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Tetrayttrium difluoride disilicate orthosilicate, $Y_4F_2[Si_2O_7][SiO_4]$

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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{Si-O}) = 0.009$ Å; R factor = 0.055; wR factor = 0.107; data-to-parameter ratio = 13.3.

In the crystal structure of $Y_4F_2[Si_2O_7][SiO_4]$, three fundamental building blocks are present, *viz.* anionic disilicate and orthosilicate units ($[Si_2O_7]^{6-}$ and $[SiO_4]^{4-}$) and cationic $[F_2Y_4]^{10+}$ entities. The latter are built up by two $[FY_3]^{8+}$ triangles sharing a common edge. The four crystallographically independent Y^{3+} cations display coordination numbers of eight for one and of seven for the other three cations, provided by oxide and fluoride anions. The overall arrangement of the building blocks can be considered as layer-like parallel to the *ac* plane.

Related literature

For isotypic $Er_4F_2[Si_2O_7][SiO_4]$, see: Müller-Bunz & Schleid (2001). For the minor by-product phase $Y_3F[Si_3O_{10}]$, see: Müller-Bunz & Schleid (1998). For the crystal structure of allanite (old name orthite), see: Rumanova & Nikoleva (1959).

Experimental

Crystal data

 $Y_4F_2[Si_2O_7][SiO_4]$
 $M_r = 653.91$

 Triclinic, $P\bar{1}$
 $a = 6.4987$ (5) Å

 $b = 6.6196$ (5) Å

 $c = 13.2978$ (9) Å

 $\alpha = 87.418$ (4)°

 $\beta = 85.702$ (4)°

 $\gamma = 60.854$ (3)°

 $V = 498.19$ (6) Å³
 $Z = 2$

 Mo $K\alpha$ radiation

 $\mu = 23.52$ mm⁻¹
 $T = 293$ K

 $0.10 \times 0.06 \times 0.03$ mm

Data collection

Nonius KappaCCD diffractometer

Absorption correction: numerical

 (*X-SHAPE*; Stoe & Cie, 1995)

 $T_{\min} = 0.104$, $T_{\max} = 0.463$

12473 measured reflections

2427 independent reflections

 1475 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.120$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.055$
 $wR(F^2) = 0.107$
 $S = 0.98$

2427 reflections

182 parameters

 $\Delta\rho_{\max} = 1.56$ e Å⁻³
 $\Delta\rho_{\min} = -1.49$ e Å⁻³

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2768).

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supporting information

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Tetrayttrium difluoride disilicate orthosilicate, $Y_4F_2[Si_2O_7][SiO_4]$

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S1. Comment

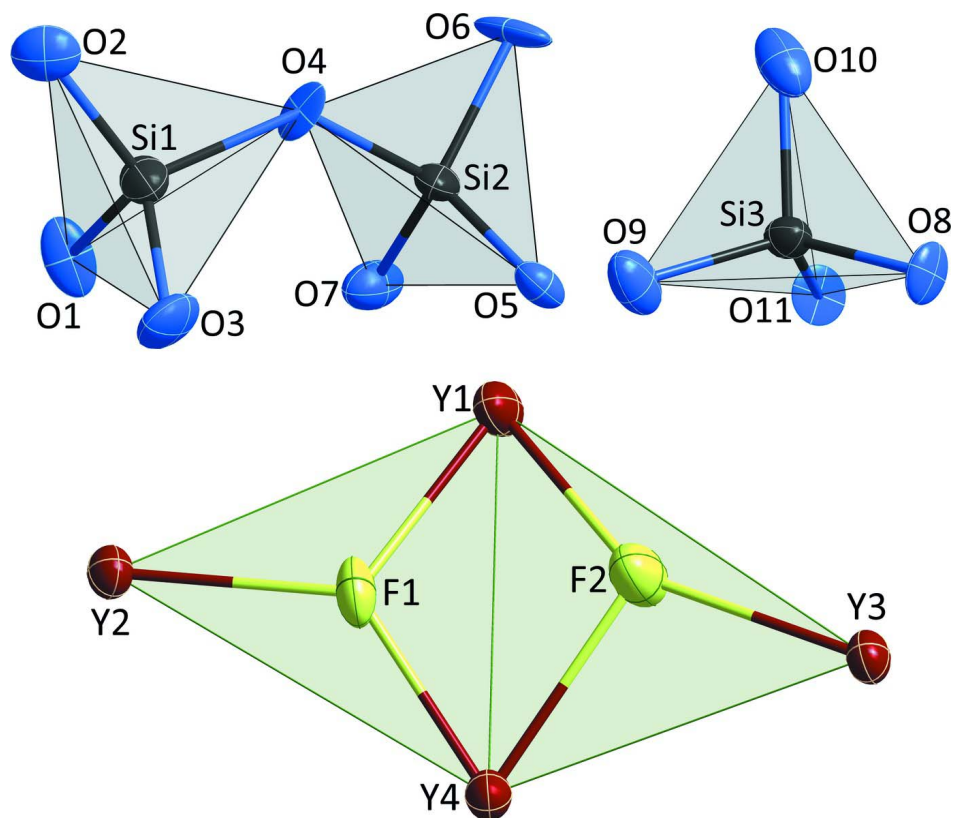
$Y_4F_2[Si_2O_7][SiO_4]$ crystallizes isotypically with the already known erbium analogue $Er_4F_2[Si_2O_7][SiO_4]$ (Müller-Bunz & Schleid, 2001). The crystal structure comprises two different oxidosilicate anions, namely a pyroanionic bitetrahedral disilicate unit $[Si_2O_7]^{6-}$ with eclipsed conformation (Fig. 1, *top left*) and an orthosilicate tetrahedron $[SiO_4]^{4-}$ (Fig. 1, *top right*), just like in the mineral allanite (old name orthite) (Rumanova & Nikoleva, 1959). Together with these two anionic building blocks, discrete cationic $[F_2Y_4]^{10+}$ entities (Fig. 1, *bottom*) complete the crystal structure of $Y_4F_2[Si_2O_7][SiO_4]$. For the formation of the latter, two almost planar $[FY_3]^{8+}$ triangles are fused together via one common edge, resulting in a butterfly-shaped $[F_2Y_4]^{10+}$ unit comprising an angle between the two triangular planes of $161.65(5)^\circ$. Two of the four crystallographically distinct Y^{3+} cations (Y2, Y3) display just one fluoride anion in their coordination sphere, while the other two (F1, F4) have contact with two F^- anions each. O^{2-} anions complete the coordination environments of the yttrium cations resulting in distorted bi- (Y1) or monocapped (Y2-4) trigonal prisms. The cationic $[F_2Y_4]^{10+}$ as well as the anionic $[Si_2O_7]^{6-}$ and $[SiO_4]^{4-}$ building blocks are arranged layer-like parallel to the *ac* plane in the crystal structure of the title compound (Fig. 2).

S2. Experimental

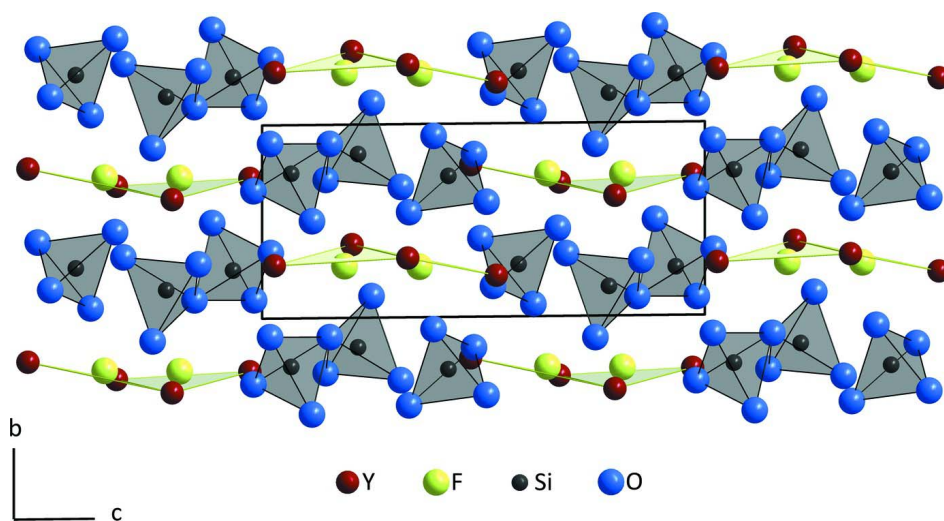
Colourless lath-shaped single crystals of $Y_4F_2[Si_2O_7][SiO_4]$ were obtained by the reaction of yttrium sesquioxide (Y_2O_3), yttrium trifluoride (YF_3), and silicon dioxide (SiO_2) in the molar ratio 2:5:3 and an excess of cesium chloride (CsCl) as flux in evacuated silica ampoules within nine days at 973 K and a cooling rate of 10 K h^{-1} . Due to the stability of the product against air and moisture, the excess flux can be removed by washing with water. Besides the title compound, single crystals of thalenite-type $Y_3F[Si_3O_{10}]$ (Müller-Bunz & Schleid, 1998) were also found in the product mixture as minor by-product.

S3. Refinement

The highest and lowest electron densities are found 1.29 \AA^{-3} from atom F2 and 1.28 \AA^{-3} from atom O8, respectively.


Figure 1

Disilicate ($[\text{Si}_2\text{O}_7]^{6-}$: *top left*) and orthosilicate units ($[\text{SiO}_4]^{4-}$: *top right*) as well as butterfly-shaped cationic $[\text{F}_2\text{Y}_4]^{10+}$ entities (*bottom*) in the crystal structure of $\text{Y}_4\text{F}_2[\text{Si}_2\text{O}_7][\text{SiO}_4]$; displacement ellipsoids are drawn at the 80 % probability level.


Figure 2

View at the crystal structure of $\text{Y}_4\text{F}_2[\text{Si}_2\text{O}_7][\text{SiO}_4]$ along $[100]$, emphasizing the layer-like arrangement as line-up of the cationic and anionic building blocks.

Tetrayttrium difluoride disilicate orthosilicate

Crystal data

Y₄F₂[Si₂O₇][SiO₄] $M_r = 653.91$ Triclinic, $P\bar{1}$

Hall symbol: -P 1

 $a = 6.4987 (5) \text{ \AA}$ $b = 6.6196 (5) \text{ \AA}$ $c = 13.2978 (9) \text{ \AA}$ $\alpha = 87.418 (4)^\circ$ $\beta = 85.702 (4)^\circ$ $\gamma = 60.854 (3)^\circ$ $V = 498.19 (6) \text{ \AA}^3$ $Z = 2$ $F(000) = 608$ $D_x = 4.359 \text{ Mg m}^{-3}$ Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 5136 reflections

 $\theta = 0.4\text{--}28.3^\circ$ $\mu = 23.52 \text{ mm}^{-1}$ $T = 293 \text{ K}$

Lath-shaped, colourless

 $0.10 \times 0.06 \times 0.03 \text{ mm}$

Data collection

Nonius KappaCCD

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

 ω and ϕ mscans

Absorption correction: numerical

 $(X\text{-SHAPE}; \text{Stoe \& Cie, 1995})$ $T_{\min} = 0.104, T_{\max} = 0.463$

12473 measured reflections

2427 independent reflections

1475 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.120$ $\theta_{\max} = 28.2^\circ, \theta_{\min} = 1.5^\circ$ $h = -8 \rightarrow 8$ $k = -8 \rightarrow 8$ $l = -17 \rightarrow 17$

Refinement

Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.055$ $wR(F^2) = 0.107$ $S = 0.98$

2427 reflections

182 parameters

0 restraints

Primary atom site location: structure-invariant

direct methods

Secondary atom site location: difference Fourier map

 $w = 1/[\sigma^2(F_o^2) + (0.0233P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} < 0.001$ $\Delta\rho_{\max} = 1.56 \text{ e \AA}^{-3}$ $\Delta\rho_{\min} = -1.49 \text{ e \AA}^{-3}$ Extinction correction: *SHELXL97* (Sheldrick, 2008), $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0029 (6)

Special details

Geometry. 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.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2 , conventional R-factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F , and R-factors based on ALL data will be even larger.

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Y1	0.32290 (19)	0.37903 (19)	0.20317 (8)	0.0102 (3)
Y2	0.94009 (19)	0.27320 (19)	0.02756 (8)	0.0083 (3)
Y3	0.21943 (19)	0.21311 (19)	0.52890 (8)	0.0083 (3)

Y4	0.82014 (19)	0.30705 (19)	0.32901 (8)	0.0084 (3)
F1	0.0366 (11)	0.2679 (11)	0.1862 (5)	0.0118 (14)
F2	0.2019 (11)	0.2616 (11)	0.3554 (5)	0.0143 (15)
Si1	0.4925 (5)	0.2508 (5)	0.9343 (2)	0.0098 (7)
Si2	0.2335 (5)	0.1526 (5)	0.7833 (2)	0.0084 (7)
Si3	0.2675 (5)	0.7298 (5)	0.4207 (2)	0.0078 (7)
O1	0.2654 (13)	0.3396 (14)	0.0197 (6)	0.0120 (17)
O2	0.2523 (13)	0.9039 (13)	0.0181 (6)	0.0117 (17)
O3	0.5550 (14)	0.5023 (14)	0.1127 (6)	0.0145 (18)
O4	0.4646 (12)	0.0987 (13)	0.8473 (5)	0.0086 (16)
O5	0.2042 (13)	0.3248 (13)	0.6867 (5)	0.0081 (16)
O6	0.6842 (13)	0.1117 (13)	0.2472 (6)	0.0122 (17)
O7	0.0069 (13)	0.7152 (13)	0.1437 (6)	0.0116 (17)
O8	0.4064 (13)	0.8414 (13)	0.4786 (6)	0.0092 (16)
O9	0.4233 (13)	0.5444 (14)	0.3321 (6)	0.0132 (18)
O10	0.8272 (13)	0.4057 (14)	0.4931 (6)	0.0135 (18)
O11	0.0157 (13)	0.9376 (13)	0.3873 (6)	0.0089 (17)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Y1	0.0090 (5)	0.0126 (6)	0.0088 (6)	-0.0050 (4)	-0.0027 (4)	0.0019 (4)
Y2	0.0088 (5)	0.0079 (6)	0.0077 (6)	-0.0035 (4)	-0.0013 (4)	-0.0008 (4)
Y3	0.0082 (5)	0.0081 (6)	0.0078 (6)	-0.0032 (4)	-0.0023 (4)	-0.0001 (4)
Y4	0.0079 (5)	0.0088 (6)	0.0076 (6)	-0.0034 (4)	-0.0011 (4)	-0.0008 (4)
F1	0.014 (3)	0.013 (4)	0.009 (3)	-0.005 (3)	-0.005 (3)	-0.001 (3)
F2	0.013 (3)	0.019 (4)	0.012 (4)	-0.009 (3)	-0.004 (3)	0.003 (3)
Si1	0.0073 (15)	0.0095 (16)	0.0107 (16)	-0.0022 (13)	-0.0022 (12)	-0.0016 (12)
Si2	0.0083 (15)	0.0058 (16)	0.0077 (16)	-0.0005 (13)	-0.0002 (12)	-0.0019 (12)
Si3	0.0079 (15)	0.0083 (16)	0.0077 (16)	-0.0044 (13)	0.0006 (12)	0.0002 (12)
O1	0.016 (4)	0.019 (4)	0.009 (4)	-0.009 (3)	0.005 (3)	-0.003 (3)
O2	0.011 (4)	0.010 (4)	0.016 (4)	-0.006 (3)	0.001 (3)	0.001 (3)
O3	0.017 (4)	0.012 (4)	0.010 (4)	-0.004 (3)	-0.003 (3)	0.006 (3)
O4	0.009 (4)	0.013 (4)	0.011 (4)	-0.006 (3)	-0.005 (3)	0.003 (3)
O5	0.010 (4)	0.009 (4)	0.009 (4)	-0.005 (3)	0.002 (3)	-0.002 (3)
O6	0.009 (4)	0.009 (4)	0.019 (4)	-0.001 (3)	-0.001 (3)	-0.004 (3)
O7	0.011 (4)	0.010 (4)	0.009 (4)	-0.002 (3)	0.002 (3)	0.002 (3)
O8	0.009 (4)	0.010 (4)	0.012 (4)	-0.006 (3)	-0.004 (3)	-0.002 (3)
O9	0.014 (4)	0.019 (4)	0.009 (4)	-0.008 (3)	0.000 (3)	-0.004 (3)
O10	0.012 (4)	0.012 (4)	0.009 (4)	0.000 (3)	-0.003 (3)	-0.001 (3)
O11	0.009 (4)	0.013 (4)	0.010 (4)	-0.005 (3)	-0.006 (3)	0.001 (3)

Geometric parameters (Å, °)

Y1—O6	2.248 (7)	Y3—Si3 ⁱⁱ	3.024 (3)
Y1—O3	2.286 (8)	Y3—Si2	3.392 (3)
Y1—O7	2.330 (7)	Y3—Y3 ⁱ	3.406 (2)
Y1—F1	2.337 (6)	Y3—Si3 ^x	3.431 (3)

Y1—F2	2.353 (6)	Y3—Y3 ⁱⁱ	3.559 (2)
Y1—O9	2.366 (7)	Y4—F1 ^{iv}	2.223 (6)
Y1—O1	2.540 (8)	Y4—O6	2.240 (8)
Y1—O4 ⁱ	2.856 (8)	Y4—O11 ^v	2.269 (8)
Y1—Si2 ⁱ	3.296 (3)	Y4—O9	2.272 (8)
Y1—Si2 ⁱⁱ	3.428 (3)	Y4—O10	2.316 (8)
Y1—Y4	3.5649 (15)	Y4—O5 ^{vi}	2.364 (7)
Y1—Y2 ⁱⁱⁱ	3.7351 (15)	Y4—F2 ^{iv}	2.400 (6)
Y2—O2 ⁱⁱⁱ	2.216 (8)	Y4—Si3 ^{vi}	3.352 (3)
Y2—F1 ^{iv}	2.239 (6)	Y4—Y3 ^{vi}	3.6603 (16)
Y2—O7 ⁱⁱⁱ	2.281 (8)	Y4—Y3 ^{iv}	3.6740 (14)
Y2—O2 ^v	2.295 (7)	Y4—Y1 ^{iv}	3.7852 (15)
Y2—O1 ⁱⁱⁱ	2.322 (8)	F1—Y4 ^{xi}	2.223 (6)
Y2—O1 ^{iv}	2.354 (7)	F1—Y2 ^{xi}	2.239 (6)
Y2—O3	2.424 (8)	F2—Y4 ^{xi}	2.400 (6)
Y2—Si1 ^{vi}	3.064 (3)	Si1—O3 ^{vi}	1.613 (8)
Y2—Si1 ^{vii}	3.316 (3)	Si1—O2 ^{vi}	1.626 (8)
Y2—Y2 ^{viii}	3.411 (2)	Si1—O4	1.644 (8)
Y2—Y2 ^{ix}	3.486 (2)	Si1—O1 ^{xiii}	1.666 (8)
Y2—Y1 ⁱⁱⁱ	3.7351 (15)	Si2—O6 ⁱ	1.622 (8)
Y3—O5	2.236 (7)	Si2—O7 ⁱⁱ	1.633 (8)
Y3—O8 ^x	2.257 (8)	Si2—O5	1.637 (8)
Y3—O8 ^{vi}	2.273 (7)	Si2—O4	1.657 (7)
Y3—O10 ^{xi}	2.305 (7)	Si3—O11	1.621 (7)
Y3—F2	2.319 (6)	Si3—O9	1.632 (8)
Y3—O11 ⁱⁱ	2.388 (8)	Si3—O8	1.660 (7)
Y3—O10 ^{vi}	2.398 (8)	Si3—O10 ^{vi}	1.684 (8)
O6—Y1—O3	78.8 (3)	O6—Y4—O10	138.3 (3)
O6—Y1—O7	163.3 (3)	O11 ^v —Y4—O10	84.6 (3)
O3—Y1—O7	85.3 (3)	O9—Y4—O10	90.6 (3)
O6—Y1—F1	119.2 (2)	F1 ^{iv} —Y4—O5 ^{vi}	78.7 (2)
O3—Y1—F1	142.5 (2)	O6—Y4—O5 ^{vi}	136.0 (3)
O7—Y1—F1	76.9 (2)	O11 ^v —Y4—O5 ^{vi}	148.0 (3)
O6—Y1—F2	83.0 (3)	O9—Y4—O5 ^{vi}	78.4 (3)
O3—Y1—F2	151.4 (2)	O10—Y4—O5 ^{vi}	75.9 (3)
O7—Y1—F2	109.4 (2)	F1 ^{iv} —Y4—F2 ^{iv}	67.0 (2)
F1—Y1—F2	66.0 (2)	O6—Y4—F2 ^{iv}	135.7 (3)
O6—Y1—O9	73.5 (3)	O11 ^v —Y4—F2 ^{iv}	77.8 (2)
O3—Y1—O9	79.2 (3)	O9—Y4—F2 ^{iv}	147.8 (3)
O7—Y1—O9	98.5 (3)	O10—Y4—F2 ^{iv}	70.5 (2)
F1—Y1—O9	135.6 (2)	O5 ^{vi} —Y4—F2 ^{iv}	71.9 (2)
F2—Y1—O9	74.6 (2)	Y4 ^{xi} —F1—Y2 ^{xi}	128.6 (3)
O6—Y1—O1	111.4 (3)	Y4 ^{xi} —F1—Y1	112.2 (2)
O3—Y1—O1	75.0 (3)	Y2 ^{xi} —F1—Y1	114.7 (3)
O7—Y1—O1	68.9 (3)	Y3—F2—Y1	149.1 (3)
F1—Y1—O1	67.9 (2)	Y3—F2—Y4 ^{xi}	102.2 (2)
F2—Y1—O1	132.7 (2)	Y1—F2—Y4 ^{xi}	105.6 (2)

O9—Y1—O1	152.0 (3)	O3 ^{vi} —Si1—O2 ^{vi}	115.4 (4)
O6—Y1—O4 ⁱ	56.4 (2)	O3 ^{vi} —Si1—O4	109.4 (4)
O3—Y1—O4 ⁱ	103.4 (3)	O2 ^{vi} —Si1—O4	108.6 (4)
O7—Y1—O4 ⁱ	133.9 (2)	O3 ^{vi} —Si1—O1 ^{xii}	99.6 (4)
F1—Y1—O4 ⁱ	68.9 (2)	O2 ^{vi} —Si1—O1 ^{xii}	113.6 (4)
F2—Y1—O4 ⁱ	84.1 (2)	O4—Si1—O1 ^{xii}	110.0 (4)
O9—Y1—O4 ⁱ	127.5 (2)	O6 ⁱ —Si2—O7 ⁱⁱ	117.1 (4)
O1—Y1—O4 ⁱ	70.1 (2)	O6 ⁱ —Si2—O5	114.0 (4)
O2 ⁱⁱⁱ —Y2—F1 ^{iv}	122.9 (3)	O7 ⁱⁱ —Si2—O5	106.6 (4)
O2 ⁱⁱⁱ —Y2—O7 ⁱⁱⁱ	79.4 (3)	O6 ⁱ —Si2—O4	97.8 (4)
F1 ^{iv} —Y2—O7 ⁱⁱⁱ	154.6 (3)	O7 ⁱⁱ —Si2—O4	109.3 (4)
O2 ⁱⁱⁱ —Y2—O2 ^v	81.8 (3)	O5—Si2—O4	111.9 (4)
F1 ^{iv} —Y2—O2 ^v	85.6 (2)	O11—Si3—O9	114.6 (4)
O7 ⁱⁱⁱ —Y2—O2 ^v	86.0 (3)	O11—Si3—O8	109.0 (4)
O2 ⁱⁱⁱ —Y2—O1 ⁱⁱⁱ	108.9 (3)	O9—Si3—O8	115.8 (4)
F1 ^{iv} —Y2—O1 ⁱⁱⁱ	106.1 (2)	O11—Si3—O10 ^{vi}	99.8 (4)
O7 ⁱⁱⁱ —Y2—O1 ⁱⁱⁱ	73.6 (3)	O9—Si3—O10 ^{vi}	107.4 (4)
O2 ^v —Y2—O1 ⁱⁱⁱ	154.3 (3)	O8—Si3—O10 ^{vi}	108.9 (4)
O2 ⁱⁱⁱ —Y2—O1 ^{iv}	153.3 (3)	Si1 ^{vii} —O1—Y2 ⁱⁱⁱ	99.1 (4)
F1 ^{iv} —Y2—O1 ^{iv}	72.8 (2)	Si1 ^{vii} —O1—Y2 ^{xi}	129.2 (4)
O7 ⁱⁱⁱ —Y2—O1 ^{iv}	82.0 (3)	Y2 ⁱⁱⁱ —O1—Y2 ^{xi}	96.4 (3)
O2 ^v —Y2—O1 ^{iv}	78.1 (3)	Si1 ^{vii} —O1—Y1	120.2 (4)
O1 ⁱⁱⁱ —Y2—O1 ^{iv}	83.6 (3)	Y2 ⁱⁱⁱ —O1—Y1	100.3 (3)
O2 ⁱⁱⁱ —Y2—O3	78.4 (3)	Y2 ^{xi} —O1—Y1	103.8 (3)
F1 ^{iv} —Y2—O3	78.6 (2)	Si1 ^{vi} —O2—Y2 ⁱⁱⁱ	118.5 (4)
O7 ⁱⁱⁱ —Y2—O3	121.1 (3)	Si1 ^{vi} —O2—Y2 ^{xiii}	139.1 (5)
O2 ^v —Y2—O3	142.0 (3)	Y2 ⁱⁱⁱ —O2—Y2 ^{xiii}	98.2 (3)
O1 ⁱⁱⁱ —Y2—O3	63.6 (3)	Si1 ^{vi} —O3—Y1	133.6 (5)
O1 ^{iv} —Y2—O3	127.9 (3)	Si1 ^{vi} —O3—Y2	96.7 (4)
O5—Y3—O8 ^x	124.4 (3)	Y1—O3—Y2	128.7 (3)
O5—Y3—O8 ^{vi}	84.1 (3)	Si1—O4—Si2	130.4 (5)
O8 ^x —Y3—O8 ^{vi}	82.5 (3)	Si1—O4—Y1 ⁱ	136.4 (4)
O5—Y3—O10 ^{xi}	102.1 (3)	Si2—O4—Y1 ⁱ	89.8 (3)
O8 ^x —Y3—O10 ^{xi}	112.7 (3)	Si2—O5—Y3	121.5 (4)
O8 ^{vi} —Y3—O10 ^{xi}	154.3 (3)	Si2—O5—Y4 ^{vi}	132.8 (4)
O5—Y3—F2	155.0 (2)	Y3—O5—Y4 ^{vi}	105.4 (3)
O8 ^x —Y3—F2	79.2 (3)	Si2 ⁱ —O6—Y4	138.9 (4)
O8 ^{vi} —Y3—F2	91.6 (2)	Si2 ⁱ —O6—Y1	115.8 (4)
O10 ^{xi} —Y3—F2	72.2 (2)	Y4—O6—Y1	105.2 (3)
O5—Y3—O11 ⁱⁱ	79.8 (3)	Si2 ⁱⁱ —O7—Y2 ⁱⁱⁱ	129.9 (4)
O8 ^x —Y3—O11 ⁱⁱ	77.4 (3)	Si2 ⁱⁱ —O7—Y1	118.8 (4)
O8 ^{vi} —Y3—O11 ⁱⁱ	140.4 (3)	Y2 ⁱⁱⁱ —O7—Y1	108.2 (3)
O10 ^{xi} —Y3—O11 ⁱⁱ	65.2 (3)	Si3—O8—Y3 ^{xiv}	121.6 (4)
F2—Y3—O11 ⁱⁱ	117.1 (2)	Si3—O8—Y3 ^{vi}	135.4 (4)
O5—Y3—O10 ^{vi}	76.7 (3)	Y3 ^{xiv} —O8—Y3 ^{vi}	97.5 (3)
O8 ^x —Y3—O10 ^{vi}	147.8 (3)	Si3—O9—Y4	125.0 (4)
O8 ^{vi} —Y3—O10 ^{vi}	75.5 (3)	Si3—O9—Y1	133.0 (4)
O10 ^{xi} —Y3—O10 ^{vi}	81.6 (3)	Y4—O9—Y1	100.4 (3)

F2—Y3—O10 ^{vi}	78.4 (3)	Si3 ^{vi} —O10—Y3 ^{iv}	97.4 (3)
O11 ⁱⁱ —Y3—O10 ^{vi}	133.8 (3)	Si3 ^{vi} —O10—Y4	112.9 (4)
F1 ^{iv} —Y4—O6	84.0 (3)	Y3 ^{iv} —O10—Y4	105.3 (3)
F1 ^{iv} —Y4—O11 ^v	99.0 (3)	Si3 ^{vi} —O10—Y3 ^{vi}	136.1 (4)
O6—Y4—O11 ^v	74.4 (3)	Y3 ^{iv} —O10—Y3 ^{vi}	98.4 (3)
F1 ^{iv} —Y4—O9	119.3 (2)	Y4—O10—Y3 ^{vi}	101.9 (3)
O6—Y4—O9	75.5 (3)	Si3—O11—Y4 ^{xiii}	145.4 (4)
O11 ^v —Y4—O9	127.5 (3)	Si3—O11—Y3 ⁱⁱ	96.1 (4)
F1 ^{iv} —Y4—O10	135.4 (2)	Y4 ^{xiii} —O11—Y3 ⁱⁱ	116.6 (3)

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