solvated $Yb(C_5H_7O_2)_3(H_2O)$ structure,[3] and confidence in the reality of such features of the polyhedron as the deviations of the ytterbium atom from the mean planes of the ligands may be obtained by comparing the two structures.

The benzene molecule is centered on the center of symmetry at 0, $^1/_2$, $^1/_2$. The mean deviation of the carbon atoms from the mean plane of the benzene ring is 0.019 Å, and the sum of the interior angles of the ring is 719.6°. Discrepancies in the carbon–carbon bond lengths (Table III) of several standard deviations must be interpreted as indicative of systematic errors in the data, such as uncorrected adsorption, rather than as implying any actual distortion of the molecule. The shortest distance between a benzene carbon atom and another carbon or oxygen atom is 3.53 Å for the CB(1)–O(4) contact.

The volume occupied by two tris(acetylacetonato)-aquoytterbium(III) molecules in the unsolvated structure[3] is 931.8 Å^3. The molecular volume of benzene, based on the density of the liquid at 25°, is 147.6 Å^3. The sum of these volumes is 1079.4 Å^3, as compared with a unit cell volume of 1077.9 Å^3 in the crystal structure of the benzene solvate. These figures suggest that the efficiency of packing of the molecules is about the same for the solvated and unsolvated structures.

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The Crystal Structure of Ammonium Hexafluorocerate(IV), $(NH_4)_2CeF_6$[1]

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Received June 5, 1968

The crystal structure of ammonium hexafluorocerate(IV), $(NH_4)_2CeF_6$, has been determined from counter measurements of 561 reflections and refined by full-matrix least squares to an R factor of 0.032. The space group is Pbcn (no. 60); D_x = 3.05 and D_m = 3.05 ± 0.02 g/cm^3. The unit cell has dimensions a = 7.026 (3), b = 12.098 (6), and c = 7.439 (8) Å; Z = 4. Of the 561 reflections measured, 389 were judged to be observed. The structure consists of infinite chains of eightfold coordinated cerium atoms parallel to the c axis, joined by NH_4^+ ions. The fluorine configuration about the Ce can be roughly described as a square antiprism. The average Ce–F distance is 2.26 Å and the average F–F distance for nearest neighbors within an antiprism is 2.77 Å. Hydrogen bonding causes this particular structure to be stabilized over the trigonal-dodecahedral arrangement found in the similar Rb_2UF_6 and K_2ZrF_6 compounds.

Introduction

The preparation of ammonium hexafluorocerate(IV) was first reported by Besse and Capestan,[2] who indexed the powder pattern on the basis of a cubic cell with a' = 10.52 Å and claimed a measured density of 3.27 g/cm^3. For Z = 8, D_x = 3.31 g/cm^3 for this cell. Penneman[3] of this laboratory noticed that these values for the volume and Z give a very low value for the fluorine volume, as compared to similar actinide fluoride compounds. Further, there is no evidence for cubic phases of any other 2:1 NH_4F–actinide(IV) fluoride complexes. He was therefore prompted to prepare this material. Optical examination showed single crystals of $(NH_4)_2CeF_6$ to be biaxial and thus this compound must have orthorhombic or lower symmetry. Subsequent examination of precession films showed the symmetry to be orthorhombic with cell dimensions which are nearly those which would permit indexing of powder data on the basis of the cubic cell of Besse and Capestan,[2] *i.e.*, $a'/a = {}^3/_2$, $a'/b = \sqrt{3}/2$, and $a'/c = \sqrt{2}$.

The single-crystal X-ray investigation of this compound was undertaken for three reasons: (1) No compound of known structure could be found with which it is isostructural. (2) Comparison of the powder patterns indicated it is isostructural with the α phase of $(NH_4)_2UF_6$ for which no single crystals were then available. (Subsequent comparisons of single-crystal data, when they became available, confirmed that the two compounds were indeed isostructural. This is of interest because of the existence of four closely related polymorphs for $(NH_4)_2UF_6$ over a narrow temperature range[4] (~70°), and the elucidation of these structures should provide information concerning the energy relationships between some of the possible coordination polyhedra for uranium.) (3) It is also of interest that after extensive investigation the only phase to be found for the Ce compound is the α phase. It is hoped that the knowledge of this structure plus the structure of the γ-$(NH_4)_2UF_6$ (room-temperature stable phase) compound currently being worked on will provide some information concerning these questions.

Experimental Section

Crystals were prepared by cooling a saturated solution of $(NH_4)_2CeF_6$ in a 15% NH_4F–H_2O solution. A needlelike crystal was selected and cut to a length suitable for examination by X-

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[1] This work was sponsored by the U. S. Atomic Energy Commission.

[2] J. P. Besse and M. Capestan, *Bull. Soc. Chim. France*, 577 (1966).

[3] R. A. Penneman, unpublished results, to be submitted for publication.

[4] R. A. Penneman, F. H. Kruse, R. S. George, and J. S. Coleman, *Inorg. Chem.*, **3**, 309 (1964).

ray methods. The resulting 0.19 × 0.11 × 0.07 mm crystal was mounted on the a axis and was coated with Fluorolube to arrest an apparent slow decomposition which took place upon contact of the material with air. The faces whose normals were perpendicular to the needle direction were of the prism $\{011\}$.

Precession photographs taken with Mo Kα radiation showed orthorhombic symmetry with the following systematic extinctions: $0kl$ reflections, k odd; $h0l$ reflections, l odd; $hk0$ reflections, $h + k$ odd. The space group is thus uniquely Pbcn (no. 60), D_{2h}^{14}. The cell constants at room temperature were obtained by least-squares calculations from 13 high-order reflections measured with a carefully aligned single-crystal orienter on a General Electroc Co. XRD-5 diffraction unit using Mo Kα_1 radiation [λ(MoKα_1) 0.70930 Å]. The cell constants are $a = 7.026$ (3), $b = 12.098$ (6), and $c = 7.439$ (8) Å, where the figure in parentheses is the least-squares standard error of the least significant digit. The calculated density with $Z = 4$ is 3.05 g/cm^3; the density measured by flotation methods in mixtures of diiodomethane and dibromomethane was 3.05 ± 0.02 g/cm^3. Four molecules per unit cell for this space group demand twofold or inversion symmetry for the cerium atom position.

ω scans through several reflections showed the crystal mosaicity was sufficiently low. Intensities of reflections with $2\theta \leq 45°$ for hkl planes were measured using Mo Kα radiation, Zr–Y balanced filters, takeoff angle of 5°, the stationary-crystal, stationary-counter mode, and a counting time of 20 sec with each filter. A few reflections from $hk\bar{l}$ planes were measured in order to have data to check the absorption correction. The counting rates were such that attenuation of the primary beam was unnecessary. Because of decomposition of the sample, the tube current was adjusted during the course of the data collection to keep the count for a standard reflection within 1% of its starting value. Without this adjustment the intensity of the standard reflection would have decreased by approximately 10% during the course of the data collection process. The crystal was checked periodically for misalignment and centering. Of the 561 reflections measured, 389 were observed according to the criterion $I > 3\sigma(I)$. The standard deviation, $\sigma(I)$, of the corrected intensity, I, was estimated from

$$\sigma(I) = [T + B + B']^{1/2}$$

where T is the total count, $I = T - (B + B')$, B is the background as measured at the reflection with the Y filter, and B' is the background taken from an empirical 2θ-dependent background curve. The empirical curve was determined by averaging the background at a given 2θ value and several values of χ and Φ for which the Bragg condition was not satisfied. The absorption correction was made by the Busing and Levy[5] method using Burnham's[6] program modified for single-crystal orienter geometry.[7] The linear absorption coefficient is 73.2 cm^{-1} and the calculated transmission factors vary from 0.561 to 0.626.

Solution and Refinement of the Structure

The position of the cerium atoms was determined from the Patterson map to be 0, 0.04, $^1/_4$ and was refined by least-squares methods to be 0, 0.0414, $^1/_4$. The structure is C-centered if only the cerium atoms are considered so that a Fourier map phased on the cerium showed a false twofold rotation axis at $y = {}^1/_2$, $z = {}^1/_2$. Since there were four atoms whose positions were unknown, there were 2^4 ways to choose the structure from the difference Fourier map. Although some of the models were slightly less desirable from a chemical point of view, the proximity of the peaks was such that none of the possible structures could be rejected on the basis of chemical evidence alone. Phasing the difference map on the C-centered cerium atom leaves one degree of freedom in fixing the origin so that the choice between two of the peaks is arbitrary. This arbitrary choice was made for F(3) and the remaining eight models were refined using anisotropic temperature factors on the cerium atom only. The nitrogen atom always refined to the same position no matter which of the two possible peaks was chosen as the starting position. Of the remaining four models, three had a conventional unweighted R factor

$$R = \frac{\sum\big||F_o| - |F_c|\big|}{\Sigma|F_o|}$$

of 0.060 and for the remaining model the R factor was 0.035. The corresponding weighted R' factors

$$R' = \frac{\sum w_i\big||F_o| - |F_c|\big|}{\Sigma w_i|F_o|}$$

were 0.050 and 0.033. The difference in R factors plus statistical tests on the ratio of the square roots of the weighted residuals[8] dictated the choice of the correct model.

The full-matrix least-squares refinement of all nonhydrogen positions and temperature factors was carried out using a newly developed program.[9] The quantity minimized was $\Sigma w_i(F_o - KF_c)_i{}^2$, where w_i is $1/\sigma^2(F_o)$.[10] Scattering factors given in the "International Critical Tables for X-Ray Crystallography," 1962, were used for fluorine and nitrogen atoms. Cromer and Waber's[11] scattering factors and Cromer's[12] anomalous dispersion terms were used for cerium. The final R with all atoms having isotropic factors was 0.059 (0.051), the R with only the cerium atom anisotropic was 0.035 (0.032), and the R with all atoms with anisotropic temperature factors was 0.032 (0.030), where the values in parentheses are the weighted R' factors. Hamilton's[8] significance tests reject the hypothesis that all atoms are isotropic at the 0.005 significance level while the hypothesis that only the cerium atoms are anisotropic can be rejected at the 0.10 level. There was no evidence of extinction effects. The final coordinates and temperature factors are listed in Tables I and II.

A final difference Fourier map showed residual electron densities which were centered around the cerium positions and ranged in value from -0.5 to $+ 1.5$ e/Å^3. The largest peaks elsewhere were about 0.5 e/Å^3 with $\sigma(\rho) = 0.8$ e/Å^3. None of these peaks was in a chemically reasonable position for a hydrogen atom.

Table III contains the observed and calculated structure factors.

Discussion

The cerium atoms are in the special positions (2c) surrounded by eight fluorine atoms in the conformation

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(5) W. R. Busing and H. A. Levy, *Acta Cryst.*, **10**, 180 (1957).

(6) C. W. Burnham, IUC World List of Crystallographic Computer Programs, Program 338, 1962.

(7) A. C. Larson, D. T. Cromer, and R. B. Roof, Jr., Report LA-3043, Los Alamos Scientific Laboratory, 1964.

(8) W. C. Hamilton, *Acta Cryst.*, **18**, 502 (1965).

(9) A. C. Larson, unpublished work.

(10) H. T. Evans, *Acta Cryst.*, **14**, 371 (1961).

(11) D. T. Cromer and J. T. Waber, *ibid.*, **18**, 104 (1965).

(12) D. T. Cromer, *ibid.*, **18**, 17 (1965).

TABLE I
FRACTIONAL COORDINATES AND LEAST-SQUARES STANDARD ERRORS

atom	x	y	z
Ce	.0 (0)	.0414(1)	.25 (0)
N	.0168(31)	.3430(10)	.4976(16)
F(1)	.2089(12)	.4816(8)	.2019(12)
F(2)	.1885(12)	.1868(7)	.2867(14)
F(3)	.9538(13)	.0979(7)	.5444(11)

TABLE II
ANISOTROPIC TEMPERATURE FACTORS AND STANDARD ERRORS ($\times 10^4$)[a]

Atom	$\beta_{11} \times 10^4$	$\beta_{22} \times 10^4$	$\beta_{33} \times 10^4$	$\beta_{12} \times 10^4$	$\beta_{13} \times 10^4$	$\beta_{23} \times 10^4$
Ce	37 (2)	30 (1)	40 (2)	0 (0)	5 (7)	0 (0)
N	63 (30)	38 (8)	72 (21)	-12 (41)	-24 (72)	-12 (23)
F (1)	64 (17)	37 (8)	127 (23)	-43 (22)	-33 (34)	29 (20)
F (2)	95 (19)	36 (6)	97 (27)	-46 (19)	-13 (35)	-10 (19)
F (3)	128 (28)	29 (6)	33 (14)	8 (20)	9 (31)	2 (16)

[a] Anisotropic temperature factors are defined by $\exp[-(\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}l^2 + \beta_{12}hk + \beta_{13}hl + \beta_{23}kl)]$.

TABLE III
OBSERVED AND CALCULATED STRUCTURE FACTORS
(COLUMN HEADINGS ARE k, l, F_o/K, $|F_c|$)

0	2	200	207
0	4	240	238
0	6	107	110
0	8	64	81
2	0	193	207
2	1	115	116
2	2	177	175
2	3	146	141
2	4	131	127
2	5	48	45
2	6	105	103
2	7	68	72
2	8	67	68
4	0	68	71
4	1	70	76
4	2	177	174
4	3	116	115
4	4	36	35
4	5	84	83
4	6	63	61
4	7	98	99
4	8	41	40
6	0	33	31
6	1	162	164
6	2	32	32
6	3	129	129
6	4	23	24
6	5	132	131
6	6	<11	11
6	7	90	84
6	8	<11	9
8	0	68	70
8	1	103	100
8	2	74	73
8	3	72	74
8	4	37	37
8	5	105	101
8	6	47	44
8	7	61	59
10	0	58	38
10	1	23	25
10	2	77	74
10	3	31	31
10	4	64	68
10	5	43	40
10	6	56	53
12	0	66	65
12	1	<11	2
12	2	88	88
12	3	13	14
12	4	61	61
14	0	71	68
14	1	45	44
14	2	61	56
H = 1			
0	2	<10	2
0	4	17	15
0	6	<11	9
0	8	<12	0
1	0	212	225
1	1	71	68
1	2	174	166
1	3	91	77
1	4	157	150
1	5	23	23
1	6	123	127
1	7	36	36
1	8	73	77
2	1	< 8	7
2	2	43	41
2	3	41	38
2	4	46	30
2	5	18	18
2	6	23	26
2	7	12	11
2	8	<12	13
3	0	143	131
3	1	112	116
3	2	72	79
3	3	142	141
3	4	112	112
3	5	66	64
3	6	70	67
3	7	57	66
3	8	72	70
4	1	< 8	10
4	2	27	27
4	3	11	6
4	4	19	16
4	5	10	10
4	6	19	19
4	7	<11	10
4	8	<11	2
5	0	<10	3
5	1	158	157
5	2	83	87
5	3	142	141
5	4	22	22
5	5	113	110
5	6	31	30
5	7	93	91
5	8	30	29
6	1	16	18
6	2	< 9	7
6	3	10	22
6	4	< 9	5
6	5	21	23
6	6	<10	4
6	7	14	13
7	0	73	76
7	1	137	137
7	2	12	16
7	3	106	110
7	4	47	47
7	5	121	120
7	6	16	16
7	7	73	67
8	1	13	12
8	2	15	16
8	3	11	10
8	4	23	23
8	5	<11	11
8	6	16	16
8	7	<12	7
9	0	59	55
9	1	82	81
9	2	102	105
9	3	59	60
9	4	52	54
9	5	74	72
9	6	63	61
10	1	<10	3
10	2	<10	5
10	3	<10	1
10	4	<10	1
10	5	<10	1
10	6	<12	6
11	0	67	66
11	1	28	28
11	2	94	93
11	3	30	32
11	4	65	67
11	5	17	15
12	1	<11	3
12	2	<11	1
12	3	17	15
12	4	<10	2
13	0	83	83
13	1	17	17
13	2	66	62
13	3	<11	6
14	1	<11	2
H = 2			
0	0	207	195
0	2	41	45
0	4	162	160
0	6	104	107
0	8	96	98
1	1	< 9	2
1	2	31	31
1	3	21	20
1	4	< 9	8
1	5	15	15
1	6	21	24
1	7	<11	5
1	8	<11	1
2	0	148	146
2	1	64	64
2	2	144	142
2	3	95	94
2	4	126	122
2	5	78	76
2	6	111	110
2	7	61	63
2	8	73	75
3	1	27	29
3	2	9	4
3	3	11	3
3	4	< 9	1
3	5	<10	11
3	6	<10	6
3	7	<11	8
3	8	<11	2
4	0	< 9	6
4	1	189	186
4	2	99	98
4	3	167	166
4	4	40	40
4	5	99	97
4	6	63	63
4	7	87	86
4	8	45	46
5	1	11	12
5	2	< 9	8
5	3	< 9	3
5	4	32	36
5	5	11	11
5	6	<10	3
5	7	<11	3
5	8	16	14
6	0	48	44
6	1	152	150
6	2	28	20
6	3	117	117
6	4	<10	3
6	5	113	0
6	6	<11	10
6	7	80	76
7	1	17	19
7	2	< 9	2
7	3	< 9	6
7	4	<10	6
7	5	<11	9
7	6	<11	4
7	7	<11	6
8	0	54	47
8	1	123	124
8	2	84	83
8	3	84	86
8	4	42	44
8	5	95	93
8	6	38	38
8	7	60	54
9	1	<10	4
9	2	<10	5
9	3	15	18
9	4	<10	6
9	5	<11	9
9	6	<11	5
10	0	89	91
10	1	64	72
10	2	94	94
10	3	56	57
10	4	76	80
10	5	46	43
11	1	<11	6
11	2	<11	9
11	3	<11	3
11	4	<11	1
11	5	<11	2
12	0	74	69
12	1	<11	2
12	2	90	87
12	3	<11	6
12	4	62	62
13	1	<11	6
13	2	<11	3
13	3	<11	2
H = 3			
0	2	30	28
0	4	10	11
0	8	<11	8
1	0	196	193
1	1	< 9	3
1	2	170	166
1	3	21	25
1	4	130	131
1	5	17	16
1	6	109	111
1	7	29	31
1	8	69	71
2	1	15	17
2	2	24	26
2	3	12	12
2	4	20	17
2	5	18	16
2	6	20	20
2	7	<11	6
2	8	<11	4
3	0	203	200
3	1	116	113
3	2	143	140
3	3	118	120
3	4	128	126
3	5	73	72
3	6	66	64
3	7	74	76
3	8	61	62
4	1	18	12
4	2	< 9	2
4	3	< 9	5
4	4	27	29
4	5	<10	2
4	6	<11	2
4	7	<11	2
5	0	<10	5
5	1	144	138
5	2	48	49
5	3	128	127
5	4	15	17
5	5	105	106
5	6	22	24
5	7	86	86
6	1	<10	7
6	2	< 9	6
6	3	17	19
6	4	15	15
6	5	<10	7
6	6	<11	8
6	7	<11	3
7	0	28	28
7	1	92	92
7	2	< 9	6
7	3	77	80
7	4	29	29
7	5	94	97
7	6	14	14
7	7	73	71
8	1	<10	7
8	2	<10	9
8	3	15	15
8	4	<11	6
8	5	<11	8
8	6	<12	9
9	0	38	39
9	1	82	83
9	2	71	75
9	3	63	68
9	4	43	46
9	5	69	68
9	6	57	56
10	1	<10	2
10	2	12	6
10	3	<11	5
10	4	<11	9
10	5	<11	0
11	0	77	79
11	1	<11	10
11	2	91	92
11	3	21	18
11	4	67	69
12	1	<11	9
12	2	<11	1
12	3	<11	3
13	0	52	62
13	1	26	25
13	2	48	47
H = 4			
0	0	214	212
0	2	143	131
0	4	152	148
0	6	88	92
1	1	16	15
1	2	< 9	9
1	3	10	10
1	4	37	39
1	5	<11	11
1	6	<11	3
1	7	15	15
2	0	154	145
2	1	69	67
2	2	143	141
2	3	76	74
2	4	105	106
2	5	49	49
2	6	89	89
2	7	68	51
3	1	21	19
3	2	< 9	4
3	3	24	26
3	4	<10	5
3	5	<10	8
3	6	<11	0
4	0	65	60
4	1	109	108
4	2	96	93
4	3	106	107
4	4	48	49
4	5	86	87
4	6	50	52
4	7	75	77
5	1	<10	2
5	2	30	31
5	3	31	21
5	4	<10	9
5	5	11	8
5	6	28	31
5	7	<11	11
6	0	19	18
6	1	114	113
6	2	<10	3
6	3	101	103
6	4	12	12
6	5	99	98
6	6	<11	8
7	1	16	19
7	2	<10	8
7	3	15	15
7	4	<10	2
7	5	<11	1
7	6	<11	8
8	0	43	46
8	1	86	87
8	2	50	48
8	3	76	77
8	4	41	43
8	5	78	78
9	1	18	18
9	2	<11	5
9	3	<10	7
9	4	<11	9
9	5	14	17
10	0	74	77
10	1	34	37
10	2	68	69
10	3	38	37
10	4	66	69
11	1	<11	7
11	2	<11	1
11	3	<12	9
12	0	65	62
12	1	<12	3
12	2	71	72
H = 5			
0	2	<10	4
0	4	24	27
0	6	<12	9
1	0	112	107
1	2	121	119
1	3	48	48
1	4	100	101
1	5	31	31
1	6	93	99
1	7	23	21
2	1	29	28
2	2	<10	3
2	3	18	18
2	4	<10	5
2	5	<11	8
2	6	<11	6
3	0	56	60
3	1	90	89
3	2	43	41
3	3	82	82
3	4	70	73
3	5	67	67
3	6	52	56
4	1	< 9	3
4	2	<10	12
4	3	14	11
4	4	<10	8
4	5	<11	10
4	6	<11	12
5	0	28	27
5	1	113	114
5	2	35	35
5	3	101	103
5	4	26	27
5	5	88	87
5	6	25	27
6	1	14	11
6	2	<10	10
6	3	11	6
6	4	<11	6
6	5	<11	3
6	6	<12	11
7	0	49	51
7	1	121	124
7	2	30	29
7	3	99	105
7	4	34	34
7	5	84	85
8	1	<11	10
8	2	<10	3
8	3	<11	1
8	4	<11	0
8	5	<11	3
9	0	64	65
9	1	60	61
9	2	75	76
9	3	53	55
9	4	31	52
10	1	<11	5
10	2	<11	3
10	3	<11	1
11	0	62	61
11	1	29	29
11	2	64	63
H = 6			
0	0	136	141
0	2	116	117
0	4	117	116
1	1	<10	0
1	2	20	21
1	3	<11	5
1	4	<11	9
1	5	<11	10
1	6	20	21
2	0	87	86
2	1	68	67
2	2	94	95
2	3	53	57
2	4	80	80
2	5	49	49
2	6	72	76
3	1	17	16
3	2	<10	3
3	3	<10	2
3	4	<11	8
3	5	<11	6
4	0	50	52
4	1	85	85
4	2	57	60
4	3	77	79
4	4	45	44
4	5	72	73
5	1	12	11
5	2	<10	4
5	3	<11	2
5	4	22	26
5	5	<12	12
6	0	18	19
6	1	107	107
6	2	<11	2
6	3	92	97
6	4	14	12
7	1	<12	14
7	2	<11	1
7	3	12	10
7	4	12	9
8	0	50	48
8	1	74	74
8	2	47	46
8	3	69	70
9	1	<11	5
9	2	<11	4
H = 7			
0	2	<12	11
0	4	<11	2
1	0	103	105
1	1	19	20
1	2	111	115
1	3	17	18
1	4	81	84
2	1	<11	14
2	2	<11	3
2	3	<12	17
2	4	<11	9
3	0	99	100
3	1	65	67
3	2	75	75
3	3	60	60
3	4	73	75
4	1	<12	3
4	2	<11	5
4	3	<11	7
5	0	33	35
5	1	84	85
5	2	20	26
5	3	78	81
6	1	<11	8
6	2	<11	2
6	3	<11	1
7	0	14	17
7	1	64	66
7	2	12	11
H = 8			
0	0	73	74
0	2	70	73
1	1	<12	3
1	2	<11	3
2	0	73	75
2	1	37	39
2	2	76	80
3	1	<11	3
4	0	39	37

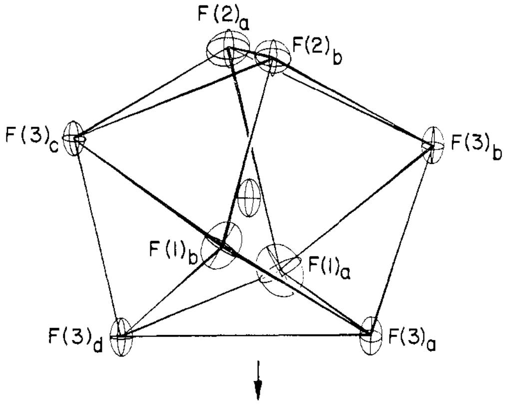

Figure 1.—Coordination around the Ce atom. The arrow indicates the twofold axis. Elipsoids are 3 times the rms amplitude.

of a slightly distorted square antiprism (see Figure 1). Each antiprism shares two fluorine atoms with each of the two neighboring antiprisms to form infinite chains in the direction of the c axis. Pertinent interatomic distances are given in Table IV. The average value of l/s for the F–F distance is 1.045, where s is the average distance between nearest atoms in the square of the antiprism and l is the average distance between nearest atoms in different squares.[13] This value is very close to the value of 1.057 for a "most favorable" antiprism as calculated by Hoard and Silverton[13] using a "neon shell" model for the ligands.

TABLE IV
INTERATOMIC DISTANCES IN $(NH_4)_2CeF_6$

Ce - F(1)	2.198 (8)	N - F' (1)	2.74 (2)
Ce - F(2)	2.219 (8)	N - F'' (1)	2.94 (2)
Ce - $\mathrm{F(3)_a}$	2.298 (8)	N - F' (2)	2.83 (2)
Ce - $\mathrm{F(3)_a}$	2.318 (8)	N - F (2)	2.74 (2)
$\mathrm{F(1)_a}$ - $\mathrm{F(2)_a}$	2.66 (1)	$\mathrm{F(2)_a}$ - $\mathrm{F(2)_b}$	2.70 (2)
$\mathrm{F(1)_a}$ - $\mathrm{F(3)_a}$	2.81 (1)	$\mathrm{F(2)_a}$ - $\mathrm{F(3)_b}$	2.87 (1)
$\mathrm{F(1)_a}$ - $\mathrm{F(3)_b}$	2.73 (1)	$\mathrm{F(2)_a}$ - $\mathrm{F(3)_c}$	2.75 (1)
$\mathrm{F(1)_a}$ - $\mathrm{F(3)_d}$	2.88 (1)	$\mathrm{F(3)_a}$ - $\mathrm{F(3)_b}$	2.54 (2)
		$\mathrm{F(3)_a}$ - $\mathrm{F(3)_d}$	3.12 (2)
F'(1) - N - F''(1)	96.0 (.5)	F''(1) - N - F'(2)	99.9 (.5)
F'(1) - N - F'(2)	85.0 (.5)	F''(1) - N - F(2)	126.4 (.8)
F'(1) - N - F(2)	111.5 (.5)	F(2) - N - F'(2)	126.6 (.5)

The nitrogen atom has four fluorine neighbors at distances of 2.74–2.94 Å plus five neighbors at distances of 3.02–3.18 Å. The six angles associated with the four shortest distances have an average value of 107.6°, which suggests that the hydrogen atoms lie near these N–F vectors.

It should also be noted that the fluorines bonded to only one cerium have the principal axis of their thermal ellipsoids tangent to the coordination polyhedron. For the shared fluorines the principal axis is perpendicular to the chaining direction. These are just the directions for which one would expect the largest vibrational amplitudes. The principal root-mean-square amplitudes of vibration for the atoms are shown in Table V.

This structure is, in its over-all features, very simi-

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(13) J. L. Hoard and J. V. Silverton, *Inorg. Chem.*, **2**, 235 (1963).

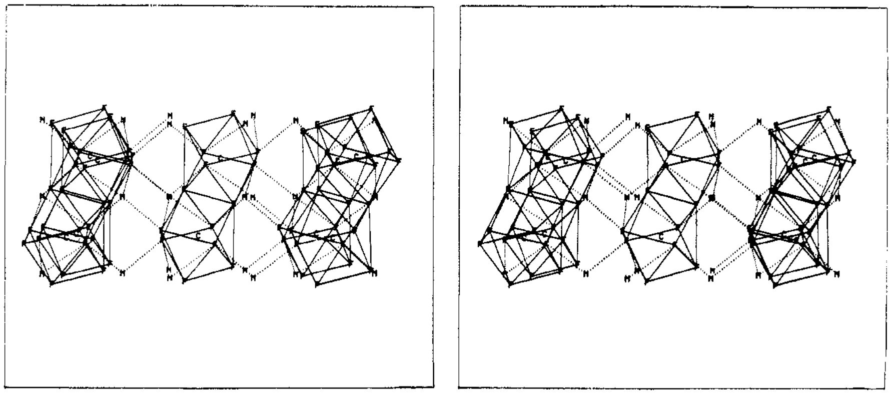

Figure 2.—Stereoview of the structure looking down the *a* axis, with the *c* direction toward the top of the picture. C indicates the Ce position.

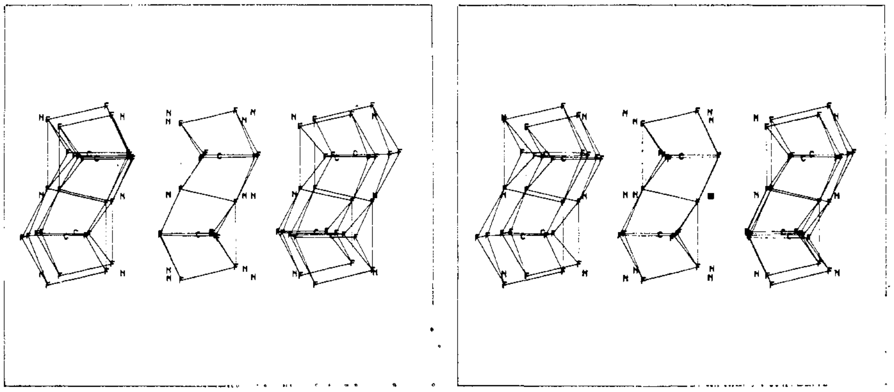

Figure 3.—Stereoview of the closely related Rb_2UF_6 structure[15] with the same orientation as Figure 2. N indicates an Rb position and C indicates a uranium position.

TABLE V

PRINCIPAL ROOT-MEAN-SQUARE AMPLITUDES

	Minimum	Intermediate	Maximum
Ce	.71	.89	1.78
N	1.05	1.72	2.29
F(1)	1.01	2.49	3.90
F(2)	1.14	2.19	2.78
F(3)	.73	1.70	2.55

lar to that of both K_2ZrF_6[14] and Rb_2UF_6,[15] the principal difference being in the coordination polyhedra making up the chains. In the latter two compounds the coordination polyhedra can best be described as somewhat distorted trigonal dodecahedra. Comparison of Figures 2 and 3 shows that distortion from what would be a trigonal dodecahedron in this structure to the existing antiprism is just that necessary to make maximum use of H···F bonding of the fluorines to the ammonium ions.

Acknowledgment.—Acknowledgment is due Dr. D. T. Cromer for his generous assistance and advice, as well as Dr. R. A. Penneman for the preparation of the compound.

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(14) H. Bode and G. Teufer, *Acta Cryst.*, **9**, 929 (1956).

(15) F. H. Kruse, to be submitted for publication.