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

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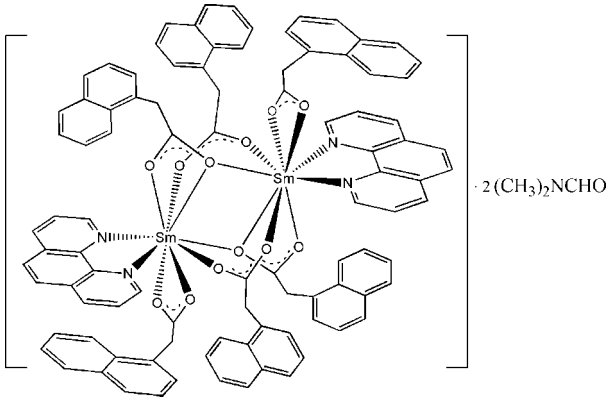
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.019 Å; R factor = 0.062; wR factor = 0.133; data-to-parameter ratio = 13.4.

The title complex, $[Sm_2(C_{12}H_9O_2)_6(C_{12}H_8N_2)_2]\cdot 2C_3H_7NO$, is centrosymmetric. The Sm atom is nine-coordinate in a distorted monocapped square-antiprismatic coordination geometry. 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. The combination of these 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, Liu, Wang & Chen (2007); Xia, Liu, Wang & Yang (2007).



Experimental

Crystal data

$[Sm_2(C_{12}H_9O_2)_6(C_{12}H_8N_2)_2]\cdot 2C_3H_7NO$
M_r = 1918.45
Monoclinic, $P2_1/c$
a = 13.4961 (17) Å
b = 15.096 (2) Å
c = 22.150 (2) Å
β = 103.720 (2)°
V = 4384.0 (10) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.40 mm^{-1}
T = 298 (2) K
0.43 × 0.13 × 0.10 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.585, T_{max} = 0.873
19845 measured reflections
7486 independent reflections
3943 reflections with $I > 2\sigma(I)$
R_{int} = 0.083

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.062
$wR(F^2)$ = 0.133
S = 1.03
7486 reflections
559 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.07 e Å^{-3}
$\Delta\rho_{min}$ = −1.39 e Å^{-3}

Table 1
Selected bond lengths (Å).

Sm1—O1^{i}	2.351 (6)	Sm1—O5	2.486 (6)
Sm1—O3	2.379 (5)	Sm1—N2	2.559 (7)
Sm1—O4^{i}	2.386 (6)	Sm1—O1	2.560 (6)
Sm1—O6	2.456 (7)	Sm1—N1	2.616 (7)
Sm1—O2	2.478 (6)		

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

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

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

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6···O7^{ii}	0.93	2.55	3.438 (18)	159
C37—H37···O4^{i}	0.93	2.37	3.036 (12)	129
C46—H46···O3	0.93	2.48	3.074 (13)	122
C47—H47···O2^{iii}	0.93	2.46	3.314 (13)	153
C50—H50*A*···O6^{iv}	0.96	2.58	3.369 (16)	139
C18—H18···*Cg*1^{v}	0.93	2.88	3.661 (15)	143

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: *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: AT2419).

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supplementary materials

Acta Cryst. (2007). E**63**, m2708-m2709 [**doi:10.1107/S1600536807049203**]

Tetrakis(*μ*-naphthalene-1-acetato)bis[(naphthalene-1-acetato)(1,10-phenanthroline)samarium(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 forth complexes $[Eu(NAA)_3(phen)]_2\cdot 2DMF$ (II), $[Gd(NAA)_3(phen)]_2\cdot 2DMF$ (III) (Liu *et al.*, 2007*a*,*b*), $[Pr(NAA)_3(phen)]_2\cdot DMF$ and $[Tb(NAA)_3(phen)]_2\cdot 2DMF$ (IV) (Xia, Liu, Wang & Chen, 2007; Xia, Liu, Wang & Yang, 2007). We repot here a similar structure of Hexakis(*μ*-naphthalene-1-acetato)bis- [(1,10-phenanthroline)samarium(III)] *N*,*N*-dimethylformamide disolvate, (I) (Fig. 1).

In the title complex, the coordination environment of Sm atom and coordination modes of the NNA ligands coordinated to the Sm^{III} ion are in agreement with the complex (II), (III) and (IV) (Fig. 1). The average bond lengths of between the samarium center and carboxylic oxygen atoms are 2.456 (7) Å, shorter than that (2.4725 (5) Å) of complex (II), longer than that 2.441 (7) of complex (III) and that 2.450 (7) of complex (IV). The dihedral angles between the least-square-plane Sm_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 plane and phen ring is 81.45 (12)°.

In (I), the molecules 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 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) 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.

*Cg*1 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 $Sm(NO_3)_3\cdot 6H_2O$ (0.364 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

The space group was uniquely assigned from the systematic absences. 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), 0.97 Å (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

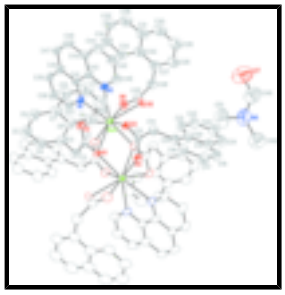


Fig. 1. The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are at the 30% probability level. Unlabelled atoms in the molecular are related to labelled atoms by (1 − *x*, 1 − *y*, 2 − *z*).

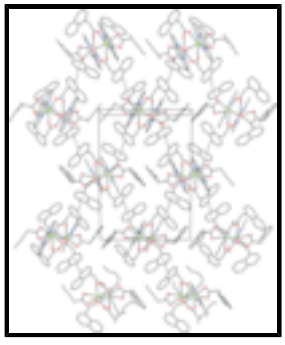


Fig. 2. A larger portion of the crystal structure of (I), showing the formation of a hydrogen-bonded chain built from C—H···π. For clarity, H atoms not involved in the hydrogen bonding have been omitted. Dashed lines indicate hydrogen bonds. [Symmetry codes: (A) 1 − *x*, −1/2 + *y*, 3/2 − *z*, (B) 1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

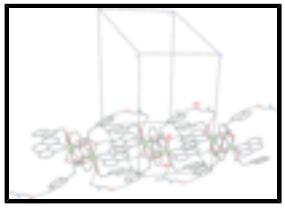


Fig. 3. A larger portion of the crystal structure of (I), showing the formation of a hydrogen-bonded chain built from C—H···O. For clarity, H atoms not involved in the hydrogen bonding have been omitted. Dashed lines indicate hydrogen bonds. [Symmetry codes: (C) *x*, *y*, 1 + *z*,, (D) − *x*, 1 − *y*,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

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

Crystal data

$[Sm_2(C_{12}H_9O_2)_6(C_{12}H_8N_2)_2]\cdot 2C_3H_7NO$	F_{000} = 1948
M_r = 1918.45	D_x = 1.453 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 3404 reflections
a = 13.4961 (17) Å	θ = 2.4–25.3º
b = 15.096 (2) Å	μ = 1.40 mm^{-1}
c = 22.150 (2) Å	*T* = 298 (2) K
β = 103.720 (2)º	Block, colourless
V = 4384.0 (10) Å^3	0.43 × 0.13 × 0.10 mm
Z = 2	

Data collection

Siemens SMART 1000 CCD area-detector	7486 independent reflections

diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

T = 298(2) K

φ and ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

T_{min} = 0.585, T_{max} = 0.873

19845 measured reflections

3943 reflections with $I > 2\sigma(I)$

R_{int} = 0.083

θ_{max} = 25.0º

θ_{min} = 1.6º

$h = -14 \rightarrow 16$

$k = -17 \rightarrow 17$

$l = -21 \rightarrow 26$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.062

$wR(F^2)$ = 0.133

S = 1.03

7486 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

$w = 1/[\sigma^2(F_o^2) + 31.99P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max}$ = 0.001

$\Delta\rho_{max}$ = 1.07 e Å^{-3}

$\Delta\rho_{min}$ = −1.39 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}
Sm1	0.38257 (3)	0.42941 (3)	1.01172 (2)	0.03850 (16)
N1	0.2294 (6)	0.4434 (5)	1.0647 (4)	0.046 (2)
N2	0.2116 (5)	0.3639 (6)	0.9536 (4)	0.052 (2)
N3	0.3672 (11)	0.3362 (9)	0.2530 (6)	0.097 (4)
O1	0.4406 (4)	0.5797 (4)	0.9790 (3)	0.0421 (15)
O2	0.2765 (4)	0.5553 (4)	0.9616 (3)	0.0493 (17)
O3	0.4038 (4)	0.4246 (5)	0.9082 (3)	0.0488 (16)
O4	0.5490 (5)	0.4870 (4)	0.8964 (3)	0.0445 (17)
O5	0.4123 (5)	0.2716 (4)	0.9893 (4)	0.060 (2)

O6	0.4040 (5)	0.3033 (5)	1.0837 (3)	0.061 (2)
O7	0.2330 (10)	0.2449 (9)	0.2356 (6)	0.162 (5)
C1	0.3480 (8)	0.5986 (7)	0.9516 (4)	0.047 (3)
C2	0.3348 (7)	0.6731 (7)	0.9059 (5)	0.064 (3)
H2A	0.3765	0.6611	0.8767	0.076*
H2B	0.3605	0.7268	0.9282	0.076*
C3	0.2263 (8)	0.6899 (8)	0.8693 (5)	0.060 (3)
C4	0.1777 (9)	0.7626 (8)	0.8802 (5)	0.071 (3)
H4	0.2113	0.8020	0.9105	0.085*
C5	0.0766 (10)	0.7825 (9)	0.8474 (6)	0.080 (4)
H5	0.0448	0.8342	0.8558	0.096*
C6	0.0269 (10)	0.7249 (10)	0.8035 (6)	0.080 (4)
H6	−0.0401	0.7366	0.7826	0.096*
C7	0.0746 (10)	0.6487 (10)	0.7892 (6)	0.074 (4)
C8	0.1752 (9)	0.6295 (9)	0.8234 (6)	0.068 (3)
C9	0.2213 (10)	0.5514 (9)	0.8093 (6)	0.079 (4)
H9	0.2874	0.5379	0.8311	0.095*
C10	0.1710 (12)	0.4948 (10)	0.7643 (7)	0.101 (5)
H10	0.2030	0.4437	0.7552	0.121*
C11	0.0702 (12)	0.5144 (11)	0.7317 (6)	0.102 (5)
H11	0.0353	0.4755	0.7015	0.123*
C12	0.0244 (11)	0.5892 (10)	0.7440 (6)	0.091 (4)
H12	−0.0419	0.6015	0.7220	0.110*
C13	0.4737 (7)	0.4361 (7)	0.8807 (4)	0.047 (2)
C14	0.4631 (8)	0.3846 (7)	0.8206 (5)	0.063 (3)
H14A	0.4150	0.3368	0.8203	0.076*
H14B	0.4333	0.4238	0.7863	0.076*
C15	0.5586 (9)	0.3455 (8)	0.8080 (5)	0.065 (3)
C16	0.5889 (9)	0.3721 (8)	0.7559 (5)	0.075 (4)
H16	0.5513	0.4143	0.7295	0.090*
C17	0.6784 (10)	0.3346 (9)	0.7423 (6)	0.083 (4)
H17	0.7009	0.3548	0.7082	0.099*
C18	0.7296 (10)	0.2710 (9)	0.7782 (6)	0.083 (4)
H18	0.7868	0.2465	0.7680	0.099*
C19	0.7002 (10)	0.2398 (9)	0.8307 (6)	0.074 (4)
C20	0.6132 (9)	0.2797 (8)	0.8467 (6)	0.067 (3)
C21	0.5844 (10)	0.2474 (9)	0.8989 (6)	0.075 (4)
H21	0.5290	0.2729	0.9105	0.090*
C22	0.6350 (11)	0.1795 (9)	0.9335 (6)	0.089 (4)
H22	0.6133	0.1584	0.9677	0.106*
C23	0.7203 (11)	0.1415 (9)	0.9173 (7)	0.094 (4)
H23	0.7550	0.0953	0.9409	0.113*
C24	0.7516 (10)	0.1709 (9)	0.8686 (7)	0.086 (4)
H24	0.8089	0.1455	0.8591	0.103*
C25	0.4099 (9)	0.2486 (8)	1.0423 (7)	0.068 (3)
C26	0.4134 (9)	0.1489 (8)	1.0564 (6)	0.079 (4)
H26A	0.4801	0.1258	1.0553	0.095*
H26B	0.4035	0.1395	1.0979	0.095*
C27	0.3334 (12)	0.0998 (9)	1.0106 (7)	0.086 (4)

C28	0.3594 (12)	0.0468 (9)	0.9656 (7)	0.097 (4)
H28	0.4272	0.0401	0.9640	0.116*
C29	0.2805 (15)	0.0029 (10)	0.9220 (8)	0.109 (5)
H29	0.2975	−0.0360	0.8935	0.131*
C30	0.1813 (15)	0.0166 (11)	0.9212 (8)	0.112 (5)
H30	0.1315	−0.0090	0.8897	0.135*
C31	0.1520 (14)	0.0667 (12)	0.9650 (9)	0.102 (5)
C32	0.2301 (13)	0.1107 (9)	1.0113 (7)	0.090 (4)
C33	0.1993 (11)	0.1620 (9)	1.0567 (7)	0.092 (4)
H33	0.2485	0.1889	1.0879	0.110*
C34	0.0965 (12)	0.1730 (9)	1.0558 (7)	0.097 (5)
H34	0.0768	0.2076	1.0857	0.116*
C35	0.0237 (13)	0.1313 (11)	1.0093 (9)	0.111 (5)
H35	−0.0449	0.1367	1.0094	0.133*
C36	0.0496 (14)	0.0842 (11)	0.9652 (8)	0.110 (5)
H36	−0.0017	0.0619	0.9330	0.132*
C37	0.2354 (8)	0.4826 (7)	1.1180 (5)	0.063 (3)
H37	0.2986	0.5050	1.1386	0.075*
C38	0.1539 (9)	0.4936 (8)	1.1466 (6)	0.073 (4)
H38	0.1631	0.5219	1.1848	0.087*
C39	0.0609 (9)	0.4615 (7)	1.1166 (6)	0.068 (3)
H39	0.0053	0.4672	1.1343	0.082*
C40	0.0497 (8)	0.4205 (8)	1.0598 (6)	0.064 (3)
C41	0.1359 (8)	0.4122 (7)	1.0347 (5)	0.061 (3)
C42	0.1273 (8)	0.3709 (8)	0.9755 (6)	0.065 (3)
C43	0.0312 (9)	0.3377 (8)	0.9432 (7)	0.076 (4)
C44	0.0264 (10)	0.2988 (9)	0.8859 (7)	0.086 (4)
H44	−0.0356	0.2778	0.8625	0.103*
C45	0.1104 (10)	0.2911 (9)	0.8639 (6)	0.087 (4)
H45	0.1071	0.2645	0.8256	0.104*
C46	0.2031 (9)	0.3236 (8)	0.8995 (6)	0.077 (4)
H46	0.2614	0.3166	0.8845	0.092*
C47	−0.0459 (9)	0.3862 (8)	1.0251 (6)	0.072 (4)
H47	−0.1033	0.3908	1.0413	0.087*
C48	−0.0539 (9)	0.3479 (8)	0.9704 (7)	0.080 (4)
H48	−0.1173	0.3270	0.9489	0.096*
C49	0.3091 (15)	0.2754 (14)	0.2198 (9)	0.123 (6)
H49	0.3249	0.2546	0.1836	0.148*
C50	0.4569 (11)	0.3668 (9)	0.2338 (7)	0.112 (5)
H50A	0.4696	0.3286	0.2018	0.168*
H50B	0.5147	0.3658	0.2687	0.168*
H50C	0.4458	0.4261	0.2181	0.168*
C51	0.3411 (13)	0.3732 (11)	0.3057 (7)	0.145 (7)
H51A	0.2716	0.3587	0.3051	0.217*
H51B	0.3487	0.4364	0.3051	0.217*
H51C	0.3852	0.3497	0.3427	0.217*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sm1	0.0269 (2)	0.0437 (3)	0.0476 (3)	−0.0026 (3)	0.0142 (2)	−0.0031 (3)
N1	0.039 (5)	0.049 (5)	0.057 (5)	0.004 (4)	0.022 (4)	0.007 (4)
N2	0.023 (4)	0.072 (6)	0.056 (6)	−0.009 (4)	−0.002 (4)	−0.014 (5)
N3	0.106 (11)	0.100 (10)	0.091 (10)	0.017 (8)	0.034 (8)	0.017 (8)
O1	0.032 (3)	0.044 (4)	0.054 (4)	−0.005 (3)	0.018 (3)	−0.001 (3)
O2	0.027 (3)	0.061 (5)	0.062 (4)	0.005 (3)	0.014 (3)	0.011 (4)
O3	0.044 (4)	0.067 (4)	0.040 (4)	−0.008 (4)	0.020 (3)	−0.007 (4)
O4	0.036 (4)	0.056 (4)	0.043 (4)	−0.011 (3)	0.012 (3)	−0.010 (3)
O5	0.073 (5)	0.027 (4)	0.085 (6)	−0.004 (4)	0.029 (5)	−0.009 (4)
O6	0.069 (5)	0.059 (5)	0.060 (5)	−0.005 (4)	0.024 (4)	0.002 (4)
O7	0.123 (10)	0.177 (13)	0.181 (13)	−0.013 (9)	0.026 (9)	0.053 (10)
C1	0.038 (6)	0.061 (8)	0.047 (6)	0.003 (5)	0.016 (5)	0.001 (5)
C2	0.052 (7)	0.072 (8)	0.065 (8)	−0.004 (6)	0.011 (6)	0.024 (6)
C3	0.051 (7)	0.071 (9)	0.058 (8)	0.003 (7)	0.011 (6)	0.023 (7)
C4	0.056 (8)	0.080 (10)	0.070 (9)	0.005 (7)	0.002 (7)	0.016 (7)
C5	0.072 (9)	0.086 (10)	0.079 (10)	0.016 (8)	0.009 (7)	0.020 (8)
C6	0.064 (9)	0.096 (11)	0.074 (10)	0.008 (8)	0.005 (7)	0.026 (8)
C7	0.068 (9)	0.085 (10)	0.063 (9)	−0.006 (8)	0.003 (7)	0.019 (8)
C8	0.060 (8)	0.079 (10)	0.061 (8)	0.001 (7)	0.008 (7)	0.022 (7)
C9	0.074 (9)	0.086 (11)	0.067 (9)	0.004 (8)	−0.002 (7)	0.011 (8)
C10	0.105 (12)	0.102 (12)	0.084 (11)	0.008 (10)	0.000 (9)	0.002 (9)
C11	0.096 (12)	0.104 (13)	0.086 (11)	−0.006 (10)	−0.020 (9)	0.008 (10)
C12	0.084 (10)	0.100 (13)	0.079 (10)	−0.004 (9)	−0.003 (8)	0.019 (9)
C13	0.051 (6)	0.048 (6)	0.048 (6)	0.003 (6)	0.026 (5)	−0.007 (6)
C14	0.069 (8)	0.068 (8)	0.058 (7)	−0.006 (6)	0.027 (6)	−0.020 (6)
C15	0.073 (8)	0.070 (9)	0.063 (8)	−0.003 (7)	0.036 (7)	−0.023 (7)
C16	0.082 (9)	0.072 (9)	0.075 (9)	0.001 (7)	0.030 (7)	−0.017 (7)
C17	0.092 (10)	0.089 (11)	0.079 (10)	−0.004 (8)	0.044 (8)	−0.021 (8)
C18	0.081 (10)	0.086 (11)	0.088 (11)	−0.001 (8)	0.033 (9)	−0.029 (8)
C19	0.078 (9)	0.072 (9)	0.079 (10)	−0.002 (7)	0.029 (8)	−0.021 (8)
C20	0.072 (8)	0.065 (8)	0.071 (9)	0.000 (7)	0.029 (7)	−0.016 (7)
C21	0.078 (9)	0.073 (9)	0.077 (9)	0.003 (7)	0.024 (8)	−0.012 (7)
C22	0.094 (11)	0.082 (11)	0.091 (11)	0.003 (9)	0.026 (9)	−0.010 (9)
C23	0.092 (11)	0.084 (11)	0.102 (12)	0.002 (9)	0.017 (9)	−0.009 (9)
C24	0.084 (10)	0.082 (11)	0.094 (11)	0.001 (8)	0.027 (9)	−0.023 (9)
C25	0.055 (8)	0.060 (9)	0.088 (10)	−0.007 (6)	0.017 (7)	0.010 (8)
C26	0.075 (9)	0.061 (8)	0.103 (10)	−0.001 (7)	0.024 (8)	0.011 (8)
C27	0.098 (12)	0.061 (9)	0.101 (12)	−0.005 (8)	0.025 (10)	0.010 (8)
C28	0.110 (12)	0.073 (11)	0.108 (12)	−0.012 (9)	0.027 (10)	0.007 (9)
C29	0.127 (15)	0.082 (11)	0.117 (14)	−0.011 (12)	0.025 (13)	0.006 (10)
C30	0.123 (16)	0.085 (13)	0.119 (15)	−0.020 (12)	0.009 (13)	0.015 (11)
C31	0.106 (14)	0.076 (11)	0.121 (14)	−0.012 (11)	0.019 (12)	0.018 (11)
C32	0.095 (12)	0.068 (10)	0.104 (12)	−0.018 (9)	0.021 (10)	0.015 (8)
C33	0.087 (11)	0.073 (10)	0.117 (13)	−0.011 (8)	0.025 (10)	0.010 (9)

C34	0.085 (11)	0.082 (11)	0.123 (13)	−0.016 (9)	0.021 (10)	0.015 (9)
C35	0.097 (13)	0.094 (14)	0.134 (16)	−0.018 (11)	0.012 (12)	0.017 (11)
C36	0.108 (15)	0.088 (13)	0.125 (15)	−0.020 (11)	0.011 (12)	0.012 (11)
C37	0.049 (7)	0.076 (8)	0.072 (8)	0.005 (6)	0.032 (6)	0.009 (7)
C38	0.063 (8)	0.085 (9)	0.082 (9)	0.008 (7)	0.040 (7)	0.007 (7)
C39	0.057 (8)	0.070 (9)	0.089 (10)	0.009 (6)	0.040 (7)	0.016 (7)
C40	0.047 (7)	0.066 (8)	0.086 (9)	−0.004 (6)	0.031 (6)	0.018 (7)
C41	0.045 (7)	0.062 (8)	0.083 (9)	−0.008 (6)	0.029 (6)	0.010 (7)
C42	0.046 (7)	0.069 (8)	0.084 (10)	−0.010 (6)	0.024 (7)	0.007 (7)
C43	0.056 (8)	0.078 (9)	0.095 (10)	−0.015 (7)	0.019 (8)	0.010 (8)
C44	0.065 (9)	0.086 (10)	0.101 (11)	−0.026 (8)	0.009 (8)	−0.001 (9)
C45	0.070 (9)	0.095 (11)	0.091 (10)	−0.024 (8)	0.009 (8)	−0.012 (8)
C46	0.057 (8)	0.085 (10)	0.087 (10)	−0.021 (7)	0.014 (7)	−0.012 (8)
C47	0.048 (8)	0.073 (9)	0.102 (11)	−0.010 (6)	0.029 (8)	0.022 (8)
C48	0.053 (8)	0.082 (10)	0.106 (11)	−0.021 (7)	0.018 (8)	0.015 (9)
C49	0.112 (16)	0.137 (18)	0.126 (16)	0.002 (13)	0.036 (13)	0.024 (13)
C50	0.113 (13)	0.107 (12)	0.115 (13)	0.002 (10)	0.024 (10)	0.028 (10)
C51	0.177 (18)	0.146 (16)	0.125 (15)	0.038 (13)	0.062 (13)	−0.004 (12)

Geometric parameters (Å, °)

Sm1—O1^{i}	2.351 (6)	C19—C24	1.411 (16)
Sm1—O3	2.379 (5)	C19—C20	1.438 (15)
Sm1—O4^{i}	2.386 (6)	C20—C21	1.393 (15)
Sm1—O6	2.456 (7)	C21—C22	1.362 (15)
Sm1—O2	2.478 (6)	C21—H21	0.9300
Sm1—O5	2.486 (6)	C22—C23	1.407 (16)
Sm1—N2	2.559 (7)	C22—H22	0.9300
Sm1—O1	2.560 (6)	C23—C24	1.325 (16)
Sm1—N1	2.616 (7)	C23—H23	0.9300
Sm1—Sm1^{i}	3.9547 (10)	C24—H24	0.9300
N1—C37	1.306 (12)	C25—C26	1.536 (15)
N1—C41	1.364 (12)	C26—C27	1.491 (16)
N2—C46	1.325 (13)	C26—H26A	0.9700
N2—C42	1.342 (12)	C26—H26B	0.9700
N3—C49	1.314 (19)	C27—C28	1.387 (17)
N3—C51	1.412 (16)	C27—C32	1.408 (18)
N3—C50	1.450 (16)	C28—C29	1.420 (18)
O1—C1	1.285 (10)	C28—H28	0.9300
O1—Sm1^{i}	2.351 (6)	C29—C30	1.350 (19)
O2—C1	1.229 (10)	C29—H29	0.9300
O3—C13	1.251 (9)	C30—C31	1.36 (2)
O4—C13	1.255 (10)	C30—H30	0.9300
O4—Sm1^{i}	2.386 (6)	C31—C36	1.41 (2)
O5—C25	1.231 (13)	C31—C32	1.446 (19)
O6—C25	1.251 (13)	C32—C33	1.408 (17)
O7—C49	1.250 (17)	C33—C34	1.392 (16)
C1—C2	1.495 (12)	C33—H33	0.9300

C2—C3	1.517 (13)	C34—C35	1.394 (18)
C2—H2A	0.9700	C34—H34	0.9300
C2—H2B	0.9700	C35—C36	1.321 (19)
C3—C4	1.330 (14)	C35—H35	0.9300
C3—C8	1.419 (15)	C36—H36	0.9300
C4—C5	1.418 (14)	C37—C38	1.404 (13)
C4—H4	0.9300	C37—H37	0.9300
C5—C6	1.357 (16)	C38—C39	1.363 (14)
C5—H5	0.9300	C38—H38	0.9300
C6—C7	1.391 (16)	C39—C40	1.376 (14)
C6—H6	0.9300	C39—H39	0.9300
C7—C12	1.395 (16)	C40—C41	1.409 (13)
C7—C8	1.419 (15)	C40—C47	1.434 (14)
C8—C9	1.403 (15)	C41—C42	1.432 (14)
C9—C10	1.364 (16)	C42—C43	1.417 (15)
C9—H9	0.9300	C43—C44	1.385 (16)
C10—C11	1.413 (17)	C43—C48	1.427 (16)
C10—H10	0.9300	C44—C45	1.340 (16)
C11—C12	1.346 (17)	C44—H44	0.9300
C11—H11	0.9300	C45—C46	1.401 (14)
C12—H12	0.9300	C45—H45	0.9300
C13—C14	1.519 (12)	C46—H46	0.9300
C14—C15	1.503 (13)	C47—C48	1.323 (15)
C14—H14A	0.9700	C47—H47	0.9300
C14—H14B	0.9700	C48—H48	0.9300
C15—C16	1.373 (14)	C49—H49	0.9300
C15—C20	1.400 (15)	C50—H50A	0.9600
C16—C17	1.428 (15)	C50—H50B	0.9600
C16—H16	0.9300	C50—H50C	0.9600
C17—C18	1.332 (16)	C51—H51A	0.9600
C17—H17	0.9300	C51—H51B	0.9600
C18—C19	1.395 (16)	C51—H51C	0.9600
C18—H18	0.9300		
$O1^{i}$—Sm1—O3	74.35 (19)	C17—C16—H16	120.1
$O1^{i}$—Sm1—$O4^{i}$	77.1 (2)	C18—C17—C16	120.3 (13)
O3—Sm1—$O4^{i}$	136.7 (2)	C18—C17—H17	119.8
$O1^{i}$—Sm1—O6	86.4 (2)	C16—C17—H17	119.8
O3—Sm1—O6	125.4 (2)	C17—C18—C19	122.1 (13)
$O4^{i}$—Sm1—O6	83.9 (2)	C17—C18—H18	119.0
$O1^{i}$—Sm1—O2	123.4 (2)	C19—C18—H18	119.0
O3—Sm1—O2	77.3 (2)	C18—C19—C24	123.2 (13)
$O4^{i}$—Sm1—O2	92.4 (2)	C18—C19—C20	118.3 (13)
O6—Sm1—O2	148.4 (2)	C24—C19—C20	118.5 (13)
$O1^{i}$—Sm1—O5	75.7 (2)	C21—C20—C15	123.2 (11)
O3—Sm1—O5	73.5 (3)	C21—C20—C19	117.5 (12)
$O4^{i}$—Sm1—O5	129.0 (2)	C15—C20—C19	119.2 (12)
O6—Sm1—O5	52.2 (2)	C22—C21—C20	122.0 (13)

O2—Sm1—O5	138.5 (2)	C22—C21—H21	119.0
O1^{i}—Sm1—N2	142.8 (2)	C20—C21—H21	119.0
O3—Sm1—N2	78.7 (2)	C21—C22—C23	119.6 (14)
O4^{i}—Sm1—N2	138.9 (2)	C21—C22—H22	120.2
O6—Sm1—N2	88.9 (3)	C23—C22—H22	120.2
O2—Sm1—N2	73.4 (2)	C24—C23—C22	120.7 (15)
O5—Sm1—N2	72.4 (3)	C24—C23—H23	119.7
O1^{i}—Sm1—O1	72.8 (2)	C22—C23—H23	119.7
O3—Sm1—O1	68.9 (2)	C23—C24—C19	121.6 (14)
O4^{i}—Sm1—O1	71.9 (2)	C23—C24—H24	119.2
O6—Sm1—O1	150.9 (2)	C19—C24—H24	119.2
O2—Sm1—O1	51.43 (19)	O5—C25—O6	122.3 (12)
O5—Sm1—O1	135.9 (2)	O5—C25—C26	117.6 (12)
N2—Sm1—O1	120.0 (2)	O6—C25—C26	120.1 (12)
O1^{i}—Sm1—N1	149.3 (2)	C27—C26—C25	111.5 (11)
O3—Sm1—N1	136.4 (2)	C27—C26—H26A	109.3
O4^{i}—Sm1—N1	76.2 (2)	C25—C26—H26A	109.3
O6—Sm1—N1	75.8 (2)	C27—C26—H26B	109.3
O2—Sm1—N1	72.8 (2)	C25—C26—H26B	109.3
O5—Sm1—N1	110.4 (2)	H26A—C26—H26B	108.0
N2—Sm1—N1	62.8 (3)	C28—C27—C32	119.7 (15)
O1—Sm1—N1	112.5 (2)	C28—C27—C26	120.6 (15)
O1^{i}—Sm1—Sm1^{i}	38.21 (15)	C32—C27—C26	119.6 (14)
O3—Sm1—Sm1^{i}	66.81 (15)	C27—C28—C29	118.8 (15)
O4^{i}—Sm1—Sm1^{i}	70.53 (14)	C27—C28—H28	120.6
O6—Sm1—Sm1^{i}	121.89 (17)	C29—C28—H28	120.6
O2—Sm1—Sm1^{i}	85.64 (14)	C30—C29—C28	121.3 (17)
O5—Sm1—Sm1^{i}	108.53 (16)	C30—C29—H29	119.4
N2—Sm1—Sm1^{i}	142.88 (19)	C28—C29—H29	119.4
O1—Sm1—Sm1^{i}	34.61 (13)	C29—C30—C31	122.0 (18)
N1—Sm1—Sm1^{i}	139.33 (19)	C29—C30—H30	119.0
C37—N1—C41	116.6 (9)	C31—C30—H30	119.0
C37—N1—Sm1	123.8 (7)	C30—C31—C36	123.9 (19)
C41—N1—Sm1	119.5 (7)	C30—C31—C32	118.3 (17)
C46—N2—C42	117.7 (9)	C36—C31—C32	117.6 (18)
C46—N2—Sm1	120.4 (7)	C27—C32—C33	122.2 (15)
C42—N2—Sm1	121.9 (7)	C27—C32—C31	119.7 (16)
C49—N3—C51	120.4 (16)	C33—C32—C31	118.1 (16)
C49—N3—C50	119.1 (15)	C34—C33—C32	121.1 (15)
C51—N3—C50	120.4 (15)	C34—C33—H33	119.5
C1—O1—Sm1^{i}	155.2 (6)	C32—C33—H33	119.5
C1—O1—Sm1	90.1 (5)	C33—C34—C35	118.9 (16)
Sm1^{i}—O1—Sm1	107.2 (2)	C33—C34—H34	120.6
C1—O2—Sm1	95.4 (6)	C35—C34—H34	120.6
C13—O3—Sm1	138.0 (6)	C36—C35—C34	121.7 (18)

C13—O4—Sm1^{i}	133.2 (6)	C36—C35—H35	119.1
C25—O5—Sm1	92.1 (7)	C34—C35—H35	119.1
C25—O6—Sm1	93.1 (7)	C35—C36—C31	122.3 (19)
O2—C1—O1	120.9 (9)	C35—C36—H36	118.8
O2—C1—C2	123.3 (9)	C31—C36—H36	118.8
O1—C1—C2	115.7 (9)	N1—C37—C38	125.1 (11)
C1—C2—C3	115.7 (9)	N1—C37—H37	117.5
C1—C2—H2A	108.4	C38—C37—H37	117.5
C3—C2—H2A	108.4	C39—C38—C37	117.9 (12)
C1—C2—H2B	108.4	C39—C38—H38	121.1
C3—C2—H2B	108.4	C37—C38—H38	121.1
H2A—C2—H2B	107.4	C38—C39—C40	119.6 (10)
C4—C3—C8	118.9 (11)	C38—C39—H39	120.2
C4—C3—C2	119.8 (12)	C40—C39—H39	120.2
C8—C3—C2	121.3 (11)	C39—C40—C41	118.6 (11)
C3—C4—C5	122.6 (13)	C39—C40—C47	122.8 (11)
C3—C4—H4	118.7	C41—C40—C47	118.5 (12)
C5—C4—H4	118.7	N1—C41—C40	122.2 (11)
C6—C5—C4	118.9 (13)	N1—C41—C42	117.4 (9)
C6—C5—H5	120.5	C40—C41—C42	120.4 (11)
C4—C5—H5	120.5	N2—C42—C43	122.8 (11)
C5—C6—C7	121.1 (13)	N2—C42—C41	118.3 (10)
C5—C6—H6	119.5	C43—C42—C41	118.8 (11)
C7—C6—H6	119.5	C44—C43—C42	116.8 (12)
C6—C7—C12	121.6 (13)	C44—C43—C48	124.5 (13)
C6—C7—C8	119.0 (13)	C42—C43—C48	118.7 (13)
C12—C7—C8	119.4 (14)	C45—C44—C43	120.7 (13)
C9—C8—C7	118.2 (13)	C45—C44—H44	119.7
C9—C8—C3	122.3 (12)	C43—C44—H44	119.7
C7—C8—C3	119.5 (13)	C44—C45—C46	119.0 (13)
C10—C9—C8	121.2 (13)	C44—C45—H45	120.5
C10—C9—H9	119.4	C46—C45—H45	120.5
C8—C9—H9	119.4	N2—C46—C45	122.9 (11)
C9—C10—C11	119.7 (14)	N2—C46—H46	118.5
C9—C10—H10	120.2	C45—C46—H46	118.5
C11—C10—H10	120.2	C48—C47—C40	121.1 (11)
C12—C11—C10	120.3 (15)	C48—C47—H47	119.4
C12—C11—H11	119.8	C40—C47—H47	119.4
C10—C11—H11	119.8	C47—C48—C43	122.3 (12)
C11—C12—C7	121.2 (14)	C47—C48—H48	118.8
C11—C12—H12	119.4	C43—C48—H48	118.8
C7—C12—H12	119.4	O7—C49—N3	121 (2)
O3—C13—O4	127.1 (9)	O7—C49—H49	119.3
O3—C13—C14	115.5 (9)	N3—C49—H49	119.3
O4—C13—C14	117.3 (8)	N3—C50—H50A	109.5
C15—C14—C13	117.1 (9)	N3—C50—H50B	109.5
C15—C14—H14A	108.0	H50A—C50—H50B	109.5
C13—C14—H14A	108.0	N3—C50—H50C	109.5
C15—C14—H14B	108.0	H50A—C50—H50C	109.5

C13—C14—H14B	108.0	H50B—C50—H50C	109.5
H14A—C14—H14B	107.3	N3—C51—H51A	109.5
C16—C15—C20	120.2 (11)	N3—C51—H51B	109.5
C16—C15—C14	118.7 (12)	H51A—C51—H51B	109.5
C20—C15—C14	121.0 (10)	N3—C51—H51C	109.5
C15—C16—C17	119.8 (12)	H51A—C51—H51C	109.5
C15—C16—H16	120.1	H51B—C51—H51C	109.5
$O1^{i}$—Sm1—N1—C37	28.3 (10)	C4—C3—C8—C9	−180.0 (11)
O3—Sm1—N1—C37	−148.2 (7)	C2—C3—C8—C9	0.1 (17)
$O4^{i}$—Sm1—N1—C37	−2.2 (8)	C4—C3—C8—C7	1.4 (16)
O6—Sm1—N1—C37	84.9 (8)	C2—C3—C8—C7	−178.5 (9)
O2—Sm1—N1—C37	−99.2 (8)	C7—C8—C9—C10	−0.4 (18)
O5—Sm1—N1—C37	124.6 (8)	C3—C8—C9—C10	−179.1 (12)
N2—Sm1—N1—C37	−179.0 (9)	C8—C9—C10—C11	−1(2)
O1—Sm1—N1—C37	−65.7 (8)	C9—C10—C11—C12	1(2)
$Sm1^{i}$—Sm1—N1—C37	−38.0 (9)	C10—C11—C12—C7	0(2)
$O1^{i}$—Sm1—N1—C41	−154.8 (7)	C6—C7—C12—C11	−178.2 (13)
O3—Sm1—N1—C41	28.7 (9)	C8—C7—C12—C11	−1(2)
$O4^{i}$—Sm1—N1—C41	174.6 (8)	Sm1—O3—C13—O4	−30.4 (17)
O6—Sm1—N1—C41	−98.3 (7)	Sm1—O3—C13—C14	151.9 (7)
O2—Sm1—N1—C41	77.7 (7)	$Sm1^{i}$—O4—C13—O3	10.6 (16)
O5—Sm1—N1—C41	−58.5 (8)	$Sm1^{i}$—O4—C13—C14	−171.8 (6)
N2—Sm1—N1—C41	−2.1 (7)	O3—C13—C14—C15	−140.4 (10)
O1—Sm1—N1—C41	111.2 (7)	O4—C13—C14—C15	41.7 (14)
$Sm1^{i}$—Sm1—N1—C41	138.9 (6)	C13—C14—C15—C16	−119.5 (11)
$O1^{i}$—Sm1—N2—C46	−21.8 (11)	C13—C14—C15—C20	63.9 (14)
O3—Sm1—N2—C46	22.2 (8)	C20—C15—C16—C17	−2.2 (17)
$O4^{i}$—Sm1—N2—C46	176.3 (7)	C14—C15—C16—C17	−178.8 (10)
O6—Sm1—N2—C46	−104.3 (9)	C15—C16—C17—C18	3.4 (19)
O2—Sm1—N2—C46	102.2 (9)	C16—C17—C18—C19	−1(2)
O5—Sm1—N2—C46	−53.9 (8)	C17—C18—C19—C24	178.3 (13)
O1—Sm1—N2—C46	79.5 (9)	C17—C18—C19—C20	−1.5 (19)
N1—Sm1—N2—C46	−179.0 (9)	C16—C15—C20—C21	−177.5 (11)
$Sm1^{i}$—Sm1—N2—C46	43.8 (10)	C14—C15—C20—C21	−0.9 (18)
$O1^{i}$—Sm1—N2—C42	160.0 (7)	C16—C15—C20—C19	−0.8 (17)
O3—Sm1—N2—C42	−156.0 (8)	C14—C15—C20—C19	175.8 (10)
$O4^{i}$—Sm1—N2—C42	−1.9 (10)	C18—C19—C20—C21	179.5 (11)
O6—Sm1—N2—C42	77.5 (8)	C24—C19—C20—C21	−0.3 (17)
O2—Sm1—N2—C42	−76.0 (8)	C18—C19—C20—C15	2.6 (17)
O5—Sm1—N2—C42	127.9 (9)	C24—C19—C20—C15	−177.2 (11)
O1—Sm1—N2—C42	−98.7 (8)	C15—C20—C21—C22	175.8 (12)
N1—Sm1—N2—C42	2.8 (8)	C19—C20—C21—C22	−1.0 (18)
$Sm1^{i}$—Sm1—N2—C42	−134.4 (7)	C20—C21—C22—C23	1(2)
$O1^{i}$—Sm1—O1—C1	161.9 (6)	C21—C22—C23—C24	0(2)
O3—Sm1—O1—C1	82.4 (5)	C22—C23—C24—C19	−1(2)

$O4^{i}$—Sm1—O1—C1	−116.5 (5)	C18—C19—C24—C23	−178.4 (13)
O6—Sm1—O1—C1	−151.9 (6)	C20—C19—C24—C23	1(2)
O2—Sm1—O1—C1	−8.0 (5)	Sm1—O5—C25—O6	−5.8 (12)
O5—Sm1—O1—C1	115.6 (5)	Sm1—O5—C25—C26	173.6 (9)
N2—Sm1—O1—C1	20.2 (6)	Sm1—O6—C25—O5	5.9 (12)
N1—Sm1—O1—C1	−50.4 (5)	Sm1—O6—C25—C26	−173.5 (10)
$Sm1^{i}$—Sm1—O1—C1	161.9 (6)	O5—C25—C26—C27	−52.8 (16)
$O1^{i}$—Sm1—O1—$Sm1^{i}$	0.0	O6—C25—C26—C27	126.7 (13)
O3—Sm1—O1—$Sm1^{i}$	−79.4 (2)	C25—C26—C27—C28	107.0 (14)
$O4^{i}$—Sm1—O1—$Sm1^{i}$	81.7 (2)	C25—C26—C27—C32	−70.1 (16)
O6—Sm1—O1—$Sm1^{i}$	46.2 (5)	C32—C27—C28—C29	−1.5 (19)
O2—Sm1—O1—$Sm1^{i}$	−169.9 (3)	C26—C27—C28—C29	−178.5 (12)
O5—Sm1—O1—$Sm1^{i}$	−46.2 (4)	C27—C28—C29—C30	4(2)
N2—Sm1—O1—$Sm1^{i}$	−141.7 (3)	C28—C29—C30—C31	−6(2)
N1—Sm1—O1—$Sm1^{i}$	147.7 (2)	C29—C30—C31—C36	178.6 (15)
$O1^{i}$—Sm1—O2—C1	−3.2 (6)	C29—C30—C31—C32	4(2)
O3—Sm1—O2—C1	−64.5 (6)	C28—C27—C32—C33	178.5 (12)
$O4^{i}$—Sm1—O2—C1	72.9 (6)	C26—C27—C32—C33	−4.4 (19)
O6—Sm1—O2—C1	155.2 (6)	C28—C27—C32—C31	0(2)
O5—Sm1—O2—C1	−110.6 (6)	C26—C27—C32—C31	176.9 (12)
N2—Sm1—O2—C1	−146.3 (6)	C30—C31—C32—C27	−1(2)
O1—Sm1—O2—C1	8.4 (5)	C36—C31—C32—C27	−175.9 (13)
N1—Sm1—O2—C1	147.7 (6)	C30—C31—C32—C33	−179.7 (14)
$Sm1^{i}$—Sm1—O2—C1	2.6 (5)	C36—C31—C32—C33	5(2)
$O1^{i}$—Sm1—O3—C13	−17.0 (10)	C27—C32—C33—C34	178.8 (12)
$O4^{i}$—Sm1—O3—C13	33.6 (11)	C31—C32—C33—C34	−3(2)
O6—Sm1—O3—C13	−90.7 (10)	C32—C33—C34—C35	1(2)
O2—Sm1—O3—C13	113.6 (10)	C33—C34—C35—C36	−2(2)
O5—Sm1—O3—C13	−96.3 (10)	C34—C35—C36—C31	6(3)
N2—Sm1—O3—C13	−171.1 (10)	C30—C31—C36—C35	178.3 (16)
O1—Sm1—O3—C13	60.3 (10)	C32—C31—C36—C35	−7(2)
N1—Sm1—O3—C13	161.2 (9)	C41—N1—C37—C38	0.9 (16)
$Sm1^{i}$—Sm1—O3—C13	22.9 (10)	Sm1—N1—C37—C38	177.9 (8)
$O1^{i}$—Sm1—O5—C25	99.8 (7)	N1—C37—C38—C39	−0.4 (17)
O3—Sm1—O5—C25	177.4 (7)	C37—C38—C39—C40	−0.5 (17)
$O4^{i}$—Sm1—O5—C25	40.0 (8)	C38—C39—C40—C41	0.7 (17)
O6—Sm1—O5—C25	3.2 (7)	C38—C39—C40—C47	−179.1 (11)
O2—Sm1—O5—C25	−135.4 (7)	C37—N1—C41—C40	−0.7 (15)
N2—Sm1—O5—C25	−99.5 (7)	Sm1—N1—C41—C40	−177.7 (8)
O1—Sm1—O5—C25	145.2 (6)	C37—N1—C41—C42	178.6 (10)
N1—Sm1—O5—C25	−48.5 (7)	Sm1—N1—C41—C42	1.5 (13)
$Sm1^{i}$—Sm1—O5—C25	119.6 (7)	C39—C40—C41—N1	−0.2 (17)
$O1^{i}$—Sm1—O6—C25	−77.7 (7)	C47—C40—C41—N1	179.7 (10)
O3—Sm1—O6—C25	−9.9 (7)	C39—C40—C41—C42	−179.4 (11)
$O4^{i}$—Sm1—O6—C25	−155.1 (7)	C47—C40—C41—C42	0.5 (16)

O2—Sm1—O6—C25	120.1 (7)	C46—N2—C42—C43	−0.4 (17)
O5—Sm1—O6—C25	−3.1 (6)	Sm1—N2—C42—C43	177.8 (8)
N2—Sm1—O6—C25	65.4 (7)	C46—N2—C42—C41	178.4 (10)
O1—Sm1—O6—C25	−121.5 (7)	Sm1—N2—C42—C41	−3.3 (14)
N1—Sm1—O6—C25	127.6 (7)	N1—C41—C42—N2	1.1 (16)
Sm1^{i}—Sm1—O6—C25	−92.6 (7)	C40—C41—C42—N2	−179.6 (10)
Sm1—O2—C1—O1	−15.4 (9)	N1—C41—C42—C43	−180.0 (10)
Sm1—O2—C1—C2	162.3 (9)	C40—C41—C42—C43	−0.7 (17)
Sm1^{i}—O1—C1—O2	149.8 (10)	N2—C42—C43—C44	−1.6 (18)
Sm1—O1—C1—O2	14.8 (9)	C41—C42—C43—C44	179.6 (11)
Sm1^{i}—O1—C1—C2	−28 (2)	N2—C42—C43—C48	179.7 (11)
Sm1—O1—C1—C2	−163.1 (8)	C41—C42—C43—C48	0.9 (17)
O2—C1—C2—C3	−3.1 (15)	C42—C43—C44—C45	2(2)
O1—C1—C2—C3	174.8 (9)	C48—C43—C44—C45	−179.4 (13)
C1—C2—C3—C4	110.1 (12)	C43—C44—C45—C46	0(2)
C1—C2—C3—C8	−69.9 (13)	C42—N2—C46—C45	2.1 (18)
C8—C3—C4—C5	−0.3 (17)	Sm1—N2—C46—C45	−176.2 (9)
C2—C3—C4—C5	179.6 (10)	C44—C45—C46—N2	−2(2)
C3—C4—C5—C6	0.5 (18)	C39—C40—C47—C48	179.4 (12)
C4—C5—C6—C7	−1.8 (19)	C41—C40—C47—C48	−0.5 (18)
C5—C6—C7—C12	−179.8 (12)	C40—C47—C48—C43	1(2)
C5—C6—C7—C8	2.9 (18)	C44—C43—C48—C47	−179.5 (13)
C6—C7—C8—C9	178.6 (11)	C42—C43—C48—C47	−0.9 (19)
C12—C7—C8—C9	1.3 (17)	C51—N3—C49—O7	−4(3)
C6—C7—C8—C3	−2.7 (17)	C50—N3—C49—O7	177.6 (15)
C12—C7—C8—C3	179.9 (11)		

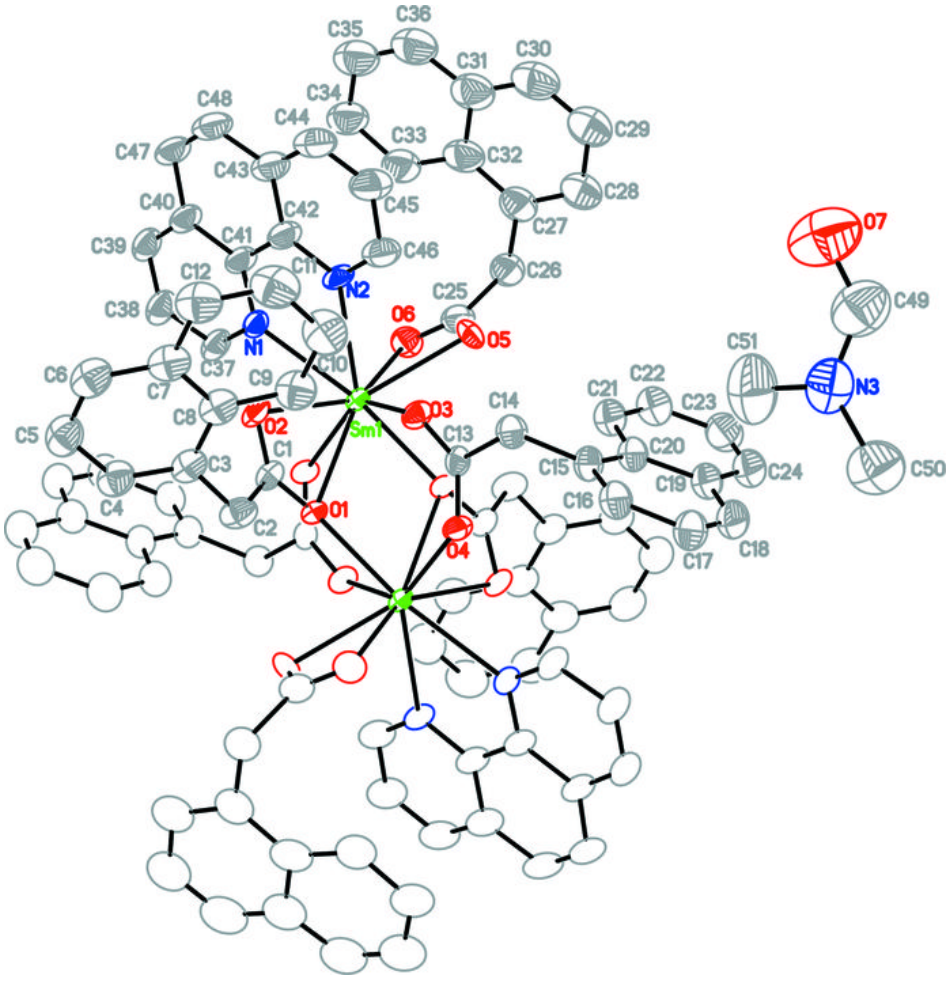
Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6···O7^{ii}	0.93	2.55	3.438 (18)	159
C37—H37···O4^{i}	0.93	2.37	3.036 (12)	129
C46—H46···O3	0.93	2.48	3.074 (13)	122
C47—H47···O2^{iii}	0.93	2.46	3.314 (13)	153
C50—H50A···O6^{iv}	0.96	2.58	3.369 (16)	139
C18—H18···Cg1^{v}	0.93	2.88	3.661 (15)	143

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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C5
C1
C13
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C16
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Fig. 2

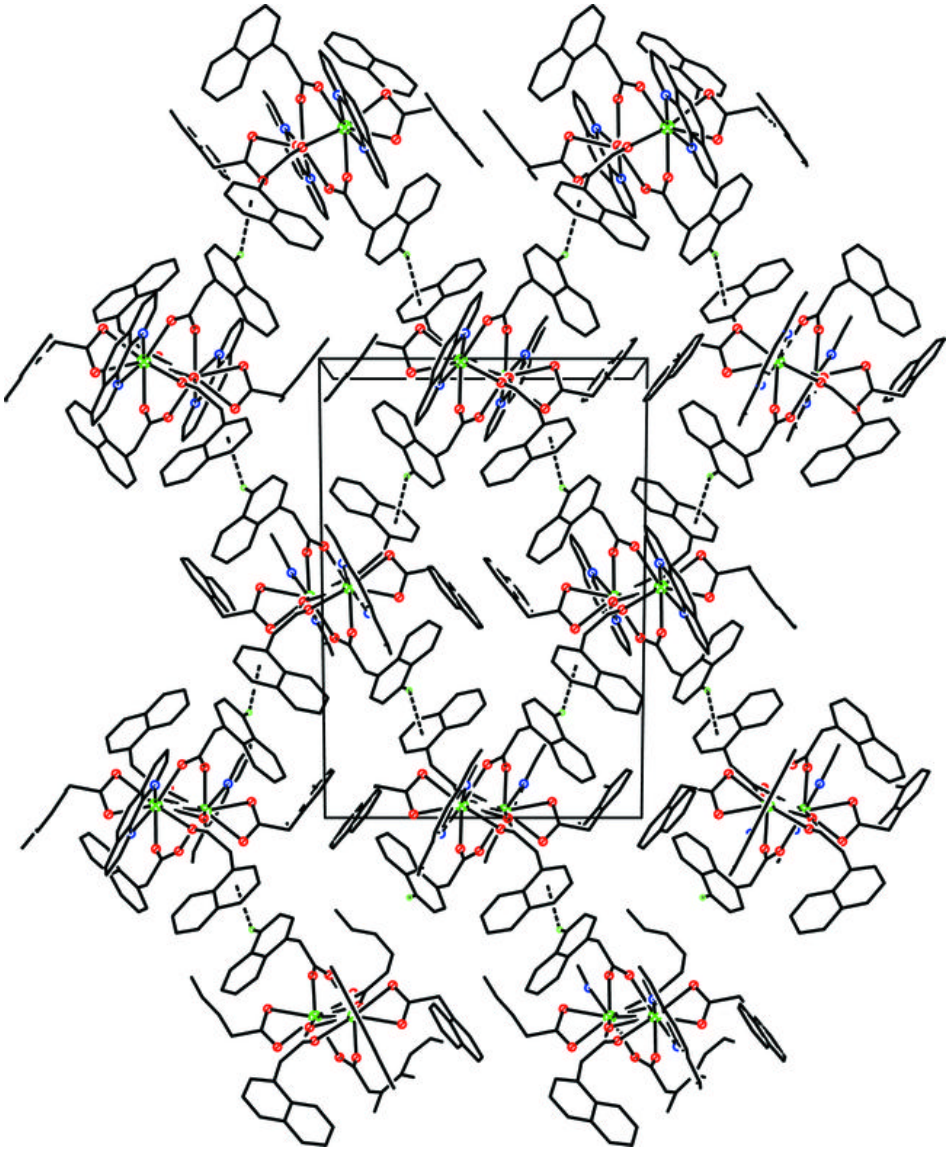

Fig. 3