Crystal structure of poly[[hexaaquatris(μ-3,6-di-oxocyclohexa-1,4-diene-1,4-diolato)dierbium(III)] octadecahydrate]

Nutcha Ponjan,[a] Kenika Kodchasanthong,[a] Suwadee Jiajaroen[b] and Kittipong Chainok[a]*

[a]Materials and Textile Technology, Faculty of Science and Technology, Thammasat University, Khlong Luang, Pathum Thani 12121, Thailand, and [b]Division of Chemistry, Faculty of Science and Technology, Thammasat University, Khlong Luang, Pathum Thani 12121, Thailand. *Correspondence e-mail: kc@tu.ac.th

The title lanthanide complex, $[Er_2(C_6H_2O_4)_3(H_2O)_6]\cdot 18H_2O$, is isostructural with its La, Gd, Yb and Lu analogues. The Er^{3+} ion, located on a threefold rotation axis, is nine-coordinated in a distorted tricapped trigonal–prismatic geometry, which is completed by six oxygen atoms from three $dhbq^{2-}$ ligands and three oxygen atoms from coordinated water molecules. Each $dhbq^{2-}$ ligand acts in a μ_2-bis(bidentate) bridging mode to connect two Er^{3+} ions to form honeycomb (6,3) two-dimensional sheets extending in the ab plane, having an $Er\cdots Er$ separation of 8.7261 (2) Å. In the crystal, extensive O—H$\cdots$O hydrogen-bonding interactions involving the coordinated water molecules and the water molecules of crystallization, as well as the oxygen atoms of the $dhbq^{2-}$ ligands, generate an overall three-dimensional supramolecular network.

1. Chemical context

Over the past few decades, lanthanide-based coordination polymers (LnCPs) have attracted significant attention because their high photoluminescence efficiency and long luminescence lifetime in lighting and full-colour displays (Parker, 2000; Bünzli & Piguet, 2005; Cui et al., 2018). Besides transition metal ions, lanthanide ions feature high coordination numbers and flexible coordination geometries, which facilitate the formation of diverse extended structures. Since lanthanide(III) ions have a high affinity to hard donor atoms, ligands containing oxygen atoms such as carboxylic acids (Xu et al., 2016), phosphoric acids (Mao, 2007), calixarenes (Ovsyannikov et al., 2017) and β-diketones (Vigato et al., 2009) have been used extensively in the synthesis of new types of LnCPs. On the basis of the above considerations, we selected 2,5-dihydroxy-1,4-benzoquinone (H_2dhbq) as the ligand to react with erbium(III) nitrate hexahydrate under solvothermal conditions to construct a new erbium(III)-based CP, $[Er_2(dhbq)_3(H_2O)_6]\cdot 18H_2O$, (I), which is isotypic with its La, Gd, Yb and Lu analogues (Abrahams et al., 2002). Herein, we report its structure.

2. Structural commentary

The asymmetric unit of (I) contains one third of an Er^{3+} ion, half of a $dhbq^{2-}$ ligand, one coordinated water molecule and three water molecules of crystallization. The Er^{3+} ion is located on a threefold rotation axis, whereas the complete
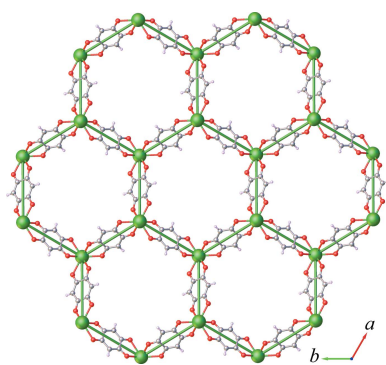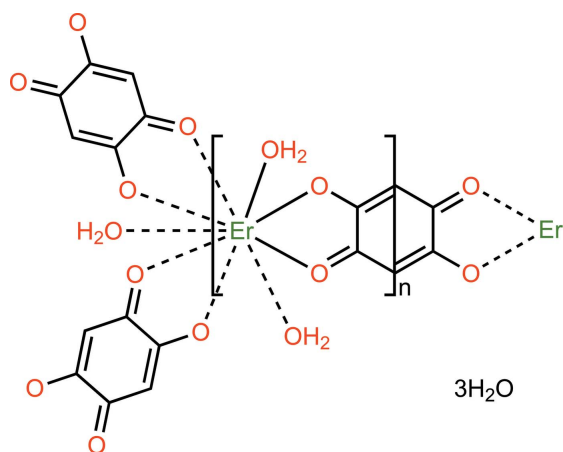
Table 1
Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O3—H3A···O6^i	0.83 (1)	1.94 (1)	2.769 (3)	174 (3)
O3—H3B···O5^{ii}	0.84 (1)	1.94 (1)	2.758 (3)	165 (3)
O4—H4A···O2^{iii}	0.84 (1)	1.92 (1)	2.738 (3)	167 (4)
O4—H4B···O4^{iv}	0.84 (1)	1.98 (1)	2.803 (3)	164 (4)
O5—H5A···O1^v	0.85 (1)	2.09 (3)	2.870 (3)	153 (5)
O5—H5B···O6^{vi}	0.84 (1)	1.95 (1)	2.794 (3)	174 (5)
O6—H6A···O4^{vii}	0.85 (1)	1.88 (1)	2.725 (3)	174 (4)
O6—H6B···O5	0.84 (1)	1.91 (1)	2.747 (3)	169 (5)

Symmetry codes: (i) $x-y+\frac{2}{3}, x+\frac{1}{3}, -z+\frac{4}{3}$; (ii) $-x+\frac{2}{3}, -y+\frac{1}{3}, -z+\frac{4}{3}$; (iii) $-x+y+1, -x+1, z$; (iv) $x-y+\frac{1}{3}, x-\frac{1}{3}, -z+\frac{2}{3}$; (v) $-y+1, x-y, z$; (vi) $y, -x+y, -z+1$; (vii) $-x+1, -y+1, -z+1$.
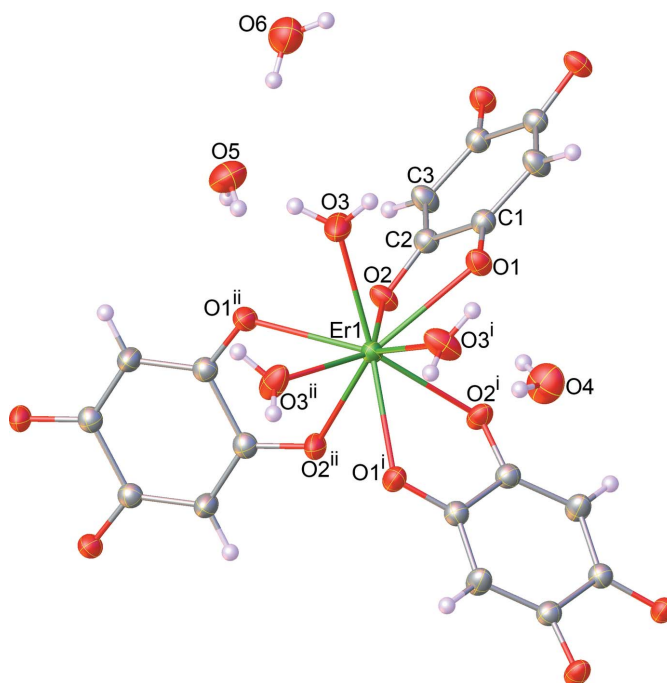

Figure 1
The molecular structure of the title complex, showing selected atom labels. Displacement ellipsoids are drawn at the 50% probability level. Symmetry codes: (i) $1 + y - x, 1 - x, z$; (ii) $1 - y, x - y, z$.

dhbq^{2-} anion is generated by a crystallographic inversion center. As can be seen from Fig. 1, the Er^{3+} ion is nine-coordinated by six oxygen atoms from three different dhbq^{2-} ligands and three other oxygen atoms from three coordinated water molecules. The coordination polyhedron of the central Er^{3+} ion can best be described as having a distorted tricapped trigonal–prismatic geometry, as depicted in Fig. 2, in which the O—Er—O bond angles range from 65.01 (5) to 139.97 (7)°. The Er—O bond lengths in the title complex lie between 2.3577 (15) and 2.4567 (15) Å, mean 2.393 Å. The whole dhbq^{2-} anion is nearly planar: the r.m.s. deviation from the mean plane through all of the non-H atoms is 0.021 Å, with a maximum displacement from this plane of 0.033 (2) Å for atom C2. As can be seen from Fig. 3, the dhbq^{2-} ligand acts in a μ_2-bis-(bidentate) bridging mode, connecting two Er^{3+} ions to form a honeycomb (6,3) sheet extending in the ab plane, having a Er···Er separation of 8.7261 (2) Å.

interaction further links neighbouring sheets into a three-dimensional supramolecular structure (Fig. 4).

4. Database survey

A search of the Cambridge Structural Database (Version 5.39 update February 2018; Groom *et al.*, 2016) for complexes of

Figure 2
View of the distorted tricapped trigonal–prismatic geometry of the central Er^{III} ion in the title complex. Symmetry codes: (i) $1 + y - x, 1 - x, z$; (ii) $1 - y, x - y, z$.

3. Supramolecular features

In the crystal, extensive O—H···O hydrogen-bonding interactions (Table 1) are observed between the oxygen atoms of the coordinated (O3) and lattice (O4 and O5) water molecules as well as between the water (O5 and O6) molecules of crystallization. Other O—H···O hydrogen-bonding interactions involve O6 and the dhbq^{2-} oxygen atom, and this

Figure 3
View of the honeycomb (6,3) sheet extending normal to the *c*-axis direction.

dhbq^{2-} ligand gave 94 hits. They include the isotypic crystal structures (Abrahams *et al.*, 2002) with La (MIZXAU), Gd (MIZXEY), Yb (MIZXIC) and Lu (MIZXOI). In most cases, the dhbq^{2-} ligand acts in a μ_2-bis(bidentate) bridging mode to the central metal ions. Comparing the mean $Ln-O$ bond length and the unit-cell volume for the title complex with the La, Gd, Yb and Lu analogues (Abrahams *et al.*, 2002), the values decrease as the ionic radius of the Ln^{3+} ions decreases in the order La [La$-$O = 2.54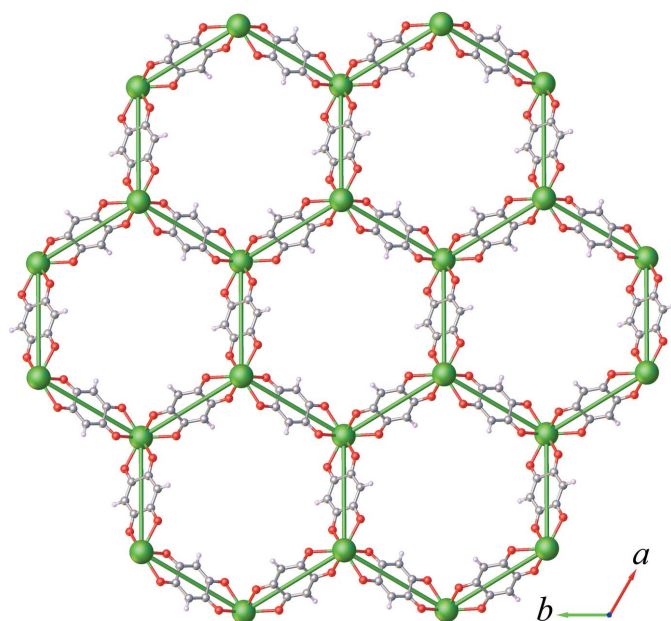0 Å, V = 3289.3 (16) Å^3] > Gd [Gd$-$O = 2.438 Å, V = 3162.7 (7) Å^3] > Er [Er$-$O = 2.393 Å, V = 3107.18 (13) Å^3] > Yb [Yb$-$O = 2.377 Å, V = 3087.1 (4) Å^3] > Lu [Lu$-$O = 2.368 Å, V = 3074.2 (4) Å^3], which is consistent with the lanthanide contraction effect.
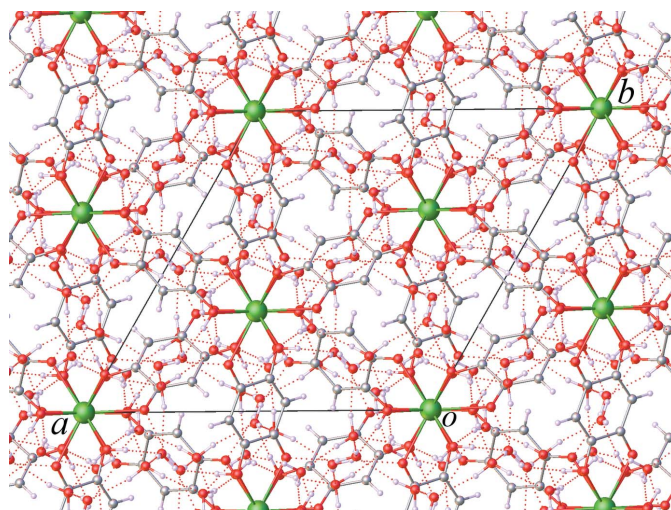

Figure 4
View of the packing in the unit cell of the title complex along the *c* axis. Hydrogen-bonding interactions are shown as dashed lines.

Table 2
Experimental details.

Crystal data	
Chemical formula	[Er$_2$(C$_6$H$_2$O$_4$)$_3$(H$_2$O)$_6$]·18H$_2$O
M_r	1181.13
Crystal system, space group	Trigonal, $R\bar{3}$
Temperature (K)	296
a, c (Å)	14.0947 (3), 18.0603 (5)
V (Å^3)	3107.18 (13)
Z	3
Radiation type	Mo $K\alpha$
μ (mm^{-1})	4.13
Crystal size (mm)	0.28 × 0.22 × 0.2
Data collection	
Diffractometer	Bruker D8 QUEST CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.677, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	32360, 2522, 2108
R_{int}	0.065
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.758
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.023, 0.042, 1.08
No. of reflections	2522
No. of parameters	118
No. of restraints	8
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.67, −1.39

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015a), *SHELXL* (Sheldrick, 2015b) and *OLEX2* (Dolomanov *et al.*, 2009).

5. Synthesis and crystallization

A mixture of Er(NO$_3$)$_3$·6H$_2$O (46.2 mg, 0.1 mmol) and H$_2$dhbq (14.2 mg, 0.1 mmol) in distilled H$_2$O (4 ml) and DMF (1 ml) was placed in a 20 ml vial and stirred at room temperature for 10 min. The mixture was sealed tightly, placed in an oven and then heated to 358 K under autogenous pressure for 12 h. After the reactor was cooled to room temperature, block-shaped dark-red crystals were filtered off, washed with deionized H$_2$O and dried in air at room temperature. Yield: 57% based on Er^{III} source.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The carbon-bound H atoms were placed in geometrically calculated positions and refined as riding with C$-$H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C). The hydrogen atoms of the water molecules were located from difference-Fourier maps but were refined with distance restraints of O$-$H = 0.84 Å and U_{iso}(H) = 1.5U_{eq}(O).

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supporting information

Crystal structure of poly[[hexaaquatris(*µ*-3,6-dioxocyclohexa-1,4-diene-1,4-diolato)dierbium(III)] octadecahydrate]

Nutcha Ponjan, Kenika Kodchasanthong, Suwadee Jiajaroen and Kittipong Chainok

Computing details

Data collection: *APEX3* (Bruker, 2016); cell refinement: *SAINT* (Bruker, 2016); data reduction: *SAINT* (Bruker, 2016); program(s) used to solve structure: SHELXT (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL* (Sheldrick, 2015b); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009).

Poly[[hexaaquatris(*µ*-3,6-dioxocyclohexa-1,4-diene-1,4-diolato)dierbium(III)] octadecahydrate]

Crystal data

$[Er_2(C_6H_2O_4)_3(H_2O)_6] \cdot 18H_2O$	$D_x = 1.894$ Mg m^{-3}
$M_r = 1181.13$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Trigonal, $R\bar{3}$	Cell parameters from 8655 reflections
$a = 14.0947$ (3) Å	$\theta = 2.8–31.7°$
$c = 18.0603$ (5) Å	$\mu = 4.13$ mm^{-1}
$V = 3107.18$ (13) Å^3	$T = 296$ K
$Z = 3$	Hexagonal prism, dark red
$F(000) = 1758$	$0.28 \times 0.22 \times 0.2$ mm

Data collection

Bruker D8 QUEST CMOS diffractometer	$T_{min} = 0.677$, $T_{max} = 0.746$
Radiation source: microfocus sealed x-ray tube, Incoatec Iμus	32360 measured reflections
	2522 independent reflections
GraphiteDouble Bounce Multilayer Mirror monochromator	2108 reflections with $I > 2\sigma(I)$
	$R_{int} = 0.065$
Detector resolution: 10.5 pixels mm^{-1}	$\theta_{max} = 32.6°$, $\theta_{min} = 2.8°$
φ and ω scans	$h = -21 \rightarrow 21$
Absorption correction: multi-scan (SADABS; Bruker, 2016)	$k = -19 \rightarrow 21$
	$l = -27 \rightarrow 27$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.023$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.042$	
$S = 1.08$	H atoms treated by a mixture of independent and constrained refinement
2522 reflections	
118 parameters	$w = 1/[\sigma^2(F_o^2) + (0.0042P)^2 + 10.2637P]$
8 restraints	where $P = (F_o^2 + 2F_c^2)/3$
Primary atom site location: dual	$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 1.67$ e Å^{-3}

$\Delta\rho_{min} = -1.39$ e Å^{-3}

Extinction correction: SHELXL (Sheldrick,
  2015b), Fc*=kFc[1+0.001xFc$^2\lambda^3$/sin(2θ)]$^{-1/4}$

Extinction coefficient: 0.00020 (2)

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 > 2sigma(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_{iso}*/U_{eq}
Er1	0.6667	0.3333	0.587213 (10)	0.01773 (5)
O1	0.65928 (12)	0.50374 (13)	0.58327 (9)	0.0236 (3)
O2	0.54678 (13)	0.33698 (13)	0.49769 (9)	0.0247 (3)
O3	0.54011 (16)	0.33067 (15)	0.67424 (11)	0.0355 (4)
H3A	0.557 (3)	0.3878 (16)	0.6975 (16)	0.055 (10)*
H3B	0.4856 (17)	0.2781 (17)	0.6941 (15)	0.046 (9)*
O4	0.7266 (2)	0.52214 (19)	0.37540 (12)	0.0455 (5)
H4A	0.736 (3)	0.494 (3)	0.4136 (13)	0.075 (13)*
H4B	0.6643 (16)	0.489 (3)	0.356 (2)	0.079 (14)*
O5	0.29245 (18)	0.15371 (19)	0.57009 (14)	0.0452 (5)
H5A	0.354 (2)	0.167 (5)	0.587 (3)	0.15 (2)*
H5B	0.285 (4)	0.138 (4)	0.5247 (8)	0.103 (17)*
O6	0.18028 (19)	0.2663 (2)	0.57759 (14)	0.0470 (5)
H6A	0.213 (3)	0.3315 (15)	0.594 (2)	0.091 (16)*
H6B	0.222 (3)	0.240 (4)	0.576 (2)	0.104 (18)*
C1	0.58618 (18)	0.50816 (18)	0.54547 (12)	0.0212 (4)
C2	0.51755 (18)	0.40906 (18)	0.49646 (12)	0.0216 (4)
C3	0.43354 (19)	0.40401 (19)	0.45415 (13)	0.0256 (5)
H3	0.3902	0.3424	0.4255	0.031*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Er1	0.01570 (6)	0.01570 (6)	0.02179 (9)	0.00785 (3)	0.000	0.000
O1	0.0218 (8)	0.0214 (8)	0.0293 (8)	0.0121 (7)	−0.0056 (6)	−0.0019 (6)
O2	0.0270 (8)	0.0222 (8)	0.0309 (8)	0.0168 (7)	−0.0069 (7)	−0.0050 (6)
O3	0.0371 (11)	0.0239 (9)	0.0394 (11)	0.0106 (8)	0.0163 (8)	−0.0025 (8)
O4	0.0474 (13)	0.0517 (13)	0.0376 (12)	0.0249 (11)	−0.0043 (10)	0.0091 (10)
O5	0.0335 (11)	0.0505 (13)	0.0505 (14)	0.0202 (10)	0.0094 (10)	0.0035 (11)
O6	0.0434 (13)	0.0436 (14)	0.0534 (14)	0.0212 (11)	0.0057 (10)	0.0082 (11)
C1	0.0202 (10)	0.0208 (10)	0.0221 (10)	0.0099 (9)	0.0003 (8)	0.0004 (8)
C2	0.0215 (10)	0.0217 (10)	0.0226 (10)	0.0115 (9)	0.0011 (8)	0.0015 (8)

C3	0.0259 (11)	0.0216 (11)	0.0318 (12)	0.0137 (10)	−0.0077 (9)	−0.0069 (9)

Geometric parameters (Å, º)

Er1—O1^i	2.4567 (15)	O3—H3B	0.836 (10)
Er1—O1	2.4567 (15)	O4—H4A	0.838 (10)
Er1—O1^{ii}	2.4567 (15)	O4—H4B	0.842 (10)
Er1—O2^{ii}	2.3578 (15)	O5—H5A	0.845 (10)
Er1—O2^i	2.3577 (15)	O5—H5B	0.844 (10)
Er1—O2	2.3578 (15)	O6—H6A	0.848 (10)
Er1—O3	2.3636 (18)	O6—H6B	0.843 (10)
Er1—O3^i	2.3636 (18)	C1—C2	1.523 (3)
Er1—O3^{ii}	2.3637 (18)	C1—C3^{iii}	1.398 (3)
O1—C1	1.263 (3)	C2—C3	1.381 (3)
O2—C2	1.273 (3)	C3—C1^{iii}	1.398 (3)
O3—H3A	0.831 (10)	C3—H3	0.9300
O1^i—Er1—O1	119.917 (4)	O3—Er1—O1^{ii}	139.97 (6)
O1^{ii}—Er1—O1^i	119.917 (4)	O3—Er1—O1	68.54 (6)
O1^{ii}—Er1—O1	119.916 (4)	O3^{ii}—Er1—O1^{ii}	68.54 (6)
O2^i—Er1—O1^i	65.01 (5)	O3^i—Er1—O1^{ii}	70.00 (6)
O2^{ii}—Er1—O1	69.91 (5)	O3^i—Er1—O1^i	68.54 (6)
O2^{ii}—Er1—O1^{ii}	65.01 (5)	O3—Er1—O1^i	70.00 (6)
O2—Er1—O1	65.01 (5)	O3^i—Er1—O3^{ii}	80.60 (8)
O2—Er1—O1^{ii}	134.93 (5)	O3^i—Er1—O3	80.60 (8)
O2^i—Er1—O1^{ii}	69.91 (5)	O3—Er1—O3^{ii}	80.60 (8)
O2^{ii}—Er1—O1^i	134.93 (5)	C1—O1—Er1	119.88 (14)
O2—Er1—O1^i	69.91 (5)	C2—O2—Er1	123.42 (14)
O2^i—Er1—O1	134.93 (5)	Er1—O3—H3A	118 (2)
O2^i—Er1—O2^{ii}	78.15 (6)	Er1—O3—H3B	131 (2)
O2^i—Er1—O2	78.15 (6)	H3A—O3—H3B	109 (3)
O2^{ii}—Er1—O2	78.15 (6)	H4A—O4—H4B	117 (4)
O2^{ii}—Er1—O3^{ii}	85.01 (7)	H5A—O5—H5B	112 (5)
O2—Er1—O3^{ii}	134.96 (6)	H6A—O6—H6B	112 (4)
O2^i—Er1—O3^{ii}	138.45 (6)	O1—C1—C2	115.38 (19)
O2^i—Er1—O3	134.96 (6)	O1—C1—C3^{iii}	124.7 (2)
O2—Er1—O3	85.01 (7)	C3^{iii}—C1—C2	119.92 (19)
O2^{ii}—Er1—O3	138.45 (6)	O2—C2—C1	114.28 (19)
O2^i—Er1—O3^i	85.01 (7)	O2—C2—C3	125.4 (2)
O2^{ii}—Er1—O3^i	134.96 (6)	C3—C2—C1	120.26 (19)
O2—Er1—O3^i	138.46 (6)	C1^{iii}—C3—H3	120.1
O3^{ii}—Er1—O1^i	139.97 (7)	C2—C3—C1^{iii}	119.8 (2)
O3^i—Er1—O1	139.97 (6)	C2—C3—H3	120.1
O3^{ii}—Er1—O1	70.00 (6)		
Er1—O1—C1—C2	−8.1 (2)	O2^{ii}—Er1—O1—C1	96.59 (16)
Er1—O1—C1—C3^{iii}	172.37 (18)	O2^{ii}—Er1—O2—C2	−86.3 (2)
Er1—O2—C2—C1	13.9 (3)	O2^i—Er1—O2—C2	−166.47 (17)

Er1—O2—C2—C3	−167.71 (18)	O2—C2—C3—C1ⁱⁱⁱ	−176.2 (2)
O1ⁱⁱ—Er1—O1—C1	139.76 (13)	O3ⁱⁱ—Er1—O1—C1	−171.43 (17)
O1ⁱ—Er1—O1—C1	−34.5 (2)	O3ⁱ—Er1—O1—C1	−126.15 (16)
O1ⁱⁱ—Er1—O2—C2	−121.30 (16)	O3—Er1—O1—C1	−83.94 (16)
O1—Er1—O2—C2	−13.10 (16)	O3ⁱⁱ—Er1—O2—C2	−15.9 (2)
O1ⁱ—Er1—O2—C2	126.04 (18)	O3—Er1—O2—C2	55.53 (17)
O1—C1—C2—O2	−3.1 (3)	O3ⁱ—Er1—O2—C2	125.30 (17)
O1—C1—C2—C3	178.4 (2)	C1—C2—C3—C1ⁱⁱⁱ	2.1 (4)
O2ⁱ—Er1—O1—C1	48.94 (18)	C3ⁱⁱⁱ—C1—C2—O2	176.4 (2)
O2—Er1—O1—C1	10.65 (15)	C3ⁱⁱⁱ—C1—C2—C3	−2.1 (4)

Symmetry codes: (i) −*y*+1, *x*−*y*, *z*; (ii) −*x*+*y*+1, −*x*+1, *z*; (iii) −*x*+1, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3*A*···O6ⁱᵛ	0.83 (1)	1.94 (1)	2.769 (3)	174 (3)
O3—H3*B*···O5ᵛ	0.84 (1)	1.94 (1)	2.758 (3)	165 (3)
O4—H4*A*···O2ⁱⁱ	0.84 (1)	1.92 (1)	2.738 (3)	167 (4)
O4—H4*B*···O4ᵛⁱ	0.84 (1)	1.98 (1)	2.803 (3)	164 (4)
O5—H5*A*···O1ⁱ	0.85 (1)	2.09 (3)	2.870 (3)	153 (5)
O5—H5*B*···O6ᵛⁱⁱ	0.84 (1)	1.95 (1)	2.794 (3)	174 (5)
O6—H6*A*···O4ⁱⁱⁱ	0.85 (1)	1.88 (1)	2.725 (3)	174 (4)
O6—H6*B*···O5	0.84 (1)	1.91 (1)	2.747 (3)	169 (5)

Symmetry codes: (i) −*y*+1, *x*−*y*, *z*; (ii) −*x*+*y*+1, −*x*+1, *z*; (iii) −*x*+1, −*y*+1, −*z*+1; (iv) *x*−*y*+2/3, *x*+1/3, −*z*+4/3; (v) −*x*+2/3, −*y*+1/3, −*z*+4/3; (vi) *x*−*y*+1/3, *x*−1/3, −*z*+2/3; (vii) *y*, −*x*+*y*, −*z*+1.