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Tetrakis(μ-naphthalene-1-acetato)-bis(naphthalene-1-acetato)bis(1,10-phenanthroline)samarium(III)terbium(III) *N*,*N*-dimethylformamide disolvate

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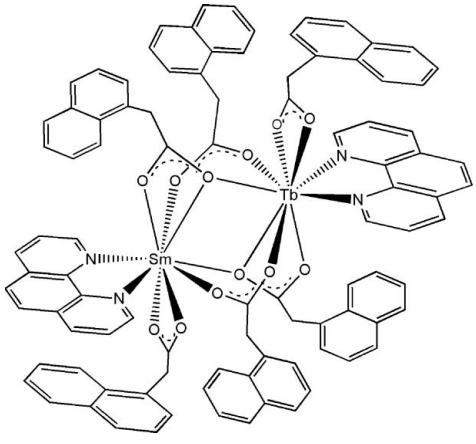
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.013 Å; disorder in main residue; R factor = 0.053; wR factor = 0.118; data-to-parameter ratio = 13.8.

Molecules of the title complex, $[SmTb(C_{12}H_9O_2)_6(C_{12}H_8N_2)_2]\cdot 2C_3H_7NO$, are centrosymmetric with equal disorder of the Sm and Tb atoms. Each Sm^{III} and Tb^{III} ion is nine-coordinate. The Sm and Tb atoms have a distorted monocapped square-antiprismatic coordination geometry. The molecules are linked into a chain by C—H···O and C—H···π hydrogen bonds parallel to the *a* axis, and into a sheet by C—H···π hydrogen bonds parallel to the (100) plane. The combination of the chains and sheets generates a three-dimensional framework structure.

Related literature

For related literature, see: Bernstein *et al.* (1995); Liu *et al.* (2007*a*,*b*); Xia *et al.* (2007); Xia *et al.* (2007*a*,*b*).



·2 $(CH_3)_2NCHO$

Experimental

Crystal data

$[SmTb(C_{12}H_9O_2)_6(C_{12}H_8N_2)_2]\cdot 2C_3H_7NO$
M_r = 1927.02
Monoclinic, $P2_1/c$
a = 13.4985 (14) Å
b = 15.1320 (17) Å
c = 22.181 (2) Å
β = 103.723 (2)°
V = 4401.3 (8) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.53 mm^{-1}
T = 298 (2) K
0.59 × 0.11 × 0.08 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.466, T_{max} = 0.888
21723 measured reflections
7724 independent reflections
6069 reflections with $I > 2\sigma(I)$
R_{int} = 0.040

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.118
S = 1.11
7724 reflections
559 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.98 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6···O7^{i}	0.93	2.57	3.459 (13)	160
C33—H33···O3	0.93	2.59	3.404 (10)	147
C37—H37···O6^{ii}	0.93	2.36	3.023 (8)	128
C46—H46···O5	0.93	2.47	3.074 (9)	122
C47—H47···O2^{iii}	0.93	2.47	3.328 (9)	153
C50—H50*A*···O4^{iv}	0.96	2.54	3.376 (12)	146
C51—H51*A*···O7	0.96	2.29	2.718 (16)	106
C39—H39···*Cg*1^{iii}	0.93	2.98	3.853 (15)	157
C30—H30···*Cg*2^{v}	0.93	2.89	3.663 (17)	142

Symmetry codes: (i) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$; (ii) $-x, -y+2, -z+1$; (iii) $-x+1, -y+2, -z+1$; (iv) $x, -y+\frac{3}{2}, z+\frac{1}{2}$; (v) $-x, y-\frac{1}{2}, -z+\frac{3}{2}$. Note: *Cg*1 and *Cg*2 are the centroids of the C7–C12 and C3–C8 rings, respectively.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; 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: AT2428).

References

Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Liu, Y.-F., Xia, H.-T., Wang, D.-Q. & Yang, S.-P. (2007*a*). *Acta Cryst.* E**63**, m2608–m2609.
Liu, Y.-F., Xia, H.-T., Wang, D.-Q. & Yang, S.-P. (2007*b*). *Acta Cryst.* E**63**, m2625–m2626.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*a*). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.

Siemens. (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Xia, H.-T., Liu, Y.-F., Wang, D.-Q. & Chen, L. (2007). *Acta Cryst.* E**63**, m2610–m2611.
Xia, H.-T., Liu, Y.-F., Wang, D.-Q. & Yang, S.-P. (2007*a*). *Acta Cryst.* E**63**, m2708–m2709.
Xia, H.-T., Liu, Y.-F., Wang, D.-Q. & Yang, S.-P. (2007*b*). *Acta Cryst.* E**63**, m2624.

supplementary materials

Acta Cryst. (2007). E**63**, m2797-m2798 [**doi:10.1107/S1600536807051720**]

Tetrakis(μ-naphthalene-1-acetato)bis(naphthalene-1-acetato)bis(1,10-phenanthroline)samarium(III)terbium(III) *N*,*N*-dimethylformamide disolvate

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

Comment

As part of our ongoing research into the complexes between rare earth elements and naphthalene-1-acetato (NNA) and 1,10-phenanthroline (phen) ligands, we have recently reported the crystal structures of four complexes (Liu *et al.*, 2007*a*,*b*; Xia *et al.*, 2007; Xia *et al.*, 2007*a*,*b*). We report here the crystal structures of a new rare earth complex with NAA and phen (Fig. 1).

In the title complex, the coordination environment of the Sm and Tb atoms and coordination modes of the NNA ligands coordinated to the Sm^{III} and Tb^{III} ions are in agreement with the complexes reported above. The average bond lengths of between the samarium and terbium center and carboxylic oxygen atoms are 2.456 (7) Å. The dihedral angles between the least-square-plane Sm_2O_2 or Tb_2O_2 and naphthyl rings are 58.11 (12)°(C3—C12 ring), 43.96 (18)°(C15—C24 ring) and 71.06 (15)°(C27—C36 ring), and the dihedral angle between Sm_2O_2 or Tb_2O_2 plane and phen ring is 81.45 (12)°.

In (I), the molecules are linked into chains by means of C—H···O hydrogen bonds and C—H···π hydrogen bonds (Fig. 2 and Table 2) and parallel to the *a* axis direction with $R_4^4(30)$ rings (Bernstein *et al.*, 1995) surrounds an $R_2^2(14)$ ring centred at (*n*, 1/2, 1) (*n* = zero or integer) (Fig. 3) and into a sheet by C—H···π hydrogen bonds parallel to the [100] plane. The action of *a* chains are to link adjacent [100] sheet into the three-dimensional framework structure.

*Cg*1 is the centroid of the C7—C12 ring.

*Cg*2 is the centroid of the C3—C8 ring.

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 $Sm(NO_3)_3·6H_2O$(0.182 g, 0.5 mmol), $Tb(NO_3)_3·6H_2O$ (0.227 g, 0.5 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

The space group was uniquely assigned from the systematic absences. The Sm and Tb atoms were found to be disordered over two positions; the occupancies of the two positions for Sm and Tb refined to 0.5 and 0.5. A l l 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 1.5 U_{eq}(C) (methyl).

Figures

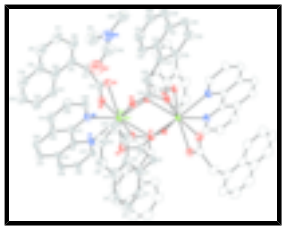

Fig. 1. The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are at the 30% probability level. Unlabelled atoms in the molecular are related to labelled atoms by (1 − *x*, 1 − *y*, 2 − *z*).

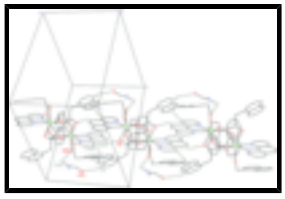

Fig. 2. A larger portion of the crystal structure of (I), showing the formation of a hydrogen-bonded chain built from C—H···O and C—H···π. For clarity, H atoms not involved in the hydrogen bonding have been omitted. Dashed lines indicate hydrogen bonds. [Symmetry codes: (A) 1 − *x*, 1/2 + *y*, 3/2 −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

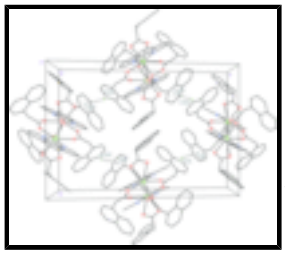

Fig. 3. A larger portion of the crystal structure of (I), showing the formation of a hydrogen-bonded sheet built from C—H···π. For clarity, H atoms not involved in the hydrogen bonding have been omitted. Dashed lines indicate hydrogen bonds. [Symmetry codes: (C) −*x*, −1/2 + *y*, 3/2 − *z*,, (D) *x*,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

Tetrakis(μ-naphthalene-1-acetato)bis(naphthalene-1-acetato)bis(1,10- phenanthroline)samarium(III)terbium(III) *N*,*N*-dimethylformamide disolvate

Crystal data

$[SmTb(C_{12}H_9O_2)_6(C_{12}H_8N_2)_2]\cdot 2C_3H_7NO$	F_{000} = 1954
M_r = 1927.02	D_x = 1.454 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 9128 reflections
a = 13.4985 (14) Å	θ = 2.4–27.9º
b = 15.1320 (17) Å	μ = 1.53 mm^{-1}
c = 22.181 (2) Å	*T* = 298 (2) K
β = 103.723 (2)º	Block, colourless
V = 4401.3 (8) Å^3	0.59 × 0.11 × 0.08 mm
Z = 2	

Data collection

Bruker SMART 1000 CCD area-detector diffractometer	7724 independent reflections
Radiation source: fine-focus sealed tube	6069 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.040
T = 298(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 1.6º

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
T_{min} = 0.466, T_{max} = 0.888
21723 measured reflections

h = −15→16
k = −17→9
l = −26→26

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.118
S = 1.11
7724 reflections
559 parameters
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0325P)^2 + 19.4345P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.98 e Å^{-3}
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}	Occ. (<1)
Sm1	0.11747 (2)	0.92966 (2)	0.488418 (14)	0.03101 (10)	0.50
Tb1	0.11747 (2)	0.92966 (2)	0.488418 (14)	0.03101 (10)	0.50
N1	0.2709 (4)	0.9436 (4)	0.4349 (3)	0.0448 (14)	
N2	0.2877 (4)	0.8639 (4)	0.5467 (3)	0.0477 (14)	
N3	0.1323 (7)	0.6639 (6)	0.7473 (4)	0.079 (2)	
O1	0.0591 (3)	1.0802 (3)	0.52069 (18)	0.0362 (10)	
O2	0.2232 (3)	1.0558 (3)	0.5387 (2)	0.0414 (11)	
O3	0.0870 (4)	0.7727 (3)	0.5111 (2)	0.0542 (13)	
O4	0.0964 (4)	0.8041 (3)	0.4168 (2)	0.0545 (13)	
O5	0.0958 (3)	0.9248 (3)	0.59139 (19)	0.0404 (10)	
O6	−0.0489 (3)	0.9875 (3)	0.60333 (19)	0.0417 (11)	
O7	0.2663 (7)	0.7560 (6)	0.7635 (4)	0.128 (3)	
C1	0.1508 (5)	1.0983 (4)	0.5481 (3)	0.0383 (15)	
C2	0.1653 (5)	1.1738 (5)	0.5945 (3)	0.0510 (18)	

H2A	0.1407	1.2278	0.5723	0.061*
H2B	0.1232	1.1626	0.6235	0.061*
C3	0.2738 (6)	1.1889 (5)	0.6310 (3)	0.0522 (19)
C4	0.3228 (6)	1.2634 (6)	0.6203 (4)	0.060 (2)
H4	0.2889	1.3031	0.5904	0.073*
C5	0.4233 (6)	1.2825 (6)	0.6531 (4)	0.070 (2)
H5	0.4551	1.3342	0.6450	0.083*
C6	0.4723 (7)	1.2256 (6)	0.6957 (4)	0.069 (2)
H6	0.5393	1.2377	0.7164	0.083*
C7	0.4257 (6)	1.1480 (6)	0.7103 (4)	0.066 (2)
C8	0.3244 (6)	1.1286 (6)	0.6772 (4)	0.057 (2)
C9	0.2783 (7)	1.0505 (6)	0.6913 (4)	0.066 (2)
H9	0.2118	1.0373	0.6701	0.079*
C10	0.3300 (8)	0.9937 (7)	0.7359 (4)	0.085 (3)
H10	0.3001	0.9414	0.7446	0.102*
C11	0.4284 (8)	1.0164 (7)	0.7678 (5)	0.089 (3)
H11	0.4629	0.9783	0.7986	0.107*
C12	0.4762 (8)	1.0900 (7)	0.7566 (4)	0.078 (3)
H12	0.5420	1.1024	0.7792	0.094*
C13	0.0899 (6)	0.7492 (5)	0.4577 (4)	0.0522 (18)
C14	0.0862 (7)	0.6504 (5)	0.4447 (4)	0.067 (2)
H14A	0.0198	0.6279	0.4467	0.081*
H14B	0.0943	0.6406	0.4029	0.081*
C15	0.1661 (8)	0.6001 (6)	0.4889 (4)	0.071 (2)
C16	0.1407 (8)	0.5477 (6)	0.5335 (5)	0.079 (3)
H16	0.0729	0.5405	0.5351	0.095*
C17	0.2207 (9)	0.5042 (7)	0.5778 (5)	0.089 (3)
H17	0.2038	0.4668	0.6071	0.107*
C18	0.3174 (10)	0.5160 (7)	0.5779 (5)	0.093 (3)
H18	0.3671	0.4886	0.6085	0.112*
C19	0.3474 (9)	0.5673 (7)	0.5344 (5)	0.087 (3)
C20	0.2703 (8)	0.6108 (6)	0.4886 (5)	0.073 (3)
C21	0.3011 (7)	0.6630 (6)	0.4440 (5)	0.076 (3)
H21	0.2524	0.6906	0.4130	0.091*
C22	0.4044 (7)	0.6739 (6)	0.4459 (5)	0.080 (3)
H22	0.4254	0.7087	0.4166	0.096*
C23	0.4738 (8)	0.6322 (7)	0.4916 (6)	0.090 (3)
H23	0.5425	0.6398	0.4927	0.108*
C24	0.4501 (9)	0.5820 (7)	0.5342 (6)	0.093 (3)
H24	0.5014	0.5560	0.5645	0.112*
C25	0.0266 (5)	0.9363 (5)	0.6194 (3)	0.0419 (15)
C26	0.0374 (6)	0.8860 (5)	0.6796 (3)	0.056 (2)
H26A	0.0863	0.8388	0.6804	0.067*
H26B	0.0661	0.9258	0.7135	0.067*
C27	−0.0580 (6)	0.8464 (6)	0.6917 (4)	0.057 (2)
C28	−0.0902 (6)	0.8723 (6)	0.7435 (4)	0.064 (2)
H28	−0.0536	0.9153	0.7695	0.077*
C29	−0.1778 (7)	0.8347 (7)	0.7580 (4)	0.073 (3)
H29	−0.1986	0.8536	0.7929	0.087*

C30	−0.2306 (7)	0.7720 (7)	0.7216 (4)	0.071 (3)
H30	−0.2886	0.7486	0.7312	0.086*
C31	−0.2004 (7)	0.7410 (6)	0.6692 (4)	0.067 (2)
C32	−0.1133 (6)	0.7798 (6)	0.6537 (4)	0.060 (2)
C33	−0.0837 (6)	0.7479 (6)	0.6008 (4)	0.062 (2)
H33	−0.0280	0.7728	0.5891	0.074*
C34	−0.1366 (7)	0.6807 (7)	0.5667 (4)	0.076 (3)
H34	−0.1165	0.6609	0.5317	0.091*
C35	−0.2201 (8)	0.6407 (7)	0.5826 (5)	0.084 (3)
H35	−0.2535	0.5939	0.5591	0.100*
C36	−0.2519 (7)	0.6702 (7)	0.6321 (5)	0.078 (3)
H36	−0.3081	0.6440	0.6423	0.093*
C37	0.2630 (6)	0.9833 (5)	0.3812 (4)	0.0524 (19)
H37	0.2000	1.0060	0.3606	0.063*
C38	0.3471 (6)	0.9927 (6)	0.3535 (4)	0.060 (2)
H38	0.3393	1.0205	0.3152	0.072*
C39	0.4385 (6)	0.9605 (5)	0.3837 (4)	0.057 (2)
H39	0.4942	0.9658	0.3661	0.069*
C40	0.4503 (5)	0.9200 (5)	0.4406 (4)	0.0533 (19)
C41	0.3636 (5)	0.9114 (5)	0.4656 (4)	0.0484 (18)
C42	0.3729 (5)	0.8697 (5)	0.5247 (4)	0.0524 (19)
C43	0.4692 (6)	0.8393 (5)	0.5574 (4)	0.060 (2)
C44	0.4731 (6)	0.8002 (6)	0.6138 (4)	0.071 (2)
H44	0.5354	0.7797	0.6371	0.085*
C45	0.3878 (6)	0.7907 (6)	0.6366 (4)	0.071 (2)
H45	0.3908	0.7631	0.6745	0.086*
C46	0.2965 (6)	0.8239 (5)	0.6008 (4)	0.060 (2)
H46	0.2382	0.8177	0.6158	0.072*
C47	0.5460 (6)	0.8855 (5)	0.4757 (4)	0.060 (2)
H47	0.6033	0.8900	0.4595	0.072*
C48	0.5544 (6)	0.8476 (6)	0.5301 (4)	0.064 (2)
H48	0.6175	0.8258	0.5513	0.077*
C49	0.1896 (9)	0.7236 (9)	0.7785 (5)	0.094 (3)
H49	0.1736	0.7443	0.8145	0.113*
C50	0.0425 (8)	0.6327 (7)	0.7665 (5)	0.094 (3)
H50A	0.0334	0.6670	0.8012	0.141*
H50B	0.0512	0.5716	0.7782	0.141*
H50C	−0.0165	0.6390	0.7327	0.141*
C51	0.1574 (10)	0.6248 (8)	0.6943 (6)	0.117 (4)
H51A	0.2183	0.6515	0.6876	0.176*
H51B	0.1023	0.6340	0.6585	0.176*
H51C	0.1683	0.5626	0.7012	0.176*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sm1	0.02274 (15)	0.03514 (17)	0.03640 (17)	0.00362 (15)	0.00952 (11)	0.00312 (16)
Tb1	0.02274 (15)	0.03514 (17)	0.03640 (17)	0.00362 (15)	0.00952 (11)	0.00312 (16)

N1	0.035 (3)	0.047 (4)	0.056 (4)	−0.002 (3)	0.019 (3)	−0.008 (3)
N2	0.034 (3)	0.050 (4)	0.061 (4)	0.009 (3)	0.014 (3)	0.003 (3)
N3	0.083 (6)	0.082 (6)	0.071 (5)	0.008 (5)	0.017 (4)	0.012 (5)
O1	0.027 (2)	0.040 (3)	0.042 (2)	−0.002 (2)	0.0095 (18)	0.004 (2)
O2	0.028 (2)	0.047 (3)	0.051 (3)	0.001 (2)	0.0127 (19)	−0.009 (2)
O3	0.053 (3)	0.048 (3)	0.064 (3)	0.005 (3)	0.019 (3)	0.004 (3)
O4	0.053 (3)	0.049 (3)	0.062 (3)	0.003 (3)	0.016 (3)	−0.005 (3)
O5	0.035 (2)	0.045 (3)	0.042 (2)	0.005 (2)	0.0116 (19)	0.010 (2)
O6	0.040 (3)	0.049 (3)	0.041 (2)	0.007 (2)	0.019 (2)	0.011 (2)
O7	0.102 (6)	0.136 (8)	0.137 (7)	−0.007 (6)	0.010 (5)	0.030 (6)
C1	0.030 (3)	0.043 (4)	0.044 (4)	−0.002 (3)	0.013 (3)	−0.002 (3)
C2	0.040 (4)	0.055 (5)	0.057 (4)	−0.001 (4)	0.010 (3)	−0.016 (4)
C3	0.044 (4)	0.056 (5)	0.056 (5)	0.000 (4)	0.012 (3)	−0.020 (4)
C4	0.054 (5)	0.061 (5)	0.063 (5)	−0.005 (4)	0.006 (4)	−0.016 (4)
C5	0.061 (5)	0.070 (6)	0.073 (6)	−0.014 (5)	0.007 (4)	−0.020 (5)
C6	0.058 (5)	0.075 (6)	0.068 (6)	−0.009 (5)	0.003 (4)	−0.024 (5)
C7	0.059 (5)	0.070 (6)	0.062 (5)	0.002 (5)	0.003 (4)	−0.022 (5)
C8	0.051 (5)	0.061 (5)	0.056 (5)	−0.003 (4)	0.008 (4)	−0.020 (4)
C9	0.061 (5)	0.066 (6)	0.064 (5)	−0.006 (4)	0.000 (4)	−0.009 (4)
C10	0.086 (7)	0.081 (7)	0.079 (6)	−0.007 (6)	−0.001 (5)	−0.006 (6)
C11	0.088 (7)	0.085 (8)	0.079 (7)	0.003 (6)	−0.011 (6)	−0.006 (6)
C12	0.072 (6)	0.079 (7)	0.071 (6)	0.001 (5)	−0.008 (5)	−0.017 (5)
C13	0.045 (4)	0.044 (4)	0.069 (5)	0.004 (4)	0.016 (4)	−0.004 (4)
C14	0.068 (5)	0.051 (5)	0.082 (6)	0.004 (4)	0.016 (5)	−0.008 (5)
C15	0.079 (6)	0.051 (5)	0.083 (6)	0.009 (5)	0.017 (5)	−0.009 (5)
C16	0.089 (7)	0.058 (6)	0.089 (7)	0.008 (5)	0.018 (6)	−0.005 (5)
C17	0.105 (9)	0.065 (6)	0.096 (8)	0.011 (6)	0.018 (7)	−0.005 (6)
C18	0.099 (9)	0.068 (7)	0.102 (8)	0.016 (6)	0.004 (7)	−0.009 (6)
C19	0.090 (8)	0.062 (6)	0.101 (8)	0.011 (6)	0.010 (6)	−0.015 (6)
C20	0.078 (7)	0.050 (5)	0.088 (7)	0.014 (5)	0.013 (5)	−0.013 (5)
C21	0.073 (6)	0.060 (6)	0.094 (7)	0.010 (5)	0.017 (5)	−0.011 (5)
C22	0.070 (6)	0.066 (6)	0.101 (7)	0.007 (5)	0.015 (6)	−0.009 (6)
C23	0.078 (7)	0.073 (7)	0.112 (9)	0.014 (6)	0.008 (7)	−0.015 (7)
C24	0.090 (8)	0.071 (7)	0.108 (9)	0.016 (6)	0.003 (7)	−0.014 (7)
C25	0.040 (4)	0.046 (4)	0.042 (4)	0.001 (4)	0.015 (3)	0.010 (3)
C26	0.053 (5)	0.064 (5)	0.052 (4)	0.003 (4)	0.016 (4)	0.018 (4)
C27	0.059 (5)	0.063 (5)	0.054 (5)	0.005 (4)	0.023 (4)	0.021 (4)
C28	0.069 (5)	0.068 (6)	0.060 (5)	0.003 (5)	0.027 (4)	0.016 (4)
C29	0.077 (6)	0.083 (7)	0.068 (6)	0.002 (5)	0.037 (5)	0.020 (5)
C30	0.069 (6)	0.078 (7)	0.073 (6)	0.000 (5)	0.029 (5)	0.026 (5)
C31	0.065 (5)	0.068 (6)	0.071 (6)	0.003 (5)	0.021 (5)	0.022 (5)
C32	0.060 (5)	0.062 (5)	0.062 (5)	0.005 (4)	0.022 (4)	0.022 (4)
C33	0.062 (5)	0.063 (5)	0.063 (5)	0.002 (4)	0.020 (4)	0.012 (4)
C34	0.074 (6)	0.076 (7)	0.076 (6)	0.002 (5)	0.014 (5)	0.008 (5)
C35	0.080 (7)	0.077 (7)	0.088 (7)	−0.002 (6)	0.008 (6)	0.009 (6)
C36	0.071 (6)	0.077 (7)	0.084 (7)	0.000 (5)	0.019 (5)	0.020 (6)
C37	0.042 (4)	0.060 (5)	0.061 (5)	−0.002 (4)	0.026 (4)	−0.005 (4)
C38	0.053 (5)	0.065 (5)	0.069 (5)	−0.004 (4)	0.031 (4)	−0.008 (4)
C39	0.046 (4)	0.060 (5)	0.074 (5)	−0.005 (4)	0.032 (4)	−0.016 (4)

C40	0.039 (4)	0.051 (5)	0.075 (5)	0.001 (4)	0.025 (4)	−0.016 (4)
C41	0.036 (4)	0.049 (5)	0.066 (5)	0.001 (3)	0.024 (3)	−0.010 (4)
C42	0.038 (4)	0.052 (5)	0.070 (5)	0.009 (3)	0.017 (4)	−0.009 (4)
C43	0.041 (4)	0.057 (5)	0.081 (6)	0.010 (4)	0.011 (4)	−0.006 (4)
C44	0.050 (5)	0.068 (6)	0.087 (6)	0.016 (4)	0.003 (4)	0.001 (5)
C45	0.054 (5)	0.073 (6)	0.080 (6)	0.017 (5)	0.003 (4)	0.014 (5)
C46	0.047 (4)	0.062 (5)	0.069 (5)	0.014 (4)	0.012 (4)	0.010 (4)
C47	0.038 (4)	0.059 (5)	0.087 (6)	0.003 (4)	0.022 (4)	−0.015 (5)
C48	0.040 (4)	0.062 (5)	0.088 (6)	0.010 (4)	0.011 (4)	−0.011 (5)
C49	0.087 (8)	0.102 (9)	0.090 (8)	0.003 (7)	0.013 (7)	0.021 (7)
C50	0.094 (8)	0.093 (8)	0.089 (7)	0.003 (6)	0.010 (6)	0.022 (6)
C51	0.126 (10)	0.116 (10)	0.112 (9)	0.021 (8)	0.034 (8)	0.002 (8)

Geometric parameters (Å, °)

Sm1—O1^{i}	2.349 (4)	C18—C19	1.372 (15)
Sm1—O5	2.371 (4)	C18—H18	0.9300
Sm1—O6^{i}	2.382 (4)	C19—C24	1.405 (15)
Sm1—O4	2.449 (5)	C19—C20	1.430 (13)
Sm1—O3	2.482 (5)	C20—C21	1.405 (13)
Sm1—O2	2.483 (4)	C21—C22	1.394 (12)
Sm1—N2	2.556 (5)	C21—H21	0.9300
Sm1—O1	2.567 (4)	C22—C23	1.362 (13)
Sm1—N1	2.628 (5)	C22—H22	0.9300
Sm1—Tb1^{i}	3.9531 (6)	C23—C24	1.310 (15)
Sm1—Sm1^{i}	3.9531 (6)	C23—H23	0.9300
N1—C37	1.316 (9)	C24—H24	0.9300
N1—C41	1.364 (9)	C25—C26	1.513 (9)
N2—C46	1.323 (9)	C26—C27	1.501 (10)
N2—C42	1.355 (9)	C26—H26A	0.9700
N3—C49	1.280 (13)	C26—H26B	0.9700
N3—C51	1.426 (13)	C27—C28	1.379 (11)
N3—C50	1.456 (12)	C27—C32	1.409 (11)
O1—C1	1.272 (7)	C28—C29	1.415 (11)
O1—Tb1^{i}	2.349 (4)	C28—H28	0.9300
O1—Sm1^{i}	2.349 (4)	C29—C30	1.336 (12)
O2—C1	1.228 (7)	C29—H29	0.9300
O3—C13	1.245 (9)	C30—C31	1.399 (12)
O4—C13	1.249 (9)	C30—H30	0.9300
O5—C25	1.251 (7)	C31—C32	1.427 (11)
O6—C25	1.262 (8)	C31—C36	1.428 (13)
O6—Tb1^{i}	2.382 (4)	C32—C33	1.412 (11)
O6—Sm1^{i}	2.382 (4)	C33—C34	1.364 (12)
O7—C49	1.259 (13)	C33—H33	0.9300
C1—C2	1.520 (9)	C34—C35	1.395 (13)
C2—C3	1.514 (9)	C34—H34	0.9300
C2—H2A	0.9700	C35—C36	1.346 (13)

C2—H2B	0.9700	C35—H35	0.9300
C3—C4	1.355 (11)	C36—H36	0.9300
C3—C8	1.419 (11)	C37—C38	1.421 (10)
C4—C5	1.409 (11)	C37—H37	0.9300
C4—H4	0.9300	C38—C39	1.348 (11)
C5—C6	1.332 (12)	C38—H38	0.9300
C5—H5	0.9300	C39—C40	1.377 (11)
C6—C7	1.406 (12)	C39—H39	0.9300
C6—H6	0.9300	C40—C41	1.416 (9)
C7—C12	1.399 (12)	C40—C47	1.438 (11)
C7—C8	1.421 (11)	C41—C42	1.433 (10)
C8—C9	1.405 (11)	C42—C43	1.408 (10)
C9—C10	1.370 (12)	C43—C44	1.373 (12)
C9—H9	0.9300	C43—C48	1.426 (11)
C10—C11	1.392 (13)	C44—C45	1.372 (12)
C10—H10	0.9300	C44—H44	0.9300
C11—C12	1.341 (14)	C45—C46	1.392 (10)
C11—H11	0.9300	C45—H45	0.9300
C12—H12	0.9300	C46—H46	0.9300
C13—C14	1.521 (10)	C47—C48	1.316 (11)
C14—C15	1.483 (12)	C47—H47	0.9300
C14—H14A	0.9700	C48—H48	0.9300
C14—H14B	0.9700	C49—H49	0.9300
C15—C16	1.375 (13)	C50—H50A	0.9600
C15—C20	1.417 (13)	C50—H50B	0.9600
C16—C17	1.435 (13)	C50—H50C	0.9600
C16—H16	0.9300	C51—H51A	0.9600
C17—C18	1.317 (14)	C51—H51B	0.9600
C17—H17	0.9300	C51—H51C	0.9600
$O1^{i}$—Sm1—O5	74.13 (14)	H14A—C14—H14B	107.8
$O1^{i}$—Sm1—$O6^{i}$	77.25 (14)	C16—C15—C20	119.1 (9)
O5—Sm1—$O6^{i}$	136.64 (15)	C16—C15—C14	120.4 (9)
$O1^{i}$—Sm1—O4	86.30 (16)	C20—C15—C14	120.4 (9)
O5—Sm1—O4	125.39 (17)	C15—C16—C17	118.8 (10)
$O6^{i}$—Sm1—O4	83.81 (17)	C15—C16—H16	120.6
$O1^{i}$—Sm1—O3	75.12 (15)	C17—C16—H16	120.6
O5—Sm1—O3	73.24 (17)	C18—C17—C16	121.7 (11)
$O6^{i}$—Sm1—O3	128.83 (17)	C18—C17—H17	119.2
O4—Sm1—O3	52.40 (17)	C16—C17—H17	119.2
$O1^{i}$—Sm1—O2	123.42 (14)	C17—C18—C19	122.1 (11)
O5—Sm1—O2	77.30 (15)	C17—C18—H18	118.9
$O6^{i}$—Sm1—O2	92.55 (15)	C19—C18—H18	118.9
O4—Sm1—O2	148.57 (15)	C18—C19—C24	123.2 (11)
O3—Sm1—O2	138.56 (16)	C18—C19—C20	118.3 (11)
$O1^{i}$—Sm1—N2	142.27 (17)	C24—C19—C20	118.5 (11)
O5—Sm1—N2	78.59 (16)	C21—C20—C15	121.8 (9)

O6^{i}—Sm1—N2	139.25 (17)	C21—C20—C19	118.2 (10)
O4—Sm1—N2	88.76 (18)	C15—C20—C19	120.0 (10)
O3—Sm1—N2	72.36 (18)	C22—C21—C20	120.4 (10)
O2—Sm1—N2	73.76 (17)	C22—C21—H21	119.8
O1^{i}—Sm1—O1	73.04 (16)	C20—C21—H21	119.8
O5—Sm1—O1	69.07 (14)	C23—C22—C21	118.3 (11)
O6^{i}—Sm1—O1	71.84 (14)	C23—C22—H22	120.9
O4—Sm1—O1	150.80 (15)	C21—C22—H22	120.9
O3—Sm1—O1	135.76 (15)	C24—C23—C22	124.3 (12)
O2—Sm1—O1	51.27 (13)	C24—C23—H23	117.8
N2—Sm1—O1	120.20 (16)	C22—C23—H23	117.8
O1^{i}—Sm1—N1	149.18 (16)	C23—C24—C19	120.3 (11)
O5—Sm1—N1	136.67 (16)	C23—C24—H24	119.9
O6^{i}—Sm1—N1	76.13 (16)	C19—C24—H24	119.9
O4—Sm1—N1	75.67 (17)	O5—C25—O6	126.3 (6)
O3—Sm1—N1	110.76 (17)	O5—C25—C26	116.2 (6)
O2—Sm1—N1	73.16 (15)	O6—C25—C26	117.4 (6)
N2—Sm1—N1	63.22 (18)	C27—C26—C25	116.8 (6)
O1—Sm1—N1	112.40 (15)	C27—C26—H26A	108.1
O1^{i}—Sm1—Tb1^{i}	38.40 (11)	C25—C26—H26A	108.1
O5—Sm1—Tb1^{i}	66.76 (10)	C27—C26—H26B	108.1
O6^{i}—Sm1—Tb1^{i}	70.52 (10)	C25—C26—H26B	108.1
O4—Sm1—Tb1^{i}	121.91 (12)	H26A—C26—H26B	107.3
O3—Sm1—Tb1^{i}	108.21 (11)	C28—C27—C32	118.3 (7)
O2—Sm1—Tb1^{i}	85.47 (10)	C28—C27—C26	119.3 (8)
N2—Sm1—Tb1^{i}	142.82 (13)	C32—C27—C26	122.3 (7)
O1—Sm1—Tb1^{i}	34.64 (9)	C27—C28—C29	121.3 (9)
N1—Sm1—Tb1^{i}	139.27 (13)	C27—C28—H28	119.3
O1^{i}—Sm1—Sm1^{i}	38.40 (11)	C29—C28—H28	119.3
O5—Sm1—Sm1^{i}	66.76 (10)	C30—C29—C28	120.2 (9)
O6^{i}—Sm1—Sm1^{i}	70.52 (10)	C30—C29—H29	119.9
O4—Sm1—Sm1^{i}	121.91 (12)	C28—C29—H29	119.9
O3—Sm1—Sm1^{i}	108.21 (11)	C29—C30—C31	121.4 (9)
O2—Sm1—Sm1^{i}	85.47 (10)	C29—C30—H30	119.3
N2—Sm1—Sm1^{i}	142.82 (13)	C31—C30—H30	119.3
O1—Sm1—Sm1^{i}	34.64 (9)	C30—C31—C32	118.7 (9)
N1—Sm1—Sm1^{i}	139.27 (13)	C30—C31—C36	122.2 (9)
Tb1^{i}—Sm1—Sm1^{i}	0.000 (8)	C32—C31—C36	119.0 (9)
C37—N1—C41	118.8 (6)	C27—C32—C33	121.8 (7)
C37—N1—Sm1	122.8 (4)	C27—C32—C31	120.0 (8)
C41—N1—Sm1	118.3 (4)	C33—C32—C31	118.2 (8)
C46—N2—C42	117.1 (6)	C34—C33—C32	120.0 (8)
C46—N2—Sm1	120.9 (5)	C34—C33—H33	120.0
C42—N2—Sm1	122.0 (5)	C32—C33—H33	120.0

C49—N3—C51	120.5 (10)	C33—C34—C35	122.1 (10)
C49—N3—C50	120.6 (10)	C33—C34—H34	118.9
C51—N3—C50	118.9 (10)	C35—C34—H34	118.9
C1—O1—Tb1^{i}	155.1 (4)	C36—C35—C34	119.7 (10)
C1—O1—Sm1^{i}	155.1 (4)	C36—C35—H35	120.2
C1—O1—Sm1	89.8 (4)	C34—C35—H35	120.2
Tb1^{i}—O1—Sm1	106.96 (16)	C35—C36—C31	120.9 (9)
Sm1^{i}—O1—Sm1	106.96 (16)	C35—C36—H36	119.6
C1—O2—Sm1	94.8 (4)	C31—C36—H36	119.6
C13—O3—Sm1	92.1 (5)	N1—C37—C38	122.4 (7)
C13—O4—Sm1	93.6 (4)	N1—C37—H37	118.8
C25—O5—Sm1	138.7 (4)	C38—C37—H37	118.8
C25—O6—Tb1^{i}	133.5 (4)	C39—C38—C37	118.6 (8)
C25—O6—Sm1^{i}	133.5 (4)	C39—C38—H38	120.7
O2—C1—O1	122.0 (6)	C37—C38—H38	120.7
O2—C1—C2	122.0 (6)	C38—C39—C40	120.7 (7)
O1—C1—C2	116.1 (6)	C38—C39—H39	119.6
C3—C2—C1	115.4 (6)	C40—C39—H39	119.6
C3—C2—H2A	108.4	C39—C40—C41	118.2 (7)
C1—C2—H2A	108.4	C39—C40—C47	123.5 (7)
C3—C2—H2B	108.4	C41—C40—C47	118.3 (8)
C1—C2—H2B	108.4	N1—C41—C40	121.2 (7)
H2A—C2—H2B	107.5	N1—C41—C42	118.9 (6)
C4—C3—C8	119.3 (7)	C40—C41—C42	119.9 (7)
C4—C3—C2	118.8 (7)	N2—C42—C43	123.5 (7)
C8—C3—C2	121.9 (7)	N2—C42—C41	117.5 (6)
C3—C4—C5	122.0 (8)	C43—C42—C41	119.0 (7)
C3—C4—H4	119.0	C44—C43—C42	116.2 (8)
C5—C4—H4	119.0	C44—C43—C48	124.4 (8)
C6—C5—C4	119.3 (9)	C42—C43—C48	119.4 (8)
C6—C5—H5	120.4	C45—C44—C43	121.9 (8)
C4—C5—H5	120.4	C45—C44—H44	119.0
C5—C6—C7	121.9 (8)	C43—C44—H44	119.0
C5—C6—H6	119.0	C44—C45—C46	117.2 (8)
C7—C6—H6	119.0	C44—C45—H45	121.4
C12—C7—C6	121.7 (8)	C46—C45—H45	121.4
C12—C7—C8	119.5 (9)	N2—C46—C45	124.1 (8)
C6—C7—C8	118.8 (8)	N2—C46—H46	118.0
C9—C8—C3	122.6 (7)	C45—C46—H46	118.0
C9—C8—C7	118.8 (8)	C48—C47—C40	121.7 (7)
C3—C8—C7	118.6 (8)	C48—C47—H47	119.1
C10—C9—C8	120.8 (8)	C40—C47—H47	119.1
C10—C9—H9	119.6	C47—C48—C43	121.7 (8)
C8—C9—H9	119.6	C47—C48—H48	119.2
C9—C10—C11	118.3 (10)	C43—C48—H48	119.2
C9—C10—H10	120.9	O7—C49—N3	124.1 (12)
C11—C10—H10	120.9	O7—C49—H49	117.9
C12—C11—C10	123.7 (10)	N3—C49—H49	117.9

C12—C11—H11	118.2	N3—C50—H50A	109.5
C10—C11—H11	118.2	N3—C50—H50B	109.5
C11—C12—C7	119.0 (9)	H50A—C50—H50B	109.5
C11—C12—H12	120.5	N3—C50—H50C	109.5
C7—C12—H12	120.5	H50A—C50—H50C	109.5
O3—C13—O4	121.6 (7)	H50B—C50—H50C	109.5
O3—C13—C14	117.0 (8)	N3—C51—H51A	109.5
O4—C13—C14	121.4 (7)	N3—C51—H51B	109.5
C15—C14—C13	113.1 (7)	H51A—C51—H51B	109.5
C15—C14—H14A	109.0	N3—C51—H51C	109.5
C13—C14—H14A	109.0	H51A—C51—H51C	109.5
C15—C14—H14B	109.0	H51B—C51—H51C	109.5
C13—C14—H14B	109.0		
O1^{i}—Sm1—N1—C37	28.8 (7)	C8—C3—C4—C5	0.9 (12)
O5—Sm1—N1—C37	−148.2 (5)	C2—C3—C4—C5	179.2 (7)
O6^{i}—Sm1—N1—C37	−2.1 (5)	C3—C4—C5—C6	0.3 (13)
O4—Sm1—N1—C37	84.9 (6)	C4—C5—C6—C7	−1.8 (13)
O3—Sm1—N1—C37	124.5 (5)	C5—C6—C7—C12	−177.8 (8)
O2—Sm1—N1—C37	−99.2 (6)	C5—C6—C7—C8	1.9 (13)
N2—Sm1—N1—C37	−179.1 (6)	C4—C3—C8—C9	179.4 (7)
O1—Sm1—N1—C37	−65.4 (6)	C2—C3—C8—C9	1.2 (11)
Tb1^{i}—Sm1—N1—C37	−37.7 (6)	C4—C3—C8—C7	−0.8 (11)
Sm1^{i}—Sm1—N1—C37	−37.7 (6)	C2—C3—C8—C7	−179.0 (7)
O1^{i}—Sm1—N1—C41	−153.8 (4)	C12—C7—C8—C9	−1.1 (12)
O5—Sm1—N1—C41	29.1 (6)	C6—C7—C8—C9	179.3 (8)
O6^{i}—Sm1—N1—C41	175.2 (5)	C12—C7—C8—C3	179.1 (7)
O4—Sm1—N1—C41	−97.8 (5)	C6—C7—C8—C3	−0.6 (11)
O3—Sm1—N1—C41	−58.2 (5)	C3—C8—C9—C10	179.5 (8)
O2—Sm1—N1—C41	78.1 (5)	C7—C8—C9—C10	−0.3 (12)
N2—Sm1—N1—C41	−1.8 (5)	C8—C9—C10—C11	1.5 (14)
O1—Sm1—N1—C41	111.9 (5)	C9—C10—C11—C12	−1.3 (17)
Tb1^{i}—Sm1—N1—C41	139.6 (4)	C10—C11—C12—C7	−0.2 (16)
Sm1^{i}—Sm1—N1—C41	139.6 (4)	C6—C7—C12—C11	−179.0 (9)
O1^{i}—Sm1—N2—C46	−22.3 (7)	C8—C7—C12—C11	1.3 (14)
O5—Sm1—N2—C46	21.9 (6)	Sm1—O3—C13—O4	−5.8 (8)
O6^{i}—Sm1—N2—C46	176.3 (5)	Sm1—O3—C13—C14	173.6 (6)
O4—Sm1—N2—C46	−104.6 (6)	Sm1—O4—C13—O3	5.9 (8)
O3—Sm1—N2—C46	−53.9 (6)	Sm1—O4—C13—C14	−173.5 (7)
O2—Sm1—N2—C46	101.8 (6)	O3—C13—C14—C15	−54.3 (11)
O1—Sm1—N2—C46	79.3 (6)	O4—C13—C14—C15	125.1 (9)
N1—Sm1—N2—C46	−179.2 (6)	C13—C14—C15—C16	107.2 (10)
Tb1^{i}—Sm1—N2—C46	43.2 (7)	C13—C14—C15—C20	−67.9 (11)
Sm1^{i}—Sm1—N2—C46	43.2 (7)	C20—C15—C16—C17	−1.1 (13)
O1^{i}—Sm1—N2—C42	159.1 (5)	C14—C15—C16—C17	−176.3 (8)
O5—Sm1—N2—C42	−156.7 (6)	C15—C16—C17—C18	2.5 (15)
O6^{i}—Sm1—N2—C42	−2.3 (7)	C16—C17—C18—C19	−2.7 (17)

O4—Sm1—N2—C42	76.7 (6)	C17—C18—C19—C24	178.9 (10)
O3—Sm1—N2—C42	127.4 (6)	C17—C18—C19—C20	1.6 (16)
O2—Sm1—N2—C42	−76.8 (5)	C16—C15—C20—C21	179.6 (8)
O1—Sm1—N2—C42	−99.4 (5)	C14—C15—C20—C21	−5.2 (13)
N1—Sm1—N2—C42	2.2 (5)	C16—C15—C20—C19	0.0 (13)
$Tb1^{i}$—Sm1—N2—C42	−135.5 (5)	C14—C15—C20—C19	175.2 (8)
$Sm1^{i}$—Sm1—N2—C42	−135.5 (5)	C18—C19—C20—C21	−179.8 (9)
$O1^{i}$—Sm1—O1—C1	161.3 (4)	C24—C19—C20—C21	2.8 (13)
O5—Sm1—O1—C1	82.2 (4)	C18—C19—C20—C15	−0.2 (14)
$O6^{i}$—Sm1—O1—C1	−116.9 (4)	C24—C19—C20—C15	−177.6 (9)
O4—Sm1—O1—C1	−151.9 (4)	C15—C20—C21—C22	178.5 (8)
O3—Sm1—O1—C1	115.6 (4)	C19—C20—C21—C22	−1.9 (13)
O2—Sm1—O1—C1	−8.1 (3)	C20—C21—C22—C23	0.4 (14)
N2—Sm1—O1—C1	20.1 (4)	C21—C22—C23—C24	0.2 (16)
N1—Sm1—O1—C1	−51.0 (4)	C22—C23—C24—C19	0.7 (17)
$Tb1^{i}$—Sm1—O1—C1	161.3 (4)	C18—C19—C24—C23	−179.5 (10)
$Sm1^{i}$—Sm1—O1—C1	161.3 (4)	C20—C19—C24—C23	−2.2 (15)
$O1^{i}$—Sm1—O1—$Tb1^{i}$	0.0	Sm1—O5—C25—O6	−29.9 (12)
O5—Sm1—O1—$Tb1^{i}$	−79.08 (17)	Sm1—O5—C25—C26	152.5 (5)
$O6^{i}$—Sm1—O1—$Tb1^{i}$	81.79 (17)	$Tb1^{i}$—O6—C25—O5	10.3 (11)
O4—Sm1—O1—$Tb1^{i}$	46.8 (4)	$Sm1^{i}$—O6—C25—O5	10.3 (11)
O3—Sm1—O1—$Tb1^{i}$	−45.7 (3)	$Tb1^{i}$—O6—C25—C26	−172.1 (5)
O2—Sm1—O1—$Tb1^{i}$	−169.4 (2)	$Sm1^{i}$—O6—C25—C26	−172.1 (5)
N2—Sm1—O1—$Tb1^{i}$	−141.19 (18)	O5—C25—C26—C27	−139.4 (7)
N1—Sm1—O1—$Tb1^{i}$	147.71 (17)	O6—C25—C26—C27	42.8 (10)
$Sm1^{i}$—Sm1—O1—$Tb1^{i}$	0.0	C25—C26—C27—C28	−119.9 (8)
$O1^{i}$—Sm1—O1—$Sm1^{i}$	0.0	C25—C26—C27—C32	63.6 (10)
O5—Sm1—O1—$Sm1^{i}$	−79.08 (17)	C32—C27—C28—C29	−1.3 (12)
$O6^{i}$—Sm1—O1—$Sm1^{i}$	81.79 (17)	C26—C27—C28—C29	−177.9 (7)
O4—Sm1—O1—$Sm1^{i}$	46.8 (4)	C27—C28—C29—C30	0.8 (13)
O3—Sm1—O1—$Sm1^{i}$	−45.7 (3)	C28—C29—C30—C31	1.0 (14)
O2—Sm1—O1—$Sm1^{i}$	−169.4 (2)	C29—C30—C31—C32	−2.2 (13)
N2—Sm1—O1—$Sm1^{i}$	−141.19 (18)	C29—C30—C31—C36	175.8 (8)
N1—Sm1—O1—$Sm1^{i}$	147.71 (17)	C28—C27—C32—C33	−178.3 (8)
$Tb1^{i}$—Sm1—O1—$Sm1^{i}$	0.0	C26—C27—C32—C33	−1.8 (12)
$O1^{i}$—Sm1—O2—C1	−3.8 (4)	C28—C27—C32—C31	0.1 (11)
O5—Sm1—O2—C1	−64.8 (4)	C26—C27—C32—C31	176.6 (7)
$O6^{i}$—Sm1—O2—C1	72.6 (4)	C30—C31—C32—C27	1.6 (12)
O4—Sm1—O2—C1	154.9 (4)	C36—C31—C32—C27	−176.5 (8)
O3—Sm1—O2—C1	−110.2 (4)	C30—C31—C32—C33	−180.0 (8)
N2—Sm1—O2—C1	−146.5 (4)	C36—C31—C32—C33	2.0 (12)
O1—Sm1—O2—C1	8.4 (4)	C27—C32—C33—C34	177.2 (8)
N1—Sm1—O2—C1	147.3 (4)	C31—C32—C33—C34	−1.3 (12)

Tb1^{i}—Sm1—O2—C1	2.4 (4)	C32—C33—C34—C35	−0.6 (13)
Sm1^{i}—Sm1—O2—C1	2.4 (4)	C33—C34—C35—C36	1.8 (15)
O1^{i}—Sm1—O3—C13	100.1 (4)	C34—C35—C36—C31	−1.0 (14)
O5—Sm1—O3—C13	177.7 (5)	C30—C31—C36—C35	−178.9 (9)
O6^{i}—Sm1—O3—C13	40.6 (5)	C32—C31—C36—C35	−0.9 (13)
O4—Sm1—O3—C13	3.2 (4)	C41—N1—C37—C38	0.9 (11)
O2—Sm1—O3—C13	−135.8 (4)	Sm1—N1—C37—C38	178.2 (5)
N2—Sm1—O3—C13	−99.3 (5)	N1—C37—C38—C39	−0.7 (12)
O1—Sm1—O3—C13	145.2 (4)	C37—C38—C39—C40	−0.5 (12)
N1—Sm1—O3—C13	−48.0 (5)	C38—C39—C40—C41	1.2 (11)
Tb1^{i}—Sm1—O3—C13	119.9 (4)	C38—C39—C40—C47	−179.0 (7)
Sm1^{i}—Sm1—O3—C13	119.9 (4)	C37—N1—C41—C40	−0.1 (10)
O1^{i}—Sm1—O4—C13	−77.2 (4)	Sm1—N1—C41—C40	−177.5 (5)
O5—Sm1—O4—C13	−9.7 (5)	C37—N1—C41—C42	178.9 (7)
O6^{i}—Sm1—O4—C13	−154.8 (4)	Sm1—N1—C41—C42	1.5 (8)
O3—Sm1—O4—C13	−3.2 (4)	C39—C40—C41—N1	−1.0 (11)
O2—Sm1—O4—C13	120.5 (5)	C47—C40—C41—N1	179.3 (7)
N2—Sm1—O4—C13	65.3 (4)	C39—C40—C41—C42	−179.9 (7)
O1—Sm1—O4—C13	−121.6 (5)	C47—C40—C41—C42	0.3 (11)
N1—Sm1—O4—C13	128.0 (5)	C46—N2—C42—C43	−2.9 (11)
Tb1^{i}—Sm1—O4—C13	−92.4 (4)	Sm1—N2—C42—C43	175.7 (6)
Sm1^{i}—Sm1—O4—C13	−92.4 (4)	C46—N2—C42—C41	178.9 (7)
O1^{i}—Sm1—O5—C25	−17.5 (7)	Sm1—N2—C42—C41	−2.4 (9)
O6^{i}—Sm1—O5—C25	33.1 (8)	N1—C41—C42—N2	0.5 (10)
O4—Sm1—O5—C25	−91.0 (7)	C40—C41—C42—N2	179.5 (7)
O3—Sm1—O5—C25	−96.3 (7)	N1—C41—C42—C43	−177.7 (7)
O2—Sm1—O5—C25	113.2 (7)	C40—C41—C42—C43	1.3 (11)
N2—Sm1—O5—C25	−171.1 (7)	N2—C42—C43—C44	1.6 (12)
O1—Sm1—O5—C25	60.1 (7)	C41—C42—C43—C44	179.7 (7)
N1—Sm1—O5—C25	161.0 (6)	N2—C42—C43—C48	179.5 (7)
Tb1^{i}—Sm1—O5—C25	22.7 (7)	C41—C42—C43—C48	−2.4 (11)
Sm1^{i}—Sm1—O5—C25	22.7 (7)	C42—C43—C44—C45	0.5 (13)
Sm1—O2—C1—O1	−15.7 (7)	C48—C43—C44—C45	−177.2 (9)
Sm1—O2—C1—C2	162.4 (6)	C43—C44—C45—C46	−1.2 (14)
Tb1^{i}—O1—C1—O2	148.3 (7)	C42—N2—C46—C45	2.2 (12)
Sm1^{i}—O1—C1—O2	148.3 (7)	Sm1—N2—C46—C45	−176.5 (7)
Sm1—O1—C1—O2	15.1 (6)	C44—C45—C46—N2	−0.2 (14)
Tb1^{i}—O1—C1—C2	−29.9 (13)	C39—C40—C47—C48	179.5 (8)
Sm1^{i}—O1—C1—C2	−29.9 (13)	C41—C40—C47—C48	−0.8 (12)
Sm1—O1—C1—C2	−163.1 (5)	C40—C47—C48—C43	−0.4 (13)
O2—C1—C2—C3	−3.8 (10)	C44—C43—C48—C47	179.7 (9)
O1—C1—C2—C3	174.5 (6)	C42—C43—C48—C47	2.0 (13)
C1—C2—C3—C4	111.5 (8)	C51—N3—C49—O7	4.7 (17)
C1—C2—C3—C8	−70.3 (9)	C50—N3—C49—O7	−177.4 (10)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6···O7^{ii}	0.93	2.57	3.459 (13)	160
C33—H33···O3	0.93	2.59	3.404 (10)	147
C37—H37···O6^{i}	0.93	2.36	3.023 (8)	128
C46—H46···O5	0.93	2.47	3.074 (9)	122
C47—H47···O2^{iii}	0.93	2.47	3.328 (9)	153
C50—H50A···O4^{iv}	0.96	2.54	3.376 (12)	146
C51—H51A···O7	0.96	2.29	2.718 (16)	106
C39—H39···CG1^{iii}	0.93	2.98	3.853 (15)	157
C30—H30···CG2^{v}	0.93	2.89	3.663 (17)	142

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

Fig. 1

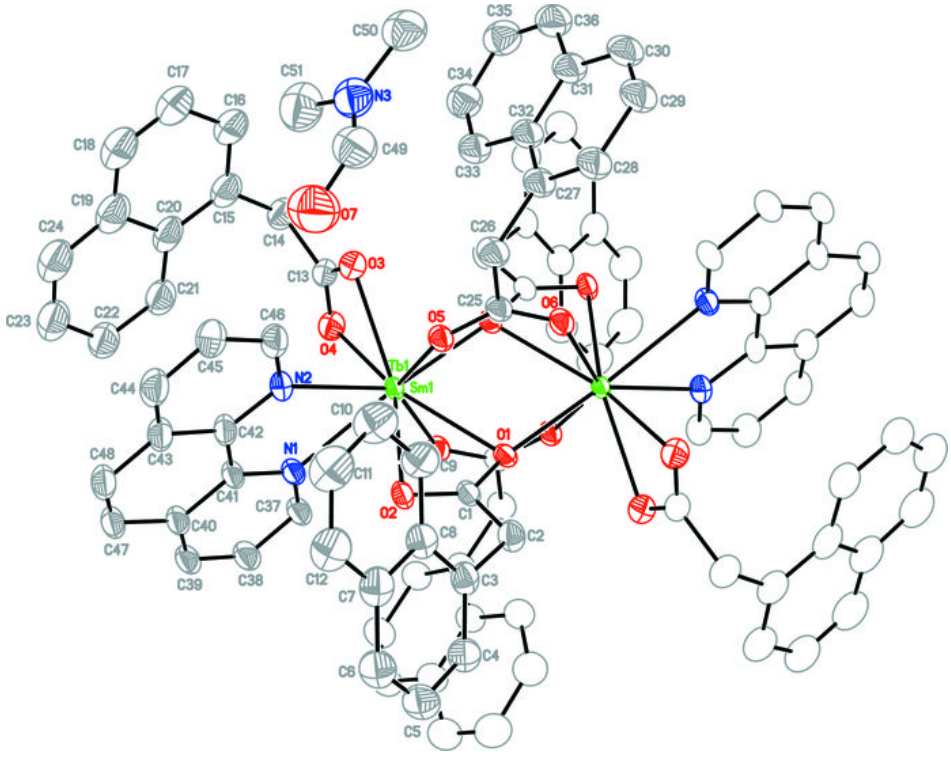
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Fig. 2

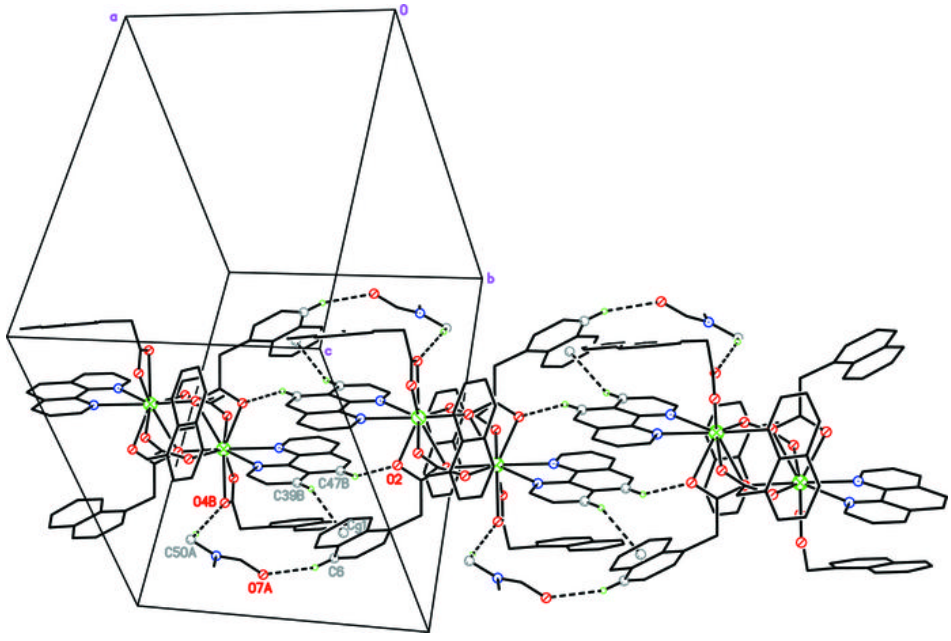

Fig. 3