Poly[diaqua-μ_2-oxalato-di-μ_4-tereph-thalato-diytterbium(III)]

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The crystal structure of the title complex, $[Yb_2(C_8H_4O_4)_2(C_2O_4)(H_2O)_2]_n$, features an extended three-dimensional framework made up of Yb^{3+} ions coordinated by terephthalate ligands, oxalate ligands and water molecules. The Yb^{3+} ion has a distorted square-antiprismatic coordination formed by one aqua ligand, two O atoms from an oxalate ligand and five O atoms belonging to four terephthalate anions. Two symmetry-independent terephthalate anions, as well as the oxalate anion, occupy special positions on inversion centers. The water molecule participates in O—H⋯O hydrogen bonding with both terephthalate anions.

Related literature

For isotypic structures, derivatives of Lu and Dy, see: Li & Wang (2009) and Li *et al.* (2009), respectively.
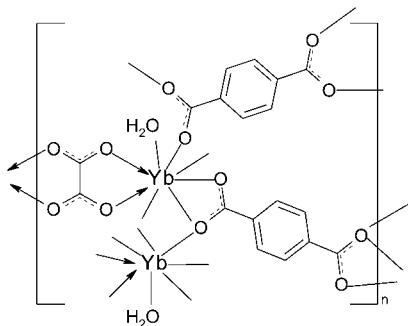
Experimental

Crystal data

$[Yb_2(C_8H_4O_4)_2(C_2O_4)(H_2O)_2]$	a = 7.034 (2) Å
M_r = 798.36	b = 7.583 (2) Å
Triclinic, $P\bar{1}$	c = 10.213 (3) Å
α = 75.372 (4)°	Mo $K\alpha$ radiation
β = 70.851 (4)°	μ = 9.43 mm^{-1}
γ = 88.126 (4)°	T = 295 K
V = 497.2 (2) Å^3	0.24 × 0.15 × 0.05 mm
Z = 1	

Data collection

Bruker SMART APEXII CCD area-detector diffractometer	2630 measured reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003) T_{min} = 0.211, T_{max} = 0.629	1882 independent reflections
	1785 reflections with $I > 2\sigma(I)$
	R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046	154 parameters
$wR(F^2)$ = 0.120	H-atom parameters constrained
S = 1.06	$\Delta\rho_{max}$ = 4.45 e Å^{-3}
1882 reflections	$\Delta\rho_{min}$ = −4.21 e Å^{-3}

Table 1
Selected bond lengths (Å).

Yb—O1	2.790 (6)	Yb—O4^{ii}	2.209 (6)
Yb—O1^{i}	2.315 (6)	Yb—O5	2.310 (6)
Yb—O2	2.314 (6)	Yb—O6^{iii}	2.321 (6)
Yb—O3	2.264 (6)	Yb—O7	2.293 (5)

Symmetry codes: (i) $-x + 1, -y, -z + 2$; (ii) $-x + 1, -y + 1, -z + 2$; (iii) $-x, -y + 1, -z + 2$.

Table 2
Hydrogen-bond geometry (Å, °).

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
O7—H7A⋯O3^{i}	0.85	1.92	2.751 (6)	167
O7—H7B⋯O2^{iv}	0.85	1.91	2.754 (6)	178

Symmetry codes: (i) $-x + 1, -y, -z + 2$; (iv) $-x, -y, -z + 2$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

References

Bruker (2004). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.

Li, Z.-F., Cheng, Q., Chen, J.-Z. & Chen, Y. (2009). *Z. Kristallogr. New Cryst. Struct.* **224**, 483–484.

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Sheldrick, G. M. (2003). *SADABS*. University of Göttingen, Germany.

Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Poly[diaqua-*μ*₂-oxalato-di-*μ*₄-terephthalato-diytterbium(III)]

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S1. Comment

The title compound is isostructural with its Lu and Dy analogues (Li & Wang, 2009; Li *et al.*, 2009). As illustrated in Fig. 1, the Yb atoms is coordinated by two oxalate O atoms and five O atoms of four terephthalate anions; an aqua ligand completes a distorted square antiprismatic geometry. The Yb-O distances are in the range of 2.208 (6)–2.790 (6) Å, with an average Yb-O bond of 2.352 Å; these parameters are similar to M-O bonds found in the above mentioned previously reported isostructural complexes.

In the title complex, both symmetry independent terephthalate (tp) anions occupy special positions on the inversion centers; nevertheless they exhibit different modes of coordination of Yb atoms. The tp1 anion (O1 to O2, C1 to C4) functions as chelating-bridging tridentate ligand: two carboxylate oxygen atoms (O1 and O2) chelate one Yb atom; the O1 atom is additionally bonded to another Yb atom; the Yb···Yb separation is 4.232 (1) Å. Two edge-sharing [YbO₈] polyhedra are bridged by the bidentate tp2 (O3 to O4, C5 to C8) ligands thus generating chains along the [010] direction. The chains are further linked by the tp1 and tp2 ligands into three-dimensional framework. The oxalate anion is also located on the inversion center and acts as a tetradentate ligand connecting the edge-sharing [YbO₈] polyhedra along the [100] direction thus even further stabilizing the three-dimensional framework. The aqua ligand provides H-bond donors which participate in H-bonds with terephthalate oxygen atoms O2 and O3.

S2. Experimental

A mixture of YbCl₃.6H₂O (1.00 mmol, 0.39 g), oxalic acid (0.50 mmol, 0.05 g), terephthalic acid (0.50 mmol, 0.09 g), NaOH (2.00 mmol, 0.08 g) and H₂O (10.0 ml) was heated in a 23 ml stainless steel reactor with a Teflon liner at 453 K for 72 h. A small amount of colorless plate-like crystals were filtered and washed with water and acetone.

S3. Refinement

H atoms attached to C atoms were included at calculated positions and treated as riding atoms [C–H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C)]. Water H atoms were located in difference Fourier maps placed at the idealized positions with O-H distance of 0.85 Å and included in the final refinement as fixed contribution with U_{iso}(H) = 1.5U_{eq}(O). The highest density peak and deepest hole are located at 0.87 Å and 1.09 Å from the Yb atom respectively.
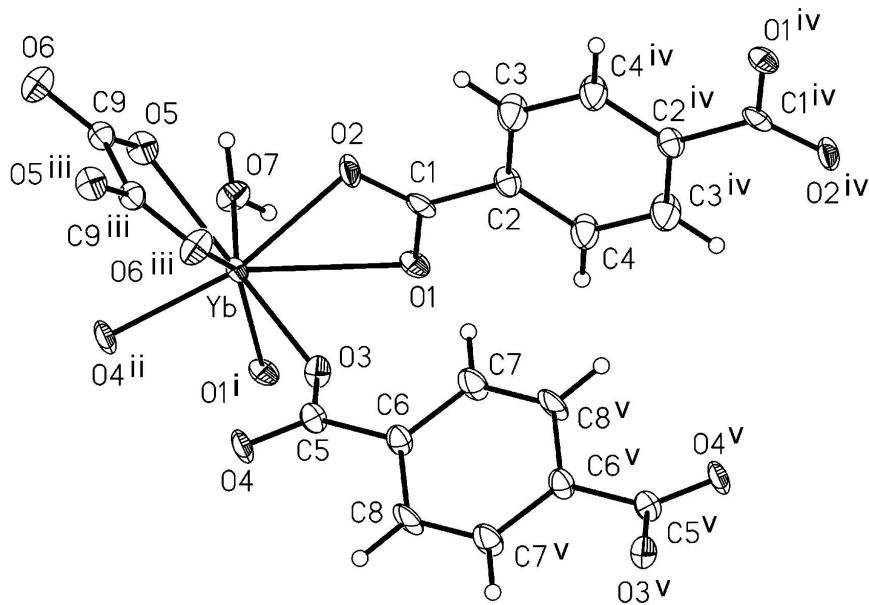
Figure 1

The fragment of the structure of the title compound, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small circles of arbitrary radii. Symmetry codes: (i) 1 -x, -y, 2 - z; (ii) 1 - x, 1 - y, 2 - z; (iii) -x, 1 - y, 2 - z; (iv) 1 - x, -y, 1 - z; (v) 2 - x, 1 - y, 1 - z.

Poly[diaqua-*μ*₂-oxalato-di-*μ*₄-terephthalato-diytterbium(III)]

Crystal data
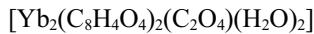
[Yb₂(C₈H₄O₄)₂(C₂O₄)(H₂O)₂]	$Z = 1$
$M_r = 798.36$	$F(000) = 372$
Triclinic, $P\overline{1}$	$D_x = 2.666$ Mg m⁻³
Hall symbol: -p 1	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 7.034$ (2) Å	Cell parameters from 196 reflections
$b = 7.583$ (2) Å	$\theta = 2.1–27.3°$
$c = 10.213$ (3) Å	$\mu = 9.43$ mm⁻¹
$\alpha = 75.372$ (4)°	$T = 295$ K
$\beta = 70.851$ (4)°	Plate, colorless
$\gamma = 88.126$ (4)°	$0.24 \times 0.15 \times 0.05$ mm
$V = 497.2$ (2) Å³	

Data collection

Bruker SMART APEXII CCD area-detector diffractometer	2630 measured reflections
	1882 independent reflections
Radiation source: fine-focus sealed tube	1785 reflections with $I > 2\sigma(I)$
Graphite monochromator	$R_{int} = 0.025$
φ and ω scans	$\theta_{max} = 26.0°$, $\theta_{min} = 2.2°$
Absorption correction: multi-scan	$h = -8 \rightarrow 8$
(*SADABS*; Sheldrick, 2003)	$k = -8 \rightarrow 9$
$T_{min} = 0.211$, $T_{max} = 0.629$	$l = -7 \rightarrow 12$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.046$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.120$	
$S = 1.06$	H-atom parameters constrained
1882 reflections	$w = 1/[\sigma^2(F_o^2) + (0.0995P)^2]$
154 parameters	where $P = (F_o^2 + 2F_c^2)/3$
0 restraints	$(\Delta/\sigma)_{max} < 0.001$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{max} = 4.45$ e Å^{-3}
	$\Delta\rho_{min} = -4.21$ e Å^{-3}

Special details

Geometry. 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.

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 $F^2 > \sigma(F^2)$ 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	$U_{iso}*/U_{eq}$
Yb	0.31071 (4)	0.22186 (3)	1.01498 (3)	0.01504 (19)
C1	0.3854 (12)	0.0294 (11)	0.7912 (9)	0.0203 (16)
C2	0.4409 (12)	0.0093 (11)	0.6438 (9)	0.0202 (16)
C3	0.3229 (16)	0.0805 (15)	0.5592 (11)	0.033 (2)
H3	0.2048	0.1355	0.5976	0.039*
C4	0.6198 (14)	−0.0700 (13)	0.5823 (10)	0.030 (2)
H4	0.7015	−0.1163	0.6370	0.036*
C5	0.7144 (12)	0.4806 (10)	0.7821 (9)	0.0189 (16)
C6	0.8607 (13)	0.4930 (11)	0.6352 (10)	0.0211 (18)
C7	0.8292 (13)	0.3852 (12)	0.5521 (10)	0.0282 (19)
H7	0.7149	0.3066	0.5875	0.034*
C8	1.0353 (13)	0.6070 (12)	0.5820 (10)	0.0275 (19)
H8	1.0602	0.6780	0.6374	0.033*
C9	−0.0833 (11)	0.4309 (10)	1.0574 (9)	0.0194 (16)
O1	0.4818 (8)	−0.0459 (8)	0.8752 (6)	0.0228 (12)
O2	0.2462 (9)	0.1353 (8)	0.8314 (6)	0.0228 (12)
O3	0.6140 (8)	0.3311 (8)	0.8501 (6)	0.0224 (12)
O4	0.6994 (9)	0.6187 (8)	0.8296 (7)	0.0248 (13)
O5	−0.0295 (9)	0.2697 (8)	1.0944 (7)	0.0246 (12)
O6	−0.2511 (8)	0.4911 (8)	1.1074 (7)	0.0254 (13)
O7	0.1351 (8)	−0.0452 (7)	1.1590 (7)	0.0242 (13)
H7B	0.0166	−0.0740	1.1644	0.036*
H7A	0.1979	−0.1429	1.1672	0.036*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Yb	0.0191 (3)	0.0156 (3)	0.0129 (3)	0.00119 (15)	−0.00688 (17)	−0.00586 (17)
C1	0.024 (4)	0.017 (4)	0.023 (5)	−0.008 (3)	−0.009 (3)	−0.007 (3)
C2	0.026 (4)	0.020 (4)	0.016 (4)	0.003 (3)	−0.008 (3)	−0.004 (3)
C3	0.036 (5)	0.043 (6)	0.023 (5)	0.015 (4)	−0.014 (4)	−0.012 (4)
C4	0.032 (4)	0.039 (5)	0.025 (5)	0.015 (4)	−0.015 (4)	−0.015 (4)
C5	0.026 (4)	0.017 (4)	0.013 (4)	0.001 (3)	−0.007 (3)	−0.002 (3)
C6	0.026 (4)	0.017 (4)	0.020 (5)	−0.001 (3)	−0.006 (4)	−0.007 (3)
C7	0.030 (4)	0.028 (4)	0.024 (5)	−0.015 (3)	0.000 (4)	−0.010 (4)
C8	0.034 (4)	0.024 (4)	0.028 (5)	−0.014 (3)	−0.007 (4)	−0.014 (4)
C9	0.022 (4)	0.017 (3)	0.021 (4)	0.004 (3)	−0.009 (3)	−0.006 (3)
O1	0.025 (3)	0.031 (3)	0.018 (3)	0.002 (2)	−0.014 (2)	−0.008 (2)
O2	0.029 (3)	0.028 (3)	0.015 (3)	0.007 (2)	−0.008 (3)	−0.013 (2)
O3	0.024 (3)	0.022 (3)	0.020 (3)	0.002 (2)	−0.004 (2)	−0.007 (2)
O4	0.032 (3)	0.026 (3)	0.019 (3)	−0.003 (2)	−0.005 (3)	−0.016 (3)
O5	0.030 (3)	0.020 (3)	0.023 (3)	0.004 (2)	−0.011 (3)	−0.003 (2)
O6	0.023 (3)	0.026 (3)	0.019 (3)	0.007 (2)	−0.004 (2)	0.003 (2)
O7	0.020 (3)	0.017 (3)	0.029 (3)	−0.001 (2)	−0.004 (3)	−0.001 (2)

Geometric parameters (Å, º)

Yb—O1	2.790 (6)	C3—H3	0.9300
Yb—O1^i	2.315 (6)	C4—H4	0.9300
Yb—O2	2.314 (6)	C5—O4	1.249 (10)
Yb—O3	2.264 (6)	C5—O3	1.264 (10)
Yb—O4^{ii}	2.209 (6)	C5—C6	1.497 (12)
Yb—O5	2.310 (6)	C6—C7	1.387 (13)
Yb—O6^{iii}	2.321 (6)	C6—C8	1.395 (11)
Yb—O7	2.293 (5)	C7—C8^v	1.377 (12)
Yb—Yb^i	4.2315 (10)	C7—H7	0.9300
C1—O2	1.274 (10)	C8—H8	0.9300
C1—O1	1.277 (10)	C9—O6	1.245 (10)
C1—C2	1.473 (12)	C9—O5	1.269 (9)
C2—C3	1.390 (13)	C9—C9^{iii}	1.550 (15)
C2—C4	1.401 (12)	O7—H7B	0.85
C3—C4^{iv}	1.390 (13)	O7—H7A	0.85
O4^{ii}—Yb—O3	98.9 (2)	O1—Yb—Yb^i	30.57 (12)
O4^{ii}—Yb—O7	102.6 (2)	C9^{iii}—Yb—Yb^i	163.60 (15)
O3—Yb—O7	141.9 (2)	O2—C1—O1	119.6 (8)
O4^{ii}—Yb—O5	79.5 (2)	O2—C1—C2	118.4 (8)
O3—Yb—O5	145.4 (2)	O1—C1—C2	121.8 (7)
O7—Yb—O5	70.19 (19)	C3—C2—C4	118.5 (8)
O4^{ii}—Yb—O2	159.4 (3)	C3—C2—C1	120.3 (8)
O3—Yb—O2	85.5 (2)	C4—C2—C1	121.1 (8)
O7—Yb—O2	85.2 (2)	C4^{iv}—C3—C2	120.5 (9)

O5—Yb—O2	85.5 (2)	C4^{iv}—C3—H3	119.8
O4^{ii}—Yb—O1^{i}	82.5 (2)	C2—C3—H3	119.8
O3—Yb—O1^{i}	80.7 (2)	C3^{iv}—C4—C2	121.0 (8)
O7—Yb—O1^{i}	71.5 (2)	C3^{iv}—C4—H4	119.5
O5—Yb—O1^{i}	132.4 (2)	C2—C4—H4	119.5
O2—Yb—O1^{i}	118.1 (2)	O4—C5—O3	124.2 (7)
O4^{ii}—Yb—O6^{iii}	79.2 (2)	O4—C5—C6	117.8 (7)
O3—Yb—O6^{iii}	75.4 (2)	O3—C5—C6	118.0 (7)
O7—Yb—O6^{iii}	139.4 (2)	C7—C6—C8	118.8 (8)
O5—Yb—O6^{iii}	70.34 (19)	C7—C6—C5	120.4 (8)
O2—Yb—O6^{iii}	82.5 (2)	C8—C6—C5	120.7 (8)
O1^{i}—Yb—O6^{iii}	147.1 (2)	C8^{v}—C7—C6	121.0 (7)
O4^{ii}—Yb—O1	150.1 (2)	C8^{v}—C7—H7	119.5
O3—Yb—O1	70.77 (19)	C6—C7—H7	119.5
O7—Yb—O1	74.9 (2)	C7^{v}—C8—C6	120.2 (9)
O5—Yb—O1	125.1 (2)	C7^{v}—C8—H8	119.9
O2—Yb—O1	50.14 (19)	C6—C8—H8	119.9
O1^{i}—Yb—O1	68.4 (2)	O6—C9—O5	127.2 (8)
O6^{iii}—Yb—O1	122.4 (2)	O6—C9—C9^{iii}	117.0 (8)
O4^{ii}—Yb—C9^{iii}	72.4 (2)	O5—C9—C9^{iii}	115.7 (8)
O3—Yb—C9^{iii}	96.2 (2)	O5—C9—Yb^{iii}	166.7 (6)
O7—Yb—C9^{iii}	120.2 (2)	C9^{iii}—C9—Yb^{iii}	76.1 (5)
O5—Yb—C9^{iii}	50.05 (19)	C1—O1—Yb^{i}	165.8 (6)
O2—Yb—C9^{iii}	87.2 (2)	C1—O1—Yb	82.4 (5)
O1^{i}—Yb—C9^{iii}	154.0 (2)	Yb^{i}—O1—Yb	111.6 (2)
O6^{iii}—Yb—C9^{iii}	21.0 (2)	C1—O2—Yb	104.7 (5)
O1—Yb—C9^{iii}	135.19 (19)	C5—O3—Yb	140.5 (5)
O4^{ii}—Yb—Yb^{i}	120.04 (17)	C5—O4—Yb^{ii}	157.0 (6)
O3—Yb—Yb^{i}	72.20 (14)	C9—O5—Yb	117.5 (5)
O7—Yb—Yb^{i}	69.81 (14)	C9—O6—Yb^{iii}	117.0 (5)
O5—Yb—Yb^{i}	138.46 (14)	Yb—O7—H7B	123.8
O2—Yb—Yb^{i}	80.49 (15)	Yb—O7—H7A	118.8
O1^{i}—Yb—Yb^{i}	37.81 (15)	H7B—O7—H7A	107.3
O6^{iii}—Yb—Yb^{i}	144.33 (15)		
O2—C1—C2—C3	−10.1 (13)	C2—C1—O2—Yb	−155.3 (6)
O1—C1—C2—C3	174.7 (9)	O4^{ii}—Yb—O2—C1	161.8 (6)
O2—C1—C2—C4	165.3 (8)	O3—Yb—O2—C1	58.4 (5)
O1—C1—C2—C4	−9.8 (12)	O7—Yb—O2—C1	−84.5 (5)
C4—C2—C3—C4^{iv}	1.1 (16)	O5—Yb—O2—C1	−155.0 (5)
C1—C2—C3—C4^{iv}	176.7 (8)	O1^{i}—Yb—O2—C1	−18.5 (6)
C3—C2—C4—C3^{iv}	−1.1 (16)	O6^{iii}—Yb—O2—C1	134.3 (5)
C1—C2—C4—C3^{iv}	−176.7 (8)	O1—Yb—O2—C1	−10.2 (5)
O4—C5—C6—C7	−152.4 (9)	C9^{iii}—Yb—O2—C1	154.9 (5)
O3—C5—C6—C7	27.6 (12)	Yb^{i}—Yb—O2—C1	−14.2 (5)
O4—C5—C6—C8	30.4 (13)	O4—C5—O3—Yb	30.8 (14)
O3—C5—C6—C8	−149.6 (9)	C6—C5—O3—Yb	−149.2 (7)
C8—C6—C7—C8^{v}	−1.5 (16)	O4^{ii}—Yb—O3—C5	−46.7 (9)

C5—C6—C7—C8ᵛ	−178.8 (8)	O7—Yb—O3—C5	−170.7 (8)
C7—C6—C8—C7ᵛ	1.5 (16)	O5—Yb—O3—C5	37.6 (11)
C5—C6—C8—C7ᵛ	178.8 (8)	O2—Yb—O3—C5	113.0 (9)
O2—C1—O1—Ybⁱ	171.7 (17)	O1ⁱ—Yb—O3—C5	−127.6 (9)
C2—C1—O1—Ybⁱ	−13 (3)	O6ⁱⁱⁱ—Yb—O3—C5	29.6 (9)
O2—C1—O1—Yb	−16.0 (7)	O1—Yb—O3—C5	162.2 (9)
C2—C1—O1—Yb	159.1 (7)	C9ⁱⁱⁱ—Yb—O3—C5	26.3 (9)
O4ⁱⁱ—Yb—O1—C1	−164.4 (5)	Ybⁱ—Yb—O3—C5	−165.5 (9)
O3—Yb—O1—C1	−90.6 (5)	O3—C5—O4—Ybⁱⁱ	50.2 (19)
O7—Yb—O1—C1	106.3 (5)	C6—C5—O4—Ybⁱⁱ	−129.7 (12)
O5—Yb—O1—C1	54.5 (5)	O6—C9—O5—Yb	−166.9 (7)
O2—Yb—O1—C1	9.9 (4)	C9ⁱⁱⁱ—C9—O5—Yb	9.8 (12)
O1ⁱ—Yb—O1—C1	−178.0 (6)	Ybⁱⁱⁱ—C9—O5—Yb	160 (2)
O6ⁱⁱⁱ—Yb—O1—C1	−33.1 (5)	O4ⁱⁱ—Yb—O5—C9	69.9 (6)
C9ⁱⁱⁱ—Yb—O1—C1	−11.5 (6)	O3—Yb—O5—C9	−20.5 (8)
Ybⁱ—Yb—O1—C1	−178.0 (6)	O7—Yb—O5—C9	177.6 (7)
O4ⁱⁱ—Yb—O1—Ybⁱ	13.6 (5)	O2—Yb—O5—C9	−95.9 (6)
O3—Yb—O1—Ybⁱ	87.4 (3)	O1ⁱ—Yb—O5—C9	139.5 (6)
O7—Yb—O1—Ybⁱ	−75.7 (3)	O6ⁱⁱⁱ—Yb—O5—C9	−12.3 (6)
O5—Yb—O1—Ybⁱ	−127.5 (2)	O1—Yb—O5—C9	−128.6 (6)
O2—Yb—O1—Ybⁱ	−172.1 (4)	C9ⁱⁱⁱ—Yb—O5—C9	−5.8 (7)
O1ⁱ—Yb—O1—Ybⁱ	0.000 (2)	Ybⁱ—Yb—O5—C9	−166.1 (5)
O6ⁱⁱⁱ—Yb—O1—Ybⁱ	144.9 (2)	O5—C9—O6—Ybⁱⁱⁱ	−169.3 (7)
C9ⁱⁱⁱ—Yb—O1—Ybⁱ	166.5 (2)	C9ⁱⁱⁱ—C9—O6—Ybⁱⁱⁱ	14.1 (12)
O1—C1—O2—Yb	19.9 (9)		

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

Hydrogen-bond geometry (Å, °)

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
O7—H7*A*⋯O3ⁱ	0.85	1.92	2.751 (6)	167
O7—H7*B*⋯O2ᵛⁱ	0.85	1.91	2.754 (6)	178

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