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CRYSTAL STRUCTURES AND LATTICE PARAMETERS
OF THE COMPOUNDS OF BERKELIUM.
IV. BERKELIUM TRIFLUORIDE

J. R. Peterson and B. B. Cunningham

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CRYSTAL STRUCTURES AND LATTICE PARAMETERS OF THE COMPOUNDS OF BERKELIUM. IV. BERKELIUM TRIFLUORIDE*

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ABSTRACT

BkF_3 has been found to exhibit a low-temperature, YF_3-type orthorhombic structure and a high-temperature, LaF_3-type trigonal structure. The lattice parameters of these two BkF_3 modifications are: $a_o = 6.70 \pm 0.01$ A, $b_o = 7.09 \pm 0.01$ A, $c_o = 4.41 \pm 0.01$ A (orthorhombic), and $a_o = 6.97 \pm 0.01$ A, $c_o = 7.14 \pm 0.01$ A (trigonal), where the error limits reflect the uncertainties in the derivation of the lattice parameters. The inversion temperature of BkF_3 lies in the range 350 to 600° C.

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*The experimental work reported here is taken from a thesis submitted by J. R. Peterson to the Graduate Division of the University of California in partial fulfillment of the requirements for the degree of Doctor of Philosophy.

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INTRODUCTION

The preparation and crystallographic characterization of two structural forms of berkelium trifluoride are described in this paper.

EXPERIMENTAL

The berkelium used in this work was derived from two separate purification cycles, both carried out as described previously.[1] Mass analyses of the two berkelium solutions showed the Ce and Nd contents to be 0.27 atom percent Ce and 0.06 atom percent Nd in one Bk solution, as contrasted with 9.53 atom percent Ce and 0.03 atom percent Nd in the other. The difference is attributed to the failure of the alcoholic HCl column, used to separate Bk and Ce, in the second purification cycle. The presence of the cerium and californium (from decay of Bk^{249} at a rate of ~0.2% per day) contaminants prevented the determination of accurate lattice parameters for BkF_3.

Berkelium trifluoride samples were prepared by treatment of the oxides (stuck on a 5-mil Pt wire inside a hole in a 1/8-in Pt rod) with a one-to-two $H_{2(g)}$-$HF_{(g)}$ mixture at 600° C for one-half hour, followed by a second, similar treatment with a fresh $H_{2(g)}$-$HF_{(g)}$ mixture. The trifluoride samples were either cooled rapidly to obtain the high-temperature, LaF_3-type trigonal modification, or cooled slowly to obtain the low-temperature, YF_3-type orthorhombic modification. In both cases the samples were cooled in the reaction gas mixture and then flushed with argon gas before removal from the all-Monel vacuum system. The very pale yellow-green trifluoride samples were

"chipped off" the Pt wire into a quartz capillary, which was subsequently evacuated and sealed off for x-ray examination. Further details of the hydrofluorination techniques can be found in reference (2).

X-ray exposure times, using the same diffraction equipment and operating conditions as reported for the oxide work,[1] were from eight to twelve hours on the 0.2 μg BkF_3 samples.

RESULTS AND DISCUSSION

Berkelium trifluoride was found to exist in both the LaF_3-type trigonal structure,[3] characteristic of the lanthanide trifluorides of La through Pm, and the YF_3-type orthorhombic structure,[4] characteristic of the lanthanide trifluorides of Sm through Lu.

All of the BkF_3 powder patterns showed the presence of more than one phase. Usually all the lines were accounted for by a trigonal trifluoride phase plus an orthorhombic trifluoride phase, but in some cases other, unaccounted-for lines were present in the powder patterns. One phase was always dominant, however, and only the more intense lines of the other phases were observed. Because of the possible superposition of lines belonging to different trifluoride phases, the observed line intensities for each separate phase are subject to error. In one case (JP-VII, Film 2691A) enough of the minor YF_3-type orthorhombic phase was observed to determine lattice parameters for it.

The observed lattice parameters of the individual trifluoride preparations along with their Cf^{249} and Ce contents are listed in Table 1.

Since CeF_3 does not exhibit an orthorhombic modification, the YF_3-type berkelium trifluoride lattice parameters were initially corrected for the known Cf content of the Bk sample in accordance with Vegard's Law.[5] The lattice parameters of orthorhombic CfF_3 (a_o = 6.653 ± 0.002 A, b_o = 7.041 ± 0.002 A, and c_o = 7.395 ± 0.001 A) were derived from a single preparation by Peterson et al.[6] These "corrected-for-Cf," orthorhombic BkF_3 lattice parameters were then plotted versus the Ce content of the berkelium sample and extrapolated to zero Ce content to obtain "best estimates" for the lattice parameters of orthorhombic BkF_3: a_o = 6.70 ± 0.01 A, b_o = 7.09 ± 0.01 A, and c_o = 4.41 ± 0.01 A, where the error limits reflect the uncertainties in the derivation of the lattice parameters.

Similarly for LaF_3-type trigonal berkelium trifluoride, since the trigonal modification of CfF_3 is unknown, the lattice parameters were corrected for the known Ce content of the Bk sample using the parameters of Swanson et al. (a_o = 7.112 A and c_o = 7.279 A).[7] These "corrected-for-Ce," trigonal BkF_3 lattice parameters did not vary in any regular fashion as the Cf content of the berkelium sample increased, so they were just averaged to obtain "best estimates" for the lattice parameters of trigonal BkF_3: a_o = 6.97 ± 0.01 A and c_o = 7.14 ± 0.01 A, where again the lattice parameters are rounded off to the nearest hundredth and the error limits reflect the uncertainties in the derivation of the lattice parameters.

The Miller indices, observed and calculated 2θ values, and observed and calculated line intensities for one sample of each type of BkF_3 are given in Tables 2 and 3.

Thoma and Brunton studied the equilibrium dimorphism of the lanthanide trifluorides.[9] Dimorphism was not observed for the trifluorides of La through Nd. They determined equilibrium inversion temperatures for the trifluorides of Sm through Lu and found them to range from 555° C for SmF_3 to 1075° C for ErF_3. The orthorhombic BkF_3 samples in this work were easily converted to the trigonal form by annealing at 600° C. The inversion temperature of BkF_3 lies between 350 and 600° C but could not be determined more precisely, since long-term annealings of trigonal BkF_3 samples failed to produce significant transformations to the orthorhombic form.

A summary of the pertinent crystallographic data of the lanthanide and actinide trifluorides along with calculated ionic radii is presented in Table 4. Crystallographic data for the high-temperature form of the heavier lanthanide trifluorides is given in reference (9). The trifluorides of Bk and Cf are the first of the actinide trifluorides to be prepared in the YF_3-type orthorhombic modification.

By comparing the Bk^{3+} ionic radius, as calculated from the LaF_3-type trifluoride, to the similarly calculated ionic radii of the light lanthanides, it is seen that the Bk^{3+} radius fits in after Pm, the last lanthanide to exhibit the trigonal trifluoride structure below ~550° C. Alternatively, by comparing the Bk^{3+} ionic radius, as calculated from the YF_3-type trifluoride, to the similarly calculated ionic radii of the heavier lanthanides, it is seen that the Bk^{3+} radius fits in before Sm, the first lanthanide to exhibit the YF_3-type orthorhombic trifluoride structure. These calculations and comparisons are consistent with the observed dimorphism in the BkF_3 system. It is important to note that comparisons of ionic radii can only be made

meaningful if the values compared are calculated in like fashion from the same type of compound, both with respect to composition and crystal structure.

From the data in Table 4 and by analogy with the work of Thoma and Brunton,[9] one can predict that CfF_3 will exhibit the LaF_3-type trigonal structure at temperatures greater than or equal to about 700° C.

The calculated density (x-ray) of YF_3-type orthorhombic BkF_3 is 9.70 g/cc, whereas for the LaF_3-type trigonal modification, it is 10.15 g/cc. These numbers reflect the general trend noted in the lanthanide trifluorides that the high-temperature, trigonal modification is the more dense one.

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Table 1. Berkelium trifluoride lattice parameters.

Sample Number	Film Number	Structure Type	Cf^{249}[a] Content (atom %)	Total Ce[b] Content (atom %)	Observed Lattice Parameters[c] (A)		
					$a_o \pm 2\sigma$	$b_o \pm 2\sigma$	$c_o \pm 2\sigma$
JRP-XXIII	2624A	YF_3	7.03	0.27	6.695 ± 0.004	7.086 ± 0.004	4.407 ± 0.003
JP-VII	2691A	YF_3	1.53	9.53	6.717 ± 0.015	7.114 ± 0.011	4.409 ± 0.005[d]
JP-X	2713A	YF_3	5.16	9.53	6.716 ± 0.001	7.103 ± 0.001	4.408 ± 0.001
JRP-XXI	2614A	LaF_3	5.26	0.27	6.973 ± 0.002		7.143 ± 0.003
JRP-XXII	2619A	LaF_3	6.20	0.27	6.965 ± 0.003		7.140 ± 0.003
JP-VII	2691A	LaF_3	1.53	9.53	6.990 ± 0.001		7.157 ± 0.001
JP-X	2716A	LaF_3	5.79	9.53	6.990 ± 0.001		7.158 ± 0.002
JP-X	2734A	LaF_3	8.05	9.53	6.988 ± 0.001		7.156 ± 0.002

[a]Calculated assuming Bk^{249} half life is 314 days.

[b]Determined by mass analysis. See text.

[c]Lattice parameters are the least squares value. The 2σ error limits represent the 95% confidence range reflecting only the internal consistency of the data for the individual preparation.

[d]The second phase in a predominantly trigonal BkF_3 powder pattern.

Table 2. Line list and indexing for YF_3-type orthorhombic BkF_3 (JP-X, Film 2713A).

hkl	2θ (deg) Observed[a]	2θ (deg) Calculated[b]	Line Intensity Observed[a]	Line Intensity Calculated[c]
011	23.67	23.75	6.5	2.0
101	24.12	24.15	9.0	5.7
020	25.02	25.07	9.0	6.3
200	26.47	26.54	1.5	0.1
111	27.27	27.26	10.0	10.0
210	29.37	29.42	10.0	7.6
201	33.51	33.55	3.5	0.4
121	35.06	35.09	9.0	3.1
211	35.90	35.91	3.0	0.1
002	40.85	40.94	6.5	1.1
221	42.25	42.34	6.5	1.4
102	43.14	43.20	4.0	0.4
031		43.38		0.1
112	44.99	45.13	6.5	1.8
301	45.44	45.44	10.0	2.4
131		45.53		3.6
230	46.84	46.95	8.5	3.2
311	47.29	47.30	7.0	1.8
022	48.54	48.61	7.0	1.5
122	50.53	50.60	7.0	1.4
212	51.23	51.21	8.0 broad	2.3
040		51.46		1.2

Table 2. (continued)

hkl	2θ (deg) Observed[a]	2θ (deg) Calculated[b]	Line Intensity Observed[a]	Line Intensity Calculated[c]
321	52.58	52.59	7.5	2.1
400	54.53	54.66	5.5	0.9
141	57.57	57.62	6.0	1.0
302	58.82	58.79	5.8	0.2
132		58.87		0.6
312	60.37	60.35	7.5	0.7
411		60.42		0.4
331		60.68		0.9
420	61.02	61.04	6.5	1.0
241	62.77	62.84	3.5	0.3
232	64.01	64.03	6.5	1.1
013	64.76	64.78	6.5	0.8
322		64.91		0.3
113	66.31	66.44	3.0	0.3
042	67.65	67.76	4.5	0.5
430	68.45	68.51	1.5	0.1
142	69.35	69.38	3.0	0.4
051		69.52		0.1
203	69.80	69.87	3.0	0.6
402	70.40	70.50	2.5	0.4
123	71.05	70.79	7.0	0.2
341		71.05		1.0
151		71.12		0.7

Table 2. (continued)

hkl	2θ (deg) Observed[a]	2θ (deg) Calculated[b]	Line Intensity Observed[a]	Line Intensity Calculated[c]
332		72.17		0.2
250	72.15	72.20	5.5	0.6
431		72.23		0.2
511	75.10	75.13	4.0	0.8
223	75.45	75.52	6.0	1.2
422	76.15	76.14	5.0	0.8
033		76.26		0.4
440	78.39	78.38	3.5	0.6
521	79.19	79.29	3.0	0.3
060	81.23	81.26	4.3	0.4
342	81.83	81.88	4.0	0.2
152		81.95		0.3
351	83.63	83.52	3.0	0.4
531		86.10		0.7
161	86.23	86.30	6.5 broad	0.4
252		86.50		0.6
610	88.28	88.40	3.5 broad	0.5
413	89.73	89.75	5.5 broad	0.8
522		89.86		0.4
114	91.78	91.63	5.0	0.4
243		91.88		0.7
352	93.96	94.05	3.5 broad	0.3
451		94.11		0.2

Table 2. (continued)

hkl	2θ (deg) Observed[a]	2θ (deg) Calculated[b]	Line Intensity Observed[a]	Line Intensity Calculated[c]
062	95.51	95.32	4.5 broad	0.2
541		95.56		0.2
124		95.69		0.4
532	96.81	96.63	1.5 broad	0.1
162		96.84		0.2
053	98.26	98.01	4.0	0.3
361		98.42		0.6
630	99.36	99.24	2.5 broad	0.4
343		99.47		0.1
153		99.54		0.1
433 α_1	100.51	100.49	3.5	0.4
304 α_1	102.36	102.34	4.0	0.1
612 α_1		102.40		0.3
134 α_1		102.41		0.3
314 α_1	103.91	103.72	4.0	0.3
171 α_1		103.87		0.3
270 α_1	104.95	104.93	3.5	0.3
460 α_1	105.50	105.52	2.0	0.3
542 α_1	106.09	106.15	1.8	0.2
542 α_2	106.59	106.53	1.3	0.1
551 α_1	107.84	107.86	4.0	0.3
324 α_1		107.92		0.2

Table 2. (continued)

hkl	2θ (deg) Observed[a]	2θ (deg) Calculated[b]	Line Intensity Observed[a]	Line Intensity Calculated[c]
551 α_2	108.29	108.25	2.0	0.1
324 α_2		108.31		0.1
362 α_1	109.09	109.12	1.0 broad	0.1
701 α_1	110.54	110.49	2.0	0.2
711 α_1	112.29	111.94	3.0 broad	0.1
144 α_1		112.30		0.3
632 α_1	113.79	113.76	2.0	0.3
533 α_1	115.04	114.76	3.5	0.1
172 α_1		115.02		0.1
334 α_1		115.17		0.4
721 α_1	116.39	116.37	3.0	0.4
371 α_1	116.78	116.76	2.3	0.2
721 α_2		116.83		0.2
263 α_1	120.13	120.09	5.5	0.5
272 α_1		120.12		0.3
080 α_1		120.34		0.1
462 α_1	120.72	120.78	3.0	0.3
650 α_1	122.27	122.34	1.8	0.3
712 α_1	123.92	123.83	5.0	0.3
453 α_1		123.94		0.5
712 α_2	124.52	124.37	3.0	0.1
561 α_1		124.43		0.1
453 α_2		124.48		0.3

Table 2. (continued)

hkl	2θ (deg) Observed[a]	2θ (deg) Calculated[b]	Line Intensity Observed[a]	Line Intensity Calculated[c]
344 α_1	126.22	126.15	5.8	0.2
623 α_1		126.20		0.4
154 α_1		126.24		0.3
181 α_1		126.34		0.2
344 α_2	126.82	126.72	3.0	0.1
623 α_2		126.76		0.2
154 α_2		126.80		0.1
181 α_2		126.90		0.1
205 α_1	129.31	129.17	4.5	0.4
372 α_1		129.30		0.1
471 α_1		129.37		0.1
504 α_1		129.39		0.3
205 α_2	129.96	129.77	2.0	0.2
372 α_2		129.90		0.1
471 α_2		129.98		0.04
504 α_2		129.99		0.1
281 α_1	132.11	132.18	0.8	0.1
281 α_2	133.01	132.82	0.8	0.1
800 α_1		133.13		0.1
073 α_1	134.65	134.58	1.8	0.3
810 α_1	135.05	135.00	1.3	0.04
633 α_1		135.09		0.03
073 α_2		135.26		0.1

Table 2. (continued)

hkl	2θ (deg) Observed[a]	2θ (deg) Calculated[b]	Line Intensity Observed[a]	Line Intensity Calculated[c]
225 α_1	136.60	136.53	6.0 broad	0.7
741 α_1		136.58		0.6
173 α_1		136.74		0.1
524 α_1		136.77		0.6
225 α_2	137.45	137.25	4.0	0.3
741 α_2		137.30		0.3
173 α_2		137.46		0.04
524 α_2		137.49		0.3
035 α_1		137.57		0.4
732 α_1	138.40	138.15	3.5 broad	0.3
035 α_2		138.31		0.2
562 α_1		138.46		0.3
082 α_1		138.54		0.2
182 α_1	141.00	140.87	4.5 broad	0.3
820 α_1		141.05		0.4
652 α_1		141.19		0.5
182 α_2	141.94	141.67	1.8 broad	0.1
820 α_2		141.86		0.2
652 α_2		142.00		0.2
354 α_1	143.44	143.28	4.5 broad	0.5
381 α_1		143.41		0.5
354 α_2	144.24	144.15	2.5 broad	0.3
381 α_2		144.28		0.2

Table 2. (continued)

hkl	2θ (deg) Observed[a]	2θ (deg) Calculated[b]	Line Intensity Observed[a]	Line Intensity Calculated[c]
164 α_1	148.19	148.20	3.3 broad	0.6
571 α_1	150.73	150.59	6.0 broad	0.8
643 α_1		150.79		0.8
571 α_2	151.83	151.69	4.0 broad	0.4
643 α_2		151.90		0.4
480 α_1	157.97	157.83	4.0 broad	0.6
802 α_1		158.10		0.4
723 α_1	159.47	158.84	3.0 broad	0.3
480 α_2		159.33		0.3
802 α_2		159.62		0.2
751 α_1		159.72		0.3
373 α_1		159.83		0.1

[a] Two independent observers' averaged readings (2θ values are ± 0.10°) and averaged intensities on a scale from 10 to 0.

[b] Based on the orthorhombic lattice parameters a_o = 6.7162 A, b_o = 7.1031 A, c_o = 4.4084 A, and $\lambda(\bar{\alpha})$ = 1.54178 A, $\lambda(\alpha_1)$ = 1.54051 A, and $\lambda(\alpha_2)$ = 1.54433 A.

[c] Calculated using the POWD intensity program,[8] assuming the atomic coordinates of YF_3[4] for those of BkF_3, and scaled such that the most intense line had I = 10.0.

Table 3. Line list and indexing for LaF_3-type trigonal BkF_3 (JP-VII, Film 2691A).

hkl	2θ (deg) Observed[a]	2θ (deg) Calculated[b]	Line Intensity Observed[a]	Line Intensity Calculated[c]
002	24.84	24.88	8.0	3.5
110	25.44	25.49	7.0	2.5
111	28.44	28.42	10.0	10.0
112	35.84	35.92	5.5	1.3
300	44.92	44.92	9.0	3.4
113	46.02	46.06	9.0	4.3
004	51.12	51.05	4.0	0.5
302	52.02	52.03	8.0	3.1
220		52.35		0.3
221	54.02	54.01	7.5	1.9
114	57.82	57.90	4.0	0.5
222	58.72	58.80	4.0	0.4
223	66.22	66.30	7.0	1.3
304	70.30	70.32	6.0	1.2
115	71.20	71.18	6.0	0.8
410		71.41		0.3
411	72.80	72.80	7.0	1.6
224	76.20	76.14	3.0	0.2
412	76.80	76.94	3.0	0.4
006	80.50	80.53	1.5	0.2
330	82.80	82.86	3.0	0.5
413	83.70	83.68	6.5	1.4
116	86.20	86.14	4.0 broad	0.2

Table 3. (continued)

hkl	2θ (deg) Observed[a]	2θ (deg) Calculated[b]	Line Intensity Observed[a]	Line Intensity Calculated[c]
332	88.20	88.20	7.0	0.8
225		88.24		0.5
414 α_1	92.90	92.91	4.0	0.2
306 α_1	97.18	97.21	5.0	0.5
600 α_1	99.58	99.54	3.5	0.2
117 α_1	103.48	103.44	3.0	0.3
334 α_1	104.18	104.18	3.0	0.4
602 α_1	104.98	104.98	6.0	0.4
415 α_1		105.02		0.6
602 α_2	105.38	105.35	4.0	0.2
415 α_2		105.39		0.3
521 α_1	106.58	106.62	5.0	0.6
521 α_2	107.08	107.00	3.0	0.3
522 α_1	110.78	110.83	2.0	0.2
523 α_1	118.08	118.12	6.0	0.7
523 α_2	118.58	118.60	4.0	0.3
416 α_1	120.98	120.93	1.5	0.3
227 α_1	121.56	121.59	3.0	0.3
604 α_1	122.36	122.44	3.0	0.5
441 α_1	125.16	125.27	4.0	0.4
118 α_1		125.44		0.1
441 α_2	125.96	125.83	2.0	0.2
118 α_2		126.00		0.1

Table 3. (continued)

hkl	2θ (deg) Observed[a]	2θ (deg) Calculated[b]	Line Intensity Observed[a]	Line Intensity Calculated[c]
524 α_1	129.36	129.31	3.5	0.2
524 α_2	130.06	129.92	1.5	0.1
336 α_1	135.06	135.10	4.0	0.6
443 α_1	139.76	139.71	3.5	0.5
308 α_1	140.66	140.73	5.0	0.6
308 α_2	141.66	141.53	3.0	0.3
417 α_1	144.56	144.61	6.0	1.1
417 α_2	145.56	145.51	4.0	0.5
525 α_1	147.26	147.36	6.0	1.2
525 α_2	148.36	148.34	4.0	0.6
711 α_1	150.24	150.33	6.0	1.3
711 α_2	151.44	151.43	4.0	0.6
444 α_1	157.74	157.67	2.5	0.3
712 α_1	159.84	159.79	3.0	0.6
712 α_2	161.44	161.45	1.5	0.3

[a] A single reading of the powder pattern (2θ readings are ± 0.10°). Observed intensities are on a scale of 10 to 0 and may be in error due to the presence of a second phase (orthorhombic BkF_3).

[b] Based on the trigonal lattice parameters a_o = 6.9899 A, c_o = 7.1566 A and $\lambda(\bar{\alpha})$ = 1.54178 A, $\lambda(\alpha_1)$ = 1.54051 A, and $\lambda(\alpha_2)$ = 1.54433 A.

[c] Calculated using the POWD intensity program,[8] assuming the atomic coordinates of LaF_3[3] for those of BkF_3, and scaled such that the most intense line had I = 10.0.

Table 4. Lattice parameters and ionic radii derived from the lanthanide and actinide trifluorides.

Trifluoride	Structure Type	Lattice Parameters (A) a_o	b_o	c_o	Reference	M^{3+} Ionic Radius[a] (A) (CN=6)
La	LaF_3	7.186		7.352	10	1.006
Ce	LaF_3	7.112		7.279	7	0.982
Pr	LaF_3	7.075		7.238	11	0.968
Nd	LaF_3	7.030		7.200	10	0.955
Pm	LaF_3	6.970		7.188	12	0.945
Sm	YF_3	6.669	7.059	4.405	4	0.921
Eu	YF_3	6.622	7.019	4.396	4	0.909
Gd	YF_3	6.570	6.984	4.393	4	0.900
Tb	YF_3	6.513	6.949	4.384	4	0.888
Dy	YF_3	6.460	6.906	4.376	4	0.877
Ho	YF_3	6.404	6.875	4.379	4	0.868
Er	YF_3	6.354	6.846	4.380	4	0.860
Tm	YF_3	6.283	6.811	4.408	4	0.855
Yb	YF_3	6.216	6.786	4.434	4	0.851
Lu	YF_3	6.151	6.758	4.467	4	0.848
Ac	LaF_3	7.41		7.55	13	1.076
U	LaF_3	7.181		7.348	13	1.005
Np	LaF_3	7.129		7.288	13	0.986
Pu	LaF_3	7.093		7.254	13	0.974

Table 4. (Continued)

Trifluoride	Structure Type	Lattice Parameters (A) a_o	b_o	c_o	Reference	M^{3+} Ionic Radius[a] (A) (CN=6)
Am	LaF_3	7.044		7.225	14	0.962
Cm	LaF_3	6.999		7.179	14	0.946
Bk	LaF_3	6.97		7.14	This Work	0.935
Bk	YF_3	6.70	7.09	4.41	This Work	0.928
Cf	YF_3	6.653	7.041	4.395	6	0.915

[a]Calculated according to the following formula:

Ionic Radius = (Weight - averaged M-F bond distance) - 1.33 - 0.11

where the fluoride ionic radius is taken to be 1.33 A[13] and the 9-fold to 6-fold coordination correction number is taken to be 0.11 A.[13]

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