% ^6H; 23% ^4I	19/2	22,194	53% ^4L; 29% ^4M; 14% ^2M
11/2	7,550	45% ^6F; 27% ^4G; 17% ^6H	9/2	22,616	34% ^6F; 28% ^6H; 16% ^4F; 11% ^2G
9/2	7,629	39% ^4F; 32% ^6F; 14% ^4G	11/2	22,990	43% ^4G; 31% ^6H; 12% ^2H
13/2	7,906	84% ^6H; 12% ^4I	5/2	23,097	38% ^4P; 32% ^6P; 13% ^2D; 10% ^6H
11/2	11,782	45% ^6H; 35% ^6F; 11% ^4G	13/2	23,795	33% ^4I; 25% ^4K; 17% ^4H
9/2	13,417	51% ^6H; 21% ^6F; 19% ^4G	3/2	24,174	42% ^6F; 25% ^4P; 14% ^2P; 11% ^6P
3/2	13,526	32% ^4D; 27% ^6F; 17% ^2P	7/2	24,945	34% ^4D; 27% ^6P; 16% ^4F; 14% ^6H
7/2	14,151	60% ^6F; 22% ^4F	11/2	25,871	33% ^4I; 17% ^2H; 16% ^4G; 13% ^4K; 12% ^2I
7/2	15,299	53% ^6H; 23% ^4G	9/2	27,186	27% ^4F; 19% ^2H; 16% ^4I; 14% ^4H; 13% ^4G
15/2	16,176	25% ^2K; 18% ^6H; 17% ^2L; 13% ^4I; 13% ^4K	15/2	28,044	26% ^4M; 23% ^2L; 22% ^4K; 15% ^4I; 11% ^2K
5/2	16,300	30% ^6F; 26% ^6H; 15% ^4G	9/2	28,894	38% ^4I; 24% ^2H; 13% ^4H; 11% ^2G
5/2	17,254	37% ^6F; 29% ^6H; 13% ^4G; 12% ^4D	15/2	29,202	32% ^4I; 19% ^4L; 15% ^2K; 12% ^4K; 11% ^4M
1/2	17,697	56% ^6F; 37% ^4D	3/2	29,324	32% ^4F; 24% ^2D; 15% ^6P; 14% ^6F; 11% ^4P
17/2	20,790	48% ^4K; 26% ^4L; 14% ^2L; 13% ^4M	7/2	29,561	33% ^4G; 17% ^6P; 16% ^4H
21/2	21,691	76% ^4M; 21% ^2N	5/2	29,978	33% ^4D; 30% ^4F; 11% ^4G; 10% ^6F

[a] Only components amounting to 10% or greater are shown.

Table 4

ELECTRONIC ENERGY LEVELS OF Es^{+3}
(0 to 30,000 cm^{-1})

J	Calculated Energy (cm^{-1})	% Composition of States[a]	J	Calculated Energy (cm^{-1})	% Composition of States[a]
8	0	77% ^5I; 20% ^3K	2	22,603	51% ^5S; 15% ^5F; 11% ^3D
7	10,554	90% ^5I	3	23,711	68% ^5F; 17% ^3D; 14% ^3F
5	11,733	40% ^3G; 32% ^5F; 14% ^3H	4	23,734	27% ^5G; 27% ^3G; 22% ^3F
6	13,975	55% ^5I; 29% ^3H	1	24,696	45% ^5F; 44% ^3D; 11% ^3P
2	14,277	27% ^3D; 25% ^3P; 15% ^5S; 15% ^1D	5	25,353	39% ^5G; 31% ^5F; 16% ^3G
4	18,809	43% ^5F; 28% ^3F	9	27,000	84% ^3L; 16% ^3M
5	19,332	50% ^5I; 26% ^5F; 18% ^3H	7	28,000	55% ^3K; 21% ^3I; 16% ^3L
4	19,752	32% ^5I; 24% ^3H; 19% ^5F; 11% ^3F	2	28,412	43% ^3F; 18% ^5G; 18% ^1D
8	20,251	41% ^3K; 19% ^5I; 19% ^1L; 16% ^3L	4	28,878	26% ^3F; 24% ^5I; 23% ^5D; 17% ^3G
6	21,837	67% ^5G; 23% ^5I			

[a] Only components amounting to 10% or greater are shown.

Table 5

ELECTRONIC ENERGY LEVELS OF Fm^{+3}
(0 to 30,000 cm^{-1})

J	Calculated Energy (cm^{-1})	% Composition of States[a]	J	Calculated Energy (cm^{-1})	% Composition of States[a]
15/2	0	91% ^4I	5/2	22,582	48% ^4F; 43% ^2D
9/2	9,848	40% ^2G; 39% ^4F; 16% ^2H	7/2	23,410	85% ^4F; 12% ^2G
11/2	11,686	52% ^2H; 25% ^4I; 21% ^4G	3/2	25,025	44% ^4S; 32% ^4F; 23% ^2D
13/2	12,341	97% ^4I	15/2	27,680	78% ^2K; 13% ^2L
3/2	15,262	34% ^2P; 30% ^4S; 27% ^2D	7/2	27,792	36% ^4G; 35% ^2G; 20% ^2F
9/2	20,236	37% ^4I; 31% ^4F; 30% ^2H	9/2	28,259	59% ^4G; 18% ^4F; 14% ^2G
11/2	22,409	48% ^4I; 48% ^4G			

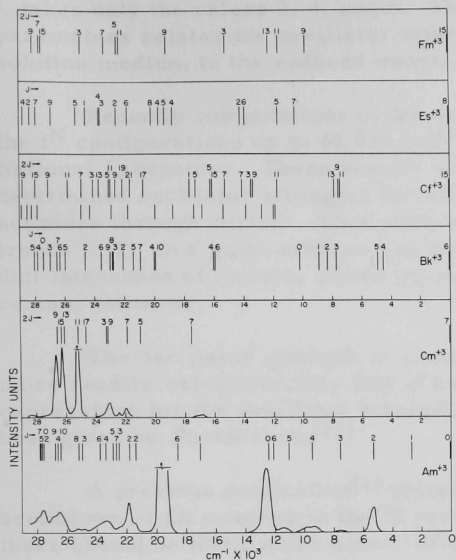[a] Only components amounting to 10% or greater are shown.

Fig. 3

Calculated Free-ion Levels of Am^{+3}, Cm^{+3}, Bk^{+3}, Cf^{+3}, Es^{+3}, and Fm^{+3}. Experimental results for Am^{+3} and Cm^{+3} are from Ref. 1. Those for Cf^{+3}, indicated below the calculated values for that element, are from Ref. 4.

These computations indicate the energies at which absorption bands are expected, but they give no information with respect to the probable intensities of the transitions. Attempts to observe the solution absorption spectrum of Bk^{+3} in the 4500 to 7500 Å region have been unsuccessful; however, it was concluded that any bands in this region have a molar absorptivity (ϵ) less than 20.[11] In contrast to these results, several absorption bands of Cf^{+3}, primarily as $CfCl_3$ in $LaCl_3$ crystals, have been observed in the course of experiments in which microgram amounts of the element were used.[4] Only two absorption bands were observed in aqueous solution. On the basis of this work, it was concluded that ϵ was less than 20 for any Cf^{+3} bands in the region 4500-7500 Å.[11]

Recent theoretical developments[12,13] indicate that in the near future it may also be possible to predict oscillator strengths of transitions in the transcurium elements.

Electronic transitions within an f^N-configuration may be classified as induced electric dipole, magnetic dipole, or electric quadrupole in nature. Of these, electric dipole transitions have been shown to be primarily responsible for observed intensities in the spectra of the trivalent lanthanide and actinide elements.[14] However, in a limited number of cases magnetic dipole or electric quadrupole contributions can also become important. Judd[13] has derived an expression for the oscillator strength of an electric dipole transition $\psi_J \rightarrow \psi_{J'}$, in terms of its reduced matrix elements, its frequency, and a complicated function, T_λ, which in part is dependent upon the crystal field experienced by the ion under consideration. In practice,

λ takes only the values 2, 4, and 6. This means that a set of only three parameters relates the oscillator strengths for all transitions in a given solution medium to the reduced matrix elements for the transitions.

Recently computations of the oscillator strengths for transitions in the f^N configurations up to 40,000 cm^{-1} were initiated at the Argonne National Laboratory. These results will be related to experimentally-determined oscillator strengths for all the lanthanides, and for the trivalent actinides through curium. This work will test the theory. If, as expected, trends in T_λ in a given medium are revealed, it should be possible to predict intensities of electric dipole transitions in that medium for the trans-curium elements.

The oscillator strength of a magnetic dipole transition is much more readily calculated than that of an electric dipole transition. Suitable expressions for the oscillator strength of magnetic dipole transitions have been given by Pasternack.[15]

A previous publication[1] pointed out that as a result of the greater breakdown of LS coupling in the 5f series as contrasted to the 4f series, there should be many more possibilities for observing magnetic dipole transitions in the actinides. The oscillator strengths (P) for the relevant magnetic dipole transitions for Bk^{+3}, Cf^{+3}, Es^{+3}, and Fm^{+3} have been calculated; the results are tabulated in Table 6. Thus if the electric dipole character of the J = 5 level of Bk^{+3}, which is expected to be found near 4946 cm^{-1}, were negligible, an absorption band with P = 2.7×10^{-7} would be anticipated. For comparison, in the case of Eu^{+3}, the band observed near 19,000 cm^{-1}[16] has an experimental value of P = 1.3×10^{-8}; thus, an equally sharp Bk^{+3} band at 4,946 cm^{-1} might be expected to be twentyfold as intense as the observed Eu^{+3} band. If this Bk^{+3} transition were also to have appreciable electric dipole character, the observed band would be proportionally more intense. Magnetic dipole transitions determine only the lower limits of the oscillator strengths expected for the electronic levels concerned.

Table 6

MAGNETIC DIPOLE OSCILLATOR STRENGTHS (P$_{M.D.}$)[a]
FOR Bk^{+3} THROUGH Fm^{+3}

Species	J	Calculated Energy (cm^{-1})	P$_{M.D.}$ x 10^{-9}	Species	J	Calculated Energy (cm^{-1})	P$_{M.D.}$ x 10^{-9}
Bk^{+3}	5	4,946	267	Cf^{+3}	13/2	7,906	460
	6	15,937	210		15/2	16,176	250
	7	20,938	14		17/2	20,790	20
	5	21,451	25		13/2	23,795	36
	6	23,594	34		15/2	28,044	3.8
	5	26,026	71		15/2	29,202	26
	6	26,373	26	Es^{+3}	7	10,554	565
	7	26,584	5.3		8	20,251	216
	5	28,070	0.3		9	27,000	12
	7	28,828	0.4		7	28,000	16
				Fm^{+3}	13/2	12,341	560
					15/2	27,680	115

[a] All magnetic dipole transitions in the energy range 0-30,000 cm^{-1}.

While it may not be feasible to observe the absorption spectra of all of the heavy actinide elements, it may be possible to do magnetic measurements on very small quantities, as illustrated by Cunningham's measurement of the magnetic susceptibility of Es^{253} on a submicrogram scale.[17] Therefore, the g-values of the ground-state eigenvector have been calculated for the various heavy actinides; the results are listed in Table 7.

Table 7

CALCULATED g-VALUES FOR THE GROUND STATES OF
Bk^{+3}, Cf^{+3}, Es^{+3}, AND Fm^{+3}

Species	J	% Composition of States[a]	% Accounted	Calculated g-value
Bk^{+3}	6	74.4% ^7F; 20.8% ^5G; 3.1% ^3H	99.79	1.44573
Cf^{+3}	15/2	71.5% ^6H; 23.0% ^4I; 3.4% ^2K; 1.3% ^4K	100.00	1.28590
Es^{+3}	8	77.3% ^5I; 20.2% ^3K; 1.3% ^1L; 1.0% ^3L	99.99	1.21856
Fm^{+3}	15/2	90.7% ^4I; 9.0% ^2K; 0.3% ^2L	100.00	1.18202

[a] Components of 1% or greater, rounded to the nearest 1/10 are shown.

Acknowledgement

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While it may not be feasible to observe the absorption spectra of all of the heavy actinide elements, it may be possible to do magnetic measurements on very small quantities, as illustrated by Cunningham's measurement of the magnetic susceptibility of Es^{3+} on a submicrogram scale.[?] Therefore, the g-values of the ground-state eigenvector have been calculated for the various heavy actinides; the results are listed in Table 7.

Table 7

CALCULATED g-VALUES FOR THE GROUND STATES OF
Bk^{4+}, Cf^{3+}, Es^{3+}, AND Fm^{3+}

Species	T	% Composition of States^a	% Accounted	Calculated g-value
Bk^{4+}	6	74.4% ^7F, 20.8% ^5G, 3.40% ^5H	99.19	1.46574
Cf^{3+}	15/2	71.58% ^6H, 22.04% ^6I, 1.49% ^4K, 1.35% ^2K	100.00	1.28590
Es^{3+}	8	77.34% ^5I, 20.26% ^5K, 1.39% ^3L, 1.04% ^3L	99.99	1.11848
Fm^{3+}	15/2	90.7% ^6H, 8.63% ^6K, 0.35% ^2L	100.00	1.19701

^a Components of 1% or greater, rounded to the nearest 1/10 are shown.

Acknowledgement

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