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Bis(μ-4-hydroxybenzoato-κ²O:O′)bis[triaquabis(4-hydroxybenzoato)-κO;κ²O,O′-terbium(III)] decahydrate

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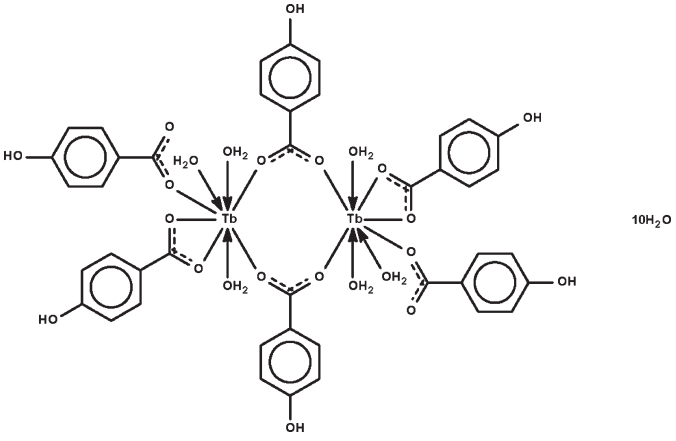
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.003 Å; R factor = 0.018; wR factor = 0.059; data-to-parameter ratio = 14.1.

The title dinuclear compound, $[Tb_2(C_7H_5O_3)_6(H_2O)_6]\cdot 10H_2O$, lies on a center of inversion and the two Tb^{III} atoms are bridged by two 4-hydroxybenzoate anions; each metal atom is further coordinated by one monodentate anion and chelated by the third anion. The eight-coordinate geometry approximates a square antiprism. Hydrogen bonds of the O—H···O type connect the uncoordinated water molecules to the dinuclear species, forming a three-dimensional network.

Related literature

For a related structure, $Tb_2(H_2O)_2(DMF)_2(C_7H_5O_3)_6$, see: Zhou *et al.* (2008).



Experimental

Crystal data

$[Tb_2(C_7H_5O_3)_6(H_2O)_6]\cdot 10H_2O$
M_r = 1428.76
Triclinic, $P\overline{1}$
a = 10.8308 (5) Å
b = 11.3337 (6) Å
c = 11.5128 (6) Å
α = 90.463 (1)°
β = 101.690 (1)°
γ = 105.249 (1)°
V = 1332.37 (12) Å³
Z = 1
Mo $K\alpha$ radiation
μ = 2.73 mm^{-1}
T = 173 K
0.47 × 0.30 × 0.19 mm

Data collection

Bruker SMART area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.360, T_{max} = 0.625
12836 measured reflections
5756 independent reflections
5391 reflections with $I > 2\sigma(I)$
R_{int} = 0.018

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.018
$wR(F^2)$ = 0.059
S = 1.09
5756 reflections
409 parameters
27 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.67 e Å^{-3}
$\Delta\rho_{min}$ = −0.64 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···O7w^{i}	0.84 (1)	1.82 (2)	2.612 (3)	158 (3)
O6—H6···O6w^{ii}	0.83 (1)	1.87 (1)	2.678 (3)	165 (4)
O9—H9···O4w^{iii}	0.84 (1)	1.98 (2)	2.763 (3)	156 (3)
O1w—H11···O4w	0.84 (1)	2.04 (1)	2.870 (3)	171 (3)
O1w—H12···O9^{iv}	0.83 (1)	1.96 (1)	2.766 (3)	164 (3)
O2w—H22···O5w	0.83 (1)	1.86 (1)	2.678 (3)	167 (3)
O2w—H21···O5w^{v}	0.84 (1)	2.20 (2)	2.952 (3)	150 (3)
O3w—H31···O3^{ii}	0.84 (1)	1.95 (1)	2.777 (3)	171 (3)
O3w—H32···O7^{vi}	0.84 (1)	2.25 (2)	2.916 (2)	137 (3)
O4w—H41···O8w^{vii}	0.84 (1)	1.94 (1)	2.753 (3)	163 (3)
O4w—H42···O5^{viii}	0.84 (1)	2.10 (1)	2.927 (3)	169 (3)
O5w—H52···O7w	0.85 (1)	2.01 (2)	2.811 (3)	157 (3)
O5w—H51···O8w^{ix}	0.86 (1)	1.96 (1)	2.791 (3)	163 (3)
O6w—H61···O2	0.85 (1)	1.90 (1)	2.743 (2)	172 (3)
O6w—H62···O5	0.84 (1)	1.95 (1)	2.785 (2)	171 (3)
O7w—H71···O6w	0.84 (1)	1.90 (1)	2.732 (3)	172 (3)
O7w—H72···O5^{x}	0.83 (1)	1.89 (1)	2.725 (3)	175 (3)
O8w—H81···O1^{xi}	0.84 (1)	2.10 (2)	2.818 (3)	144 (3)
O8w—H82···O6	0.84 (1)	1.90 (1)	2.713 (3)	164 (3)

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2706).

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Zhou, Y.-X., Shen, X.-Q., Zhang, H.-Y., Du, C.-X. & Hou, H.-W. (2008). *J. Coord. Chem.* **61**, 3981–3992.

supplementary materials

Acta Cryst. (2010). E**66**, m54-m55 [**doi:10.1107/S1600536809052489**]

Bis(μ-4-hydroxybenzoato-κ^2O:O')bis[triaquabis(4-hydroxybenzoato)-κO;κ^2O,O'-terbium(III)] decahydrate

Y.-M. Zhu, P.-P. Feng, Y.-Y. Yang and S. W. Ng

Experimental

4-Hydroxybenzoic acid (0.3 mmol) and sodium hydroxide (0.3 mmol) were dissolved in water (5 ml) and this was mixed with a solution of terbium chloride (0.1 mmol) dissolved in water (5 ml). The white precipitate that formed was removed by filtration. Colorless crystals were isolated from the filtrated after two weeks.

Refinement

Carbon-bound hydrogen atoms were generated geometrically and were constrained to ride on their parent atoms [C–H = 0.95, U_{iso}(H) = 1.2U_{eq}(C)]. The hydroxy and water H-atoms were located in a difference Fourier map, and were refined with distance restraints of O–H 0.84±0.01 Å and H···H 1.37±0.01 Å. Their temperature factors were tied by a factor of 1.5.

Figures

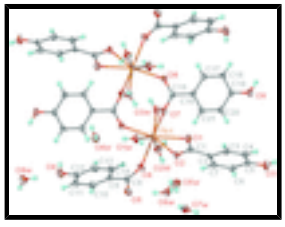

Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of $Tb_2(H_2O)_6(C_7H_5O_3)_6\cdot 10H_2O$ at the 70% probability level; hydrogen atoms are drawn as sphere of arbitrary radius.

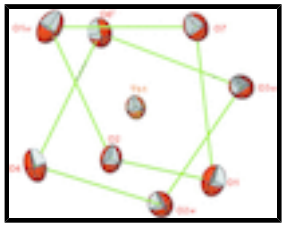

Fig. 2. Detail of the coordination environment of the terbium(III) atom.

Bis(μ-4-hydroxybenzoato-κ^2O:O')bis[triaquabis(4- hydroxybenzoato)-κO;κ^2O,O'-terbium(III)] decahydrate

Crystal data

$[Tb_2(C_7H_5O_3)_6(H_2O)_6]\cdot 10H_2O$	Z = 1
M_r = 1428.76	F(000) = 716
Triclinic, $P\overline{1}$	D_x = 1.781 Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation, λ = 0.71073 Å
a = 10.8308 (5) Å	Cell parameters from 5392 reflections
b = 11.3337 (6) Å	θ = 2.3–27.0°

c = 11.5128 (6) Å	μ = 2.73 mm^{-1}
α = 90.463 (1)°	T = 173 K
β = 101.690 (1)°	Block, colorless
γ = 105.249 (1)°	0.47 × 0.30 × 0.19 mm
V = 1332.37 (12) Å^3	

Data collection

Bruker SMART area-detector diffractometer	5756 independent reflections
Radiation source: fine-focus sealed tube	5391 reflections with $I > 2\sigma(I)$
graphite	R_{int} = 0.018
φ and ω scans	θ_{max} = 27.0°, θ_{min} = 1.8°
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	h = −13→13
T_{min} = 0.360, T_{max} = 0.625	k = −13→14
12836 measured reflections	l = −14→14

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)]$ = 0.018	Hydrogen site location: inferred from neighbouring sites
$wR(F^2)$ = 0.059	H atoms treated by a mixture of independent and constrained refinement
S = 1.09	$w = 1/[\sigma^2(F_o^2) + (0.0407P)^2 + 0.0925P]$ where $P = (F_o^2 + 2F_c^2)/3$
5756 reflections	$(\Delta/\sigma)_{max}$ = 0.001
409 parameters	$\Delta\rho_{max}$ = 0.67 e Å^{-3}
27 restraints	$\Delta\rho_{min}$ = −0.64 e Å^{-3}

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

	x	y	z	U_{iso}*/U_{eq}
Tb1	0.521099 (9)	0.392335 (9)	0.316629 (8)	0.01393 (5)
O1	0.68247 (16)	0.52500 (16)	0.22113 (15)	0.0219 (4)
O2	0.71938 (16)	0.35118 (15)	0.28025 (15)	0.0189 (3)
O3	1.25530 (17)	0.60503 (18)	0.13235 (17)	0.0243 (4)
H3	1.262 (3)	0.6687 (19)	0.095 (3)	0.036*
O4	0.44616 (17)	0.20553 (16)	0.21445 (16)	0.0233 (4)
O5	0.44536 (17)	0.00991 (16)	0.21119 (16)	0.0236 (4)
O6	−0.15974 (18)	−0.03603 (17)	0.16884 (18)	0.0280 (4)
H6	−0.192 (3)	0.023 (2)	0.171 (3)	0.042*
O7	0.66267 (16)	0.51402 (16)	0.47709 (14)	0.0207 (3)
O8	0.65933 (16)	0.66801 (16)	0.59555 (15)	0.0209 (4)
O9	1.23480 (17)	0.85877 (17)	0.50180 (16)	0.0220 (4)

H9	1.262 (3)	0.9320 (13)	0.529 (3)	0.033*
O1w	0.56576 (17)	0.25542 (17)	0.47360 (16)	0.0241 (4)
H11	0.509 (2)	0.206 (2)	0.502 (3)	0.036*
H12	0.6353 (16)	0.234 (3)	0.487 (3)	0.036*
O2w	0.40382 (18)	0.41807 (17)	0.12181 (15)	0.0233 (4)
H21	0.405 (3)	0.4895 (13)	0.102 (2)	0.035*
H22	0.426 (3)	0.380 (2)	0.071 (2)	0.035*
O3w	0.44922 (17)	0.57723 (16)	0.32029 (15)	0.0201 (3)
H31	0.397 (2)	0.593 (3)	0.2625 (14)	0.030*
H32	0.428 (3)	0.593 (3)	0.3838 (13)	0.030*
O4w	0.39635 (19)	0.08545 (18)	0.59456 (16)	0.0267 (4)
H41	0.358 (3)	0.130 (3)	0.624 (2)	0.040*
H42	0.450 (3)	0.066 (3)	0.6490 (19)	0.040*
O5w	0.4872 (2)	0.3305 (2)	−0.05591 (17)	0.0309 (4)
H51	0.421 (2)	0.294 (3)	−0.111 (2)	0.046*
H52	0.530 (3)	0.278 (2)	−0.037 (3)	0.046*
O6w	0.69870 (17)	0.12258 (17)	0.18465 (16)	0.0235 (4)
H61	0.711 (3)	0.1957 (12)	0.211 (3)	0.035*
H62	0.6246 (17)	0.082 (2)	0.194 (3)	0.035*
O7w	0.6606 (2)	0.18314 (17)	−0.04660 (16)	0.0286 (4)
H71	0.676 (3)	0.160 (3)	0.0230 (11)	0.043*
H72	0.627 (3)	0.1215 (18)	−0.0936 (19)	0.043*
O8w	−0.30680 (19)	−0.22701 (18)	0.26414 (18)	0.0301 (4)
H81	−0.280 (3)	−0.2897 (17)	0.276 (3)	0.045*
H82	−0.249 (2)	−0.172 (2)	0.242 (3)	0.045*
C1	0.7539 (2)	0.4523 (2)	0.2315 (2)	0.0169 (5)
C2	0.8802 (2)	0.4855 (2)	0.19285 (19)	0.0163 (4)
C3	0.9139 (2)	0.5908 (2)	0.1316 (2)	0.0190 (5)
H3A	0.8513	0.6352	0.1057	0.023*
C4	1.0383 (2)	0.6307 (2)	0.1084 (2)	0.0186 (5)
H4	1.0609	0.7020	0.0660	0.022*
C5	1.1296 (2)	0.5662 (2)	0.1474 (2)	0.0177 (5)
C6	1.0956 (2)	0.4574 (2)	0.2042 (2)	0.0188 (5)
H6A	1.1572	0.4112	0.2268	0.023*
C7	0.9713 (2)	0.4181 (2)	0.22698 (19)	0.0178 (5)
H7	0.9475	0.3446	0.2661	0.021*
C8	0.3871 (2)	0.0935 (2)	0.2068 (2)	0.0184 (5)
C9	0.2416 (2)	0.0589 (2)	0.1919 (2)	0.0168 (4)
C10	0.1763 (2)	−0.0536 (2)	0.2258 (2)	0.0206 (5)
H10	0.2237	−0.1109	0.2542	0.025*
C11	0.0414 (2)	−0.0831 (2)	0.2184 (2)	0.0224 (5)
H11A	−0.0027	−0.1592	0.2440	0.027*
C12	−0.0276 (2)	−0.0015 (2)	0.1740 (2)	0.0201 (5)
C13	0.0352 (2)	0.1103 (2)	0.1364 (2)	0.0214 (5)
H13	−0.0135	0.1651	0.1034	0.026*
C14	0.1704 (2)	0.1410 (2)	0.1477 (2)	0.0207 (5)
H14	0.2146	0.2185	0.1251	0.025*
C15	0.7152 (2)	0.6180 (2)	0.53115 (19)	0.0159 (4)
C16	0.8513 (2)	0.6851 (2)	0.52099 (19)	0.0153 (4)

C17	0.9058 (2)	0.8072 (2)	0.56448 (19)	0.0167 (4)
H17	0.8550	0.8494	0.5982	0.020*
C18	1.0337 (2)	0.8673 (2)	0.5587 (2)	0.0187 (5)
H18	1.0704	0.9503	0.5883	0.022*
C19	1.1080 (2)	0.8052 (2)	0.5093 (2)	0.0177 (5)
C20	1.0543 (2)	0.6841 (2)	0.4635 (2)	0.0187 (5)
H20	1.1045	0.6427	0.4282	0.022*
C21	0.9260 (2)	0.6245 (2)	0.4702 (2)	0.0176 (5)
H21A	0.8890	0.5418	0.4398	0.021*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Tb1	0.01190 (7)	0.01180 (7)	0.01807 (7)	0.00220 (4)	0.00446 (4)	0.00005 (4)
O1	0.0188 (8)	0.0190 (9)	0.0318 (9)	0.0082 (7)	0.0104 (7)	0.0067 (7)
O2	0.0174 (8)	0.0138 (8)	0.0276 (8)	0.0042 (6)	0.0098 (6)	0.0035 (6)
O3	0.0152 (8)	0.0248 (10)	0.0348 (10)	0.0051 (7)	0.0099 (7)	0.0120 (8)
O4	0.0198 (8)	0.0152 (9)	0.0338 (9)	0.0032 (7)	0.0051 (7)	−0.0029 (7)
O5	0.0186 (8)	0.0183 (9)	0.0343 (9)	0.0062 (7)	0.0049 (7)	−0.0008 (7)
O6	0.0173 (9)	0.0201 (10)	0.0484 (11)	0.0055 (7)	0.0105 (8)	0.0042 (8)
O7	0.0160 (8)	0.0188 (9)	0.0244 (8)	0.0005 (7)	0.0032 (6)	−0.0025 (7)
O8	0.0174 (8)	0.0170 (9)	0.0302 (9)	0.0039 (7)	0.0105 (7)	−0.0001 (7)
O9	0.0134 (8)	0.0204 (9)	0.0321 (9)	0.0023 (7)	0.0079 (7)	0.0027 (7)
O1w	0.0184 (8)	0.0241 (10)	0.0337 (9)	0.0082 (7)	0.0108 (7)	0.0114 (7)
O2w	0.0316 (10)	0.0196 (9)	0.0203 (8)	0.0097 (8)	0.0058 (7)	0.0005 (7)
O3w	0.0237 (9)	0.0198 (9)	0.0195 (8)	0.0093 (7)	0.0065 (7)	0.0013 (7)
O4w	0.0262 (10)	0.0251 (10)	0.0301 (9)	0.0082 (8)	0.0067 (7)	0.0042 (8)
O5w	0.0298 (10)	0.0359 (12)	0.0292 (10)	0.0122 (9)	0.0072 (8)	−0.0007 (8)
O6w	0.0200 (9)	0.0194 (9)	0.0330 (10)	0.0057 (7)	0.0092 (7)	0.0001 (7)
O7w	0.0404 (11)	0.0183 (9)	0.0272 (9)	0.0055 (8)	0.0109 (8)	0.0021 (7)
O8w	0.0293 (10)	0.0204 (10)	0.0427 (11)	0.0062 (8)	0.0128 (8)	0.0068 (8)
C1	0.0153 (11)	0.0168 (11)	0.0172 (10)	0.0023 (9)	0.0030 (8)	−0.0022 (9)
C2	0.0156 (10)	0.0159 (11)	0.0170 (10)	0.0029 (9)	0.0047 (8)	0.0000 (8)
C3	0.0185 (11)	0.0181 (12)	0.0224 (11)	0.0074 (9)	0.0057 (9)	0.0039 (9)
C4	0.0207 (11)	0.0155 (11)	0.0206 (11)	0.0047 (9)	0.0066 (9)	0.0040 (9)
C5	0.0162 (11)	0.0183 (12)	0.0185 (11)	0.0028 (9)	0.0057 (8)	−0.0004 (9)
C6	0.0180 (11)	0.0180 (12)	0.0222 (11)	0.0066 (9)	0.0055 (9)	0.0046 (9)
C7	0.0190 (11)	0.0155 (11)	0.0182 (10)	0.0028 (9)	0.0046 (8)	0.0029 (9)
C8	0.0181 (11)	0.0172 (12)	0.0189 (10)	0.0026 (9)	0.0044 (8)	−0.0012 (9)
C9	0.0185 (11)	0.0136 (11)	0.0185 (10)	0.0046 (9)	0.0039 (8)	−0.0004 (8)
C10	0.0203 (11)	0.0158 (12)	0.0276 (12)	0.0078 (9)	0.0054 (9)	0.0029 (9)
C11	0.0222 (12)	0.0147 (12)	0.0318 (13)	0.0040 (10)	0.0102 (10)	0.0027 (10)
C12	0.0186 (11)	0.0184 (12)	0.0230 (11)	0.0036 (9)	0.0055 (9)	−0.0021 (9)
C13	0.0215 (12)	0.0185 (12)	0.0247 (12)	0.0082 (10)	0.0023 (9)	0.0034 (9)
C14	0.0216 (12)	0.0156 (12)	0.0245 (11)	0.0032 (10)	0.0064 (9)	0.0022 (9)
C15	0.0141 (10)	0.0166 (11)	0.0176 (10)	0.0052 (9)	0.0031 (8)	0.0036 (8)
C16	0.0147 (10)	0.0166 (11)	0.0142 (10)	0.0043 (9)	0.0021 (8)	0.0016 (8)
C17	0.0163 (11)	0.0163 (11)	0.0189 (10)	0.0055 (9)	0.0051 (8)	0.0024 (9)

C18	0.0188 (11)	0.0148 (11)	0.0221 (11)	0.0030 (9)	0.0053 (9)	0.0008 (9)
C19	0.0121 (10)	0.0209 (12)	0.0200 (11)	0.0036 (9)	0.0040 (8)	0.0051 (9)
C20	0.0175 (11)	0.0190 (12)	0.0217 (11)	0.0070 (9)	0.0064 (9)	0.0001 (9)
C21	0.0163 (11)	0.0161 (11)	0.0189 (10)	0.0026 (9)	0.0028 (8)	−0.0008 (9)

Geometric parameters (Å, °)

Tb1—O4	2.2791 (17)	O8w—H81	0.836 (10)
Tb1—O7	2.3162 (16)	O8w—H82	0.840 (10)
Tb1—O8^{i}	2.3276 (16)	C1—C2	1.480 (3)
Tb1—O2w	2.4042 (17)	C2—C3	1.394 (3)
Tb1—O3w	2.4227 (18)	C2—C7	1.398 (3)
Tb1—O2	2.4276 (16)	C3—C4	1.385 (3)
Tb1—O1	2.4388 (17)	C3—H3A	0.9500
Tb1—O1w	2.4482 (17)	C4—C5	1.386 (3)
O1—C1	1.262 (3)	C4—H4	0.9500
O2—C1	1.280 (3)	C5—C6	1.398 (3)
O3—C5	1.364 (3)	C6—C7	1.383 (3)
O3—H3	0.837 (10)	C6—H6A	0.9500
O4—C8	1.256 (3)	C7—H7	0.9500
O5—C8	1.265 (3)	C8—C9	1.494 (3)
O6—C12	1.370 (3)	C9—C10	1.387 (3)
O6—H6	0.833 (10)	C9—C14	1.395 (4)
O7—C15	1.262 (3)	C10—C11	1.395 (3)
O8—C15	1.262 (3)	C10—H10	0.9500
O8—Tb1^{i}	2.3276 (16)	C11—C12	1.375 (4)
O9—C19	1.368 (3)	C11—H11A	0.9500
O9—H9	0.841 (10)	C12—C13	1.389 (4)
O1w—H11	0.839 (10)	C13—C14	1.392 (3)
O1w—H12	0.834 (10)	C13—H13	0.9500
O2w—H21	0.838 (10)	C14—H14	0.9500
O2w—H22	0.832 (10)	C15—C16	1.499 (3)
O3w—H31	0.835 (10)	C16—C21	1.395 (3)
O3w—H32	0.840 (10)	C16—C17	1.397 (3)
O4w—H41	0.837 (10)	C17—C18	1.389 (3)
O4w—H42	0.840 (10)	C17—H17	0.9500
O5w—H51	0.861 (10)	C18—C19	1.394 (3)
O5w—H52	0.852 (10)	C18—H18	0.9500
O6w—H61	0.846 (10)	C19—C20	1.394 (3)
O6w—H62	0.841 (10)	C20—C21	1.394 (3)
O7w—H71	0.842 (10)	C20—H20	0.9500
O7w—H72	0.833 (10)	C21—H21A	0.9500
O4—Tb1—O7	147.98 (6)	C4—C3—H3A	119.9
O4—Tb1—O8^{i}	86.52 (6)	C2—C3—H3A	119.9
O7—Tb1—O8^{i}	97.15 (6)	C3—C4—C5	119.7 (2)
O4—Tb1—O2w	71.93 (6)	C3—C4—H4	120.2
O7—Tb1—O2w	138.23 (6)	C5—C4—H4	120.2
O8^{i}—Tb1—O2w	97.25 (6)	O3—C5—C4	122.0 (2)

O4—Tb1—O3w	136.40 (6)	O3—C5—C6	117.2 (2)
O7—Tb1—O3w	74.94 (6)	C4—C5—C6	120.8 (2)
O8^{i}—Tb1—O3w	77.43 (6)	C7—C6—C5	119.1 (2)
O2w—Tb1—O3w	70.33 (6)	C7—C6—H6A	120.4
O4—Tb1—O2	76.79 (6)	C5—C6—H6A	120.4
O7—Tb1—O2	83.64 (6)	C6—C7—C2	120.5 (2)
O8^{i}—Tb1—O2	147.37 (6)	C6—C7—H7	119.8
O2w—Tb1—O2	103.72 (6)	C2—C7—H7	119.8
O3w—Tb1—O2	133.16 (6)	O4—C8—O5	122.9 (2)
O4—Tb1—O1	108.71 (6)	O4—C8—C9	117.9 (2)
O7—Tb1—O1	78.16 (6)	O5—C8—C9	119.2 (2)
O8^{i}—Tb1—O1	158.46 (6)	C10—C9—C14	119.2 (2)
O2w—Tb1—O1	74.23 (6)	C10—C9—C8	120.3 (2)
O3w—Tb1—O1	81.06 (6)	C14—C9—C8	120.4 (2)
O2—Tb1—O1	53.69 (6)	C9—C10—C11	120.4 (2)
O4—Tb1—O1w	78.28 (6)	C9—C10—H10	119.8
O7—Tb1—O1w	73.07 (6)	C11—C10—H10	119.8
O8^{i}—Tb1—O1w	70.82 (6)	C12—C11—C10	119.7 (2)
O2w—Tb1—O1w	148.59 (6)	C12—C11—H11A	120.2
O3w—Tb1—O1w	130.93 (6)	C10—C11—H11A	120.2
O2—Tb1—O1w	78.37 (6)	O6—C12—C11	116.8 (2)
O1—Tb1—O1w	126.13 (6)	O6—C12—C13	122.2 (2)
C1—O1—Tb1	93.28 (14)	C11—C12—C13	121.0 (2)
C1—O2—Tb1	93.32 (14)	C14—C13—C12	119.1 (2)
C5—O3—H3	107 (2)	C14—C13—H13	120.5
C8—O4—Tb1	150.98 (16)	C12—C13—H13	120.5
C12—O6—H6	114 (2)	C13—C14—C9	120.6 (2)
C15—O7—Tb1	150.17 (16)	C13—C14—H14	119.7
C15—O8—Tb1^{i}	136.88 (15)	C9—C14—H14	119.7
C19—O9—H9	113 (2)	O8—C15—O7	123.1 (2)
Tb1—O1w—H11	125.7 (19)	O8—C15—C16	117.9 (2)
Tb1—O1w—H12	121.8 (19)	O7—C15—C16	119.0 (2)
H11—O1w—H12	109.2 (16)	C21—C16—C17	119.4 (2)
Tb1—O2w—H21	118 (2)	C21—C16—C15	119.8 (2)
Tb1—O2w—H22	110 (2)	C17—C16—C15	120.8 (2)
H21—O2w—H22	110.7 (16)	C18—C17—C16	120.3 (2)
Tb1—O3w—H31	121 (2)	C18—C17—H17	119.8
Tb1—O3w—H32	114.7 (19)	C16—C17—H17	119.8
H31—O3w—H32	109.5 (16)	C17—C18—C19	119.7 (2)
H41—O4w—H42	108.8 (16)	C17—C18—H18	120.1
H51—O5w—H52	105.4 (15)	C19—C18—H18	120.1
H61—O6w—H62	108.3 (16)	O9—C19—C18	122.6 (2)
H71—O7w—H72	108.9 (16)	O9—C19—C20	116.8 (2)
H81—O8w—H82	109.5 (16)	C18—C19—C20	120.6 (2)
O1—C1—O2	119.7 (2)	C21—C20—C19	119.2 (2)
O1—C1—C2	120.5 (2)	C21—C20—H20	120.4
O2—C1—C2	119.7 (2)	C19—C20—H20	120.4
C3—C2—C7	119.6 (2)	C20—C21—C16	120.7 (2)

C3—C2—C1	120.0 (2)	C20—C21—H21A	119.7
C7—C2—C1	120.2 (2)	C16—C21—H21A	119.7
C4—C3—C2	120.2 (2)		
O4—Tb1—O1—C1	−56.96 (14)	C3—C4—C5—C6	3.5 (3)
O7—Tb1—O1—C1	90.56 (14)	O3—C5—C6—C7	176.6 (2)
O8^{i}—Tb1—O1—C1	169.90 (15)	C4—C5—C6—C7	−3.4 (3)
O2w—Tb1—O1—C1	−121.11 (14)	C5—C6—C7—C2	0.5 (3)
O3w—Tb1—O1—C1	166.92 (14)	C3—C2—C7—C6	2.3 (3)
O2—Tb1—O1—C1	−0.22 (12)	C1—C2—C7—C6	−171.8 (2)
O1w—Tb1—O1—C1	31.99 (16)	Tb1—O4—C8—O5	−108.1 (3)
O4—Tb1—O2—C1	125.77 (14)	Tb1—O4—C8—C9	72.0 (4)
O7—Tb1—O2—C1	−79.74 (13)	O4—C8—C9—C10	−156.2 (2)
O8^{i}—Tb1—O2—C1	−173.07 (12)	O5—C8—C9—C10	23.8 (3)
O2w—Tb1—O2—C1	58.44 (14)	O4—C8—C9—C14	21.5 (3)
O3w—Tb1—O2—C1	−17.32 (16)	O5—C8—C9—C14	−158.5 (2)
O1—Tb1—O2—C1	0.22 (12)	C14—C9—C10—C11	−1.5 (4)
O1w—Tb1—O2—C1	−153.71 (14)	C8—C9—C10—C11	176.2 (2)
O7—Tb1—O4—C8	66.9 (4)	C9—C10—C11—C12	1.9 (4)
O8^{i}—Tb1—O4—C8	−31.0 (3)	C10—C11—C12—O6	179.8 (2)
O2w—Tb1—O4—C8	−129.8 (3)	C10—C11—C12—C13	−0.1 (4)
O3w—Tb1—O4—C8	−98.7 (3)	O6—C12—C13—C14	178.0 (2)
O2—Tb1—O4—C8	120.8 (3)	C11—C12—C13—C14	−2.1 (4)
O1—Tb1—O4—C8	164.6 (3)	C12—C13—C14—C9	2.4 (4)
O1w—Tb1—O4—C8	40.1 (3)	C10—C9—C14—C13	−0.7 (4)
O4—Tb1—O7—C15	169.6 (3)	C8—C9—C14—C13	−178.4 (2)
O8^{i}—Tb1—O7—C15	−95.6 (3)	Tb1^{i}—O8—C15—O7	14.8 (4)
O2w—Tb1—O7—C15	13.8 (3)	Tb1^{i}—O8—C15—C16	−163.99 (16)
O3w—Tb1—O7—C15	−20.7 (3)	Tb1—O7—C15—O8	81.1 (4)
O2—Tb1—O7—C15	117.3 (3)	Tb1—O7—C15—C16	−100.2 (3)
O1—Tb1—O7—C15	63.1 (3)	O8—C15—C16—C21	167.8 (2)
O1w—Tb1—O7—C15	−163.0 (3)	O7—C15—C16—C21	−11.1 (3)
Tb1—O1—C1—O2	0.4 (2)	O8—C15—C16—C17	−10.6 (3)
Tb1—O1—C1—C2	−176.78 (18)	O7—C15—C16—C17	170.5 (2)
Tb1—O2—C1—O1	−0.4 (2)	C21—C16—C17—C18	−0.9 (3)
Tb1—O2—C1—C2	176.80 (18)	C15—C16—C17—C18	177.6 (2)
O1—C1—C2—C3	−7.7 (3)	C16—C17—C18—C19	0.0 (3)
O2—C1—C2—C3	175.1 (2)	C17—C18—C19—O9	−179.5 (2)
O1—C1—C2—C7	166.3 (2)	C17—C18—C19—C20	1.2 (4)
O2—C1—C2—C7	−10.8 (3)	O9—C19—C20—C21	179.2 (2)
C7—C2—C3—C4	−2.3 (3)	C18—C19—C20—C21	−1.5 (4)
C1—C2—C3—C4	171.8 (2)	C19—C20—C21—C16	0.5 (3)
C2—C3—C4—C5	−0.6 (4)	C17—C16—C21—C20	0.6 (3)
C3—C4—C5—O3	−176.5 (2)	C15—C16—C21—C20	−177.8 (2)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*

O3—H3···O7w^{ii}	0.84 (1)	1.82 (2)	2.612 (3)	158 (3)
O6—H6···O6w^{iii}	0.83 (1)	1.87 (1)	2.678 (3)	165 (4)
O9—H9···O4w^{iv}	0.84 (1)	1.98 (2)	2.763 (3)	156 (3)
O1w—H11···O4w	0.84 (1)	2.04 (1)	2.870 (3)	171 (3)
O1w—H12···O9^{v}	0.83 (1)	1.96 (1)	2.766 (3)	164 (3)
O2w—H22···O5w	0.83 (1)	1.86 (1)	2.678 (3)	167 (3)
O2w—H21···O5w^{vi}	0.84 (1)	2.20 (2)	2.952 (3)	150 (3)
O3w—H31···O3^{iii}	0.84 (1)	1.95 (1)	2.777 (3)	171 (3)
O3w—H32···O7^{i}	0.84 (1)	2.25 (2)	2.916 (2)	137 (3)
O4w—H41···O8w^{vii}	0.84 (1)	1.94 (1)	2.753 (3)	163 (3)
O4w—H42···O5^{viii}	0.84 (1)	2.10 (1)	2.927 (3)	169 (3)
O5w—H52···O7w	0.85 (1)	2.01 (2)	2.811 (3)	157 (3)
O5w—H51···O8w^{ix}	0.86 (1)	1.96 (1)	2.791 (3)	163 (3)
O6w—H61···O2	0.85 (1)	1.90 (1)	2.743 (2)	172 (3)
O6w—H62···O5	0.84 (1)	1.95 (1)	2.785 (2)	171 (3)
O7w—H71···O6w	0.84 (1)	1.90 (1)	2.732 (3)	172 (3)
O7w—H72···O5^{x}	0.83 (1)	1.89 (1)	2.725 (3)	175 (3)
O8w—H81···O1^{xi}	0.84 (1)	2.10 (2)	2.818 (3)	144 (3)
O8w—H82···O6	0.84 (1)	1.90 (1)	2.713 (3)	164 (3)

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

Fig. 1

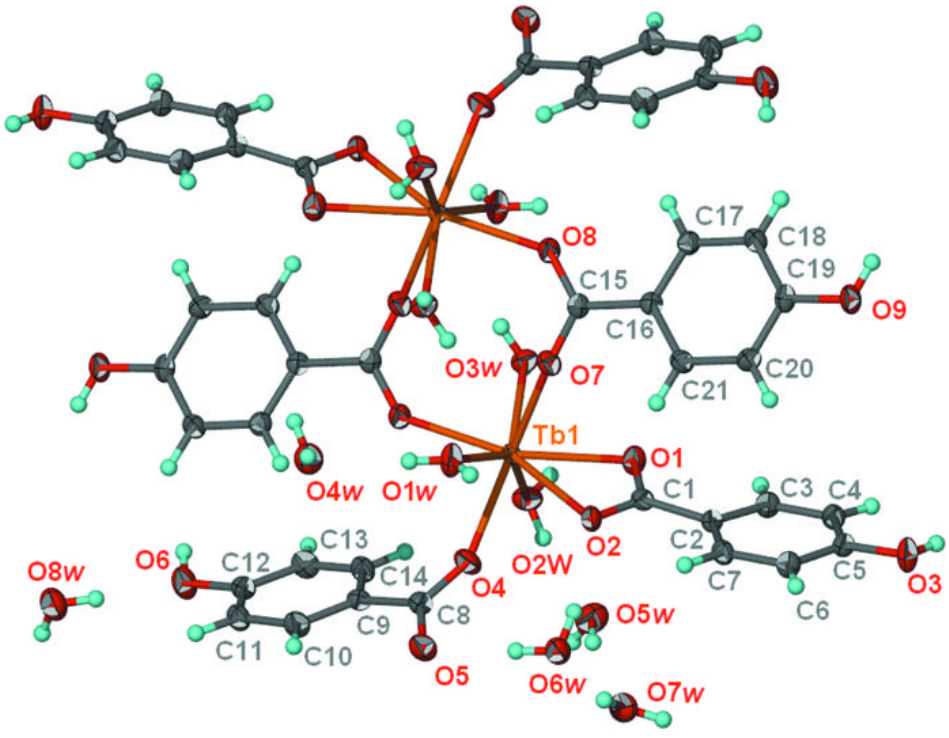
C17
C18
C19
O9
O8
C15
C16
C20
C21
O3w
O7
Tb1
O1
C1
C3
C4
O4w
O1w
O2
C2
C5
O3
C7
C6
O8w
O6
C12
C13
C14
O4
O2W
C8
O5w
C9
C11
C10
O5
O6w
O7w

Fig. 2