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Crystal structure of $[Y_6(\mu_6\text{-O})(\mu_3\text{-OH})_8(H_2O)_{24}]I_8\cdot 8H_2O$

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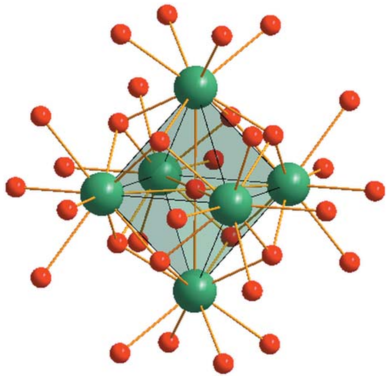
The crystal structure of the title compound {systematic name: octa-μ_3-hydroxido-μ_6-oxido-hexakis[tetraaquayttrium(III)] octaiodide octahydrate}, is characterized by the presence of the centrosymmetric molecular entity $[Y_6(\mu_6\text{-O})(\mu_3\text{-OH})_8(H_2O)_{24}]^{8+}$, in which the six Y^{3+} cations are arranged octahedrally around a μ_6-O atom at the centre of the cationic complex. Each of the eight faces of the Y_6 octahedron is capped by an μ_3-OH group in the form of a distorted cube. In the hexanuclear entity, the Y^{3+} cations are coordinated by the central μ_6-O atom, the O atoms of four μ_3-OH and of four water molecules. The resulting coordination sphere of the metal ions is a capped square-antiprism. The crystal packing is quite similar to that of the orthorhombic $[Ln_6(\mu_6\text{-O})(\mu_3\text{-OH})_8(H_2O)_{24}]I_8\cdot 8H_2O$ structures with Ln = La—Nd, Eu—Tb, Dy, except that the title compound exhibits a slight monoclinic distortion. The proximity of the cationic complexes and the lattice water molecules leads to the formation of a three-dimensional hydrogen-bonded network of medium strength.

1. Chemical context

Rare-earth-based oxido-hydroxido polynuclear complexes are of interest because of their unique luminescence (Chen *et al.*, 2010; Le Natur *et al.*, 2013; Petit *et al.*, 2009), magnetic properties (Abbas *et al.*, 2010; Xu *et al.*, 2011) or structural characteristics (Zheng, 2001; Andrews *et al.*, 2013). Actually, in this kind of complex, the spatial proximity between metal ions affords cooperative/synergetic effects or energy-transfer mechanisms workable in terms of optical properties. For more than a decade, our group has been involved in the synthesis and the characterization of such rare-earth-based hexanuclear



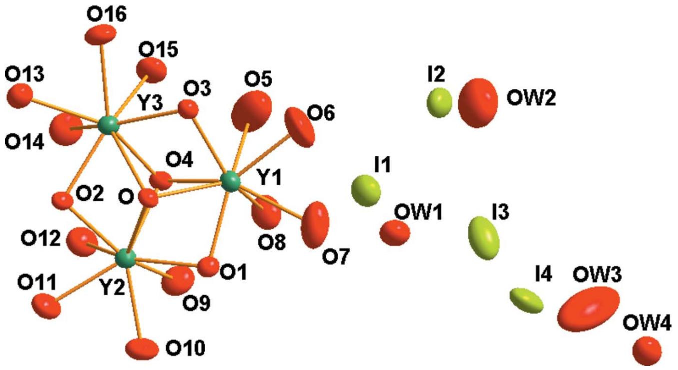


Figure 1
The asymmetric unit of the title complex. Displacement ellipsoids are drawn at the 50% probability level.

complexes (Calvez *et al.*, 2010). The hexanuclear complexes crystallize in different structures depending on the counter-anion (*e.g.* nitrate, perchlorate, iodide: Zak *et al.*, 1994; Wang *et al.*, 2000; Mudring *et al.*, 2006), the number of lattice water molecules and/or the radius of the involved lanthanide ion. Since the pioneering work of Zak *et al.* (1994), we have developed a systematic synthetic procedure for the nitrate counter-anion complex with most of the rare earth elements (Calvez *et al.*, 2008, 2010). In this context, we have undertaken the study of a series of complexes based on the iodide counter-anion which have never been obtained with heavier rare earth ions. We report here the synthesis and crystal structure of the yttrium derivative.

2. Structural commentary

In contrast to the orthorhombic $[Ln_6(\mu_6\text{-O})(\mu_3\text{-OH})_8(H_2O)_{24}]I_8\cdot 8H_2O$ structures with *Ln* = La—Nd, Eu—Tb, Dy (Mudring & Babai, 2005; Mudring *et al.*, 2006; Rukk *et al.*, 2009), the crystal structure of the yttrium member of this series has monoclinic symmetry, with the monoclinic angle close to 90° (Table 2). The asymmetric unit of $[Y_6(\mu_6\text{-O})(\mu_3\text{-OH})_8(H_2O)_{24}]I_8\cdot 8H_2O$ contains half of the formula unit because the complete complex is situated on a centre of inversion. Three independent yttrium cations (Y1, Y2 and Y3), four oxygen atoms from μ_3-hydroxyl groups (O1, O2, O3, O4), twelve oxygen atoms of terminal aqua ligands coordinating to each yttrium cation (Y1: O5, O6, O7, O8; Y2: O9, O10, O11, O12; Y3: O13, O14, O15 O16), one μ_6-bridging O atom (O) lying on an inversion centre, four iodide anions (I1, I2, I3, I4) and four oxygen atoms of lattice water molecules (O*W*1, O*W*2, O*W*3, O*W*4) are present in the crystal structure (Fig. 1). Calculations with the *SHAPE* software suite (Alvarez *et al.*, 2005) indicate that each of the coordination polyhedra surrounding the Y^{3+} ions is best described as a spherical capped square-antiprism (Ruiz-Martínez *et al.*, 2010) with idealized C_{4v} symmetry. However, the true symmetry of this structural fragment in the title structure is C_1.

Since the μ_6-O atom is located on an inversion centre and binds to six Y^{3+} cations, a slightly distorted anion-centred $[OY_6]$ octahedron results (Fig. 2). The average of the Y···Y distances between adjacent cations in the octahedron is found to be 3.536 Å. The mean Y—(μ_6-O) distance is 2.537 Å, while the averaged Y—(μ_3-OH) is 2.34 Å. The hydroxide ions are situated above the eight faces of the OY_6 octahedron and form a distorted cube around the octahedron (Fig. 2).

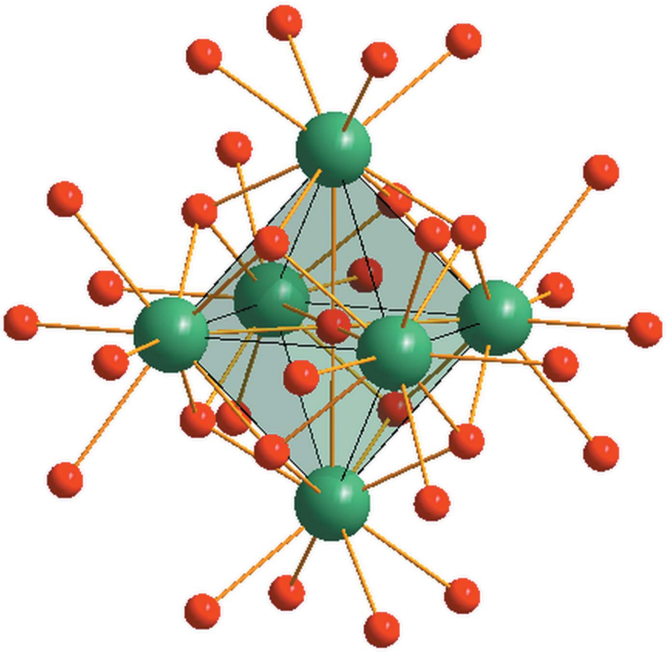


Figure 2
The OY_6 octahedron in the complex $[Y_6(\mu_6\text{-O})(\mu_3\text{-OH})_8(H_2O)_{24}]^{8+}$ cation. Y atoms are green and O atoms are red.

3. Supramolecular features

The hexanuclear $[Y_6(\mu_6\text{-O})(\mu_3\text{-OH})_8(H_2O)_{24}]^{8+}$ units are arranged in a body-centred fashion in the crystal structure. Each of these units is surrounded by twelve iodide anions, connecting the units to each other through Coulombic interactions. Although the hydrogen atoms of the water molecules and hydroxide groups could not be located, the range of O···O distances between the cationic complex and the lattice water molecules suggest the formation of medium-strength

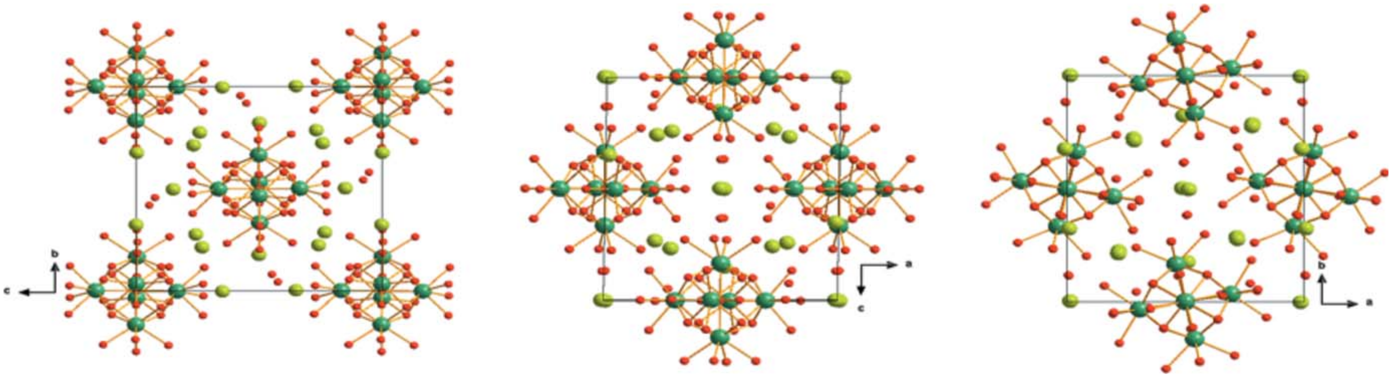


Figure 3
The crystal structure of $[Y_6(\mu_6\text{-O})(\mu_3\text{-OH})_8(H_2O)_{24}]I_8\cdot 8H_2O$ in projections along [100], [010] and [001], respectively, from left to right. Y atoms are green, O atoms are red and I atoms are yellow.

Table 1
Hydrogen-bond geometry (Å).

$D\cdots A$	$D\cdots A$
O7$\cdots$O*W*2	2.646 (4)
O10$\cdots$O*W*3	2.764 (1)
O13$\cdots$O*W*4	2.803 (8)
O15$\cdots$O*W*1	2.767 (2)
O16$\cdots$O*W*4	2.836 (2)
O16$\cdots$O*W*1	2.851 (6)

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Y_6O(OH)_8(H_2O)_{24}]I_8\cdot 8H_2O$
M_r	2277.24
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	293
a, b, c (Å)	12.9099 (2), 14.8050 (2), 14.7933 (3)
β (°)	90.821 (1)
V (Å^3)	2827.17 (8)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	10.54
Crystal size (mm)	0.18 × 0.14 × 0.1
Data collection	
Diffractometer	Nonius KappaCCD
Absorption correction	Gaussian (Coppens *et al.*, 1965)
T_{min}, T_{max}	0.018, 0.091
No. of measured, independent and observed $[I > 2\sigma(I)]$ reflections	35352, 6374, 5449
R_{int}	0.124
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.647
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.067, 0.178, 1.11
No. of reflections	6374
No. of parameters	251
	$w = 1/[\sigma^2(F_o^2) + (0.0487P)^2 + 43.8859P]$ where $P = (F_o^2 + 2F_c^2)/3$
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	2.62, −1.83

Computer programs: *COLLECT* (Nonius, 1998), *EVALCCD* (Duisenberg *et al.*, 2003), *SHELXS97* and *SHELXL97* (Sheldrick, 2008), *DIAMOND* (Brandenburg, 2006) and *publCIF* (Westrip, 2010).

hydrogen bonds (Table 1). These interactions lead to the formation of a three-dimensional network in the structure (Fig. 3).

4. Synthesis and crystallization

Yttrium oxide Y_2O_3 (2 g, Strem Chemicals 4M) was dissolved in fresh hydroiodic acid (9 ml, 57wt%, unstabilized from Acros Organics) under gentle heating (323 K). If the acid used is not fresh, it should be distilled twice. The clear solution was exposed to air under isothermal conditions (6 weeks). At this stage, the pH of the solution remains acidic. Large pale-yellow polyhedral crystals were separated manually from the solution and were mounted into a glass capillary.

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The hydrogen atoms from the water molecules or hydroxide could not be assigned reliably and thus were not included in the refinement. However, they were taken into account for the chemical formula sum, moiety, weight, as well as for the absorption coefficient and the number of electrons in the unit cell.

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Crystal structure of $[Y_6(\mu_6\text{-O})(\mu_3\text{-OH})_8(H_2O)_{24}]I_8\cdot 8H_2O$

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Computing details

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *COLLECT* (Nonius, 1998); data reduction: *EVALCCD* (Duisenberg *et al.*, 2003); 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: *publCIF* (Westrip, 2010).

Octa-μ_3-hydroxido-μ_6-oxido-hexakis[tetraaquayttrium(III)] octaiodide octahydrate

Crystal data

$[Y_6O(OH)_8(H_2O)_{24}]I_8\cdot 8H_2O$
$M_r = 2277.24$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 12.9099$ (2) Å
$b = 14.8050$ (2) Å
$c = 14.7933$ (3) Å
$\beta = 90.821$ (1)°
$V = 2827.17$ (8) Å^3
$Z = 2$
$F(000) = 2116$
$D_x = 2.675$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 62388 reflections
$\theta = 2.9$–27.5°
$\mu = 10.54$ mm^{-1}
$T = 293$ K
Block, colorless
0.18 × 0.14 × 0.1 mm

Data collection

Nonius KappaCCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
CCD rotation images, thick slices scans
Absorption correction: gaussian (Coppens *et al.*, 1965)
$T_{min} = 0.018$, $T_{max} = 0.091$
35352 measured reflections
6374 independent reflections
5449 reflections with $I > 2\sigma(I)$
$R_{int} = 0.124$
$\theta_{max} = 27.4°$, $\theta_{min} = 3.1°$
$h = -16 \rightarrow 16$
$k = -19 \rightarrow 18$
$l = -19 \rightarrow 19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.067$
$wR(F^2) = 0.178$
$S = 1.11$
6374 reflections
251 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
$w = 1/[\sigma^2(F_o^2) + (0.0487P)^2 + 43.8859P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 2.62$ e Å^{-3}
$\Delta\rho_{min} = -1.83$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00258 (19)

Special details

Experimental. 6336 sampling points

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'s 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 (Å^2)

	x	y	z	$U_{\rm iso}$*/$U_{\rm eq}$
Y1	0.50083 (7)	1.00150 (6)	1.16560 (6)	0.0335 (2)
Y2	0.46090 (7)	1.16586 (6)	0.99794 (6)	0.0317 (2)
Y3	0.30677 (7)	0.96613 (6)	0.99944 (6)	0.0323 (2)
I1	0.49148 (9)	0.82346 (8)	0.49868 (6)	0.0707 (3)
I2	0.28137 (7)	0.72379 (7)	0.24171 (7)	0.0650 (3)
I3	0.48625 (14)	0.50289 (7)	0.14980 (8)	0.0932 (4)
I4	0.78359 (8)	0.78678 (8)	0.26729 (8)	0.0792 (4)
O	0.5000	1.0000	1.0000	0.0293 (17)
O1	0.3633 (5)	1.0806 (4)	1.0999 (4)	0.0328 (13)
O2	0.4097 (5)	0.8826 (4)	1.1002 (4)	0.0313 (13)
O3	0.3622 (5)	1.0773 (4)	0.8978 (4)	0.0321 (13)
O4	0.4081 (5)	0.8803 (4)	0.9008 (4)	0.0335 (13)
O5	0.6563 (13)	1.0251 (17)	1.2721 (11)	0.150 (8)
O6	0.5306 (14)	0.8859 (13)	1.2758 (10)	0.136 (7)
O7	0.3511 (12)	0.9672 (11)	1.2711 (9)	0.106 (5)
O8	0.4775 (9)	1.1210 (7)	1.2708 (6)	0.069 (3)
O9	0.4402 (8)	1.2676 (6)	1.1305 (7)	0.064 (2)
O10	0.2918 (7)	1.2392 (6)	0.9958 (7)	0.065 (2)
O11	0.4402 (7)	1.2644 (6)	0.8649 (7)	0.060 (2)
O12	0.5819 (8)	1.2981 (6)	0.9988 (7)	0.066 (2)
O13	0.1968 (6)	0.9524 (7)	1.1339 (6)	0.058 (2)
O14	0.2216 (8)	0.8163 (7)	1.0027 (8)	0.075 (3)
O15	0.1950 (6)	0.9452 (7)	0.8664 (6)	0.059 (2)
O16	0.1578 (7)	1.0700 (7)	0.9987 (7)	0.063 (2)
OW1	−0.0079 (7)	0.8851 (8)	0.8689 (7)	0.070 (3)
OW2	0.2083 (19)	0.5431 (17)	0.0762 (13)	0.164 (8)
OW3	0.7261 (18)	0.5806 (14)	0.051 (2)	0.216 (13)
OW4	0.9948 (7)	0.8828 (8)	0.1328 (7)	0.069 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Y1	0.0380 (5)	0.0307 (5)	0.0318 (4)	0.0014 (3)	−0.0006 (3)	0.0000 (3)
Y2	0.0313 (4)	0.0271 (4)	0.0367 (5)	−0.0001 (3)	−0.0010 (3)	0.0003 (3)
Y3	0.0297 (4)	0.0292 (4)	0.0381 (5)	−0.0001 (3)	−0.0011 (3)	0.0003 (3)

I1	0.0799 (7)	0.0740 (7)	0.0580 (5)	0.0010 (5)	−0.0028 (4)	−0.0014 (4)
I2	0.0624 (5)	0.0599 (5)	0.0731 (6)	−0.0069 (4)	0.0146 (4)	0.0202 (4)
I3	0.1624 (13)	0.0473 (5)	0.0701 (7)	−0.0080 (6)	0.0074 (7)	0.0003 (4)
I4	0.0647 (6)	0.0771 (7)	0.0950 (8)	0.0062 (5)	−0.0237 (5)	0.0377 (6)
O	0.035 (4)	0.021 (4)	0.032 (4)	0.001 (3)	−0.002 (3)	0.002 (3)
O1	0.032 (3)	0.028 (3)	0.039 (3)	−0.001 (2)	0.001 (3)	−0.003 (3)
O2	0.029 (3)	0.023 (3)	0.042 (3)	0.001 (2)	0.000 (3)	0.005 (3)
O3	0.029 (3)	0.033 (3)	0.034 (3)	−0.002 (2)	−0.003 (2)	0.003 (3)
O4	0.029 (3)	0.033 (3)	0.038 (3)	0.000 (2)	−0.006 (3)	0.000 (3)
O5	0.099 (11)	0.26 (3)	0.090 (11)	0.009 (13)	−0.001 (9)	−0.023 (13)
O6	0.157 (15)	0.171 (17)	0.080 (9)	0.027 (12)	0.002 (9)	0.065 (10)
O7	0.127 (11)	0.120 (11)	0.070 (7)	−0.043 (9)	0.026 (7)	−0.005 (7)
O8	0.101 (8)	0.057 (6)	0.050 (5)	0.002 (5)	0.000 (5)	−0.018 (4)
O9	0.064 (6)	0.051 (5)	0.078 (6)	−0.003 (4)	0.004 (5)	−0.020 (5)
O10	0.054 (5)	0.052 (5)	0.089 (7)	0.018 (4)	−0.004 (5)	0.006 (5)
O11	0.058 (5)	0.047 (5)	0.075 (6)	0.001 (4)	−0.006 (4)	0.020 (4)
O12	0.067 (6)	0.048 (5)	0.082 (7)	−0.007 (4)	−0.004 (5)	0.007 (5)
O13	0.041 (4)	0.073 (6)	0.061 (5)	0.000 (4)	0.005 (4)	0.010 (4)
O14	0.062 (6)	0.065 (6)	0.098 (8)	−0.027 (5)	−0.003 (5)	0.002 (6)
O15	0.045 (4)	0.075 (6)	0.058 (5)	−0.004 (4)	−0.018 (4)	−0.005 (4)
O16	0.041 (4)	0.079 (6)	0.071 (6)	0.023 (4)	0.002 (4)	−0.006 (5)
OW1	0.051 (5)	0.086 (7)	0.072 (6)	−0.006 (5)	−0.004 (4)	−0.009 (5)
OW2	0.19 (2)	0.19 (2)	0.114 (14)	0.012 (17)	0.028 (13)	−0.005 (14)
OW3	0.158 (19)	0.091 (13)	0.40 (4)	0.027 (13)	0.09 (2)	0.004 (19)
OW4	0.052 (5)	0.086 (7)	0.068 (6)	−0.010 (5)	−0.006 (4)	0.010 (5)

Geometric parameters (Å, º)

Y1—O2	2.321 (6)	Y2—O11	2.462 (9)
Y1—O3$^{\rm i}$	2.326 (6)	Y2—O9	2.490 (9)
Y1—O1	2.328 (7)	Y2—O12	2.506 (9)
Y1—O4$^{\rm i}$	2.332 (7)	Y2—O	2.5070 (9)
Y1—O8	2.378 (9)	Y3—O2	2.336 (6)
Y1—O6	2.390 (14)	Y3—O3	2.347 (6)
Y1—O	2.4497 (9)	Y3—O4	2.348 (7)
Y1—O7	2.553 (13)	Y3—O1	2.362 (6)
Y1—O5	2.557 (18)	Y3—O15	2.443 (8)
Y2—O2$^{\rm i}$	2.341 (6)	Y3—O16	2.462 (8)
Y2—O3	2.341 (6)	Y3—O13	2.469 (8)
Y2—O4$^{\rm i}$	2.344 (6)	Y3—O14	2.477 (10)
Y2—O1	2.347 (6)	Y3—O	2.5444 (9)
Y2—O10	2.438 (9)		
O2—Y1—O3$^{\rm i}$	80.5 (2)	O10—Y2—O	128.0 (2)
O2—Y1—O1	80.1 (2)	O11—Y2—O	127.6 (2)
O3$^{\rm i}$—Y1—O1	131.5 (2)	O9—Y2—O	127.3 (3)
O2—Y1—O4$^{\rm i}$	130.4 (2)	O12—Y2—O	129.8 (2)
O3$^{\rm i}$—Y1—O4$^{\rm i}$	79.4 (2)	O2—Y3—O3	127.1 (2)

O1—Y1—O4^{i}	80.4 (2)	O2—Y3—O4	78.1 (2)
O2—Y1—O8	140.2 (3)	O3—Y3—O4	78.7 (2)
O3^{i}—Y1—O8	137.8 (3)	O2—Y3—O1	79.1 (2)
O1—Y1—O8	78.2 (3)	O3—Y3—O1	78.8 (2)
O4^{i}—Y1—O8	77.7 (3)	O4—Y3—O1	127.5 (2)
O2—Y1—O6	79.4 (5)	O2—Y3—O15	140.4 (3)
O3^{i}—Y1—O6	78.5 (5)	O3—Y3—O15	75.8 (3)
O1—Y1—O6	139.4 (5)	O4—Y3—O15	76.0 (3)
O4^{i}—Y1—O6	138.4 (5)	O1—Y3—O15	140.5 (3)
O8—Y1—O6	96.2 (6)	O2—Y3—O16	140.4 (3)
O2—Y1—O	65.23 (16)	O3—Y3—O16	78.7 (3)
O3^{i}—Y1—O	65.46 (16)	O4—Y3—O16	141.0 (3)
O1—Y1—O	66.07 (16)	O1—Y3—O16	77.8 (3)
O4^{i}—Y1—O	65.21 (16)	O15—Y3—O16	67.9 (3)
O8—Y1—O	131.5 (3)	O2—Y3—O13	76.8 (3)
O6—Y1—O	132.4 (5)	O3—Y3—O13	139.3 (3)
O2—Y1—O7	73.7 (4)	O4—Y3—O13	142.0 (3)
O3^{i}—Y1—O7	137.2 (4)	O1—Y3—O13	74.2 (3)
O1—Y1—O7	77.0 (4)	O15—Y3—O13	107.4 (3)
O4^{i}—Y1—O7	142.9 (4)	O16—Y3—O13	66.2 (3)
O8—Y1—O7	69.2 (4)	O2—Y3—O14	76.3 (3)
O6—Y1—O7	63.7 (6)	O3—Y3—O14	141.2 (3)
O—Y1—O7	128.1 (3)	O4—Y3—O14	77.2 (3)
O2—Y1—O5	138.5 (6)	O1—Y3—O14	139.8 (3)
O3^{i}—Y1—O5	73.9 (4)	O15—Y3—O14	69.2 (4)
O1—Y1—O5	140.9 (6)	O16—Y3—O14	102.3 (4)
O4^{i}—Y1—O5	76.2 (5)	O13—Y3—O14	69.5 (4)
O8—Y1—O5	66.5 (5)	O2—Y3—O	63.48 (15)
O6—Y1—O5	64.0 (7)	O3—Y3—O	63.63 (15)
O—Y1—O5	127.5 (4)	O4—Y3—O	63.47 (15)
O7—Y1—O5	104.2 (5)	O1—Y3—O	64.06 (15)
O2^{i}—Y2—O3	79.8 (2)	O15—Y3—O	126.5 (2)
O2^{i}—Y2—O4^{i}	78.0 (2)	O16—Y3—O	130.0 (3)
O3—Y2—O4^{i}	128.4 (2)	O13—Y3—O	126.1 (2)
O2^{i}—Y2—O1	128.9 (2)	O14—Y3—O	127.7 (3)
O3—Y2—O1	79.2 (2)	Y1^{i}—O—Y1	180.0
O4^{i}—Y2—O1	79.7 (2)	Y1^{i}—O—Y2^{i}	90.07 (3)
O2^{i}—Y2—O10	140.8 (3)	Y1—O—Y2^{i}	89.93 (3)
O3—Y2—O10	76.2 (3)	Y1^{i}—O—Y2	89.93 (3)
O4^{i}—Y2—O10	140.9 (3)	Y1—O—Y2	90.07 (3)
O1—Y2—O10	76.1 (3)	Y2^{i}—O—Y2	180.0
O2^{i}—Y2—O11	75.9 (3)	Y1^{i}—O—Y3^{i}	89.73 (3)
O3—Y2—O11	77.0 (3)	Y1—O—Y3^{i}	90.27 (3)
O4^{i}—Y2—O11	138.8 (3)	Y2^{i}—O—Y3^{i}	89.76 (3)
O1—Y2—O11	141.2 (3)	Y2—O—Y3^{i}	90.24 (3)
O10—Y2—O11	68.8 (3)	Y1^{i}—O—Y3	90.27 (3)
O2^{i}—Y2—O9	139.4 (3)	Y1—O—Y3	89.73 (3)
O3—Y2—O9	140.6 (3)	Y2^{i}—O—Y3	90.24 (3)

O4^{i}—Y2—O9	76.0 (3)	Y2—O—Y3	89.76 (3)
O1—Y2—O9	75.8 (3)	Y3^{i}—O—Y3	180.0
O10—Y2—O9	68.6 (3)	Y1—O1—Y2	97.2 (2)
O11—Y2—O9	105.1 (4)	Y1—O1—Y3	97.4 (2)
O2^{i}—Y2—O12	78.0 (3)	Y2—O1—Y3	98.4 (2)
O3—Y2—O12	140.8 (3)	Y1—O2—Y3	98.3 (2)
O4^{i}—Y2—O12	77.3 (3)	Y1—O2—Y2^{i}	97.4 (2)
O1—Y2—O12	139.3 (3)	Y3—O2—Y2^{i}	99.9 (2)
O10—Y2—O12	102.2 (3)	Y1^{i}—O3—Y2	97.3 (2)
O11—Y2—O12	66.5 (3)	Y1^{i}—O3—Y3	98.5 (2)
O9—Y2—O12	66.3 (3)	Y2—O3—Y3	99.0 (2)
O2^{i}—Y2—O	64.02 (15)	Y1^{i}—O4—Y2^{i}	97.2 (2)
O3—Y2—O	64.31 (16)	Y1^{i}—O4—Y3	98.3 (2)
O4^{i}—Y2—O	64.12 (16)	Y2^{i}—O4—Y3	99.4 (2)
O1—Y2—O	64.86 (16)		

Symmetry code: (i) −*x*+1, −*y*+2, −*z*+2.

Hydrogen-bond geometry (Å)

D—H···*A*	*D*···*A*
O7···O*W*2	2.646 (4)
O10···O*W*3	2.764 (1)
O13···O*W*4	2.803 (8)
O15···O*W*1	2.767 (2)
O16···O*W*4	2.836 (2)
O16···O*W*1	2.851 (6)