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Hexakis(μ-naphthalene-1-acetato)-bis[(1,10-phenanthroline)terbium(III)] *N*,*N*-dimethylformamide disolvate

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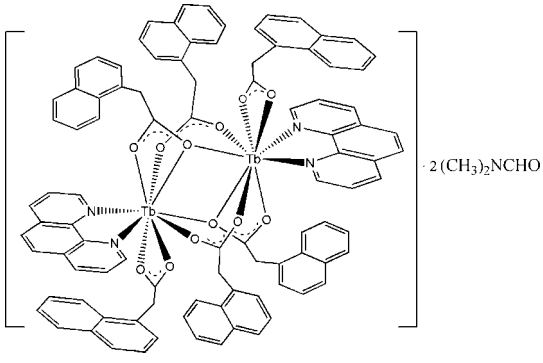
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.022 Å; R factor = 0.077; wR factor = 0.197; data-to-parameter ratio = 13.2.

The title complex, $[Tb_2(C_{12}H_9O_2)_6(C_{12}H_8N_2)_2]\cdot 2C_3H_7NO$, is centrosymmetric. The Tb atom is nine-coordinate. Molecules are linked into a chain by C—H···O hydrogen bonds parallel to the *a*-axis direction and into a sheet by C—H···π hydrogen bonds parallel to the (100) plane. A combination of the *a* chains and (100) sheets generates a three-dimensional framework structure.

Related literature

For related literature, see: Liu *et al.* (2007); Xia *et al.* (2007).



Experimental

Crystal data

$[Tb_2(C_{12}H_9O_2)_6(C_{12}H_8N_2)_2]\cdot 2C_3H_7NO$
M_r = 1935.59
Monoclinic, $P2_1/c$
a = 13.4619 (16) Å
b = 15.086 (2) Å
c = 22.166 (2) Å
β = 103.584 (2)°
V = 4375.6 (9) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.67 mm^{-1}
T = 298 (2) K
0.28 × 0.17 × 0.12 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.652, T_{max} = 0.825
21422 measured reflections
7389 independent reflections
4674 reflections with $I > 2\sigma(I)$
R_{int} = 0.193

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.077
$wR(F^2)$ = 0.197
S = 1.07
7389 reflections
559 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 2.20 e Å^{-3}
$\Delta\rho_{min}$ = −2.72 e Å^{-3}

Table 1
Selected bond lengths (Å).

Tb1—O1^{i}	2.343 (5)	Tb1—O2	2.478 (7)
Tb1—O3	2.349 (6)	Tb1—O1	2.539 (7)
Tb1—O4^{i}	2.369 (7)	Tb1—N2	2.547 (9)
Tb1—O6	2.433 (8)	Tb1—N1	2.587 (7)
Tb1—O5	2.468 (8)		

Symmetry code: (i) $-x+1, -y+1, -z+2$.

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

*Cg*1 is the centroid of the C3–C8 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6···O7^{ii}	0.93	2.56	3.44 (2)	157
C37—H37···O4^{i}	0.93	2.35	3.015 (11)	128
C46—H46···O3	0.93	2.48	3.056 (13)	120
C47—H47···O2^{iii}	0.93	2.45	3.314 (13)	154
C50—H50*A*···O6^{iv}	0.96	2.62	3.40 (2)	138
C18—H18···*Cg*1^{v}	0.93	2.90	3.673 (16)	141

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1996); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2407).

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supplementary materials

Acta Cryst. (2007). E**63**, m2624 [**doi:10.1107/S1600536807047095**]

Hexakis(*μ*-naphthalene-1-acetato)bis[(1,10-phenanthroline)terbium(III)] *N*,*N*-dimethylformamide disolvate

H.-T. Xia, Y.-F. Liu, D.-Q. Wang and S.-P. Yang

Comment

As a part of our investigation of the rare earth complexes with 1-naphthylacetic acid (NAA) and 1,10-phenanthroline (phen), we have recently reported the crystal structures of two complexes $[Eu(NAA)_3(phen)]_2{\cdot}2DMF$ (II) (Liu *et al.*, 2007) and $[Pr(NAA)_3(phen)]_2{\cdot}DMF$ (Xia *et al.*, 2007) We report here the crystal structure of terbium complexes with NAA and phen, (I).

In the title complex, the coordination environment of Tb atom and coordination modes of the NNA ligands coordinated to the Tb^{III} ion are in agreement with the complex (II) (Fig. 1). The average bond lengths of between the terbium center and carboxylic oxygen atoms are 2.441 (7) Å, shorter than that (2.4725 (5) Å) of complex (II). The dihedral angles of the least-square-plane Tb_2O_2 and naphthyl rings are 58.20 (19)° (C3—C12 ring), 43.74 (31)° (C15—C24 ring) and 71.38 (26)° (C27—C36 ring), and the dihedral angle between Tb_2O_2 plane and phen ring is 82.08 (21)°.

The molecules of (I) are linked into sheets by means of C—H···π hydrogen bond (Fig. 2 and Table 2) and chains parallel to the *a* axis direction (Fig. 3) by C—H···O hydrogen bonds (Fig. 3 and Table 2). The action of *a* chains are to link adjacent [100] sheet into the three-dimensional framework structure.

Experimental

To a stirred solution of 1-naphthylacetic acid (0.5586 g, 3 mmol) and 1,10-phenanthroline monohydrate (0.198 g, 1 mmol) in 30 ml me thanol, and a solution of $Tb(NO_3)_3{\cdot}6H_2O$ (0.453 g, 1 mmol) in water (10 ml) was added. The mixed solution was heated to 333 K and stirred for 3 h, and then cooled to room temperature. The precipitate was washed with water and then dissolved in DMF. A colourless crystal suitable for X-ray diffraction was obtained by evaporation of DMF solution.

Refinement

All H atoms were located in difference Fourier maps. H atoms bonded to C atoms were treated as riding atoms, with C—H distances of 0.93 Å (aryl, formyl), 0.97Å (methylene) and 0.96 Å (methyl), and with $U_{iso}(H) = 1.2U_{eq}(C)$ (aryl, formyl, methylene) or $1.5U_{eq}(C)$ (methyl).

Figures

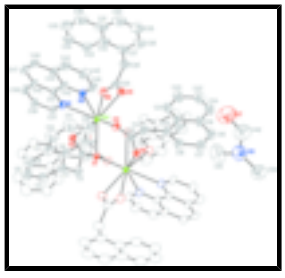


Fig. 1. The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are at the 30% probability level. Unlabelled atoms in the molecular are related to labelled atoms by (1 − *x*, 1 − *y*, 2 − *z*).

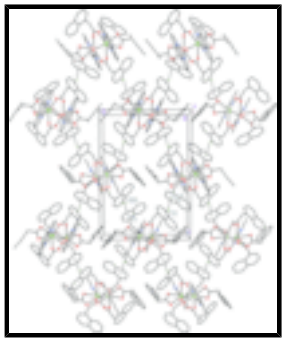


Fig. 2. A larger portion of the crystal structure of (I), showing the formation of a hydrogen-bonded sheets built from C—H···π. For clarity, H atoms not involved in the hydrogen bonding have been omitted. Dashed lines indicate hydrogen bonds. [Symmetry codes: (A) 1 − *x*, −1/2 + *y*, 3/2 − *z*, (B) 1 − *x*, 1/2 + *y*, 3/2 − *z*].

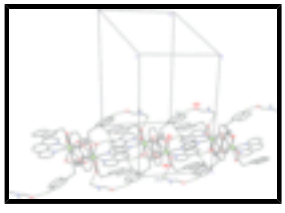


Fig. 3. A larger portion of the crystal structure of (I), showing the formation of a hydrogen-bonded chain built from C—H···O. For clarity, H atoms not involved in the hydrogen bonding have been omitted. Dashed lines indicate hydrogen bonds. [Symmetry codes: (C) *x*, *y*, 1 + *z*,, (D) − *x*, 1 − *y*, 1 − *z*, (E) − *x*, 1 − *y*, 2 − *z*].

Hexakis(μ-naphthalene-1-acetato)bis[(1,10-phenanthroline)terbium(III)] *N*,*N*-dimethylformamide disolvate

Crystal data

$[Tb_2(C_{12}H_9O_2)_6(C_{12}H_8N_2)_2]\cdot 2C_3H_7NO$	F_{000} = 1960
M_r = 1935.59	D_x = 1.469 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 6504 reflections
a = 13.4619 (16) Å	θ = 2.4–25.3°
b = 15.086 (2) Å	μ = 1.67 mm^{-1}
c = 22.166 (2) Å	*T* = 298 (2) K
β = 103.584 (2)°	Block, colourless
V = 4375.6 (9) Å^3	0.28 × 0.17 × 0.12 mm
Z = 2	

Data collection

Bruker SMART 1000 CCD area-detector diffractometer	7389 independent reflections
Radiation source: fine-focus sealed tube	4674 reflections with $I > 2\sigma(I)$

Monochromator: graphite	R_{int} = 0.193
T = 298(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 1.6º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −14→16
T_{min} = 0.652, T_{max} = 0.825	k = −17→17
21422 measured reflections	l = −21→26

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.077	H-atom parameters constrained
$wR(F^2)$ = 0.197	$w = 1/[\sigma^2(F_o^2) + (0.0648P)^2 + 17.4888P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.07	$(\Delta/\sigma)_{max}$ = 0.010
7389 reflections	$\Delta\rho_{max}$ = 2.20 e Å^{-3}
559 parameters	$\Delta\rho_{min}$ = −2.72 e Å^{-3}
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 $F^2 > \sigma(F^2)$ 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}
Tb1	0.38253 (3)	0.43006 (3)	1.01126 (2)	0.03377 (19)
N1	0.2316 (6)	0.4439 (6)	1.0645 (4)	0.043 (2)
N2	0.2134 (6)	0.3634 (6)	0.9529 (4)	0.045 (2)
N3	0.3685 (12)	0.3365 (11)	0.2523 (6)	0.089 (4)
O1	0.4406 (4)	0.5791 (5)	0.9788 (3)	0.0361 (15)
O2	0.2766 (5)	0.5556 (5)	0.9603 (3)	0.0419 (17)
O3	0.4044 (5)	0.4251 (5)	0.9092 (3)	0.0405 (16)
O4	0.5497 (5)	0.4868 (5)	0.8977 (3)	0.0426 (18)
O5	0.4125 (6)	0.2737 (5)	0.9880 (4)	0.052 (2)
O6	0.4021 (6)	0.3048 (5)	1.0822 (4)	0.055 (2)
O7	0.2327 (12)	0.2428 (11)	0.2366 (8)	0.141 (5)

C1	0.3510 (7)	0.5982 (7)	0.9521 (5)	0.041 (3)
C2	0.3350 (8)	0.6742 (9)	0.9067 (6)	0.058 (3)
H2A	0.3780	0.6646	0.8778	0.070*
H2B	0.3583	0.7282	0.9295	0.070*
C3	0.2269 (9)	0.6888 (9)	0.8697 (6)	0.056 (3)
C4	0.1766 (10)	0.7654 (9)	0.8805 (6)	0.067 (4)
H4	0.2098	0.8065	0.9096	0.080*
C5	0.0754 (11)	0.7809 (11)	0.8473 (7)	0.076 (4)
H5	0.0416	0.8312	0.8563	0.091*
C6	0.0274 (10)	0.7262 (11)	0.8041 (7)	0.073 (4)
H6	−0.0388	0.7391	0.7822	0.088*
C7	0.0743 (10)	0.6496 (11)	0.7907 (7)	0.069 (4)
C8	0.1752 (9)	0.6298 (9)	0.8235 (6)	0.059 (3)
C9	0.2205 (12)	0.5507 (11)	0.8086 (7)	0.076 (4)
H9	0.2872	0.5378	0.8297	0.092*
C10	0.1713 (13)	0.4931 (13)	0.7650 (8)	0.095 (5)
H10	0.2021	0.4410	0.7563	0.114*
C11	0.0680 (13)	0.5166 (14)	0.7324 (8)	0.097 (5)
H11	0.0321	0.4781	0.7023	0.116*
C12	0.0236 (13)	0.5897 (13)	0.7436 (8)	0.086 (5)
H12	−0.0419	0.6029	0.7207	0.103*
C13	0.4733 (7)	0.4365 (7)	0.8814 (5)	0.041 (2)
C14	0.4627 (9)	0.3853 (9)	0.8215 (6)	0.055 (3)
H14A	0.4148	0.3372	0.8213	0.066*
H14B	0.4328	0.4244	0.7873	0.066*
C15	0.5584 (10)	0.3469 (9)	0.8091 (6)	0.061 (3)
C16	0.5901 (10)	0.3733 (10)	0.7564 (6)	0.069 (4)
H16	0.5521	0.4155	0.7303	0.082*
C17	0.6774 (11)	0.3380 (11)	0.7418 (7)	0.077 (4)
H17	0.6988	0.3583	0.7073	0.092*
C18	0.7313 (11)	0.2728 (11)	0.7791 (7)	0.075 (4)
H18	0.7897	0.2494	0.7696	0.090*
C19	0.7003 (10)	0.2412 (10)	0.8305 (7)	0.070 (4)
C20	0.6141 (9)	0.2793 (9)	0.8467 (6)	0.061 (3)
C21	0.5847 (11)	0.2480 (10)	0.8994 (7)	0.067 (4)
H21	0.5300	0.2742	0.9117	0.081*
C22	0.6357 (12)	0.1798 (11)	0.9324 (8)	0.083 (4)
H22	0.6131	0.1582	0.9662	0.100*
C23	0.7221 (13)	0.1400 (12)	0.9176 (9)	0.091 (5)
H23	0.7569	0.0941	0.9415	0.110*
C24	0.7519 (12)	0.1707 (11)	0.8680 (8)	0.081 (5)
H24	0.8085	0.1451	0.8576	0.098*
C25	0.4093 (9)	0.2508 (8)	1.0418 (7)	0.054 (3)
C26	0.4137 (11)	0.1524 (9)	1.0563 (7)	0.073 (4)
H26A	0.4806	0.1296	1.0550	0.088*
H26B	0.4041	0.1433	1.0978	0.088*
C27	0.3350 (13)	0.1034 (11)	1.0117 (8)	0.079 (4)
C28	0.3615 (15)	0.0497 (11)	0.9671 (9)	0.089 (5)
H28	0.4296	0.0429	0.9659	0.107*

C29	0.2822 (17)	0.0045 (12)	0.9227 (9)	0.101 (6)
H29	0.3005	−0.0333	0.8939	0.121*
C30	0.1862 (18)	0.0149 (13)	0.9216 (10)	0.106 (6)
H30	0.1374	−0.0131	0.8908	0.127*
C31	0.1539 (15)	0.0682 (12)	0.9665 (10)	0.096 (5)
C32	0.2307 (13)	0.1116 (11)	1.0113 (8)	0.080 (4)
C33	0.1998 (12)	0.1637 (10)	1.0553 (9)	0.084 (5)
H33	0.2489	0.1919	1.0857	0.100*
C34	0.0975 (12)	0.1744 (11)	1.0547 (9)	0.088 (5)
H34	0.0774	0.2093	1.0843	0.106*
C35	0.0270 (15)	0.1323 (13)	1.0095 (11)	0.100 (6)
H35	−0.0414	0.1387	1.0103	0.120*
C36	0.0473 (16)	0.0840 (13)	0.9654 (11)	0.104 (6)
H36	−0.0046	0.0604	0.9342	0.125*
C37	0.2364 (8)	0.4819 (9)	1.1177 (6)	0.056 (3)
H37	0.2998	0.5037	1.1386	0.067*
C38	0.1546 (10)	0.4932 (9)	1.1467 (7)	0.066 (4)
H38	0.1633	0.5215	1.1848	0.080*
C39	0.0600 (9)	0.4596 (9)	1.1153 (7)	0.065 (4)
H39	0.0040	0.4647	1.1330	0.078*
C40	0.0490 (8)	0.4191 (8)	1.0584 (6)	0.055 (3)
C41	0.1391 (8)	0.4124 (8)	1.0345 (6)	0.050 (3)
C42	0.1272 (8)	0.3709 (9)	0.9741 (6)	0.056 (3)
C43	0.0315 (8)	0.3372 (9)	0.9417 (7)	0.064 (4)
C44	0.0268 (10)	0.2992 (10)	0.8847 (8)	0.077 (4)
H44	−0.0352	0.2787	0.8608	0.092*
C45	0.1130 (10)	0.2920 (11)	0.8639 (7)	0.080 (4)
H45	0.1106	0.2662	0.8255	0.095*
C46	0.2051 (9)	0.3232 (9)	0.8997 (7)	0.063 (4)
H46	0.2638	0.3151	0.8851	0.075*
C47	−0.0462 (9)	0.3862 (10)	1.0248 (8)	0.065 (4)
H47	−0.1035	0.3925	1.0410	0.078*
C48	−0.0549 (9)	0.3465 (10)	0.9703 (7)	0.068 (4)
H48	−0.1181	0.3238	0.9498	0.082*
C49	0.3092 (17)	0.2712 (17)	0.2221 (10)	0.108 (6)
H49	0.3275	0.2459	0.1880	0.129*
C50	0.4600 (14)	0.3654 (13)	0.2341 (8)	0.100 (6)
H50A	0.4724	0.3271	0.2020	0.151*
H50B	0.5172	0.3631	0.2693	0.151*
H50C	0.4508	0.4251	0.2187	0.151*
C51	0.3405 (18)	0.3704 (16)	0.3046 (10)	0.136 (8)
H51A	0.2707	0.3550	0.3030	0.205*
H51B	0.3475	0.4337	0.3054	0.205*
H51C	0.3839	0.3457	0.3414	0.205*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}

Tb1	0.0240 (2)	0.0402 (3)	0.0367 (3)	−0.0027 (2)	0.00618 (17)	−0.0022 (3)
N1	0.033 (4)	0.050 (5)	0.047 (5)	0.004 (4)	0.014 (4)	0.004 (5)
N2	0.028 (4)	0.060 (6)	0.047 (5)	−0.009 (4)	0.006 (4)	−0.011 (5)
N3	0.108 (11)	0.096 (10)	0.063 (8)	0.027 (9)	0.021 (8)	0.033 (9)
O1	0.019 (3)	0.047 (4)	0.038 (4)	0.001 (3)	−0.001 (3)	−0.005 (4)
O2	0.030 (3)	0.050 (4)	0.045 (4)	0.005 (3)	0.006 (3)	0.011 (4)
O3	0.028 (3)	0.049 (4)	0.041 (4)	−0.005 (3)	0.002 (3)	−0.001 (4)
O4	0.044 (4)	0.051 (4)	0.036 (4)	−0.003 (4)	0.016 (3)	−0.012 (4)
O5	0.063 (5)	0.045 (4)	0.050 (5)	−0.014 (4)	0.020 (4)	−0.009 (4)
O6	0.051 (4)	0.054 (5)	0.061 (5)	−0.005 (4)	0.017 (4)	0.000 (5)
O7	0.110 (11)	0.150 (13)	0.155 (13)	0.000 (10)	0.014 (9)	0.046 (13)
C1	0.029 (5)	0.044 (6)	0.051 (6)	−0.003 (4)	0.013 (5)	−0.007 (6)
C2	0.042 (6)	0.066 (8)	0.062 (8)	−0.001 (6)	0.004 (5)	0.020 (8)
C3	0.044 (6)	0.065 (8)	0.058 (8)	0.005 (6)	0.009 (6)	0.018 (7)
C4	0.058 (8)	0.067 (9)	0.069 (9)	0.008 (7)	0.003 (6)	0.020 (8)
C5	0.065 (8)	0.081 (10)	0.077 (10)	0.018 (8)	0.007 (7)	0.020 (10)
C6	0.053 (7)	0.086 (11)	0.073 (10)	0.010 (8)	0.000 (7)	0.025 (10)
C7	0.058 (8)	0.078 (10)	0.062 (9)	−0.008 (8)	−0.001 (6)	0.022 (9)
C8	0.048 (7)	0.072 (9)	0.056 (8)	−0.001 (6)	0.009 (6)	0.021 (8)
C9	0.071 (9)	0.076 (10)	0.069 (10)	0.005 (8)	−0.009 (7)	0.010 (10)
C10	0.092 (12)	0.090 (12)	0.087 (12)	0.004 (10)	−0.013 (9)	0.007 (12)
C11	0.092 (12)	0.097 (14)	0.081 (12)	−0.004 (11)	−0.022 (9)	0.010 (12)
C12	0.073 (10)	0.091 (12)	0.078 (11)	−0.002 (9)	−0.016 (8)	0.015 (11)
C13	0.033 (5)	0.047 (6)	0.042 (6)	−0.011 (5)	0.009 (4)	−0.012 (6)
C14	0.054 (7)	0.064 (8)	0.051 (7)	0.001 (6)	0.019 (6)	−0.016 (7)
C15	0.062 (7)	0.068 (8)	0.058 (8)	−0.010 (7)	0.024 (6)	−0.028 (8)
C16	0.074 (9)	0.075 (9)	0.062 (8)	−0.005 (7)	0.027 (7)	−0.024 (8)
C17	0.080 (10)	0.090 (11)	0.069 (9)	−0.009 (9)	0.036 (8)	−0.026 (10)
C18	0.069 (9)	0.085 (11)	0.078 (10)	−0.006 (8)	0.028 (8)	−0.034 (10)
C19	0.065 (8)	0.073 (9)	0.076 (10)	−0.005 (7)	0.022 (7)	−0.035 (9)
C20	0.057 (7)	0.064 (8)	0.064 (8)	−0.006 (7)	0.020 (6)	−0.029 (8)
C21	0.067 (8)	0.066 (9)	0.069 (9)	−0.006 (7)	0.017 (7)	−0.021 (9)
C22	0.080 (10)	0.079 (11)	0.086 (11)	0.005 (9)	0.008 (9)	−0.014 (11)
C23	0.082 (11)	0.085 (11)	0.096 (13)	0.005 (9)	−0.003 (9)	−0.017 (12)
C24	0.069 (9)	0.078 (11)	0.094 (12)	0.000 (8)	0.014 (9)	−0.030 (11)
C25	0.039 (6)	0.051 (7)	0.074 (9)	−0.005 (5)	0.015 (6)	0.010 (8)
C26	0.072 (9)	0.065 (9)	0.080 (10)	−0.004 (8)	0.011 (8)	0.014 (9)
C27	0.091 (11)	0.056 (8)	0.087 (11)	−0.012 (8)	0.016 (9)	0.022 (9)
C28	0.102 (12)	0.066 (10)	0.095 (12)	−0.015 (9)	0.014 (10)	0.013 (11)
C29	0.125 (17)	0.076 (11)	0.097 (14)	−0.012 (12)	0.015 (12)	0.014 (12)
C30	0.116 (16)	0.077 (12)	0.109 (15)	−0.023 (12)	−0.006 (12)	0.023 (13)
C31	0.101 (14)	0.069 (11)	0.109 (15)	−0.018 (10)	0.006 (11)	0.023 (12)
C32	0.086 (11)	0.058 (8)	0.090 (12)	−0.016 (8)	0.007 (9)	0.019 (10)
C33	0.077 (10)	0.067 (9)	0.106 (13)	−0.012 (8)	0.019 (9)	0.019 (11)
C34	0.075 (10)	0.075 (10)	0.109 (13)	−0.007 (9)	0.011 (9)	0.018 (11)
C35	0.087 (12)	0.078 (12)	0.125 (17)	−0.020 (10)	0.003 (12)	0.018 (14)
C36	0.102 (15)	0.081 (13)	0.114 (16)	−0.021 (11)	−0.004 (11)	0.023 (13)
C37	0.036 (6)	0.076 (8)	0.061 (8)	0.004 (6)	0.025 (6)	0.010 (8)
C38	0.056 (8)	0.078 (9)	0.074 (9)	0.009 (7)	0.033 (7)	0.011 (9)

C39	0.052 (7)	0.072 (8)	0.079 (9)	0.007 (7)	0.033 (7)	0.017 (9)
C40	0.031 (5)	0.063 (8)	0.077 (9)	0.004 (5)	0.024 (6)	0.017 (8)
C41	0.032 (5)	0.059 (7)	0.066 (7)	−0.001 (5)	0.023 (5)	0.008 (7)
C42	0.034 (6)	0.063 (8)	0.070 (9)	−0.007 (5)	0.015 (6)	0.008 (7)
C43	0.034 (6)	0.067 (8)	0.090 (10)	−0.010 (6)	0.012 (6)	0.005 (9)
C44	0.052 (8)	0.079 (10)	0.093 (11)	−0.019 (7)	0.004 (7)	−0.001 (10)
C45	0.052 (8)	0.094 (11)	0.084 (10)	−0.020 (8)	−0.001 (7)	−0.009 (10)
C46	0.039 (6)	0.076 (9)	0.074 (9)	−0.006 (6)	0.014 (6)	−0.005 (8)
C47	0.035 (6)	0.067 (8)	0.096 (11)	−0.001 (6)	0.023 (7)	0.025 (9)
C48	0.033 (6)	0.072 (9)	0.096 (11)	−0.015 (6)	0.008 (6)	0.014 (10)
C49	0.101 (14)	0.126 (18)	0.089 (13)	0.005 (13)	0.007 (11)	0.029 (15)
C50	0.108 (13)	0.103 (13)	0.091 (12)	0.015 (11)	0.025 (10)	0.039 (12)
C51	0.16 (2)	0.14 (2)	0.113 (17)	0.043 (17)	0.030 (15)	−0.003 (18)

Geometric parameters (Å, °)

Tb1—O1^{i}	2.343 (5)	C19—C20	1.415 (16)
Tb1—O3	2.349 (6)	C19—C24	1.43 (2)
Tb1—O4^{i}	2.369 (7)	C20—C21	1.400 (18)
Tb1—O6	2.433 (8)	C21—C22	1.35 (2)
Tb1—O5	2.468 (8)	C21—H21	0.9300
Tb1—O2	2.478 (7)	C22—C23	1.41 (2)
Tb1—O1	2.539 (7)	C22—H22	0.9300
Tb1—N2	2.547 (9)	C23—C24	1.34 (2)
Tb1—N1	2.587 (7)	C23—H23	0.9300
Tb1—Tb1^{i}	3.9302 (9)	C24—H24	0.9300
N1—C37	1.299 (14)	C25—C26	1.518 (18)
N1—C41	1.352 (15)	C26—C27	1.47 (2)
N2—C46	1.306 (15)	C26—H26A	0.9700
N2—C42	1.356 (12)	C26—H26B	0.9700
N3—C49	1.34 (2)	C27—C28	1.39 (2)
N3—C51	1.40 (2)	C27—C32	1.41 (2)
N3—C50	1.45 (2)	C28—C29	1.44 (2)
O1—C1	1.247 (12)	C28—H28	0.9300
O1—Tb1^{i}	2.343 (5)	C29—C30	1.30 (2)
O2—C1	1.239 (11)	C29—H29	0.9300
O3—C13	1.241 (10)	C30—C31	1.43 (3)
O4—C13	1.262 (11)	C30—H30	0.9300
O4—Tb1^{i}	2.369 (7)	C31—C32	1.41 (3)
O5—C25	1.252 (15)	C31—C36	1.45 (3)
O6—C25	1.231 (14)	C32—C33	1.39 (2)
O7—C49	1.23 (2)	C33—C34	1.38 (2)
C1—C2	1.507 (16)	C33—H33	0.9300
C2—C3	1.509 (16)	C34—C35	1.37 (3)
C2—H2A	0.9700	C34—H34	0.9300
C2—H2B	0.9700	C35—C36	1.30 (3)
C3—C4	1.388 (18)	C35—H35	0.9300
C3—C8	1.411 (18)	C36—H36	0.9300

C4—C5	1.407 (19)	C37—C38	1.410 (13)
C4—H4	0.9300	C37—H37	0.9300
C5—C6	1.31 (2)	C38—C39	1.395 (19)
C5—H5	0.9300	C38—H38	0.9300
C6—C7	1.38 (2)	C39—C40	1.378 (19)
C6—H6	0.9300	C39—H39	0.9300
C7—C8	1.413 (18)	C40—C47	1.412 (19)
C7—C12	1.43 (2)	C40—C41	1.437 (12)
C8—C9	1.41 (2)	C41—C42	1.453 (17)
C9—C10	1.35 (2)	C42—C43	1.413 (17)
C9—H9	0.9300	C43—C44	1.375 (19)
C10—C11	1.45 (2)	C43—C48	1.456 (16)
C10—H10	0.9300	C44—C45	1.351 (17)
C11—C12	1.31 (2)	C44—H44	0.9300
C11—H11	0.9300	C45—C46	1.388 (18)
C12—H12	0.9300	C45—H45	0.9300
C13—C14	1.513 (15)	C46—H46	0.9300
C14—C15	1.495 (15)	C47—C48	1.328 (19)
C14—H14A	0.9700	C47—H47	0.9300
C14—H14B	0.9700	C48—H48	0.9300
C15—C16	1.393 (17)	C49—H49	0.9300
C15—C20	1.416 (19)	C50—H50A	0.9600
C16—C17	1.395 (17)	C50—H50B	0.9600
C16—H16	0.9300	C50—H50C	0.9600
C17—C18	1.38 (2)	C51—H51A	0.9600
C17—H17	0.9300	C51—H51B	0.9600
C18—C19	1.39 (2)	C51—H51C	0.9600
C18—H18	0.9300		
$O1^{i}$—Tb1—O3	74.6 (2)	C17—C16—H16	119.1
$O1^{i}$—Tb1—$O4^{i}$	76.8 (2)	C18—C17—C16	119.0 (13)
O3—Tb1—$O4^{i}$	136.6 (2)	C18—C17—H17	120.5
$O1^{i}$—Tb1—O6	86.6 (2)	C16—C17—H17	120.5
O3—Tb1—O6	125.4 (3)	C17—C18—C19	121.4 (13)
$O4^{i}$—Tb1—O6	84.2 (3)	C17—C18—H18	119.3
$O1^{i}$—Tb1—O5	75.6 (2)	C19—C18—H18	119.3
O3—Tb1—O5	72.9 (2)	C18—C19—C20	119.5 (15)
$O4^{i}$—Tb1—O5	129.4 (3)	C18—C19—C24	122.4 (13)
O6—Tb1—O5	52.7 (3)	C20—C19—C24	118.2 (13)
$O1^{i}$—Tb1—O2	123.5 (2)	C21—C20—C19	119.0 (14)
O3—Tb1—O2	77.0 (2)	C21—C20—C15	121.3 (11)
$O4^{i}$—Tb1—O2	92.8 (2)	C19—C20—C15	119.7 (12)
O6—Tb1—O2	148.4 (2)	C22—C21—C20	120.0 (13)
O5—Tb1—O2	137.8 (3)	C22—C21—H21	120.0
$O1^{i}$—Tb1—O1	72.8 (3)	C20—C21—H21	120.0
O3—Tb1—O1	68.8 (2)	C21—C22—C23	122.5 (16)
$O4^{i}$—Tb1—O1	72.0 (2)	C21—C22—H22	118.7

O6—Tb1—O1	151.3 (3)	C23—C22—H22	118.7
O5—Tb1—O1	135.3 (2)	C24—C23—C22	117.8 (18)
O2—Tb1—O1	51.5 (2)	C24—C23—H23	121.1
O1^{i}—Tb1—N2	142.4 (2)	C22—C23—H23	121.1
O3—Tb1—N2	78.3 (2)	C23—C24—C19	122.5 (14)
O4^{i}—Tb1—N2	139.6 (2)	C23—C24—H24	118.8
O6—Tb1—N2	88.3 (3)	C19—C24—H24	118.8
O5—Tb1—N2	71.7 (3)	O6—C25—O5	122.5 (11)
O2—Tb1—N2	73.8 (3)	O6—C25—C26	120.0 (12)
O1—Tb1—N2	120.3 (3)	O5—C25—C26	117.5 (13)
O1^{i}—Tb1—N1	148.4 (3)	C27—C26—C25	111.4 (13)
O3—Tb1—N1	137.0 (3)	C27—C26—H26A	109.4
O4^{i}—Tb1—N1	75.8 (3)	C25—C26—H26A	109.4
O6—Tb1—N1	75.2 (3)	C27—C26—H26B	109.4
O5—Tb1—N1	110.9 (3)	C25—C26—H26B	109.4
O2—Tb1—N1	73.5 (2)	H26A—C26—H26B	108.0
O1—Tb1—N1	112.7 (2)	C28—C27—C32	118.1 (17)
N2—Tb1—N1	63.9 (3)	C28—C27—C26	120.5 (15)
O1^{i}—Tb1—Tb1^{i}	38.12 (17)	C32—C27—C26	121.4 (16)
O3—Tb1—Tb1^{i}	66.94 (16)	C27—C28—C29	119.3 (18)
O4^{i}—Tb1—Tb1^{i}	70.35 (15)	C27—C28—H28	120.3
O6—Tb1—Tb1^{i}	122.06 (18)	C29—C28—H28	120.3
O5—Tb1—Tb1^{i}	108.12 (16)	C30—C29—C28	122 (2)
O2—Tb1—Tb1^{i}	85.76 (15)	C30—C29—H29	119.0
O1—Tb1—Tb1^{i}	34.72 (13)	C28—C29—H29	119.0
N2—Tb1—Tb1^{i}	142.9 (2)	C29—C30—C31	121 (2)
N1—Tb1—Tb1^{i}	139.2 (2)	C29—C30—H30	119.3
C37—N1—C41	116.4 (8)	C31—C30—H30	119.3
C37—N1—Tb1	124.9 (7)	C32—C31—C30	117.4 (19)
C41—N1—Tb1	118.6 (7)	C32—C31—C36	120 (2)
C46—N2—C42	116.9 (10)	C30—C31—C36	123 (2)
C46—N2—Tb1	121.3 (6)	C33—C32—C27	120.6 (16)
C42—N2—Tb1	121.8 (8)	C33—C32—C31	117.7 (17)
C49—N3—C51	115.9 (18)	C27—C32—C31	121.8 (18)
C49—N3—C50	121.6 (16)	C34—C33—C32	121.4 (17)
C51—N3—C50	122 (2)	C34—C33—H33	119.3
C1—O1—Tb1^{i}	155.2 (6)	C32—C33—H33	119.3
C1—O1—Tb1	90.6 (6)	C35—C34—C33	118.1 (19)
Tb1^{i}—O1—Tb1	107.2 (2)	C35—C34—H34	120.9
C1—O2—Tb1	93.7 (6)	C33—C34—H34	120.9
C13—O3—Tb1	138.8 (7)	C36—C35—C34	125 (2)
C13—O4—Tb1^{i}	133.5 (6)	C36—C35—H35	117.3
C25—O5—Tb1	91.2 (7)	C34—C35—H35	117.3
C25—O6—Tb1	93.3 (7)	C35—C36—C31	118 (2)
O2—C1—O1	122.4 (10)	C35—C36—H36	121.2
O2—C1—C2	119.9 (9)	C31—C36—H36	121.2

O1—C1—C2	117.6 (8)	N1—C37—C38	126.1 (12)
C1—C2—C3	116.3 (9)	N1—C37—H37	116.9
C1—C2—H2A	108.2	C38—C37—H37	116.9
C3—C2—H2A	108.2	C39—C38—C37	116.7 (13)
C1—C2—H2B	108.2	C39—C38—H38	121.7
C3—C2—H2B	108.2	C37—C38—H38	121.7
H2A—C2—H2B	107.4	C40—C39—C38	120.4 (10)
C4—C3—C8	118.2 (12)	C40—C39—H39	119.8
C4—C3—C2	118.4 (13)	C38—C39—H39	119.8
C8—C3—C2	123.4 (11)	C39—C40—C47	121.9 (10)
C3—C4—C5	120.0 (15)	C39—C40—C41	116.7 (11)
C3—C4—H4	120.0	C47—C40—C41	121.3 (13)
C5—C4—H4	120.0	N1—C41—C40	123.7 (11)
C6—C5—C4	121.8 (14)	N1—C41—C42	119.6 (8)
C6—C5—H5	119.1	C40—C41—C42	116.7 (11)
C4—C5—H5	119.1	N2—C42—C43	123.1 (12)
C5—C6—C7	120.7 (14)	N2—C42—C41	116.0 (10)
C5—C6—H6	119.7	C43—C42—C41	120.9 (10)
C7—C6—H6	119.7	C44—C43—C42	117.2 (10)
C6—C7—C8	119.9 (15)	C44—C43—C48	124.8 (12)
C6—C7—C12	121.4 (15)	C42—C43—C48	118.0 (13)
C8—C7—C12	118.7 (14)	C45—C44—C43	119.3 (13)
C3—C8—C7	119.4 (13)	C45—C44—H44	120.3
C3—C8—C9	122.4 (13)	C43—C44—H44	120.3
C7—C8—C9	118.2 (14)	C44—C45—C46	120.0 (15)
C10—C9—C8	122.9 (15)	C44—C45—H45	120.0
C10—C9—H9	118.5	C46—C45—H45	120.0
C8—C9—H9	118.5	N2—C46—C45	123.3 (11)
C9—C10—C11	116.7 (17)	N2—C46—H46	118.3
C9—C10—H10	121.6	C45—C46—H46	118.3
C11—C10—H10	121.6	C48—C47—C40	121.0 (10)
C12—C11—C10	122.6 (19)	C48—C47—H47	119.5
C12—C11—H11	118.7	C40—C47—H47	119.5
C10—C11—H11	118.7	C47—C48—C43	122.0 (12)
C11—C12—C7	120.8 (17)	C47—C48—H48	119.0
C11—C12—H12	119.6	C43—C48—H48	119.0
C7—C12—H12	119.6	O7—C49—N3	124 (2)
O3—C13—O4	126.5 (9)	O7—C49—H49	117.9
O3—C13—C14	116.1 (9)	N3—C49—H49	117.9
O4—C13—C14	117.4 (8)	N3—C50—H50A	109.5
C15—C14—C13	116.8 (10)	N3—C50—H50B	109.5
C15—C14—H14A	108.1	H50A—C50—H50B	109.5
C13—C14—H14A	108.1	N3—C50—H50C	109.5
C15—C14—H14B	108.1	H50A—C50—H50C	109.5
C13—C14—H14B	108.1	H50B—C50—H50C	109.5
H14A—C14—H14B	107.3	N3—C51—H51A	109.5
C16—C15—C20	118.4 (11)	N3—C51—H51B	109.5
C16—C15—C14	119.3 (13)	H51A—C51—H51B	109.5
C20—C15—C14	122.1 (10)	N3—C51—H51C	109.5

C15—C16—C17	121.8 (15)	H51A—C51—H51C	109.5
C15—C16—H16	119.1	H51B—C51—H51C	109.5
O1^{i}—Tb1—N1—C37	27.9 (11)	C6—C7—C8—C3	0.1 (18)
O3—Tb1—N1—C37	−148.8 (8)	C12—C7—C8—C3	179.2 (11)
O4^{i}—Tb1—N1—C37	−2.9 (9)	C6—C7—C8—C9	179.9 (12)
O6—Tb1—N1—C37	84.7 (9)	C12—C7—C8—C9	−0.9 (18)
O5—Tb1—N1—C37	124.3 (9)	C3—C8—C9—C10	179.2 (14)
O2—Tb1—N1—C37	−100.2 (9)	C7—C8—C9—C10	−1(2)
O1—Tb1—N1—C37	−66.0 (9)	C8—C9—C10—C11	1(2)
N2—Tb1—N1—C37	−179.8 (10)	C9—C10—C11—C12	0(3)
Tb1^{i}—Tb1—N1—C37	−37.6 (10)	C10—C11—C12—C7	−2(3)
O1^{i}—Tb1—N1—C41	−154.6 (7)	C6—C7—C12—C11	−178.6 (16)
O3—Tb1—N1—C41	28.7 (10)	C8—C7—C12—C11	2(2)
O4^{i}—Tb1—N1—C41	174.6 (8)	Tb1—O3—C13—O4	−28.8 (18)
O6—Tb1—N1—C41	−97.8 (8)	Tb1—O3—C13—C14	152.1 (8)
O5—Tb1—N1—C41	−58.2 (8)	Tb1^{i}—O4—C13—O3	8.6 (17)
O2—Tb1—N1—C41	77.3 (8)	Tb1^{i}—O4—C13—C14	−172.3 (7)
O1—Tb1—N1—C41	111.4 (8)	O3—C13—C14—C15	−140.2 (12)
N2—Tb1—N1—C41	−2.3 (8)	O4—C13—C14—C15	40.6 (16)
Tb1^{i}—Tb1—N1—C41	139.9 (7)	C13—C14—C15—C16	−119.7 (13)
O1^{i}—Tb1—N2—C46	−22.3 (11)	C13—C14—C15—C20	65.3 (16)
O3—Tb1—N2—C46	22.3 (9)	C20—C15—C16—C17	−3(2)
O4^{i}—Tb1—N2—C46	176.7 (8)	C14—C15—C16—C17	−178.4 (13)
O6—Tb1—N2—C46	−104.4 (9)	C15—C16—C17—C18	3(2)
O5—Tb1—N2—C46	−53.3 (9)	C16—C17—C18—C19	0(2)
O2—Tb1—N2—C46	102.0 (9)	C17—C18—C19—C20	−3(2)
O1—Tb1—N2—C46	79.1 (10)	C17—C18—C19—C24	176.8 (14)
N1—Tb1—N2—C46	−178.7 (10)	C18—C19—C20—C21	−178.8 (12)
Tb1^{i}—Tb1—N2—C46	42.8 (11)	C24—C19—C20—C21	1.6 (19)
O1^{i}—Tb1—N2—C42	160.4 (8)	C18—C19—C20—C15	2.2 (19)
O3—Tb1—N2—C42	−155.0 (9)	C24—C19—C20—C15	−177.4 (12)
O4^{i}—Tb1—N2—C42	−0.6 (11)	C16—C15—C20—C21	−178.2 (13)
O6—Tb1—N2—C42	78.3 (9)	C14—C15—C20—C21	−3.2 (18)
O5—Tb1—N2—C42	129.4 (9)	C16—C15—C20—C19	0.7 (18)
O2—Tb1—N2—C42	−75.3 (9)	C14—C15—C20—C19	175.7 (12)
O1—Tb1—N2—C42	−98.2 (9)	C19—C20—C21—C22	−3(2)
N1—Tb1—N2—C42	3.9 (8)	C15—C20—C21—C22	176.1 (13)
Tb1^{i}—Tb1—N2—C42	−134.5 (8)	C20—C21—C22—C23	3(2)
O1^{i}—Tb1—O1—C1	162.4 (7)	C21—C22—C23—C24	−1(2)
O3—Tb1—O1—C1	82.7 (6)	C22—C23—C24—C19	0(2)
O4^{i}—Tb1—O1—C1	−116.3 (6)	C18—C19—C24—C23	−179.9 (15)
O6—Tb1—O1—C1	−151.6 (6)	C20—C19—C24—C23	0(2)
O5—Tb1—O1—C1	115.4 (6)	Tb1—O6—C25—O5	5.3 (11)
O2—Tb1—O1—C1	−7.3 (5)	Tb1—O6—C25—C26	−174.2 (11)
N2—Tb1—O1—C1	21.2 (6)	Tb1—O5—C25—O6	−5.3 (11)

N1—Tb1—O1—C1	−50.8 (6)	Tb1—O5—C25—C26	174.3 (10)
Tb1^{i}—Tb1—O1—C1	162.4 (7)	O6—C25—C26—C27	125.9 (14)
O1^{i}—Tb1—O1—Tb1^{i}	0.0	O5—C25—C26—C27	−53.6 (16)
O3—Tb1—O1—Tb1^{i}	−79.7 (3)	C25—C26—C27—C28	107.4 (16)
O4^{i}—Tb1—O1—Tb1^{i}	81.3 (3)	C25—C26—C27—C32	−70.4 (17)
O6—Tb1—O1—Tb1^{i}	46.0 (6)	C32—C27—C28—C29	0(2)
O5—Tb1—O1—Tb1^{i}	−47.0 (4)	C26—C27—C28—C29	−178.1 (14)
O2—Tb1—O1—Tb1^{i}	−169.7 (4)	C27—C28—C29—C30	2(3)
N2—Tb1—O1—Tb1^{i}	−141.2 (3)	C28—C29—C30—C31	−3(3)
N1—Tb1—O1—Tb1^{i}	146.8 (3)	C29—C30—C31—C32	2(2)
O1^{i}—Tb1—O2—C1	−4.4 (7)	C29—C30—C31—C36	177.6 (17)
O3—Tb1—O2—C1	−65.8 (6)	C28—C27—C32—C33	179.3 (14)
O4^{i}—Tb1—O2—C1	71.5 (6)	C26—C27—C32—C33	−3(2)
O6—Tb1—O2—C1	155.0 (6)	C28—C27—C32—C31	−1(2)
O5—Tb1—O2—C1	−111.0 (6)	C26—C27—C32—C31	176.6 (14)
O1—Tb1—O2—C1	7.4 (6)	C30—C31—C32—C33	−180.0 (14)
N2—Tb1—O2—C1	−147.2 (6)	C36—C31—C32—C33	4(2)
N1—Tb1—O2—C1	145.9 (7)	C30—C31—C32—C27	1(2)
Tb1^{i}—Tb1—O2—C1	1.5 (6)	C36—C31—C32—C27	−175.5 (14)
O1^{i}—Tb1—O3—C13	−17.2 (10)	C27—C32—C33—C34	178.3 (14)
O4^{i}—Tb1—O3—C13	33.3 (11)	C31—C32—C33—C34	−1(2)
O6—Tb1—O3—C13	−91.4 (10)	C32—C33—C34—C35	0(2)
O5—Tb1—O3—C13	−96.6 (10)	C33—C34—C35—C36	−2(3)
O2—Tb1—O3—C13	113.4 (10)	C34—C35—C36—C31	5(3)
O1—Tb1—O3—C13	60.0 (10)	C32—C31—C36—C35	−6(2)
N2—Tb1—O3—C13	−170.8 (11)	C30—C31—C36—C35	178.6 (17)
N1—Tb1—O3—C13	161.0 (9)	C41—N1—C37—C38	0.0 (18)
Tb1^{i}—Tb1—O3—C13	22.5 (10)	Tb1—N1—C37—C38	177.6 (10)
O1^{i}—Tb1—O5—C25	99.6 (7)	N1—C37—C38—C39	0(2)
O3—Tb1—O5—C25	177.6 (7)	C37—C38—C39—C40	−1.0 (19)
O4^{i}—Tb1—O5—C25	40.6 (7)	C38—C39—C40—C47	−178.6 (12)
O6—Tb1—O5—C25	2.8 (6)	C38—C39—C40—C41	1.0 (18)
O2—Tb1—O5—C25	−136.1 (6)	C37—N1—C41—C40	−0.1 (16)
O1—Tb1—O5—C25	145.7 (6)	Tb1—N1—C41—C40	−177.8 (8)
N2—Tb1—O5—C25	−99.4 (7)	C37—N1—C41—C42	178.6 (11)
N1—Tb1—O5—C25	−47.9 (7)	Tb1—N1—C41—C42	0.9 (14)
Tb1^{i}—Tb1—O5—C25	119.7 (6)	C39—C40—C41—N1	−0.5 (17)
O1^{i}—Tb1—O6—C25	−77.4 (6)	C47—C40—C41—N1	179.1 (11)
O3—Tb1—O6—C25	−9.0 (7)	C39—C40—C41—C42	−179.1 (11)
O4^{i}—Tb1—O6—C25	−154.4 (7)	C47—C40—C41—C42	0.4 (17)
O5—Tb1—O6—C25	−2.9 (6)	C46—N2—C42—C43	0.4 (18)
O2—Tb1—O6—C25	119.7 (7)	Tb1—N2—C42—C43	177.8 (10)
O1—Tb1—O6—C25	−120.9 (7)	C46—N2—C42—C41	177.5 (11)
N2—Tb1—O6—C25	65.4 (7)	Tb1—N2—C42—C41	−5.1 (14)
N1—Tb1—O6—C25	128.7 (7)	N1—C41—C42—N2	2.7 (16)

Tb1^{i}—Tb1—O6—C25	−92.0 (7)	C40—C41—C42—N2	−178.6 (11)
Tb1—O2—C1—O1	−14.0 (10)	N1—C41—C42—C43	179.9 (12)
Tb1—O2—C1—C2	163.7 (9)	C40—C41—C42—C43	−1.4 (17)
Tb1^{i}—O1—C1—O2	150.2 (11)	N2—C42—C43—C44	−3(2)
Tb1—O1—C1—O2	13.6 (10)	C41—C42—C43—C44	179.7 (12)
Tb1^{i}—O1—C1—C2	−28 (2)	N2—C42—C43—C48	177.8 (12)
Tb1—O1—C1—C2	−164.1 (9)	C41—C42—C43—C48	0.8 (19)
O2—C1—C2—C3	−4.7 (16)	C42—C43—C44—C45	3(2)
O1—C1—C2—C3	173.1 (10)	C48—C43—C44—C45	−178.0 (14)
C1—C2—C3—C4	112.9 (13)	C43—C44—C45—C46	0(2)
C1—C2—C3—C8	−68.9 (15)	C42—N2—C46—C45	2.7 (19)
C8—C3—C4—C5	2.3 (18)	Tb1—N2—C46—C45	−174.7 (11)
C2—C3—C4—C5	−179.4 (11)	C44—C45—C46—N2	−3(2)
C3—C4—C5—C6	−3(2)	C39—C40—C47—C48	−179.2 (13)
C4—C5—C6—C7	2(2)	C41—C40—C47—C48	1.3 (19)
C5—C6—C7—C8	0(2)	C40—C47—C48—C43	−2(2)
C5—C6—C7—C12	−179.6 (13)	C44—C43—C48—C47	−177.9 (15)
C4—C3—C8—C7	−1.0 (17)	C42—C43—C48—C47	1(2)
C2—C3—C8—C7	−179.3 (11)	C51—N3—C49—O7	2(3)
C4—C3—C8—C9	179.1 (12)	C50—N3—C49—O7	178.1 (19)
C2—C3—C8—C9	0.9 (18)		

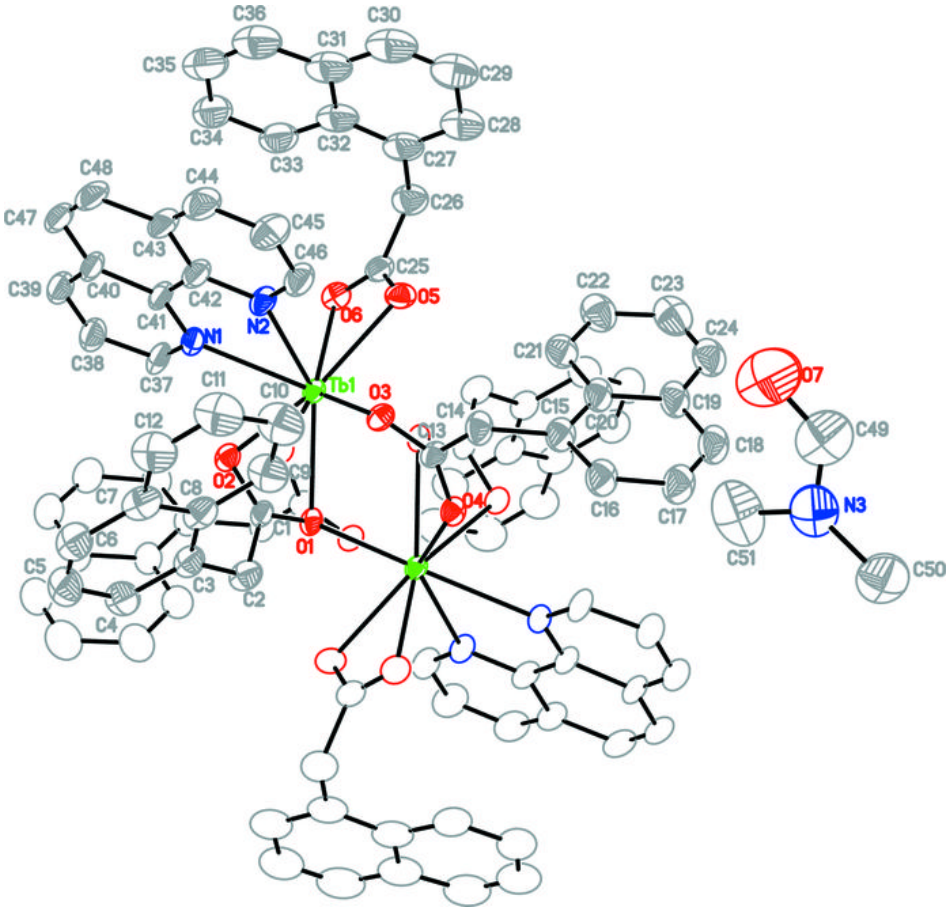
Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6···O7^{ii}	0.93	2.56	3.44 (2)	157
C37—H37···O4^{i}	0.93	2.35	3.015 (11)	128
C46—H46···O3	0.93	2.48	3.056 (13)	120
C47—H47···O2^{iii}	0.93	2.45	3.314 (13)	154
C50—H50A···O6^{iv}	0.96	2.62	3.40 (2)	138
C18—H18···Cg1^{v}	0.93	2.90	3.673 (16)	141

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

Fig. 1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C9
C7
C8
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Fig. 2

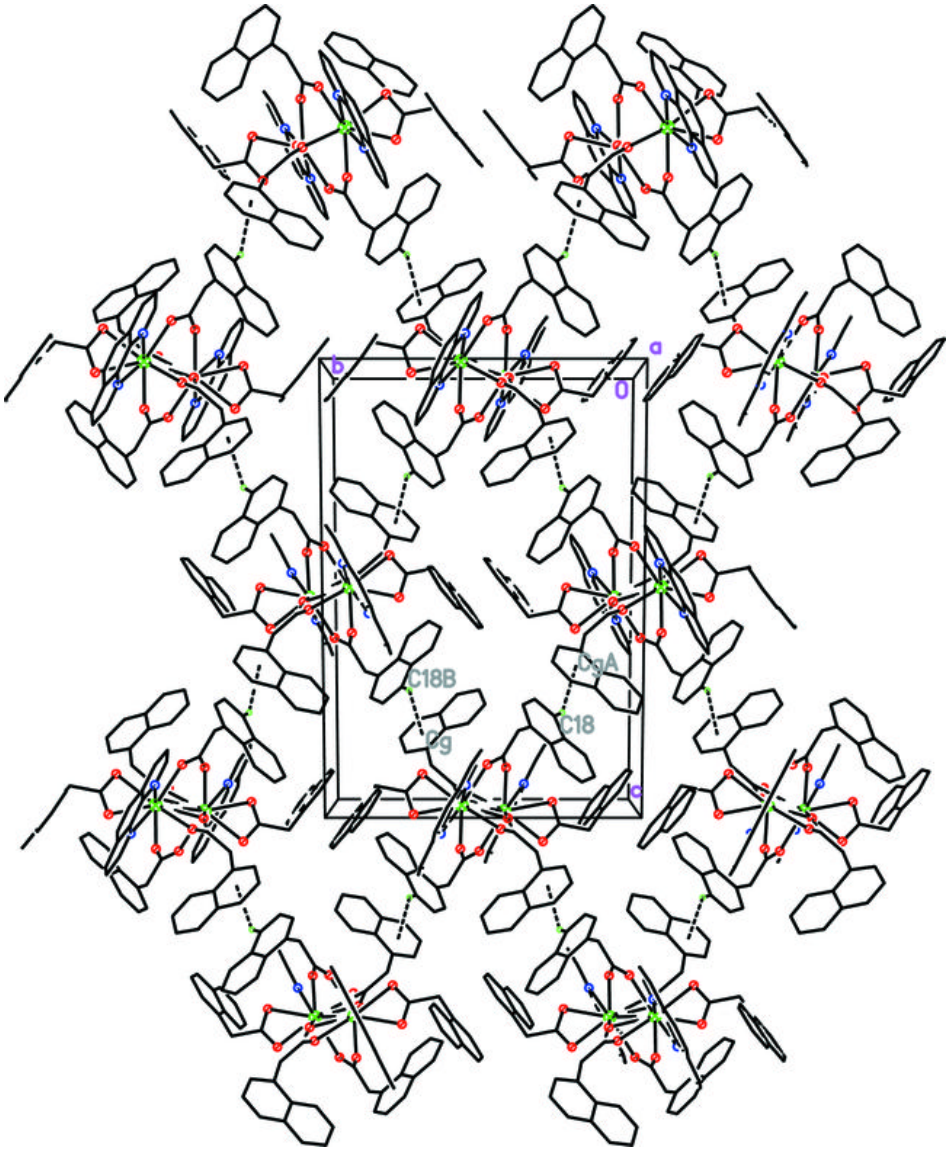

Fig. 3