Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

catena-Poly[[[diaqua(6-carboxypyridine-2-carboxylato)terbium(III)]-μ-pyridine-2,6-dicarboxylato] tetrahydrate]

Lu-Jiang Hao* and Tong-Li Yu

College of Food and Biological Engineering, Shandong Institute of Light Industry, Jinan 250353, People's Republic of China
Correspondence e-mail: lujianghao001@yahoo.com.cn

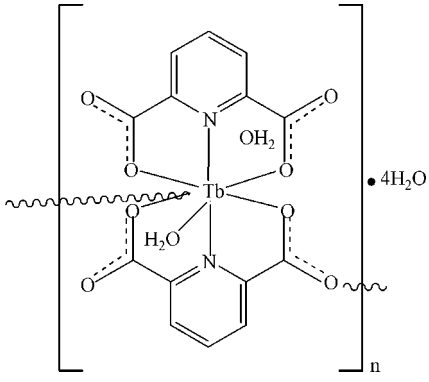
Received 11 July 2007; accepted 16 July 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.011 Å; R factor = 0.042; wR factor = 0.131; data-to-parameter ratio = 11.0.

The title compound, $[Tb(C_7H_3NO_4)(C_7H_4NO_4)(H_2O)_2]\cdot 4H_2O$, is isostructural with its La^{3+}, Ce^{3+}, Pr^{3+}, Nd^{3+}, Sm^{3+} and Gd^{3+} analogues. The Tb^{3+} ion is nine-coordinated by two O and one N atoms from a tridentate 6-carboxypyridine-2-carboxylate ligand, two O and one N atoms from a tridentate pyridine-2,6-dicarboxylate ligand, one O atom belonging to a neighbouring pyridine-2,6-dicarboxylate ligand, and two water molecules. The bridging pyridine-2,6-dicarboxylate ligand gives rise to infinite chains. The crystal structure involves O—H···O hydrogen bonds.

Related literature

The isostructural lanthanide compounds are those with La^{3+} (Guerriero *et al.*, 1987; Ghosh & Bharadwaj, 2005), Ce^{3+} (Okabe *et al.*, 2002; Ghosh & Bharadwaj, 2003; Rafizadeh *et al.*, 2005; Ramezanipour *et al.*, 2005), Pr^{3+} (Ghosh & Bharadwaj, 2003; Zhao *et al.*, 2005), Nd^{3+} (Miao *et al.*, 1992), Sm^{3+} (Liu *et al.*, 2005, 2006; Rafizadeh *et al.*, 2005; Song *et al.*, 2005), Eu^{3+} (Brayshaw *et al.*, 2005) and Gd^{3+} (Hao & Yu, 2007).



Experimental

Crystal data

$[Tb(C_7H_3NO_4)(C_7H_4NO_4)(H_2O)_2]\cdot 4H_2O$
M_r = 598.24
Monoclinic, $P2_1/c$
a = 13.9986 (3) Å
b = 11.3819 (2) Å
c = 12.8982 (2) Å
β = 102.0126 (10)°
V = 2010.08 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 3.60 mm^{-1}
T = 293 (2) K
0.10 × 0.10 × 0.10 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.715, T_{max} = 0.715
7168 measured reflections
3499 independent reflections
3237 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.131
S = 1.00
3499 reflections
317 parameters
189 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.20 e Å^{-3}
$\Delta\rho_{min}$ = −2.00 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O5—H1W···O11^{i}	0.81 (6)	2.08 (5)	2.743 (7)	138 (7)
O6—H3W···O1^{ii}	0.81 (8)	1.97 (4)	2.714 (7)	154 (9)
O6—H4W···O9^{iii}	0.81 (10)	2.05 (7)	2.719 (7)	140 (11)
O11—H5W···O7^{iii}	0.80 (11)	2.15 (11)	2.913 (7)	159 (11)
O11—H6W···O8^{iv}	0.81 (10)	2.10 (10)	2.893 (7)	167 (13)
O14—H9W···O11^{v}	0.810 (12)	2.15 (4)	2.926 (8)	159 (11)
O14—H10W···O8^{vi}	0.81 (9)	1.92 (9)	2.690 (7)	157 (11)
O4—H4···O13^{vii}	0.82	1.74	2.522 (12)	160

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RK2026).

References

Brayshaw, P. A., Hall, A. K., Harrison, W. T. A., Harrowfield, J. M., Pearce, D., Shand, T. M., Skelton, B. W., Whitaker, C. R. & White, A. H. (2005). *Eur. J. Inorg. Chem.* pp. 1127–1167.
Bruker (2001). *SADABS*, *SAINT-Plus* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2004). *APEX2*. Bruker AXS Inc., Madison, Wisconsin, USA.
Ghosh, S. K. & Bharadwaj, P. K. (2003). *Inorg. Chem.* **42**, 8250–8261.
Ghosh, S. K. & Bharadwaj, P. K. (2005). *Inorg. Chem.* **44**, 3156–3162.
Guerriero, P., Casellato, U., Sitran, S., Vigato, P. & Graziani, R. (1987). *Inorg. Chim. Acta*, **133**, 337–339.
Hao, L.-J. & Yu, T.-L. (2007). *Acta Cryst.* E**63**, m1967.
Liu, S.-H., Li, Y.-Z. & Meng, Q.-J. (2005). *Acta Cryst.* E**61**, m1111–m1113.

  doi:10.1107/S1600536807034629

Liu, Y., Dou, J.-M., Wang, D.-Q., Zhang, X.-X. & Zhou, L. (2006). *Acta Cryst.* E**62**, m2794–m2795.
Miao, F., Wang, J., Jin, T., Liu, J., Zhang, H. & Huang, C. (1992). *Chin. J. Inorg. Chem.* **8**, 180–186.
Okabe, N., Kyoyama, H. & Fujimoto, A. (2002). *Acta Cryst.* E**58**, m354–m356.
Rafizadeh, M., Amani, V., Iravani, E. & Neumuller, B. (2005). *Z. Anorg. Allg. Chem.* **631**, 952–934.
Ramezanipour, F., Aghabozorg, H., Shokrollahi, A., Shamsipur, M., Stoeckli-Evans, H., Soleimannejad, J. & Sheshmani, S. (2005). *J. Mol. Struct.* **779**, 77–92.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Song, Y., Yan, B. & Chen, Z. (2005). *J. Mol. Struct.* **750**, 101–107.
Zhao, B., Yi, L., Dai, Y., Chen, X., Cheng, P., Liao, D., Yan, S. & Jiang, Z. (2005). *Inorg. Chem.* **44**, 911–926.

supplementary materials

Acta Cryst. (2007). E**63**, m2182-m2183 [**doi:10.1107/S1600536807034629**]

catena-Poly[[[diaqua(6-carboxypyridine-2-carboxylato)terbium(III)]-μ-pyridine-2,6-dicarboxylato] tetrahydrate]

L.-J. Hao and T.-L. Yu

Comment

The title compound is isostructural those with its La^{3+} (Guerriero *et al.*, 1987; Ghosh & Bharadwaj, 2005), Ce^{3+} (Okabe *et al.*, 2002; Ghosh & Bharadwaj, 2003; Rafizadeh *et al.*, 2005; Ramezanipour *et al.*, 2005), Pr^{3+} (Ghosh & Bharadwaj, 2003; Zhao *et al.*, 2005), Nd^{3+} (Miao *et al.*, 1992), Sm^{3+} (Liu *et al.*, 2005, 2006; Rafizadeh *et al.*, 2005; Song *et al.*, 2005), Eu^{3+} (Brayshaw *et al.*, 2005) and Gd^{3+} (Hao & Yu, 2007) analogues.

The Tb^{3+} ion is nine-coordinated by four O and two N atoms from two independent tridentate pyridine-2,6-dicarboxyate ligands, one O atom belonging pyridine-2,6-dicarboxylate ligand and two water molecules (Fig. 1). The bridging pyridine-2,6-dicarboxylate ligand gives rise to infinite chains along the *c*-axis (Fig. 2). An extensive network of hydrogen bonds exists between water molecules.

Experimental

A mixture of $Tb(NO_3)_3$ (0.5 mmol), Sodium hydroxide(0.5 mmol), pyridine-2,6-dicarboxylic acid (0.5 mmol), H_2O (8 ml) and ethanol (8 ml) in a 25 ml teflon-lined stainless steel autoclave was kept at 433 K for three days. Colorless crystals were obtained after cooling to room temperature with a yield of 36%. Anal. Calc. for $C_{14}H_{19}N_2O_{14}Tb$: C 28.09, H 3.18, N 4.68%; Found: C 28.01, H 3.23, N 4.61%.

Refinement

The H atoms of the water molecules were located from difference density maps and were refined with distance restraints of d(H···H) = 1.38 (2) Å and d(O–H) = 0.82 (2) Å. All other H atoms were placed in calculated positions with a C–H bond distance of 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C).

Figures

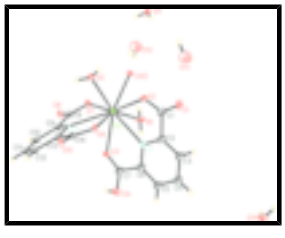


Fig. 1. The asymmetric unit of the title compound showing 30% probability displacement ellipsoids. H atoms shown as spheres of arbitrary radius. Atom O10i is generated by the symmetry code: (x, $-y$ + 3/2, z + 1/2).

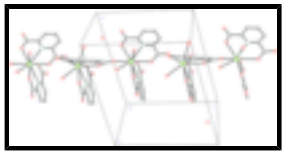


Fig. 2. Part of an infinite chain running along the *c*-axis. H atoms omitted for clarity.

catena-Poly[[[diaqua(6-carboxypyridine-2-carboxylato)terbium(III)]-μ- pyridine-2,6-dicarboxylato] tetrahydrate]

Crystal data

$[Tb(C_7H_3NO_4)(C_7H_4NO_4)(H_2O)_2]\cdot 4H_2O$	$F_{000} = 1176$
$M_r = 598.24$	$D_x = 1.977$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 3499 reflections
$a = 13.9986$ (3) Å	$\theta = 1.5$–25.0º
$b = 11.3819$ (2) Å	$\mu = 3.60$ mm^{-1}
$c = 12.8982$ (2) Å	$T = 293$ (2) K
$\beta = 102.0126$ (10)º	Cube, colourless
$V = 2010.08$ (6) Å^3	0.10 × 0.10 × 0.10 mm
$Z = 4$	

Data collection

Bruker APEXII CCD area-detector diffractometer	3499 independent reflections
Radiation source: fine-focus sealed tube	3237 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.022$
$T = 293(2)$ K	$\theta_{max} = 25.2$º
φ and ω scans	$\theta_{min} = 1.5$º
Absorption correction: multi-scan (SADABS; Bruker, 2001)	$h = -16\rightarrow16$
$T_{min} = 0.715$, $T_{max} = 0.715$	$k = -13\rightarrow13$
7168 measured reflections	$l = -7\rightarrow15$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.042$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.131$	$w = 1/[\sigma^2(F_o^2) + (0.0953P)^2 + 13.066P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{max} < 0.001$
3499 reflections	$\Delta\rho_{max} = 1.20$ e Å^{-3}
317 parameters	$\Delta\rho_{min} = -2.00$ e Å^{-3}

189 restraints
Primary atom site location: structure-invariant direct methods
Extinction correction: none

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 $F^2 > 2\sigma(F^2)$ 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}
C1	0.5673 (6)	0.5764 (8)	0.8725 (7)	0.0353 (9)
C2	0.5029 (6)	0.6849 (8)	0.8698 (7)	0.0358 (8)
C3	0.4056 (6)	0.6786 (8)	0.8673 (7)	0.0363 (8)
H3	0.3749	0.6062	0.8679	0.044*
C4	0.3521 (7)	0.7840 (7)	0.8636 (8)	0.0369 (8)
H4A	0.2852	0.7815	0.8610	0.044*
C5	0.3989 (6)	0.8910 (8)	0.8638 (7)	0.0364 (8)
H5	0.3648	0.9614	0.8617	0.044*
C6	0.4975 (6)	0.8894 (8)	0.8671 (7)	0.0360 (8)
C7	0.5573 (6)	0.9998 (8)	0.8682 (7)	0.0358 (9)
C8	0.8806 (5)	1.0253 (6)	0.8263 (5)	0.0179 (7)
C9	0.8732 (5)	1.0388 (6)	0.9408 (5)	0.0176 (6)
C10	0.9082 (5)	1.1397 (6)	1.0001 (5)	0.0180 (6)
H10	0.9344	1.2028	0.9696	0.022*
C11	0.9018 (5)	1.1406 (6)	1.1065 (5)	0.0182 (6)
H11	0.9247	1.2050	1.1488	0.022*
C12	0.8619 (5)	1.0469 (6)	1.1489 (5)	0.0178 (6)
H12	0.8585	1.0464	1.2201	0.021*
C13	0.8264 (5)	0.9519 (6)	1.0829 (5)	0.0175 (6)
C14	0.7743 (5)	0.8473 (6)	1.1189 (5)	0.0173 (7)
H1W	0.909 (4)	0.718 (4)	0.987 (5)	0.080*
H2W	0.863 (3)	0.612 (4)	0.952 (8)	0.080*
H3W	0.595 (6)	0.899 (7)	0.672 (3)	0.080*
H4W	0.665 (8)	0.841 (10)	0.629 (6)	0.080*
H5W	0.924 (8)	0.676 (10)	0.190 (8)	0.080*
H6W	0.988 (9)	0.753 (7)	0.158 (9)	0.080*
H7W	0.788 (10)	0.465 (5)	0.888 (8)	0.080*
H8W	0.791 (12)	0.397 (10)	0.977 (5)	0.080*
H9W	0.023 (10)	0.4869 (17)	0.898 (8)	0.080*
H10W	0.038 (10)	0.589 (8)	0.847 (5)	0.080*

H11W	0.608 (9)	0.300 (12)	0.826 (4)	0.080*
H12W	0.674 (6)	0.238 (11)	0.899 (9)	0.080*
N1	0.5474 (5)	0.7881 (5)	0.8674 (5)	0.0201 (13)
N2	0.8315 (4)	0.9488 (4)	0.9813 (4)	0.0111 (10)
O1	0.5308 (4)	0.4780 (5)	0.8764 (5)	0.0400 (15)
O2	0.6558 (4)	0.5971 (4)	0.8704 (4)	0.0227 (10)
O3	0.6432 (4)	0.9921 (4)	0.8649 (4)	0.0257 (11)
O4	0.5122 (5)	1.0991 (5)	0.8733 (6)	0.0464 (16)
H4	0.5471	1.1535	0.8619	0.070*
O5	0.8754 (4)	0.6841 (5)	0.9368 (4)	0.0255 (11)
O6	0.6333 (4)	0.8452 (6)	0.6743 (4)	0.0372 (15)
O7	0.8449 (4)	0.9295 (4)	0.7819 (3)	0.0224 (10)
O8	0.9207 (4)	1.1044 (5)	0.7853 (4)	0.0303 (12)
O9	0.7268 (4)	0.7815 (4)	1.0468 (4)	0.0175 (10)
O10	0.7813 (4)	0.8336 (4)	1.2163 (3)	0.0200 (10)
O11	0.9581 (4)	0.6919 (5)	0.1491 (4)	0.0251 (12)
O12	0.7991 (8)	0.4014 (7)	0.9163 (9)	0.086 (3)
O13	0.6236 (7)	0.2750 (8)	0.8855 (10)	0.082 (3)
O14	0.0299 (5)	0.5576 (5)	0.9011 (4)	0.0338 (13)
Tb1	0.73015 (2)	0.79481 (3)	0.85156 (2)	0.01780 (18)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0230 (18)	0.039 (2)	0.044 (2)	0.0056 (14)	0.0088 (15)	0.0012 (15)
C2	0.0236 (17)	0.0396 (19)	0.0450 (19)	0.0060 (13)	0.0087 (14)	0.0012 (14)
C3	0.0239 (17)	0.0399 (19)	0.0458 (19)	0.0059 (13)	0.0087 (14)	0.0013 (14)
C4	0.0242 (17)	0.0403 (19)	0.0469 (19)	0.0061 (13)	0.0086 (14)	0.0012 (14)
C5	0.0241 (17)	0.0399 (19)	0.0456 (19)	0.0064 (13)	0.0086 (14)	0.0011 (14)
C6	0.0239 (17)	0.0396 (19)	0.0451 (19)	0.0063 (13)	0.0087 (14)	0.0010 (14)
C7	0.0241 (18)	0.039 (2)	0.045 (2)	0.0065 (14)	0.0085 (15)	0.0007 (15)
C8	0.0207 (15)	0.0176 (14)	0.0149 (14)	−0.0021 (12)	0.0024 (12)	−0.0008 (12)
C9	0.0205 (13)	0.0172 (13)	0.0146 (13)	−0.0022 (11)	0.0024 (10)	−0.0009 (10)
C10	0.0209 (13)	0.0175 (13)	0.0149 (13)	−0.0024 (11)	0.0023 (10)	−0.0009 (10)
C11	0.0212 (14)	0.0176 (13)	0.0150 (13)	−0.0024 (11)	0.0019 (10)	−0.0011 (11)
C12	0.0208 (13)	0.0174 (13)	0.0146 (13)	−0.0024 (11)	0.0022 (10)	−0.0009 (10)
C13	0.0204 (13)	0.0172 (13)	0.0145 (13)	−0.0022 (11)	0.0024 (10)	−0.0008 (10)
C14	0.0201 (15)	0.0170 (14)	0.0142 (14)	−0.0023 (12)	0.0026 (12)	−0.0006 (12)
N1	0.018 (3)	0.026 (3)	0.015 (3)	−0.002 (2)	0.001 (2)	−0.001 (2)
N2	0.011 (2)	0.013 (3)	0.010 (2)	−0.0026 (19)	0.0016 (18)	−0.0017 (19)
O1	0.030 (3)	0.021 (3)	0.065 (4)	−0.013 (2)	0.003 (3)	0.002 (3)
O2	0.020 (2)	0.017 (2)	0.031 (3)	−0.0016 (19)	0.004 (2)	−0.002 (2)
O3	0.027 (3)	0.017 (2)	0.032 (3)	0.007 (2)	0.002 (2)	−0.003 (2)
O4	0.048 (4)	0.029 (3)	0.060 (4)	0.015 (3)	0.008 (3)	−0.004 (3)
O5	0.026 (3)	0.035 (3)	0.013 (2)	0.007 (2)	−0.002 (2)	−0.005 (2)
O6	0.041 (3)	0.056 (4)	0.012 (2)	0.033 (3)	0.000 (2)	0.001 (2)
O7	0.035 (3)	0.022 (2)	0.012 (2)	−0.011 (2)	0.010 (2)	−0.0040 (18)
O8	0.047 (3)	0.025 (3)	0.023 (3)	−0.016 (2)	0.017 (2)	0.000 (2)

O9	0.021 (2)	0.021 (2)	0.009 (2)	−0.0107 (18)	0.0010 (18)	−0.0008 (17)
O10	0.027 (3)	0.021 (2)	0.010 (2)	−0.008 (2)	0.0006 (19)	0.0020 (19)
O11	0.026 (3)	0.030 (3)	0.018 (3)	−0.003 (2)	0.003 (2)	0.000 (2)
O12	0.069 (6)	0.039 (4)	0.135 (9)	0.014 (4)	−0.014 (7)	0.000 (5)
O13	0.068 (6)	0.044 (5)	0.128 (10)	0.003 (4)	0.008 (6)	0.003 (5)
O14	0.048 (4)	0.029 (3)	0.030 (3)	0.010 (3)	0.022 (3)	0.001 (2)
Tb1	0.0184 (3)	0.0198 (3)	0.0146 (2)	−0.00110 (11)	0.00191 (15)	−0.00124 (11)

Geometric parameters (Å, °)

C1—O1	1.237 (10)	C13—C14	1.518 (9)
C1—O2	1.267 (10)	C14—O10	1.249 (8)
C1—C2	1.525 (11)	C14—O9	1.269 (8)
C2—N1	1.332 (11)	N1—Tb1	2.610 (6)
C2—C3	1.358 (12)	N2—Tb1	2.626 (5)
C3—C4	1.410 (12)	O2—Tb1	2.512 (5)
C3—H3	0.9300	O3—Tb1	2.578 (5)
C4—C5	1.382 (13)	O4—H4	0.8200
C4—H4A	0.9300	O5—Tb1	2.449 (5)
C5—C6	1.373 (11)	O5—H1W	0.81 (6)
C5—H5	0.9300	O5—H2W	0.87 (5)
C6—N1	1.347 (10)	O6—Tb1	2.470 (5)
C6—C7	1.509 (12)	O6—H3W	0.81 (8)
C7—O3	1.214 (10)	O6—H4W	0.81 (10)
C7—O4	1.303 (10)	O7—Tb1	2.517 (5)
C8—O8	1.237 (8)	O9—Tb1	2.533 (5)
C8—O7	1.284 (8)	O10—Tb1^{i}	2.493 (4)
C8—C9	1.510 (9)	O11—H5W	0.80 (11)
C9—N2	1.337 (8)	O11—H6W	0.81 (10)
C9—C10	1.410 (9)	O12—H7W	0.81 (7)
C10—C11	1.393 (9)	O12—H8W	0.82 (7)
C10—H10	0.9300	O13—H11W	0.81 (8)
C11—C12	1.369 (9)	O13—H12W	0.81 (10)
C11—H11	0.9300	O14—H9W	0.810 (12)
C12—C13	1.403 (9)	O14—H10W	0.81 (9)
C12—H12	0.9300	Tb1—O10^{ii}	2.493 (4)
C13—N2	1.328 (8)	Tb1—H2W	2.91 (4)
O1—C1—O2	125.7 (8)	Tb1—O6—H4W	112 (8)
O1—C1—C2	119.1 (7)	H3W—O6—H4W	119 (9)
O2—C1—C2	115.2 (7)	C8—O7—Tb1	125.2 (4)
N1—C2—C3	121.1 (8)	C14—O9—Tb1	125.3 (4)
N1—C2—C1	116.0 (7)	C14—O10—Tb1^{i}	143.4 (4)
C3—C2—C1	122.9 (8)	H5W—O11—H6W	118 (11)
C2—C3—C4	118.7 (9)	H7W—O12—H8W	116 (11)
C2—C3—H3	120.6	H11W—O13—H12W	116 (12)
C4—C3—H3	120.7	H9W—O14—H10W	116 (10)
C5—C4—C3	120.1 (9)	O5—Tb1—O6	141.19 (17)
C5—C4—H4A	120.0	O5—Tb1—O10^{ii}	71.34 (16)

C3—C4—H4A	120.0	O6—Tb1—O10^{ii}	70.77 (16)
C6—C5—C4	117.5 (8)	O5—Tb1—O2	79.49 (18)
C6—C5—H5	121.3	O6—Tb1—O2	98.0 (2)
C4—C5—H5	121.2	O10^{ii}—Tb1—O2	74.20 (16)
N1—C6—C5	121.9 (8)	O5—Tb1—O7	86.65 (18)
N1—C6—C7	115.3 (7)	O6—Tb1—O7	78.3 (2)
C5—C6—C7	122.8 (8)	O10^{ii}—Tb1—O7	79.02 (16)
O3—C7—O4	123.9 (8)	O2—Tb1—O7	152.60 (16)
O3—C7—C6	119.4 (7)	O5—Tb1—O9	73.05 (17)
O4—C7—C6	116.7 (7)	O6—Tb1—O9	144.46 (17)
O8—C8—O7	126.7 (6)	O10^{ii}—Tb1—O9	136.75 (15)
O8—C8—C9	118.3 (6)	O2—Tb1—O9	75.91 (15)
O7—C8—C9	115.0 (6)	O7—Tb1—O9	122.43 (14)
N2—C9—C10	122.9 (6)	O5—Tb1—O3	141.05 (17)
N2—C9—C8	115.4 (5)	O6—Tb1—O3	71.56 (17)
C10—C9—C8	121.8 (6)	O10^{ii}—Tb1—O3	140.01 (16)
C11—C10—C9	117.0 (6)	O2—Tb1—O3	124.28 (17)
C11—C10—H10	121.5	O7—Tb1—O3	80.72 (16)
C9—C10—H10	121.5	O9—Tb1—O3	83.04 (16)
C12—C11—C10	120.2 (6)	O5—Tb1—N1	133.26 (18)
C12—C11—H11	119.9	O6—Tb1—N1	73.8 (2)
C10—C11—H11	119.9	O10^{ii}—Tb1—N1	117.83 (17)
C11—C12—C13	118.8 (6)	O2—Tb1—N1	62.20 (16)
C11—C12—H12	120.6	O7—Tb1—N1	139.00 (17)
C13—C12—H12	120.6	O9—Tb1—N1	72.47 (17)
N2—C13—C12	122.3 (6)	O3—Tb1—N1	62.35 (17)
N2—C13—C14	114.2 (5)	O5—Tb1—N2	76.67 (17)
C12—C13—C14	123.4 (6)	O6—Tb1—N2	123.7 (2)
O10—C14—O9	125.7 (6)	O10^{ii}—Tb1—N2	129.89 (16)
O10—C14—C13	117.6 (6)	O2—Tb1—N2	135.72 (16)
O9—C14—C13	116.7 (6)	O7—Tb1—N2	61.35 (15)
C2—N1—C6	120.7 (7)	O9—Tb1—N2	61.70 (14)
C2—N1—Tb1	119.8 (5)	O3—Tb1—N2	64.91 (16)
C6—N1—Tb1	119.3 (5)	N1—Tb1—N2	112.22 (16)
C13—N2—C9	118.9 (5)	O5—Tb1—H2W	15.9 (5)
C13—N2—Tb1	120.9 (4)	O6—Tb1—H2W	139 (2)
C9—N2—Tb1	119.0 (4)	O10^{ii}—Tb1—H2W	69 (2)
C1—O2—Tb1	126.5 (5)	O2—Tb1—H2W	63.6 (5)
C7—O3—Tb1	123.3 (5)	O7—Tb1—H2W	101.4 (7)
C7—O4—H4	109.5	O9—Tb1—H2W	70 (2)
Tb1—O5—H1W	114 (3)	O3—Tb1—H2W	149 (2)
Tb1—O5—H2W	114 (3)	N1—Tb1—H2W	119.4 (9)
H1W—O5—H2W	112 (7)	N2—Tb1—H2W	89.0 (16)
Tb1—O6—H3W	116 (3)		

Symmetry codes: (i) *x*, −*y*+3/2, *z*+1/2; (ii) *x*, −*y*+3/2, *z*−1/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H1W···O11^{iii}	0.81 (6)	2.08 (5)	2.743 (7)	138 (7)
O6—H3W···O1^{iv}	0.81 (8)	1.97 (4)	2.714 (7)	154 (9)
O6—H4W···O9^{ii}	0.81 (10)	2.05 (7)	2.719 (7)	140 (11)
O11—H5W···O7^{ii}	0.80 (11)	2.15 (11)	2.913 (7)	159 (11)
O11—H6W···O8^{v}	0.81 (10)	2.10 (10)	2.893 (7)	167 (13)
O14—H9W···O11^{vi}	0.810 (12)	2.15 (4)	2.926 (8)	159 (11)
O14—H10W···O8^{vii}	0.81 (9)	1.92 (9)	2.690 (7)	157 (11)
O4—H4···O13^{viii}	0.82	1.74	2.522 (12)	160

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

Fig. 1

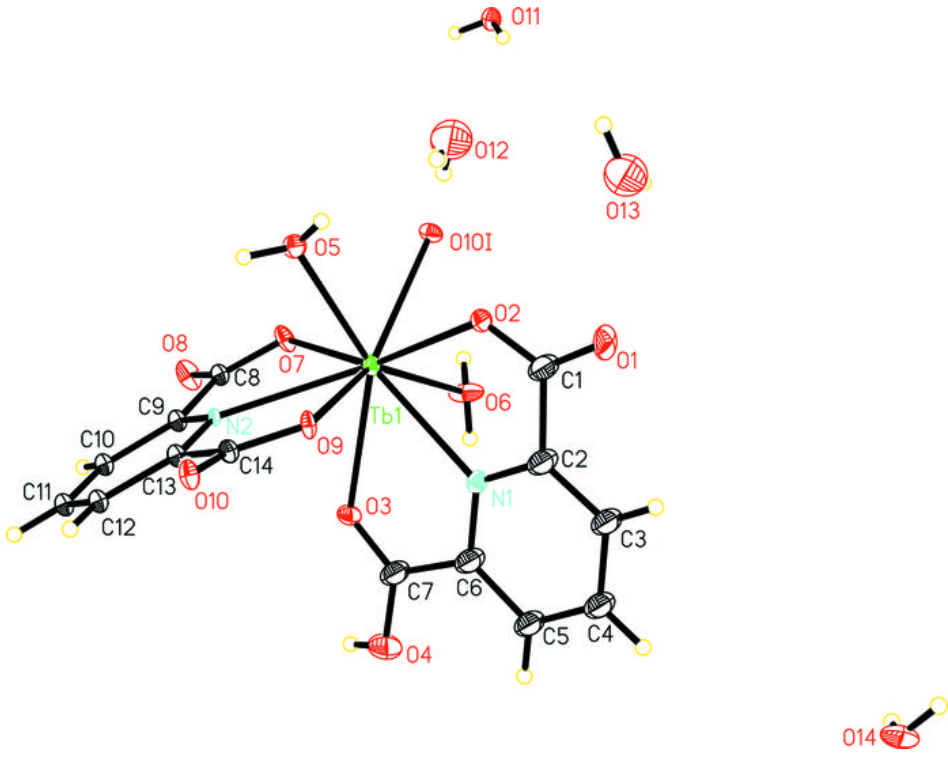

O11
O12
O13
O5
O10I
O2
O8
O7
C8
C1
O1
C9
N2
Tb1
O6
C10
O9
C2
C14
C13
O10
N1
C11
O3
C3
C12
C7
C6
C5
C4
O4
O14

Fig. 2