Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Expanding Pentafluorouranates: Hydrothermal Synthesis and Characterization of β-NaUF5 and β-NaUF5•H2O

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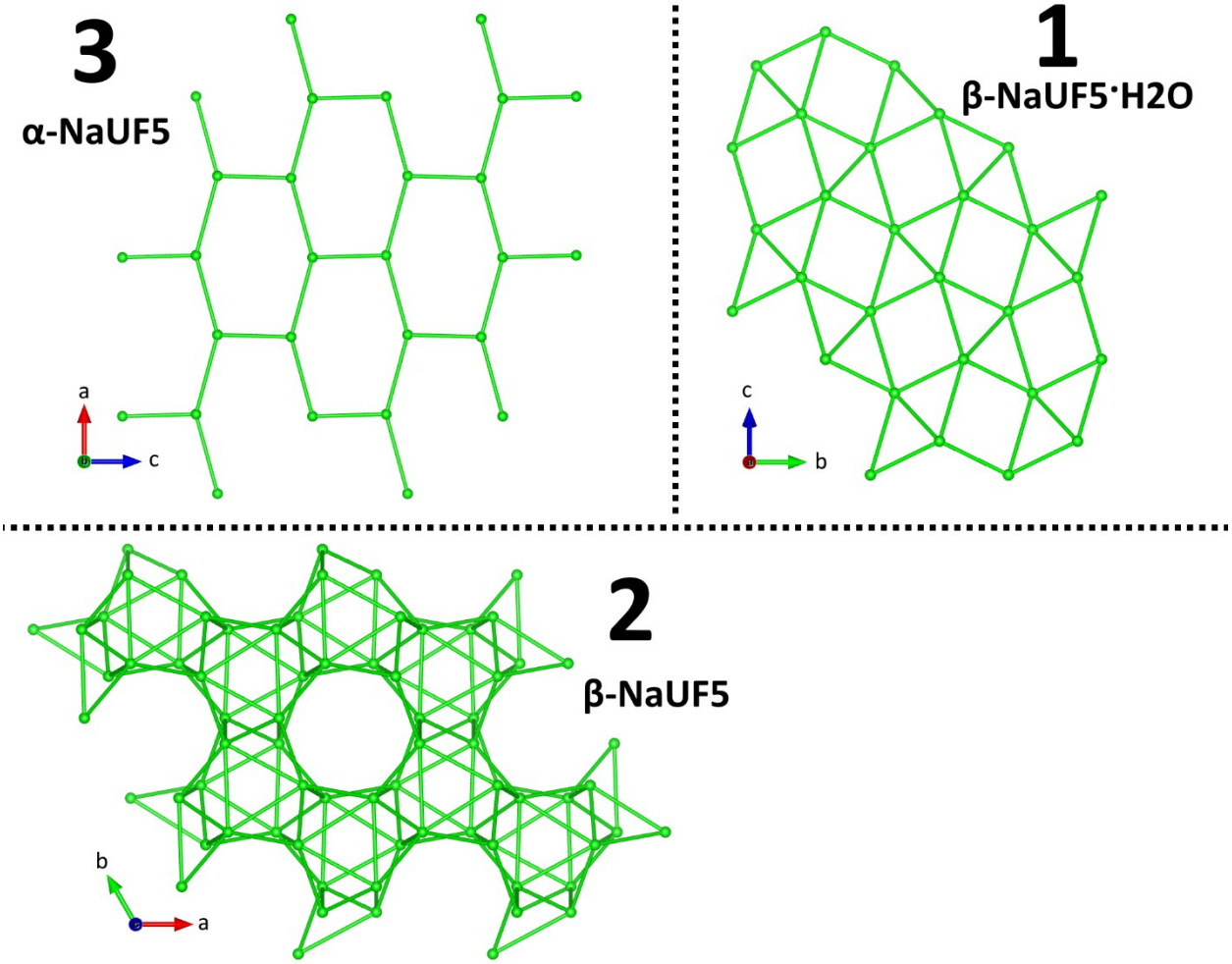
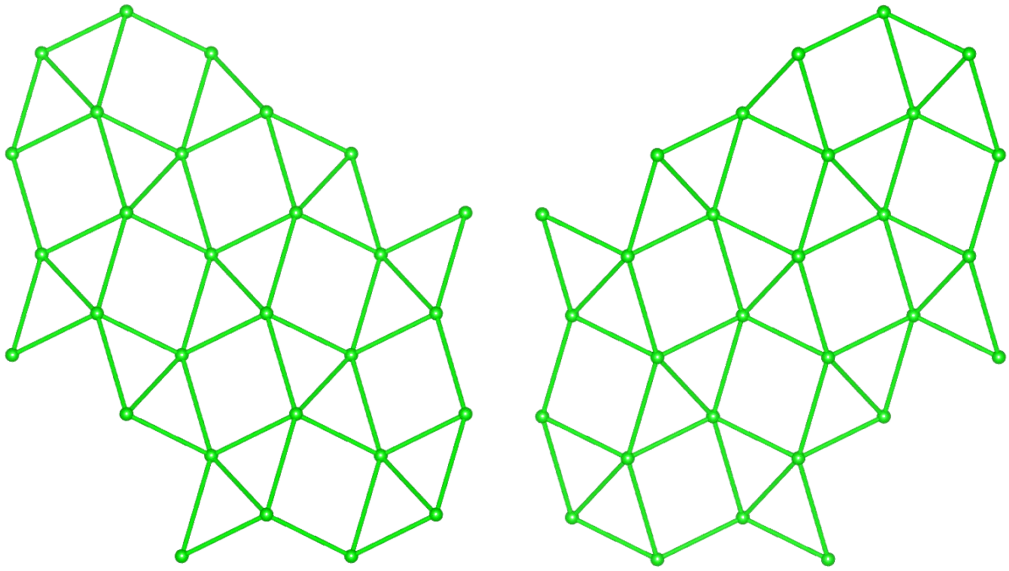
Supporting Information Figure 1

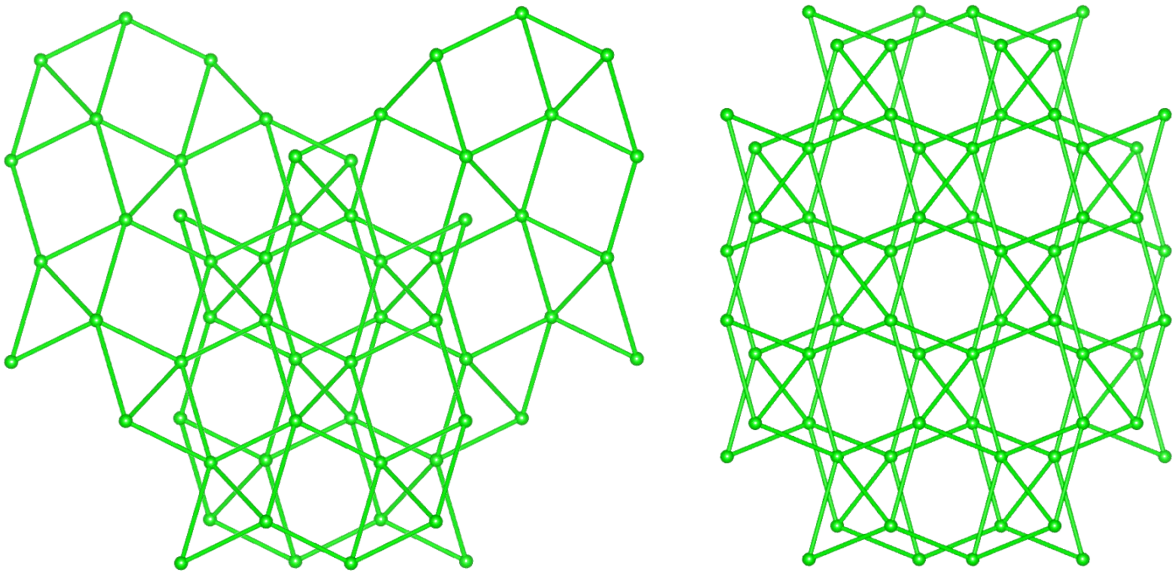


SI Figure 1: Wireframe comparison of the uranium networks in all three products. Particularly note that, although the absorption spectra of 1 and 3 are nearly identical (Figure 4 in the text), and they have similar uranium coordination environments, they have very different uranium networks.

Supporting Information Figure 2



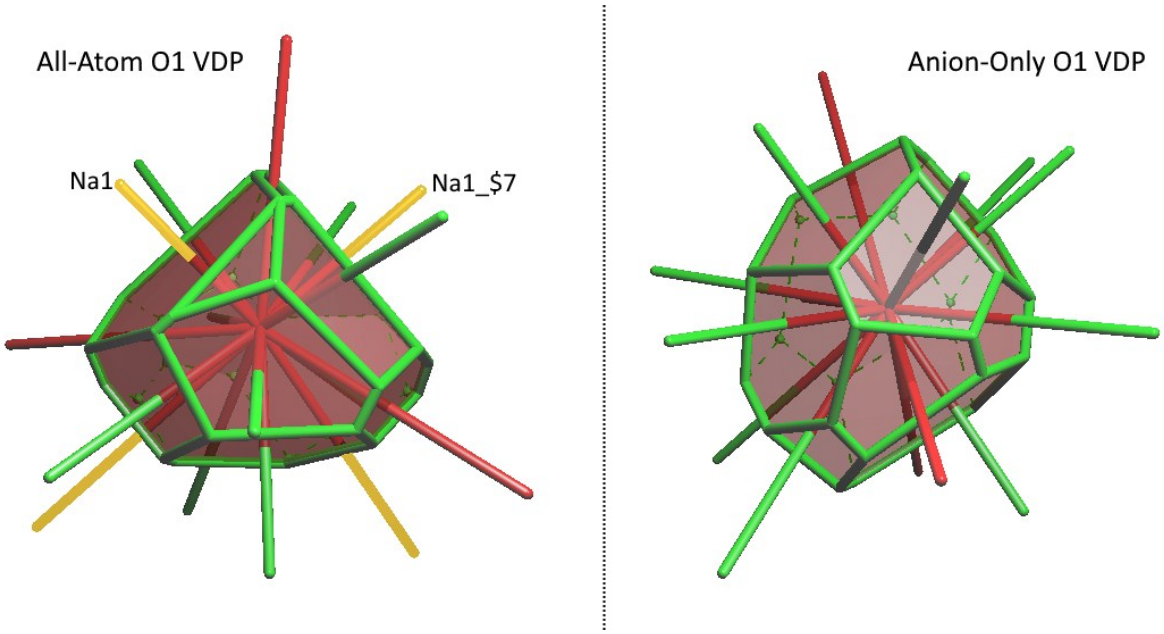
These layers of **1** are mirror images.



SI Figure 2: The generation of the layer structure of the alpha-hydrate from the **1** motif.

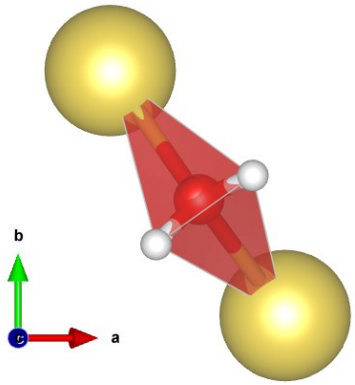
When superimposed (left), they generate the α-$NaUF_5 \cdot H_2O$ template (right).

Supporting Information Figure 3



SI Figure 3: Voronoi-Dirichlet polyhedra for O1 with all atoms considered (left) and only anions (right).

Supporting Information Figure 4



SI Figure 4: The coordination environment of O1 viewed down the c-axis, a distorted tetrahedron. Sodium atoms are yellow, and hydrogen atoms are white.

Supporting Information Table 1

All Non-Hydrogen Atoms Dirichlet Calculation of **1**

#################
1:Na, U F5, H2 O
#################
Central atom:O1 OxSt:-2 CN:2 0.998 0.511 0.810 Rsd:1.655
D(CP):0.244 (0.9819 0.5140 0.7811)
D(VDP):0.134 (0.9984 0.5114 0.7946)
Atom:2.367 < r < 3.749 <r>=3.218 Top: 1.808 < R < 2.055 <R>=1.945
CN=16:0:2 NV=32 V=18.996/93.871 S=38.109 Cpac=0.365 Ccov=1.913
G3=0.081560699
Face distribution: {4/2 5/8 6/8 }
Vertex distribution: {3/32 }

	Atom	x	y	z	Distance (Å)	D1	D2	Solid Angle %
1	Na1	1.13	0.30	1.02	2.37	1.66	0.71	16.34
2	Na1	0.87	0.70	0.98	2.48	1.66	0.83	13.86
3	F_3	1.13	0.66	0.57	2.87	1.66	1.22	10.12
4	F_2	0.65	0.49	0.84	2.91	1.66	1.25	6.64
5	F_4	0.65	0.58	0.55	2.99	1.66	1.34	8.32
6	F_3	0.87	0.16	0.93	3.04	1.66	1.39	5.40
7	F_5	1.37	0.71	0.89	3.15	1.66	1.49	6.96
8	F_1	1.34	0.36	0.74	3.16	1.66	1.50	6.70
9	F_3	1.13	0.85	1.07	3.20	1.66	1.54	4.55
10	O_1	1.00	0.49	1.19	3.34	1.66	1.68	0.80
11	F_3	0.87	0.35	0.43	3.34	1.66	1.69	5.37
12	Na1	0.87	0.80	0.48	3.42	1.66	1.76	2.65
*13	F_2	1.35	0.51	1.16	3.45	1.66	1.79	1.37
*14	F_1	0.66	0.86	0.76	3.56	1.66	1.91	1.05
15	F_5	0.63	0.21	0.61	3.57	1.66	1.92	2.57
16	O_1	1.00	0.01	0.69	3.67	1.66	2.01	3.07
17	O_1	1.00	1.01	0.69	3.67	1.66	2.01	3.07
18	Na1	1.13	0.20	0.52	3.75	1.66	2.09	1.15

Elapsed time: 6.43 sec

Supporting Information Table 2

Anion-Only Dirichlet Calculation of **1**
################
1:Na, U F5, H2 O
################
Central atom:O1 OxSt:-2 CN:2 0.998 0.511 0.810 Rsd:1.773
D(CP):0.157 (1.0075 0.4913 0.8088)
D(VDP):0.066 (1.0036 0.5068 0.8163)
Atom:2.871 < r < 4.003 <r>=3.328 Top: 1.808 < R < 2.336 <R>=2.048
CN=15:0:0 NV=26 V=23.366/94.889 S=43.477 Cpac=0.530 Ccov=2.284
G3=0.080107027
Face distribution: {4/3 5/6 6/6 }
Vertex distribution: {3/26 }

	Atom	x	y	z	Distance (Å)	D1	D2	Solid Angle %
1	F_3	1.13	0.66	0.57	2.87	1.77	1.10	11.07
2	F_2	0.65	0.49	0.84	2.91	1.77	1.14	10.06
3	F_4	0.65	0.58	0.55	2.99	1.77	1.22	9.31
4	F_3	0.87	0.16	0.93	3.04	1.77	1.27	10.20
5	F_5	1.37	0.71	0.89	3.15	1.77	1.38	6.98
6	F_1	1.34	0.36	0.74	3.16	1.77	1.38	8.43
7	F_3	1.13	0.85	1.07	3.20	1.77	1.42	8.82
8	O_1	1.00	0.49	1.19	3.34	1.77	1.57	6.72
9	F_3	0.87	0.35	0.43	3.34	1.77	1.57	5.82
10	F_2	1.35	0.51	1.16	3.45	1.77	1.68	5.85
11	F_1	0.66	0.86	0.76	3.56	1.77	1.79	4.06
12	F_5	0.63	0.21	0.61	3.57	1.77	1.80	2.57
13	O_1	1.00	1.01	0.69	3.67	1.77	1.90	4.01
14	O_1	1.00	0.01	0.69	3.67	1.77	1.90	4.01
15	F_4	1.35	0.08	0.95	4.00	1.77	2.23	2.09

Elapsed time: 5.15 sec.

Supporting Information Table 3

Uranium-fluorine bond length and uranium-uranium distance comparison between $Na_4CuU_6F_{30}$ and **2**

	$Na_4CuU_6F_{30}$[17]	β-$NaUF_5$ (**2**)
U-F non-bridging bond length (Å)	2.250(4)	2.196(4)
U-F (μ^2) bond lengths (Å)	2.268(3)-2.418(3)	2.287(4)-2.435(4)
U-U double-fluoride bridge distances (Å)	4.0266(3)-4.0700(4)	4.0442(4)-4.1019(6)
U-U single-fluoride bridge distances (Å)	4.4851(3)-4.5088(2)	4.5235(5)-4.5480(7)

17 J. Yeon, M. D. Smith, J. Tapp, A. Möller and H.-C. zur Loye, Application of a Mild Hydrothermal Approach Containing an in Situ Reduction Step to the Growth of Single Crystals of the Quaternary U(IV)-Containing Fluorides $Na_4MU_6F_{30}$ (M = Mn^{2+}, Co^{2+}, Ni^{2+}, Cu^{2+}, and Zn^{2+}) Crystal Growth, Structures, and Magnetic Properties, *Journal of the American Chemical Society*, 2014, **136**, 3955–3963.

Atomic coordinates and structural information of Product 1 - β-$NaUF_5 \cdot H_2O$

Crystal data

$NaUF_5 \cdot H_2O$	Monoclinic, $P2_1/c$
M_r = 374.04	D_x = 5.334 Mg m^{-3}
a = 7.957 (3) Å	Mo Kα radiation, λ = 0.71073 Å
b = 7.027 (2) Å	Cell parameters from 996 reflections
c = 8.792 (3) Å	θ = 2.7–28.0°
β = 108.678 (7)°	μ = 34.96 mm^{-1}
V = 465.7 (3) $Å^3$	T = 297 K
Z = 4	Thin tetragonal plates, emerald green
F(000) = 632	0.05 × 0.05 × 0.02 mm
$R[F^2 > 2\sigma(F^2)]$ = 0.036	$wR(F^2)$ = 0.105
$w = 1/[\sigma^2(F_o^2) + (0.0764P)^2]$, where $P = (F_o^2 + 2F_c^2)/3$	$\Delta\rho_{max}$ = 2.84 e $Å^{-3}$, $\Delta\rho_{min}$ = −2.47 e $Å^{-3}$

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
U1	0.57881 (4)	0.16299 (5)	0.85335 (4)	0.0074 (2)
F2	0.3390 (8)	0.3605 (7)	0.7381 (8)	0.0121 (13)
F3	0.6455 (8)	0.4858 (8)	0.8413 (7)	0.0138 (12)
F1	0.8667 (10)	0.1548 (8)	0.9336 (10)	0.0236 (17)
F4	0.3451 (7)	0.0822 (9)	0.9506 (7)	0.0139 (12)
F5	0.6300 (9)	0.2883 (9)	1.1107 (7)	0.0189 (13)
Na1	1.1349 (7)	0.2974 (7)	1.0214 (6)	0.0276 (11)
O1	0.9980 (11)	0.5106 (13)	0.8115 (11)	0.0287 (19)
H1	0.915 (5)	0.471 (7)	0.730 (4)	0.11 (9)*
H2	1.064 (6)	0.585 (6)	0.778 (6)	0.03 (3)*

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
U1	0.0088 (3)	0.0065 (3)	0.0074 (3)	−0.00006 (11)	0.00308 (17)	0.00032 (10)
F2	0.007 (3)	0.012 (3)	0.014 (3)	−0.001 (2)	−0.001 (2)	0.001 (2)
F3	0.017 (3)	0.011 (3)	0.012 (3)	−0.001 (2)	0.002 (2)	0.000 (2)
F1	0.018 (4)	0.019 (4)	0.030 (4)	0.001 (2)	0.002 (3)	−0.001 (2)
F4	0.012 (3)	0.014 (3)	0.017 (3)	−0.001 (2)	0.007 (2)	0.002 (2)

F5	0.031 (4)	0.012 (3)	0.017 (3)	−0.003 (3)	0.014 (3)	−0.003 (3)
Na1	0.026 (3)	0.020 (2)	0.031 (3)	0.003 (2)	0.001 (2)	−0.002 (2)
O1	0.021 (5)	0.036 (5)	0.031 (5)	−0.007 (4)	0.011 (4)	0.003 (4)

Geometric parameters (Å, °)

U1—F1	2.171 (8)	F3—U1^{vi}	2.389 (6)
U1—F2	2.314 (6)	F1—Na1	2.258 (9)
U1—F5^{i}	2.322 (6)	F4—U1^{ii}	2.374 (6)
U1—F5	2.339 (6)	F4—Na1^{viii}	2.477 (8)
U1—F3	2.340 (6)	F5—U1^{ix}	2.322 (6)
U1—F4	2.352 (6)	Na1—F3^{vii}	2.341 (7)
U1—F4^{ii}	2.374 (6)	Na1—F2^{x}	2.349 (8)
U1—F3^{iii}	2.389 (6)	Na1—O1	2.356 (10)
U1—F2^{iii}	2.435 (6)	Na1—O1^{vii}	2.468 (10)
U1—Na1^{iv}	3.804 (5)	Na1—F4^{xi}	2.477 (8)
U1—Na1^{v}	3.906 (5)	Na1—Na1^{vii}	3.513 (10)
U1—U1^{ii}	3.9424 (11)	Na1—U1^{x}	3.804 (5)
F2—Na1^{iv}	2.349 (8)	Na1—U1^{v}	3.906 (5)
F2—U1^{vi}	2.435 (6)	O1—Na1^{vii}	2.468 (10)
F3—Na1^{vii}	2.341 (7)		
F1—U1—F2	142.6 (2)	F5^{i}—U1—U1^{ii}	150.80 (16)
F1—U1—F5^{i}	79.9 (3)	F5—U1—U1^{ii}	65.12 (17)
F2—U1—F5^{i}	82.6 (2)	F3—U1—U1^{ii}	135.83 (15)
F1—U1—F5	81.8 (3)	F4—U1—U1^{ii}	33.65 (14)
F2—U1—F5	93.5 (2)	F4^{ii}—U1—U1^{ii}	33.29 (14)
F5^{i}—U1—F5	143.69 (18)	F3^{iii}—U1—U1^{ii}	81.05 (14)
F1—U1—F3	79.0 (2)	F2^{iii}—U1—U1^{ii}	83.35 (15)
F2—U1—F3	64.3 (2)	Na1^{iv}—U1—U1^{ii}	97.63 (9)
F5^{i}—U1—F3	72.9 (2)	Na1^{v}—U1—U1^{ii}	67.25 (9)
F5—U1—F3	73.0 (2)	U1—F2—Na1^{iv}	109.3 (3)
F1—U1—F4	138.6 (3)	U1—F2—U1^{vi}	113.4 (3)
F2—U1—F4	70.5 (2)	Na1^{iv}—F2—U1^{vi}	109.5 (3)
F5^{i}—U1—F4	139.6 (2)	U1—F3—Na1^{vii}	138.6 (3)
F5—U1—F4	69.6 (2)	U1—F3—U1^{vi}	114.2 (2)
F3—U1—F4	117.9 (2)	Na1^{vii}—F3—U1^{vi}	107.0 (2)
F1—U1—F4^{ii}	75.4 (2)	U1—F1—Na1	152.0 (3)

F2—U1—F4^{ii}	137.4 (2)	U1—F4—U1^{ii}	113.1 (2)
F5^{i}—U1—F4^{ii}	134.0 (2)	U1—F4—Na1^{viii}	128.3 (3)
F5—U1—F4^{ii}	69.3 (2)	U1^{ii}—F4—Na1^{viii}	107.2 (3)
F3—U1—F4^{ii}	136.7 (2)	U1^{ix}—F5—U1	156.5 (3)
F4—U1—F4^{ii}	66.9 (2)	F1—Na1—F3^{vii}	158.8 (4)
F1—U1—F3^{iii}	133.4 (2)	F1—Na1—F2^{x}	113.6 (3)
F2—U1—F3^{iii}	71.1 (2)	F3^{vii}—Na1—F2^{x}	71.4 (2)
F5^{i}—U1—F3^{iii}	74.3 (2)	F1—Na1—O1	82.2 (3)
F5—U1—F3^{iii}	138.4 (2)	F3^{vii}—Na1—O1	94.1 (3)
F3—U1—F3^{iii}	126.94 (14)	F2^{x}—Na1—O1	164.2 (4)
F4—U1—F3^{iii}	68.8 (2)	F1—Na1—O1^{vii}	84.7 (3)
F4^{ii}—U1—F3^{iii}	95.7 (2)	F3^{vii}—Na1—O1^{vii}	74.2 (3)
F1—U1—F2^{iii}	73.6 (2)	F2^{x}—Na1—O1^{vii}	95.3 (3)
F2—U1—F2^{iii}	130.53 (11)	O1—Na1—O1^{vii}	86.5 (3)
F5^{i}—U1—F2^{iii}	71.4 (2)	F1—Na1—F4^{xi}	106.5 (3)
F5—U1—F2^{iii}	131.8 (2)	F3^{vii}—Na1—F4^{xi}	94.3 (3)
F3—U1—F2^{iii}	137.9 (2)	F2^{x}—Na1—F4^{xi}	64.4 (2)
F4—U1—F2^{iii}	103.7 (2)	O1—Na1—F4^{xi}	111.8 (3)
F4^{ii}—U1—F2^{iii}	64.7 (2)	O1^{vii}—Na1—F4^{xi}	159.3 (3)
F3^{iii}—U1—F2^{iii}	61.7 (2)	F1—Na1—Na1^{vii}	81.1 (3)
F1—U1—Na1^{iv}	151.1 (2)	F3^{vii}—Na1—Na1^{vii}	81.8 (2)
F2—U1—Na1^{iv}	35.64 (16)	F2^{x}—Na1—Na1^{vii}	135.2 (3)
F5^{i}—U1—Na1^{iv}	71.17 (19)	O1—Na1—Na1^{vii}	44.5 (2)
F5—U1—Na1^{iv}	123.10 (19)	O1^{vii}—Na1—Na1^{vii}	42.0 (2)
F3—U1—Na1^{iv}	93.58 (16)	F4^{xi}—Na1—Na1^{vii}	155.0 (3)
F4—U1—Na1^{iv}	69.43 (17)	F1—Na1—U1^{x}	147.0 (3)
F4^{ii}—U1—Na1^{iv}	124.63 (16)	F3^{vii}—Na1—U1^{x}	36.90 (16)
F3^{iii}—U1—Na1^{iv}	36.05 (15)	F2^{x}—Na1—U1^{x}	35.03 (16)
F2^{iii}—U1—Na1^{iv}	95.28 (16)	O1—Na1—U1^{x}	129.6 (3)
F1—U1—Na1^{v}	55.05 (16)	O1^{vii}—Na1—U1^{x}	88.4 (2)
F2—U1—Na1^{v}	160.85 (16)	F4^{xi}—Na1—U1^{x}	72.64 (18)
F5^{i}—U1—Na1^{v}	97.07 (19)	Na1^{vii}—Na1—U1^{x}	114.1 (2)
F5—U1—Na1^{v}	97.68 (18)	F1—Na1—U1^{v}	97.5 (2)
F3—U1—Na1^{v}	134.06 (18)	F3^{vii}—Na1—U1^{v}	97.0 (2)
F4—U1—Na1^{v}	98.93 (17)	F2^{x}—Na1—U1^{v}	36.00 (16)

F4^{ii}—U1—Na1^{v}	37.27 (17)	O1—Na1—U1^{v}	146.0 (3)
F3^{iii}—U1—Na1^{v}	90.27 (16)	O1^{vii}—Na1—U1^{v}	127.4 (3)
F2^{iii}—U1—Na1^{v}	34.54 (16)	F4^{xi}—Na1—U1^{v}	35.48 (15)
Na1^{iv}—U1—Na1^{v}	126.25 (12)	Na1^{vii}—Na1—U1^{v}	169.3 (3)
F1—U1—U1^{ii}	107.2 (2)	U1^{x}—Na1—U1^{v}	61.96 (8)
F2—U1—U1^{ii}	104.14 (16)	Na1—O1—Na1^{vii}	93.5 (3)

Symmetry codes: (i) *x*, −*y*+1/2, *z*−1/2; (ii) −*x*+1, −*y*, −*z*+2; (iii) −*x*+1, *y*−1/2, −*z*+3/2; (iv) *x*−1, −*y*+1/2, *z*−1/2; (v) −*x*+2, −*y*, −*z*+2; (vi) −*x*+1, *y*+1/2, −*z*+3/2; (vii) −*x*+2, −*y*+1, −*z*+2; (viii) *x*−1, *y*, *z*; (ix) *x*, −*y*+1/2, *z*+1/2; (x) *x*+1, −*y*+1/2, *z*+1/2; (xi) *x*+1, *y*, *z*.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···F1^{i}	0.85 (2)	2.66 (3)	3.356 (12)	140 (4)
O1—H1···F4^{vi}	0.85 (2)	2.30 (4)	2.998 (11)	139 (4)
O1—H2···F1^{xii}	0.86 (2)	2.16 (3)	2.884 (12)	142 (5)
O1—H2···F5^{vii}	0.86 (2)	2.48 (4)	3.151 (11)	136 (4)
O1—H1···F1^{i}	0.85 (2)	2.66 (3)	3.356 (12)	140 (4)
O1—H1···F4^{vi}	0.85 (2)	2.30 (4)	2.998 (11)	139 (4)
O1—H2···F1^{xii}	0.86 (2)	2.16 (3)	2.884 (12)	142 (5)
O1—H2···F5^{vii}	0.86 (2)	2.48 (4)	3.151 (11)	136 (4)

Symmetry codes: (i) *x*, −*y*+1/2, *z*−1/2; (vi) −*x*+1, *y*+1/2, −*z*+3/2; (vii) −*x*+2, −*y*+1, −*z*+2; (xii) −*x*+2, *y*+1/2, −*z*+3/2.

All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Atomic coordinates and structural information of Product 2 - β-$NaUF_5$

Crystal data

$NaUF_5$	Trigonal, *P*-3*c*1
M_r = 1068.06	D_x = 6.276 Mg m^{-3}

a = 10.0029 (12) Å	Mo *K*α radiation, λ = 0.71073 Å
c = 13.0457 (16) Å	Cell parameters from 883 reflections
V = 1130.4 (3) Å^3	θ = 2.4–27.8°
Z = 4	μ = 43.18 mm^{-1}
F(000) = 1776	T = 120 K
$R[F^2 > 2\sigma(F^2)]$ = 0.020	Blocky green hexagon, emerald green
$wR(F^2)$ = 0.038	0.07 × 0.07 × 0.05 mm
w = 1/[σ^2(F$_o^2$) + (0.0023P)^2 + 17.4221P], where P = (F$_o^2$ + 2F$_c^2$)/3	Δρ$_{max}$ =C:\Users\atche\Desktop\Fluorides\NaUF5 drafts\aaa _refine_diff_density_max 1.14 e Å^{-3}, Δρ$_{min}$ = −1.74 e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U$_{iso}$*/U$_{eq}$	Occ. (<1)
U1	0.07583 (2)	0.39943 (2)	0.89893 (2)	0.00251 (9)	
Na1	−0.3333	0.3333	0.8421 (3)	0.0086 (9)	
Na2	0.0000	0.0000	0.7500	0.0246 (17)	
Na3	0.0000	0.0000	1.0000	0.045 (3)	
Na4	0.3289 (15)	0.2861 (14)	0.7907 (10)	0.041 (3)	0.3333
F1	−0.4140 (4)	0.1165 (4)	0.9466 (3)	0.0070 (7)	
F2	−0.1224 (4)	0.1896 (4)	0.9777 (3)	0.0088 (7)	
F3	−0.1318 (4)	0.3091 (5)	0.7833 (3)	0.0106 (8)	
F4	0.0895 (5)	0.2007 (5)	0.8406 (3)	0.0184 (9)	
F5	0.3417 (4)	0.5116 (4)	0.8631 (3)	0.0109 (8)	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
U1	0.00250 (12)	0.00270 (12)	0.00201 (12)	0.00107 (9)	−0.00019 (7)	−0.00013 (7)
Na1	0.0081 (13)	0.0081 (13)	0.010 (2)	0.0041 (7)	0.000	0.000
Na2	0.024 (3)	0.024 (3)	0.026 (4)	0.0118 (13)	0.000	0.000
Na3	0.024 (3)	0.024 (3)	0.088 (8)	0.0118 (15)	0.000	0.000
Na4	0.038 (7)	0.036 (6)	0.063 (8)	0.028 (6)	−0.001 (6)	−0.015 (6)
F1	0.0057 (17)	0.0055 (17)	0.0084 (16)	0.0017 (15)	−0.0012 (14)	0.0018 (13)
F2	0.0081 (17)	0.0058 (17)	0.0119 (17)	0.0031 (15)	0.0012 (14)	0.0020 (14)
F3	0.0076 (18)	0.021 (2)	0.0038 (17)	0.0073 (16)	−0.0006 (14)	−0.0005 (15)

F4	0.026 (2)	0.015 (2)	0.017 (2)	0.0125 (19)	−0.0078 (18)	−0.0040 (17)
F5	0.0041 (17)	0.0105 (19)	0.0147 (18)	0.0012 (15)	−0.0009 (14)	0.0040 (15)

Geometric parameters (Å, °)

U1—F4	2.196 (4)	Na2—Na4	3.143 (13)
U1—F2	2.287 (4)	Na3—F4^{ii}	2.713 (4)
U1—F5^{i}	2.318 (4)	Na3—F4^{vii}	2.713 (4)
U1—F1^{ii}	2.326 (3)	Na3—F4^{xi}	2.713 (4)
U1—F3	2.351 (4)	Na3—F4^{x}	2.713 (4)
U1—F5	2.359 (4)	Na3—F4^{xii}	2.713 (4)
U1—F2^{ii}	2.376 (4)	Na3—F4	2.713 (4)
U1—F3^{iii}	2.430 (4)	Na3—F2^{xii}	2.739 (4)
U1—F1^{iv}	2.435 (4)	Na3—F2	2.739 (4)
U1—Na4^{v}	3.539 (12)	Na3—F2^{ii}	2.739 (4)
U1—Na4	3.543 (11)	Na3—F2^{vii}	2.739 (4)
U1—Na4^{i}	3.743 (12)	Na3—F2^{xi}	2.739 (4)
Na1—F3	2.281 (4)	Na3—F2^{x}	2.739 (4)
Na1—F3^{vi}	2.281 (4)	Na4—Na4^{v}	1.29 (3)
Na1—F3^{iv}	2.281 (4)	Na4—F4	2.200 (13)
Na1—F1^{iv}	2.337 (4)	Na4—F3^{x}	2.319 (12)
Na1—F1	2.337 (4)	Na4—F5	2.389 (12)
Na1—F1^{vi}	2.338 (4)	Na4—F4^{v}	2.434 (13)
Na1—Na4^{vii}	3.240 (12)	Na4—F5^{v}	2.580 (14)
Na1—Na4^{i}	3.240 (12)	Na4—F1^{x}	2.695 (13)
Na1—Na4^{viii}	3.240 (12)	Na4—F2^{x}	2.896 (14)
Na1—U1^{vi}	3.8771 (10)	Na4—Na1^{xiii}	3.240 (12)
Na1—U1^{iv}	3.8771 (10)	Na4—U1^{v}	3.539 (12)
Na2—F4	2.105 (4)	F1—U1^{xi}	2.326 (3)
Na2—F4^{ix}	2.105 (4)	F1—U1^{vi}	2.435 (4)
Na2—F4^{x}	2.105 (4)	F1—Na4^{vii}	2.695 (13)
Na2—F4^{iii}	2.105 (4)	F2—U1^{xi}	2.376 (4)
Na2—F4^{vii}	2.105 (4)	F2—Na4^{vii}	2.896 (14)
Na2—F4^{v}	2.105 (4)	F3—Na4^{vii}	2.319 (12)
Na2—Na4^{v}	3.143 (13)	F3—U1^{iii}	2.430 (4)
Na2—Na4^{iii}	3.143 (13)	F4—Na4^{v}	2.434 (13)
Na2—Na4^{ix}	3.143 (13)	F5—U1^{xiv}	2.318 (4)

Na2—Na4^{x}	3.143 (13)	F5—Na4^{v}	2.580 (14)
Na2—Na4^{vii}	3.143 (13)		
F4—U1—F2	75.09 (15)	F4^{v}—Na2—Na4^{vii}	140.9 (2)
F4—U1—F5^{i}	140.11 (15)	Na4^{v}—Na2—Na4^{vii}	107.5 (4)
F2—U1—F5^{i}	142.87 (13)	Na4^{iii}—Na2—Na4^{vii}	23.7 (5)
F4—U1—F1^{ii}	137.54 (13)	Na4^{ix}—Na2—Na4^{vii}	134.4 (4)
F2—U1—F1^{ii}	87.43 (13)	Na4^{x}—Na2—Na4^{vii}	117.21 (14)
F5^{i}—U1—F1^{ii}	71.71 (13)	F4—Na2—Na4	44.3 (2)
F4—U1—F3	82.68 (15)	F4^{ix}—Na2—Na4	140.9 (2)
F2—U1—F3	75.03 (13)	F4^{x}—Na2—Na4	76.0 (3)
F5^{i}—U1—F3	95.01 (14)	F4^{iii}—Na2—Na4	98.1 (3)
F1^{ii}—U1—F3	130.12 (13)	F4^{vii}—Na2—Na4	132.3 (3)
F4—U1—F5	78.23 (16)	F4^{v}—Na2—Na4	50.7 (3)
F2—U1—F5	141.18 (13)	Na4^{v}—Na2—Na4	23.7 (5)
F5^{i}—U1—F5	72.39 (19)	Na4^{iii}—Na2—Na4	134.4 (4)
F1^{ii}—U1—F5	93.76 (13)	Na4^{ix}—Na2—Na4	107.5 (4)
F3—U1—F5	128.66 (13)	Na4^{x}—Na2—Na4	117.21 (14)
F4—U1—F2^{ii}	69.09 (14)	Na4^{vii}—Na2—Na4	117.21 (14)
F2—U1—F2^{ii}	73.30 (14)	F4^{ii}—Na3—F4^{vii}	180.0
F5^{i}—U1—F2^{ii}	123.12 (14)	F4^{ii}—Na3—F4^{xi}	67.58 (14)
F1^{ii}—U1—F2^{ii}	68.88 (12)	F4^{vii}—Na3—F4^{xi}	112.42 (14)
F3—U1—F2^{ii}	141.86 (14)	F4^{ii}—Na3—F4^{x}	112.42 (14)
F5—U1—F2^{ii}	71.09 (13)	F4^{vii}—Na3—F4^{x}	67.58 (14)
F4—U1—F3^{iii}	72.67 (14)	F4^{xi}—Na3—F4^{x}	180.0
F2—U1—F3^{iii}	128.02 (13)	F4^{ii}—Na3—F4^{xii}	67.58 (14)
F5^{i}—U1—F3^{iii}	71.46 (13)	F4^{vii}—Na3—F4^{xii}	112.42 (14)
F1^{ii}—U1—F3^{iii}	142.28 (13)	F4^{xi}—Na3—F4^{xii}	67.58 (14)
F3—U1—F3^{iii}	61.42 (16)	F4^{x}—Na3—F4^{xii}	112.42 (14)
F5—U1—F3^{iii}	67.45 (13)	F4^{ii}—Na3—F4	112.42 (14)
F2^{ii}—U1—F3^{iii}	127.86 (13)	F4^{vii}—Na3—F4	67.58 (14)
F4—U1—F1^{iv}	139.92 (15)	F4^{xi}—Na3—F4	112.42 (14)
F2—U1—F1^{iv}	72.68 (13)	F4^{x}—Na3—F4	67.58 (14)
F5^{i}—U1—F1^{iv}	70.59 (13)	F4^{xii}—Na3—F4	180.00 (11)
F1^{ii}—U1—F1^{iv}	63.72 (14)	F4^{ii}—Na3—F2^{xii}	72.96 (12)
F3—U1—F1^{iv}	66.51 (12)	F4^{vii}—Na3—F2^{xii}	107.04 (12)

F5—U1—F1^{iv}	141.15 (13)	F4^{xi}—Na3—F2^{xii}	123.10 (11)
F2^{ii}—U1—F1^{iv}	121.72 (12)	F4^{x}—Na3—F2^{xii}	56.90 (11)
F3^{iii}—U1—F1^{iv}	110.40 (12)	F4^{xii}—Na3—F2^{xii}	60.17 (12)
F4—U1—Na4^{v}	42.7 (2)	F4—Na3—F2^{xii}	119.82 (12)
F2—U1—Na4^{v}	117.4 (2)	F4^{ii}—Na3—F2	107.04 (12)
F5^{i}—U1—Na4^{v}	97.6 (2)	F4^{vii}—Na3—F2	72.96 (12)
F1^{ii}—U1—Na4^{v}	139.8 (2)	F4^{xi}—Na3—F2	56.90 (11)
F3—U1—Na4^{v}	88.5 (2)	F4^{x}—Na3—F2	123.10 (11)
F5—U1—Na4^{v}	46.8 (2)	F4^{xii}—Na3—F2	119.82 (12)
F2^{ii}—U1—Na4^{v}	87.6 (2)	F4—Na3—F2	60.18 (12)
F3^{iii}—U1—Na4^{v}	40.6 (2)	F2^{xii}—Na3—F2	180.0
F1^{iv}—U1—Na4^{v}	150.5 (2)	F4^{ii}—Na3—F2^{ii}	60.18 (12)
F4—U1—Na4	36.3 (2)	F4^{vii}—Na3—F2^{ii}	119.82 (12)
F2—U1—Na4	108.4 (2)	F4^{xi}—Na3—F2^{ii}	72.95 (12)
F5^{i}—U1—Na4	108.7 (2)	F4^{x}—Na3—F2^{ii}	107.05 (12)
F1^{ii}—U1—Na4	125.0 (2)	F4^{xii}—Na3—F2^{ii}	123.10 (11)
F3—U1—Na4	104.8 (2)	F4—Na3—F2^{ii}	56.90 (11)
F5—U1—Na4	42.1 (2)	F2^{xii}—Na3—F2^{ii}	118.89 (3)
F2^{ii}—U1—Na4	66.6 (2)	F2—Na3—F2^{ii}	61.11 (3)
F3^{iii}—U1—Na4	61.6 (2)	F4^{ii}—Na3—F2^{vii}	119.82 (12)
F1^{iv}—U1—Na4	171.0 (2)	F4^{vii}—Na3—F2^{vii}	60.18 (12)
Na4^{v}—U1—Na4	21.0 (4)	F4^{xi}—Na3—F2^{vii}	107.05 (12)
F4—U1—Na4^{i}	135.4 (2)	F4^{x}—Na3—F2^{vii}	72.95 (12)
F2—U1—Na4^{i}	113.1 (2)	F4^{xii}—Na3—F2^{vii}	56.90 (11)
F5^{i}—U1—Na4^{i}	38.0 (2)	F4—Na3—F2^{vii}	123.10 (11)
F1^{ii}—U1—Na4^{i}	87.0 (2)	F2^{xii}—Na3—F2^{vii}	61.11 (3)
F3—U1—Na4^{i}	59.8 (2)	F2—Na3—F2^{vii}	118.89 (3)
F5—U1—Na4^{i}	105.7 (2)	F2^{ii}—Na3—F2^{vii}	180.0
F2^{ii}—U1—Na4^{i}	155.1 (2)	F4^{ii}—Na3—F2^{xi}	123.10 (11)
F3^{iii}—U1—Na4^{i}	68.7 (2)	F4^{vii}—Na3—F2^{xi}	56.90 (11)
F1^{iv}—U1—Na4^{i}	45.9 (2)	F4^{xi}—Na3—F2^{xi}	60.17 (12)
Na4^{v}—U1—Na4^{i}	108.47 (13)	F4^{x}—Na3—F2^{xi}	119.83 (12)
Na4—U1—Na4^{i}	128.2 (4)	F4^{xii}—Na3—F2^{xi}	72.96 (12)
F3—Na1—F3^{vi}	109.29 (14)	F4—Na3—F2^{xi}	107.04 (12)
F3—Na1—F3^{iv}	109.29 (14)	F2^{xii}—Na3—F2^{xi}	118.89 (3)

F3^{vi}—Na1—F3^{iv}	109.29 (14)	F2—Na3—F2^{xi}	61.11 (3)
F3—Na1—F1^{iv}	69.27 (13)	F2^{ii}—Na3—F2^{xi}	118.88 (3)
F3^{vi}—Na1—F1^{iv}	158.69 (19)	F2^{vii}—Na3—F2^{xi}	61.12 (3)
F3^{iv}—Na1—F1^{iv}	90.62 (14)	F4^{ii}—Na3—F2^{x}	56.90 (11)
F3—Na1—F1	90.62 (14)	F4^{vii}—Na3—F2^{x}	123.10 (11)
F3^{vi}—Na1—F1	69.27 (13)	F4^{xi}—Na3—F2^{x}	119.83 (12)
F3^{iv}—Na1—F1	158.68 (19)	F4^{x}—Na3—F2^{x}	60.17 (12)
F1^{iv}—Na1—F1	89.41 (17)	F4^{xii}—Na3—F2^{x}	107.04 (12)
F3—Na1—F1^{vi}	158.69 (19)	F4—Na3—F2^{x}	72.96 (12)
F3^{vi}—Na1—F1^{vi}	90.62 (14)	F2^{xii}—Na3—F2^{x}	61.11 (3)
F3^{iv}—Na1—F1^{vi}	69.27 (13)	F2—Na3—F2^{x}	118.89 (3)
F1^{iv}—Na1—F1^{vi}	89.41 (17)	F2^{ii}—Na3—F2^{x}	61.12 (3)
F1—Na1—F1^{vi}	89.41 (17)	F2^{vii}—Na3—F2^{x}	118.88 (3)
F3—Na1—Na4^{vii}	45.7 (2)	F2^{xi}—Na3—F2^{x}	180.0
F3^{vi}—Na1—Na4^{vii}	70.2 (2)	Na4^{v}—Na4—F4	84.1 (7)
F3^{iv}—Na1—Na4^{vii}	145.9 (3)	Na4^{v}—Na4—F3^{x}	122.4 (12)
F1^{iv}—Na1—Na4^{vii}	97.7 (3)	F4—Na4—F3^{x}	123.2 (6)
F1—Na1—Na4^{vii}	55.0 (2)	Na4^{v}—Na4—F5	83.3 (9)
F1^{vi}—Na1—Na4^{vii}	143.3 (2)	F4—Na4—F5	77.5 (4)
F3—Na1—Na4^{i}	70.2 (2)	F3^{x}—Na4—F5	146.0 (6)
F3^{vi}—Na1—Na4^{i}	145.9 (3)	Na4^{v}—Na4—F4^{v}	64.0 (7)
F3^{iv}—Na1—Na4^{i}	45.7 (2)	F4—Na4—F4^{v}	82.1 (5)
F1^{iv}—Na1—Na4^{i}	55.0 (2)	F3^{x}—Na4—F4^{v}	70.6 (3)
F1—Na1—Na4^{i}	143.3 (2)	F5—Na4—F4^{v}	143.1 (6)
F1^{vi}—Na1—Na4^{i}	97.7 (3)	Na4^{v}—Na4—F5^{v}	66.8 (9)
Na4^{vii}—Na1—Na4^{i}	115.83 (17)	F4—Na4—F5^{v}	146.1 (6)
F3—Na1—Na4^{viii}	145.9 (3)	F3^{x}—Na4—F5^{v}	65.5 (3)
F3^{vi}—Na1—Na4^{viii}	45.7 (2)	F5—Na4—F5^{v}	114.0 (5)
F3^{iv}—Na1—Na4^{viii}	70.2 (2)	F4^{v}—Na4—F5^{v}	69.9 (4)
F1^{iv}—Na1—Na4^{viii}	143.3 (2)	Na4^{v}—Na4—F1^{x}	139.0 (5)
F1—Na1—Na4^{viii}	97.7 (3)	F4—Na4—F1^{x}	111.8 (5)
F1^{vi}—Na1—Na4^{viii}	55.0 (2)	F3^{x}—Na4—F1^{x}	81.4 (4)
Na4^{vii}—Na1—Na4^{viii}	115.83 (17)	F5—Na4—F1^{x}	65.1 (3)
Na4^{i}—Na1—Na4^{viii}	115.83 (17)	F4^{v}—Na4—F1^{x}	151.8 (5)
F3—Na1—U1^{vi}	108.36 (10)	F5^{v}—Na4—F1^{x}	101.7 (4)

F3^{vi}—Na1—U1^{vi}	33.74 (10)	Na4^{v}—Na4—F2^{x}	160.4 (5)
F3^{iv}—Na1—U1^{vi}	135.20 (11)	F4—Na4—F2^{x}	77.7 (4)
F1^{iv}—Na1—U1^{vi}	125.26 (15)	F3^{x}—Na4—F2^{x}	64.5 (3)
F1—Na1—U1^{vi}	36.52 (9)	F5—Na4—F2^{x}	99.3 (5)
F1^{vi}—Na1—U1^{vi}	83.79 (10)	F4^{v}—Na4—F2^{x}	106.1 (4)
Na4^{vii}—Na1—U1^{vi}	62.7 (2)	F5^{v}—Na4—F2^{x}	127.7 (4)
Na4^{i}—Na1—U1^{vi}	178.5 (3)	F1^{x}—Na4—F2^{x}	56.7 (3)
Na4^{viii}—Na1—U1^{vi}	65.0 (2)	Na4^{v}—Na4—Na2	78.1 (2)
F3—Na1—U1	33.74 (10)	F4—Na4—Na2	41.9 (2)
F3^{vi}—Na1—U1	135.20 (11)	F3^{x}—Na4—Na2	91.2 (4)
F3^{iv}—Na1—U1	108.36 (10)	F5—Na4—Na2	117.7 (4)
F1^{iv}—Na1—U1	36.52 (9)	F4^{v}—Na4—Na2	42.0 (2)
F1—Na1—U1	83.79 (10)	F5^{v}—Na4—Na2	111.8 (4)
F1^{vi}—Na1—U1	125.26 (15)	F1^{x}—Na4—Na2	138.9 (5)
Na4^{vii}—Na1—U1	65.0 (2)	F2^{x}—Na4—Na2	83.6 (3)
Na4^{i}—Na1—U1	62.7 (2)	Na4^{v}—Na4—Na1^{xiii}	127.9 (8)
Na4^{viii}—Na1—U1	178.5 (3)	F4—Na4—Na1^{xiii}	148.0 (6)
U1^{vi}—Na1—U1	116.43 (4)	F3^{x}—Na4—Na1^{xiii}	44.7 (2)
F3—Na1—U1^{iv}	135.20 (11)	F5—Na4—Na1^{xiii}	102.7 (4)
F3^{vi}—Na1—U1^{iv}	108.36 (10)	F4^{v}—Na4—Na1^{xiii}	110.7 (4)
F3^{iv}—Na1—U1^{iv}	33.74 (10)	F5^{v}—Na4—Na1^{xiii}	63.6 (3)
F1^{iv}—Na1—U1^{iv}	83.79 (10)	F1^{x}—Na4—Na1^{xiii}	45.2 (2)
F1—Na1—U1^{iv}	125.26 (15)	F2^{x}—Na4—Na1^{xiii}	70.7 (3)
F1^{vi}—Na1—U1^{iv}	36.51 (9)	Na2—Na4—Na1^{xiii}	135.1 (4)
Na4^{vii}—Na1—U1^{iv}	178.5 (3)	Na4^{v}—Na4—U1^{v}	79.6 (10)
Na4^{i}—Na1—U1^{iv}	65.0 (2)	F4—Na4—U1^{v}	118.5 (5)
Na4^{viii}—Na1—U1^{iv}	62.7 (2)	F3^{x}—Na4—U1^{v}	43.0 (2)
U1^{vi}—Na1—U1^{iv}	116.43 (4)	F5—Na4—U1^{v}	154.8 (5)
U1—Na1—U1^{iv}	116.43 (4)	F4^{v}—Na4—U1^{v}	37.72 (19)
F4—Na2—F4^{ix}	174.1 (2)	F5^{v}—Na4—U1^{v}	41.79 (19)
F4—Na2—F4^{x}	91.55 (16)	F1^{x}—Na4—U1^{v}	119.0 (4)
F4^{ix}—Na2—F4^{x}	92.8 (2)	F2^{x}—Na4—U1^{v}	103.0 (3)
F4—Na2—F4^{iii}	84.4 (2)	Na2—Na4—U1^{v}	76.7 (3)
F4^{ix}—Na2—F4^{iii}	91.55 (16)	Na1^{xiii}—Na4—U1^{v}	74.2 (2)
F4^{x}—Na2—F4^{iii}	174.1 (3)	Na4^{v}—Na4—U1	79.3 (9)

F4—Na2—F4^{vii}	91.55 (16)	F4—Na4—U1	36.3 (2)
F4^{ix}—Na2—F4^{vii}	84.4 (2)	F3^{x}—Na4—U1	152.8 (6)
F4^{x}—Na2—F4^{vii}	91.55 (16)	F5—Na4—U1	41.4 (2)
F4^{iii}—Na2—F4^{vii}	92.8 (3)	F4^{v}—Na4—U1	111.5 (4)
F4—Na2—F4^{v}	92.8 (3)	F5^{v}—Na4—U1	141.6 (5)
F4^{ix}—Na2—F4^{v}	91.55 (16)	F1^{x}—Na4—U1	91.8 (3)
F4^{x}—Na2—F4^{v}	84.4 (2)	F2^{x}—Na4—U1	89.8 (3)
F4^{iii}—Na2—F4^{v}	91.55 (16)	Na2—Na4—U1	76.6 (3)
F4^{vii}—Na2—F4^{v}	174.1 (2)	Na1^{xiii}—Na4—U1	136.9 (4)
F4—Na2—Na4^{v}	50.7 (3)	U1^{v}—Na4—U1	148.8 (4)
F4^{ix}—Na2—Na4^{v}	132.3 (3)	U1^{xi}—F1—Na1	133.12 (17)
F4^{x}—Na2—Na4^{v}	98.1 (3)	U1^{xi}—F1—U1^{vi}	116.28 (14)
F4^{iii}—Na2—Na4^{v}	76.0 (3)	Na1—F1—U1^{vi}	108.65 (14)
F4^{vii}—Na2—Na4^{v}	140.9 (2)	U1^{xi}—F1—Na4^{vii}	109.1 (3)
F4^{v}—Na2—Na4^{v}	44.3 (2)	Na1—F1—Na4^{vii}	79.8 (3)
F4—Na2—Na4^{iii}	98.1 (3)	U1^{vi}—F1—Na4^{vii}	93.6 (3)
F4^{ix}—Na2—Na4^{iii}	76.0 (3)	U1—F2—U1^{xi}	151.86 (18)
F4^{x}—Na2—Na4^{iii}	140.9 (2)	U1—F2—Na3	101.58 (13)
F4^{iii}—Na2—Na4^{iii}	44.3 (2)	U1^{xi}—F2—Na3	99.29 (12)
F4^{vii}—Na2—Na4^{iii}	50.7 (3)	U1—F2—Na4^{vii}	95.6 (3)
F4^{v}—Na2—Na4^{iii}	132.3 (3)	U1^{xi}—F2—Na4^{vii}	101.5 (3)
Na4^{v}—Na2—Na4^{iii}	117.21 (14)	Na3—F2—Na4^{vii}	94.2 (3)
F4—Na2—Na4^{ix}	140.9 (2)	Na1—F3—Na4^{vii}	89.5 (3)
F4^{ix}—Na2—Na4^{ix}	44.3 (2)	Na1—F3—U1	113.65 (18)
F4^{x}—Na2—Na4^{ix}	50.7 (3)	Na4^{vii}—F3—U1	111.6 (4)
F4^{iii}—Na2—Na4^{ix}	132.3 (3)	Na1—F3—U1^{iii}	120.80 (19)
F4^{vii}—Na2—Na4^{ix}	98.1 (3)	Na4^{vii}—F3—U1^{iii}	96.3 (4)
F4^{v}—Na2—Na4^{ix}	76.0 (3)	U1—F3—U1^{iii}	118.16 (15)
Na4^{v}—Na2—Na4^{ix}	117.21 (14)	Na2—F4—U1	150.3 (2)
Na4^{iii}—Na2—Na4^{ix}	117.21 (14)	Na2—F4—Na4	93.8 (3)
F4—Na2—Na4^{x}	132.3 (3)	U1—F4—Na4	107.4 (3)
F4^{ix}—Na2—Na4^{x}	50.7 (3)	Na2—F4—Na4^{v}	87.3 (3)
F4^{x}—Na2—Na4^{x}	44.3 (2)	U1—F4—Na4^{v}	99.6 (3)
F4^{iii}—Na2—Na4^{x}	140.9 (2)	Na4—F4—Na4^{v}	31.9 (6)
F4^{vii}—Na2—Na4^{x}	76.0 (3)	Na2—F4—Na3	84.21 (14)

F4^{v}—Na2—Na4^{x}	98.1 (3)	U1—F4—Na3	104.92 (15)
Na4^{v}—Na2—Na4^{x}	134.4 (4)	Na4—F4—Na3	114.0 (4)
Na4^{iii}—Na2—Na4^{x}	107.5 (4)	Na4^{v}—F4—Na3	144.1 (3)
Na4^{ix}—Na2—Na4^{x}	23.7 (5)	U1^{xiv}—F5—U1	153.01 (19)
F4—Na2—Na4^{vii}	76.0 (3)	U1^{xiv}—F5—Na4	105.4 (3)
F4^{ix}—Na2—Na4^{vii}	98.1 (3)	U1—F5—Na4	96.5 (3)
F4^{x}—Na2—Na4^{vii}	132.3 (3)	U1^{xiv}—F5—Na4^{v}	115.4 (3)
F4^{iii}—Na2—Na4^{vii}	50.7 (3)	U1—F5—Na4^{v}	91.4 (3)
F4^{vii}—Na2—Na4^{vii}	44.3 (2)	Na4—F5—Na4^{v}	29.9 (6)

Symmetry codes: (i) −x+y, −x+1, z; (ii) y, −x+y, −z+2; (iii) −x, −x+y, −z+3/2; (iv) −y, x−y+1, z; (v) y, x, −z+3/2; (vi) −x+y−1, −x, z; (vii) −y, x−y, z; (viii) x−1, y, z; (ix) x−y, −y, −z+3/2; (x) −x+y, −x, z; (xi) x−y, x, −z+2; (xii) −x, −y, −z+2; (xiii) x+1, y, z; (xiv) −y+1, x−y+1, z.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.