

interplanar distance between pairs of hypoxanthine ligands related by a screw axis is 3.41 Å. The overlap is seen to be extensive (Fig. 3).

The methyl group is found to be almost exactly eclipsed relative to C(8)-H(8), the H(8)···H(93) distance being only 2.3 Å. There are no other short intra- or intermolecular H···H contacts in the structure.

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Preparation and Single-Crystal Structure of β -NH₄UF₅, Ammonium Pentafluorouranate(IV)

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The single-crystal structure of β -NH₄UF₅ has been determined by a three-dimensional X-ray study. It belongs to space group *P2₁/c*, with dimensions $a = 7.799$ (5), $b = 7.158$ (5), $c = 8.762$ (7) Å, $\beta = 116.45$ (5)°, $Z = 4$, $V = 437.9$ Å³, $d_{\text{calc}} = 5.32$, $d_{\text{obs}} = 5.3$ g cm⁻³. Full-matrix least-squares treatment of 1325 observed intensities, measured by counting techniques, gave an unweighted *R* value of 0.036, all atoms having anisotropic thermal parameters. The structure is composed of infinite sheets of equivalent UF₅ polyhedra, running parallel to the (100) plane. One fluorine in each polyhedron is unshared, projecting alternatively toward adjacent sheets, but not connecting them. Ammonium ions bind the sheets together. The minimum U-U distances are 3.91 Å within the sheets and 6.33 Å between closest uranium atoms in adjacent sheets. The structure differs greatly from that of isostructural α -NH₄UF₅.

Introduction

Ten years ago it was established (Benz, Douglass, Kruse & Penneman, 1963) that NH₄UF₅ exists in α and β forms. Compounds of 1:1 NH₄F/UF₄ stoichiometry are actually difficult to prepare. The usual result from aqueous precipitation is formation of 7NH₄F.6MF₄. Indeed, many compounds having this special 7:6 molar ratio of alkali fluoride to tetravalent fluoride are known (Thoma, 1962; Penneman, Ryan & Rosenzweig, 1973). The parent structure is that of 7NaF.6ZrF₄ (Burns, Ellison & Levy, 1968). In this structure the tetravalent element is surrounded by eight fluorines in an antiprism, six of which enclose a

large cubo-octahedral cavity which accommodates the 'extra' fluoride. We volatilized NH₄F from higher NH₄F/UF₄ complexes and obtained α and β forms of NH₄UF₅ in which the molar ratio of NH₄F to UF₄ was established as unity. The α form has the same X-ray powder diffraction pattern as that of 7NH₄F.6UF₄ and is thus presumed to be an NH₄F-deficient form of it. The structure of the β form was unknown; therefore it was of considerable interest to us that a patent (Allied Chemical Corporation, 1970) disclosed that both α - and β -NH₄UF₅ could be selectively precipitated from hot uranium-bearing aqueous ammonium fluoride solutions upon reduction of U(VI) to U(IV).

Experimental

We attempted to grow single crystals of $\beta\text{-NH}_4\text{UF}_5$ under conditions listed in the patent but the rapid precipitation yielded microcrystalline powders. Addition of Petroscale^R-101* to delay precipitation did yield larger dendritic crystals. However, the best success was achieved from dilute boiling solutions of formic acid, uranyl fluoride and ammonium fluoride, coupled with photochemical reduction. Clear green prismatic crystals of $\beta\text{-NH}_4\text{F}$ were grown, only occasionally twinned. They were small but adequate for single-crystal study. Optical examination established monoclinic morphology, with the forms $\{011\}$ and $\{100\}$ resulting in a pseudo-rhombohedral appearance. The crystals are biaxial negative, $2V = -55^\circ$; $N_x = 1.532$, yellow; $N_y = 1.560$; $N_z = 1.568$, blue-green; $Y = b$, $X \sim \perp(100)$. These refractive indices and the cell

* Petroscale: registered trademark of the Petrochemicals Company, Inc., Fort Worth, Texas.

volume of 438 \AA^3 ($Z=4$) give a value of 21.2 cm^3 for the molar refractivity. The X-ray powder diffraction pattern of a single crystal agreed with that from a bulk preparation of $\beta\text{-NH}_4\text{UF}_5$ whose composition was confirmed by chemical analysis.

Precession photographs of several crystals established monoclinic symmetry, space group $P2_1/c$, with extinctions: $h0l$, $l=2n+1$; $0k0$, $k=2n+1$; and hkl , no restrictions.

A single crystal of approximate dimensions $0.06 \times 0.35 \times 0.028 \text{ mm}$ was used for data collection. The cell constants were determined by least-squares refinement, using as observations the setting angles of 12 high-order reflections that had been centered on an automated four-circle Picker X-ray diffractometer using $\text{Mo K}\alpha_1$ radiation ($\lambda=0.70930 \text{ \AA}$). The values thus determined are $a=7.799(5)$, $b=7.158(5)$, $c=8.762(7) \text{ \AA}$, $\beta=116.45(5)^\circ$, $Z=4$, $d_{\text{calc}}=5.32$, $d_{\text{obs}}=5.3 \text{ g cm}^{-3}$ (by pycnometer on a bulk powder preparation).

Intensity data were collected on a Picker FACS-I system, using $\text{Mo K}\alpha$ radiation, a single-crystal graph-

Table 1. Fractional coordinates and thermal parameters (all $\times 10^4$)

Thermal parameters are defined by $\exp [-(\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}l^2 + \beta_{12}hk + \beta_{13}hl + \beta_{23}kl)]$.
Extinction factor, $g=1.6(7) \times 10^{-6}$.

The standard deviation of the least significant digit is given in parentheses.

	<i>x</i>	<i>y</i>	<i>z</i>	β_{11}	β_{22}	β_{23}	β_{12}	β_{13}	β_{23}
U	4247 (1)	1525 (1)	1456 (1)	57 (1)	32 (1)	25 (1)	3 (2)	50 (1)	-1 (1)
F(1)	3745 (10)	2015 (9)	3859 (8)	109 (15)	64 (12)	43 (9)	21 (20)	92 (20)	-16 (17)
F(2)	1104 (10)	1734 (11)	222 (9)	74 (13)	108 (16)	95 (12)	4 (26)	66 (21)	-73 (24)
F(3)	6659 (9)	714 (9)	700 (8)	91 (14)	70 (13)	43 (9)	-7 (22)	83 (19)	-16 (18)
F(4)	6603 (9)	(-)264 (9)	3538 (8)	84 (13)	53 (12)	50 (9)	-19 (22)	59 (19)	-2 (18)
F(5)	6702 (9)	1393 (10)	7810 (8)	66 (12)	61 (12)	60 (9)	12 (23)	64 (17)	23 (20)
N	9551 (15)	831 (18)	6701 (13)	96 (25)	177 (27)	88 (19)	-109 (41)	110 (37)	-81 (36)

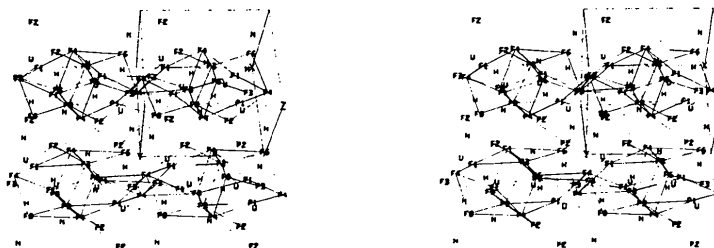


Fig. 1. Stereo view of the packing. The position of the vacancy is denoted as H.

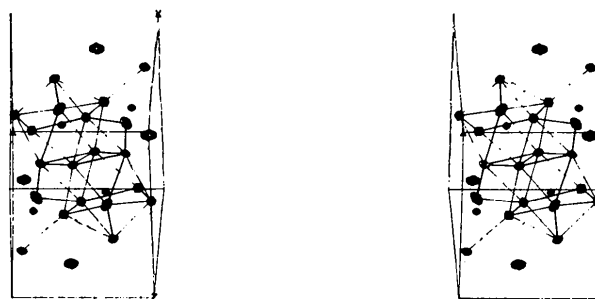


Fig. 2. Stereo view of unit cell showing coordination polyhedra.

ite monochromator (using the 002 reflection), and a take-off angle of 3.5°. The count was taken using a θ -2 θ scan over a 2 θ range of 2° (plus the α_1 - α_2 dispersion) at a scan rate of 1° min⁻¹; stationary-counter stationary-crystal background counts of 20 s were taken at each end of the scan. Intensities were collected for hkl and $\bar{h}k\bar{l}$ planes for all values of $2\theta \leq 70^\circ$; 4110 reflections were measured, equivalent reflections were averaged and 1325 were judged to be observed according to the criterion $I \geq 3\sigma(I)$, where $\sigma^2(I) = (T+B) + \sigma_s^2(T-B)^2$, T being the total count, B the estimated background. The quantity σ_s^2 was taken to be 2.5×10^{-4} , a number which we feel to be a reasonable estimate of the normalized variance of a reflection due to random variations other than counting statistics.

The intensities of two standard reflections were measured after every 20 reflections. The alignment of the crystal was examined periodically. The final intensities of the standard reflections were not significantly different from the starting values. Corrections were made for the Lorentz and polarization factors. The graphite crystal in the monochromator was assumed to be of perfect mosaicity, giving the following form for the polarization factor: $(\cos^2 2\alpha + \cos^2 2\theta)/(1 + \cos^2 2\alpha)$, where α is the angle the beam makes with the monochromator. The absorption corrections were made by the Busing & Levy (1957) method, using Burnham's (1962) program as modified by Larson, Cromer & Roof (1964). The linear absorption coefficient of β -NH₄UF₅ for Mo $K\alpha$ radiation is 554 cm⁻¹.

The Patterson function showed all the heavy-atom-light-atom vectors to be resolved, and a chemically reasonable structure could be deduced directly from it. The structure thus determined was refined using Larson's (1973) full-matrix least-squares program. The function minimized was $\sum w_i(|F_o| - |F_c^*|)^2$, where w_i is the weight defined as $1/\sigma^2(F_o)$

$$\text{and } F_c^* = kF_c / \left\{ 1 + 2g \left(\frac{e^2}{mc^2V} \right)^2 \text{Lp} \chi \right. \\ \left. \times \left[\frac{(1 + \cos^2 2\alpha)(\cos^2 2\alpha + \cos^4 2\theta)}{(\cos^2 2\alpha + \cos^2 2\theta)^2} \right]^2 F_c^2 \right\}^{1/4}.$$

The final R value [$R = \sum(|F_o| - |F_c^*|)/\sum|F_o|$] was 0.036 when anisotropic temperature factors and an extinction correction (g) were included (Larson, 1967; Zachariasen, 1963). The scattering factors for neutral U, N, and F atoms were taken from *International Tables for X-ray Crystallography* (1974) as were the dispersion corrections for uranium. Hamilton's (1965) tests showed that anisotropic temperature factors for nitrogen and the fluorine atoms and an extinction correction gave statistically significant improvements in the R value.

Discussion

The atomic parameters for β -NH₄UF₅ are listed in Table 1, and selected interatomic distances and angles in Table 2. Table 3 lists the observed and calculated

structure factors. A stereo view of the packing is shown in Fig. 1, and that of a unit cell showing coordination polyhedra, in Fig. 2.

Table 2. Bond distances (Å)

U-F distances within a single polyhedron	N-F distances (to 3.2 Å)
U-F(1) 2.373 (6)	N-F(1) 3.14 (1)
U-F(1) 2.333 (6)	N-F(2) 2.75 (1)
U-F(2) 2.200 (7) unshared fluorine	N-F(2) 2.84 (1)
U-F(3) 2.333 (6)	N-F(3) 3.20 (1)
U-F(3) 2.329 (6)	N-F(3) 3.02 (1)
U-F(4) 2.315 (7)	N-F(4) 2.81 (1)
U-F(4) 2.393 (7)	N-F(4) 3.13 (1)
U-F(5) 2.398 (7)	N-F(5) 2.82 (1)
U-F(5) 2.296 (7)	
F-F distances	
F(1)-F(2) 2.94 (1), 2.93 (1)	
F(1)-F(3) 2.67 (1), 2.71 (1) shared corner	F(1)-U-F(1) 155.4(3)°
F(1)-F(4) 2.87 (1), 2.79 (1)	
F(1)-F(5) 2.78 (1), 3.06 (1)	
F(2)-F(3) 2.83 (1)	
F(2)-F(4) 2.70 (1)	
F(2)-F(5) 2.88 (1)	
F(3)-F(3) 2.53 (1); shared edge	U-F(3)-U = 114.2 (3)°
F(4)-F(5) 2.45 (1); shared edge	U-F(4)-U = 114.2 (3)°
F(3)-F(4) 2.60 (1)	
F(3)-F(5) 2.59 (1); shared edge	U-F(5)-U = 114.7 (3)°
F and N distances to vacancy (H)	
H...F(1)	2.63
H...F(1)	2.04
H...F(3)	2.11
H...F(4)	1.89
H...F(5)	2.25
H...F(5)	2.66

The structure consists of sheets built of equivalent UF₅ polyhedra, in which three edges [involving F(3), F(4), F(5)] are shared with three adjacent polyhedra and two corners [F(1)] are shared with two additional polyhedra to form a sheet parallel to (100). The remaining corner [F(2)] of each polyhedron is unshared, and lies on the surface of the sheet. The one short U-F bond involves the unshared fluorine at a U-F distance of 2.20 Å compared with the average U-F distance of 2.35 Å to the other eight fluorines. This unshared fluorine is the cap atom of a rather squat irregular pentagonal pyramid of fluorines and has significantly larger thermal motion than the shared fluorines. The distances from this unshared fluorine to the five closest fluorines all exceed van der Waals radii. The corner-shared F(1) has van der Waals contact distances or larger. The fluorine atoms involved in edge sharing, F(3), F(4), and F(5), all have closer than van der Waals contact distances as is customarily observed (Penneman, Ryan & Rosenzweig, 1973). The sheets are bound together by ammonium ions, which link pairs of unshared fluorines in one sheet to shared fluorines in adjoining sheets. The light-atom thermal ellipsoids are chemically reasonable.

The molar refractivities of 7NH₄F.6UF₄ and of β -NH₄F.UF₄ are, respectively, 22.4 and 21.2 cm³. The

difference is 1.2 cm³ which is accounted for nicely by the 1/2 mole of NH₄F difference in stoichiometry [the empirical molar refractivity of NH₄F is 6.79 cm³ in such complexes (Penneman, 1969)]. However, the refractivity values of both structures are somewhat below the values expected for close-packed structures. In the 7:6 structure this can be ascribed to the large 'vacancy' enclosed by the six antiprisms which share extra ions among them. In the present structure there is an obvious vacancy in the surface of the fluoride sheets. As part of the nine-coordination polyhedron, rings of five fluorines coordinated to uranium atoms are capped

by an unshared fluorine. Adjacent to these is a depression in the surface which consists of a five-membered ring of fluorines containing no cation. The barycenter of this vacancy is surrounded by five fluorines in essentially a plane, plus one fluorine below it at distances ranging from 1.9 to 2.66 Å; it is 2.1 Å from an NH₄⁺ site. This vacancy is shown as H in Fig. 1. Such a site could accommodate a small cation, with slight shifts of the light-atom positions. In this regard, β-NH₄UF₅ has been reported to contain 0.9% Na/U when precipitated from solution having 3% sodium ions, compared to 0.2% Na/U contained in the α

Table 3. Observed and calculated structure factors for β-NH₄UF₅
Column headings are *l*, *F_o*/scale, and *F_c*^{*} (see text).

<i>l</i>	<i>F_o</i> /scale	<i>F_c</i> [*]	<i>l</i>	<i>F_o</i> /scale	<i>F_c</i> [*]	<i>l</i>	<i>F_o</i> /scale	<i>F_c</i> [*]
0	0	0	1	100	100	2	100	100
1	100	100	2	100	100	3	100	100
2	100	100	3	100	100	4	100	100
3	100	100	4	100	100	5	100	100
4	100	100	5	100	100	6	100	100
5	100	100	6	100	100	7	100	100
6	100	100	7	100	100	8	100	100
7	100	100	8	100	100	9	100	100
8	100	100	9	100	100	10	100	100
9	100	100	10	100	100	11	100	100
10	100	100	11	100	100	12	100	100
11	100	100	12	100	100	13	100	100
12	100	100	13	100	100	14	100	100
13	100	100	14	100	100	15	100	100
14	100	100	15	100	100	16	100	100
15	100	100	16	100	100	17	100	100
16	100	100	17	100	100	18	100	100
17	100	100	18	100	100	19	100	100
18	100	100	19	100	100	20	100	100
19	100	100	20	100	100	21	100	100
20	100	100	21	100	100	22	100	100
21	100	100	22	100	100	23	100	100
22	100	100	23	100	100	24	100	100
23	100	100	24	100	100	25	100	100
24	100	100	25	100	100	26	100	100
25	100	100	26	100	100	27	100	100
26	100	100	27	100	100	28	100	100
27	100	100	28	100	100	29	100	100
28	100	100	29	100	100	30	100	100
29	100	100	30	100	100	31	100	100
30	100	100	31	100	100	32	100	100
31	100	100	32	100	100	33	100	100
32	100	100	33	100	100	34	100	100
33	100	100	34	100	100	35	100	100
34	100	100	35	100	100	36	100	100
35	100	100	36	100	100	37	100	100
36	100	100	37	100	100	38	100	100
37	100	100	38	100	100	39	100	100
38	100	100	39	100	100	40	100	100
39	100	100	40	100	100	41	100	100
40	100	100	41	100	100	42	100	100
41	100	100	42	100	100	43	100	100
42	100	100	43	100	100	44	100	100
43	100	100	44	100	100	45	100	100
44	100	100	45	100	100	46	100	100
45	100	100	46	100	100	47	100	100
46	100	100	47	100	100	48	100	100
47	100	100	48	100	100	49	100	100
48	100	100	49	100	100	50	100	100
49	100	100	50	100	100	51	100	100
50	100	100	51	100	100	52	100	100
51	100	100	52	100	100	53	100	100
52	100	100	53	100	100	54	100	100
53	100	100	54	100	100	55	100	100
54	100	100	55	100	100	56	100	100
55	100	100	56	100	100	57	100	100
56	100	100	57	100	100	58	100	100
57	100	100	58	100	100	59	100	100
58	100	100	59	100	100	60	100	100
59	100	100	60	100	100	61	100	100
60	100	100	61	100	100	62	100	100
61	100	100	62	100	100	63	100	100
62	100	100	63	100	100	64	100	100
63	100	100	64	100	100	65	100	100
64	100	100	65	100	100	66	100	100
65	100	100	66	100	100	67	100	100
66	100	100	67	100	100	68	100	100
67	100	100	68	100	100	69	100	100
68	100	100	69	100	100	70	100	100
69	100	100	70	100	100	71	100	100
70	100	100	71	100	100	72	100	100
71	100	100	72	100	100	73	100	100
72	100	100	73	100	100	74	100	100
73	100	100	74	100	100	75	100	100
74	100	100	75	100	100	76	100	100
75	100	100	76	100	100	77	100	100
76	100	100	77	100	100	78	100	100
77	100	100	78	100	100	79	100	100
78	100	100	79	100	100	80	100	100
79	100	100	80	100	100	81	100	100
80	100	100	81	100	100	82	100	100
81	100	100	82	100	100	83	100	100
82	100	100	83	100	100	84	100	100
83	100	100	84	100	100	85	100	100
84	100	100	85	100	100	86	100	100
85	100	100	86	100	100	87	100	100
86	100	100	87	100	100	88	100	100
87	100	100	88	100	100	89	100	100
88	100	100	89	100	100	90	100	100
89	100	100	90	100	100	91	100	100
90	100	100	91	100	100	92	100	100
91	100	100	92	100	100	93	100	100
92	100	100	93	100	100	94	100	100
93	100	100	94	100	100	95	100	100
94	100	100	95	100	100	96	100	100
95	100	100	96	100	100	97	100	100
96	100	100	97	100	100	98	100	100
97	100	100	98	100	100	99	100	100
98	100	100	99	100	100	100	100	100

form (Selman, Wamser & Wilkalis, 1972). Smaller amounts of potassium ion are included.

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The Tricyclic Antidepressants: Iprindole. The Crystal and Molecular Structure of 5-[3-{Dimethylamino}propyl]-6,7,8,9,10,11-hexahydro-5H-cyclooct[b]indole Monohydrate

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Iprindole hydrochloride monohydrate is orthorhombic, space group *Pbca*, with $a=10.812$ (2), $b=28.585$ (7), $c=12.422$ (3) Å, $Z=8$. The structure was solved by tangent formula refinement of diffractometer data collected with Cu radiation. Full-matrix least-squares refinement resulted in a final R of 0.084 for 2339 reflexions. The indole system is planar. Centrosymmetrically related molecules are linked by a system of hydrogen bonds.

Introduction

Of the classes of psychotropic drugs now in clinical use for the treatment of depressive illness the most widely prescribed are the tricyclic antidepressants such as imipramine, desipramine and amitriptyline. There is considerable evidence that a functional abnormality of one of the brain's biogenic amine (noradrenaline or 5-hydroxytryptamine) systems may be involved in the aetiology of these disorders (Schildkraut & Kety, 1967; Ashcroft *et al.*, 1972). The most significant biochemical effect of the tricyclics is their ability to inhibit the amine recapture or uptake process that trans-

ports the amine back into the presynaptic nerve ending (Shaskan & Snyder, 1970; Horn, Coyle & Snyder, 1971; Iversen 1973). This process is largely responsible for the termination of the synaptic action of the biogenic amines. It has been hypothesized that this inhibition of the uptake process may be responsible for the tricyclic's ameliorative action in the depressive states (Schildkraut & Kety, 1967). It is therefore of interest to investigate what molecular or conformational features the tricyclics have that enable them to act as inhibitors of this uptake process. Valuable information can also be obtained by comparing the structures of tricyclics that, although active clinically, have differing biochemical actions. An excellent example of this is iprindole (I), which, although in clinical use as an antidepressant (El Diery, Forrest & Litt-

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