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

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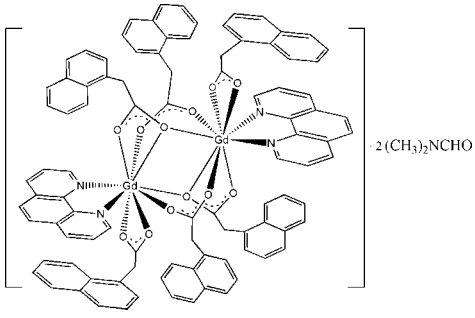
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.012 Å; R factor = 0.041; wR factor = 0.081; data-to-parameter ratio = 13.7.

The title complex, $[Gd_2(C_{12}H_9O_2)_6(C_{12}H_8N_2)_2]\cdot 2C_3H_7NO$, has a centrosymmetric structure. The Gd atom has a distorted monocapped square-antiprismatic coordination geometry. Molecules are linked into a chain by C—H···O hydrogen bonds parallel to *a* 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: Bernstein *et al.* (1995); Liu *et al.* (2007); Xia *et al.* (2007).



Experimental

Crystal data

$[Gd_2(C_{12}H_9O_2)_6(C_{12}H_8N_2)_2]\cdot 2C_3H_7NO$
M_r = 1932.25
Monoclinic, $P2_1/c$
a = 13.4762 (19) Å
b = 15.103 (2) Å
c = 22.178 (2) Å
β = 103.698 (2)°
V = 4385.4 (10) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.57 mm^{-1}
T = 298 (2) K
0.43 × 0.16 × 0.15 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.552, T_{max} = 0.799
20263 measured reflections
7696 independent reflections
4921 reflections with $I > 2\sigma(I)$
R_{int} = 0.055

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.081
S = 1.03
7696 reflections
561 parameters
36 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.01 e Å^{-3}
$\Delta\rho_{min}$ = −0.80 e Å^{-3}

Table 1
Selected bond lengths (Å).

Gd1—O1^{i}	2.349 (3)	Gd1—O5	2.480 (4)
Gd1—O3	2.368 (3)	Gd1—O1	2.551 (3)
Gd1—O4^{i}	2.378 (3)	Gd1—N2	2.552 (4)
Gd1—O6	2.445 (4)	Gd1—N1	2.608 (4)
Gd1—O2	2.478 (3)		

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

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

*Cg*1 and *Cg*2 are the centroids of the C3–C8 and C7–C12 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C50—H50*A*···O6^{ii}	0.96	2.54	3.379 (9)	146
C47—H47···O2^{iii}	0.93	2.46	3.319 (7)	153
C6—H6···O7^{iv}	0.93	2.55	3.436 (10)	159
C51—H51*C*···O7	0.96	2.30	2.713 (13)	105
C46—H46···O3	0.93	2.45	3.057 (7)	123
C37—H37···O4^{i}	0.93	2.37	3.027 (7)	127
C21—H21···O5	0.93	2.59	3.412 (8)	148
C18—H18···*Cg*1^{v}	0.93	2.88	3.66 (2)	142
C39—H39···*Cg*2^{iii}	0.93	2.99	3.858 (18)	156

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

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: AT2408).

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supplementary materials

Acta Cryst. (2007). E**63**, m2625-m2626 [**doi:10.1107/S1600536807047101**]

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

Y.-F. Liu, H.-T. Xia, 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 $[Eu(NAA)_3(phen)]_2$.2DMF (II) (Liu *et al.*, 2007) and $[Pr(NAA)_3(phen)]_2$ .DMF (Xia *et al.*, 2007). We report here the crystal structure of gadolinium complexes with NAA and phen, (I).

In the title complex, the coordination environment of Gd atom and coordination modes of the NNA ligands coordinated to the Gd^{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 2.450 (7) Å, shorter than that 2.4725 (5) Å) of complex (II). The dihedral angles of the least-square-plane Gd_2O_2 and naphthyl rings are 58.35 (20)° (C3—C12 ring), 43.84 (29)° (C15—C24 ring) and 71.45 (26)° (C27—C36 ring), and the dihedral angle between Gd_2O_2 plane and phen ring is 81.89 (20)°.

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 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.

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 $Gd(NO_3)_3·6H_2O$ (0.451 g, 1 mmol) in water (10 ml) was added. The mixed solution was heated to 333k and stirred for 3 h, and then cooled to room temperature. The precipitate was washed with water and then dissolved in DMF. A colorless 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), 0.97Å (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

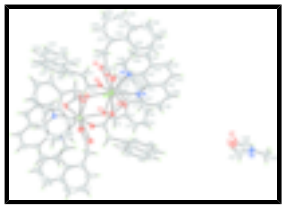

Fig. 1. The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are at the 30% probability level. Unlabelled atoms in the molecular are related to labelled atoms by (1 − *x*, 1 − *y*, 2 − *z*).

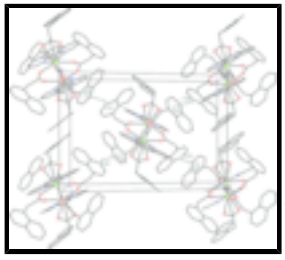

Fig. 2. A larger portion of the crystal structure of (I), showing the formation of a hydrogen-bonded chain built from C—H···π. For clarty, H atomes not involved in the hydrogen bonding have been omitted. Dashed lines indicate hydrogen bonds. [symmetry code: (A) 2 − *x*, 1 − *y*, 1 − *z*, (B) 2 − *x*,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

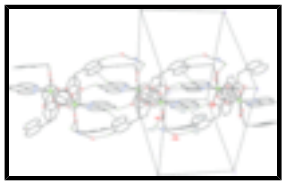

Fig. 3. A larger portion of the crystal structure of (I), showing the formation of a hydrogen-bonded chain built from C—H···O. For clarty, H atomes not involved in the hydrogen bonding have been omitted. Dashed lines indicate hydrogen bonds. [symmetry code: (F) 1 − *x*, 1 − *y*, 1 + *z*,, (G) 1 − *x*,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

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

Crystal data

$[Gd_2(C_{12}H_9O_2)_6(C_{12}H_8N_2)_2]\cdot 2C_3H_7NO$	F_{000} = 1956
M_r = 1932.25	D_x = 1.463 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 4868 reflections
a = 13.4762 (19) Å	θ = 2.4–25.3º
b = 15.103 (2) Å	μ = 1.57 mm^{-1}
c = 22.178 (2) Å	*T* = 298 (2) K
β = 103.698 (2)º	Block, colourless
V = 4385.4 (10) Å^3	0.43 × 0.16 × 0.15 mm
Z = 2	

Data collection

Bruker SMART 1000 CCD area-detector diffractometer	7696 independent reflections
Radiation source: fine-focus sealed tube	4921 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.055
T = 298(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 1.7º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −16→15

T_{min} = 0.552, T_{max} = 0.799
20263 measured reflections
k = −17→12
l = −24→26

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.081
S = 1.03
7696 reflections
561 parameters
36 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.0215P)^2 + 3.2792P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 1.01 e Å^{-3}
$\Delta\rho_{min}$ = −0.80 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}
Gd1	0.882546 (19)	0.429745 (18)	0.511490 (12)	0.03439 (9)
N1	0.7300 (3)	0.4440 (3)	0.5645 (2)	0.0422 (11)
N2	0.7124 (3)	0.3633 (3)	0.4537 (2)	0.0505 (12)
N3	0.1327 (6)	0.8355 (5)	0.7469 (3)	0.0839 (19)
O1	0.9404 (2)	0.5795 (2)	0.47896 (14)	0.0378 (8)
O2	0.7765 (2)	0.5557 (2)	0.46141 (15)	0.0457 (10)
O3	0.9045 (2)	0.4248 (2)	0.40872 (14)	0.0407 (8)
O4	1.0488 (3)	0.4869 (2)	0.39721 (15)	0.0432 (9)
O5	0.9128 (3)	0.2727 (3)	0.48857 (18)	0.0554 (11)
O6	0.9031 (3)	0.3045 (3)	0.58324 (17)	0.0555 (11)
O7	0.2671 (5)	0.7448 (5)	0.7639 (3)	0.167 (3)
C1	0.8487 (4)	0.5984 (3)	0.4517 (2)	0.0375 (13)
C2	0.8341 (4)	0.6733 (4)	0.4055 (3)	0.0562 (17)
H2A	0.8592	0.7273	0.4275	0.067*
H2B	0.8760	0.6617	0.3763	0.067*

C3	0.7266 (4)	0.6887 (4)	0.3695 (3)	0.0501 (16)
C4	0.6767 (5)	0.7631 (5)	0.3803 (3)	0.070 (2)
H4	0.7099	0.8027	0.4106	0.084*
C5	0.5768 (6)	0.7819 (5)	0.3473 (4)	0.086 (2)
H5	0.5448	0.8336	0.3555	0.103*
C6	0.5272 (5)	0.7250 (6)	0.3038 (4)	0.082 (2)
H6	0.4603	0.7371	0.2827	0.099*
C7	0.5746 (5)	0.6482 (5)	0.2899 (3)	0.0670 (19)
C8	0.6755 (5)	0.6291 (5)	0.3233 (3)	0.0557 (17)
C9	0.7209 (6)	0.5511 (5)	0.3087 (3)	0.081 (2)
H9	0.7874	0.5379	0.3300	0.097*
C10	0.6713 (8)	0.4947 (6)	0.2646 (4)	0.121 (3)
H10	0.7031	0.4433	0.2558	0.145*
C11	0.5716 (9)	0.5142 (7)	0.2324 (4)	0.126 (4)
H11	0.5369	0.4753	0.2021	0.151*
C12	0.5251 (6)	0.5889 (6)	0.2445 (4)	0.101 (3)
H12	0.4588	0.6011	0.2223	0.121*
C13	0.9738 (4)	0.4363 (4)	0.3807 (2)	0.0372 (12)
C14	0.9632 (4)	0.3856 (4)	0.3204 (2)	0.0565 (17)
H14A	0.9148	0.3379	0.3197	0.068*
H14B	0.9340	0.4253	0.2864	0.068*
C15	1.0584 (5)	0.3468 (4)	0.3082 (3)	0.0538 (16)
C16	1.0911 (6)	0.3718 (5)	0.2565 (3)	0.076 (2)
H16	1.0543	0.4146	0.2304	0.092*
C17	1.1773 (7)	0.3353 (6)	0.2419 (4)	0.097 (3)
H17	1.1981	0.3548	0.2071	0.116*
C18	1.2305 (6)	0.2718 (6)	0.2783 (4)	0.093 (3)
H18	1.2883	0.2483	0.2683	0.112*
C19	1.2010 (5)	0.2402 (5)	0.3310 (4)	0.074 (2)
C20	1.1143 (5)	0.2798 (4)	0.3467 (3)	0.0571 (17)
C21	1.0848 (6)	0.2471 (5)	0.3991 (3)	0.075 (2)
H21	1.0292	0.2721	0.4109	0.090*
C22	1.1363 (7)	0.1797 (5)	0.4324 (4)	0.095 (3)
H22	1.1152	0.1591	0.4669	0.114*
C23	1.2197 (7)	0.1402 (6)	0.4169 (5)	0.108 (3)
H23	1.2534	0.0935	0.4405	0.129*
C24	1.2515 (6)	0.1704 (6)	0.3673 (5)	0.100 (3)
H24	1.3079	0.1443	0.3570	0.120*
C25	0.9101 (4)	0.2498 (4)	0.5422 (3)	0.0506 (15)
C26	0.9136 (5)	0.1503 (4)	0.5563 (3)	0.0678 (18)
H26A	0.9808	0.1276	0.5560	0.081*
H26B	0.9026	0.1412	0.5975	0.081*
C27	0.8354 (6)	0.1001 (4)	0.5107 (3)	0.072 (2)
C28	0.8583 (8)	0.0475 (5)	0.4667 (4)	0.098 (3)
H28	0.9264	0.0398	0.4658	0.117*
C29	0.7823 (10)	0.0038 (7)	0.4221 (5)	0.133 (4)
H29	0.8010	−0.0330	0.3930	0.160*
C30	0.6834 (10)	0.0148 (8)	0.4211 (5)	0.134 (4)
H30	0.6338	−0.0128	0.3906	0.161*

C31	0.6544 (8)	0.0675 (6)	0.4657 (5)	0.105 (3)
C32	0.7308 (7)	0.1103 (5)	0.5116 (4)	0.076 (2)
C33	0.6992 (6)	0.1631 (5)	0.5555 (4)	0.095 (3)
H33	0.7479	0.1917	0.5861	0.114*
C34	0.5973 (8)	0.1733 (6)	0.5541 (5)	0.126 (4)
H34	0.5767	0.2077	0.5836	0.151*
C35	0.5259 (10)	0.1311 (8)	0.5075 (7)	0.161 (6)
H35	0.4571	0.1390	0.5065	0.194*
C36	0.5502 (11)	0.0801 (8)	0.4644 (6)	0.151 (5)
H36	0.4996	0.0533	0.4340	0.182*
C37	0.7367 (5)	0.4833 (4)	0.6186 (3)	0.0583 (17)
H37	0.7996	0.5059	0.6396	0.070*
C38	0.6537 (5)	0.4923 (5)	0.6458 (3)	0.072 (2)
H38	0.6620	0.5195	0.6842	0.086*
C39	0.5613 (5)	0.4611 (4)	0.6156 (3)	0.070 (2)
H39	0.5054	0.4678	0.6331	0.085*
C40	0.5494 (4)	0.4195 (4)	0.5590 (3)	0.0590 (17)
C41	0.6369 (4)	0.4123 (3)	0.5345 (2)	0.0414 (14)
C42	0.6274 (4)	0.3709 (4)	0.4755 (3)	0.0451 (15)
C43	0.5323 (4)	0.3381 (4)	0.4424 (3)	0.0611 (18)
C44	0.5275 (6)	0.2987 (5)	0.3857 (3)	0.084 (2)
H44	0.4654	0.2772	0.3626	0.101*
C45	0.6120 (5)	0.2912 (5)	0.3634 (3)	0.087 (2)
H45	0.6091	0.2646	0.3252	0.104*
C46	0.7043 (5)	0.3246 (4)	0.3993 (3)	0.0676 (19)
H46	0.7627	0.3192	0.3841	0.081*
C47	0.4541 (5)	0.3857 (5)	0.5243 (4)	0.073 (2)
H47	0.3967	0.3905	0.5405	0.088*
C48	0.4457 (5)	0.3476 (5)	0.4695 (4)	0.079 (2)
H48	0.3824	0.3265	0.4480	0.094*
C49	0.1908 (8)	0.7742 (7)	0.7788 (4)	0.111 (3)
H49	0.1740	0.7518	0.8142	0.134*
C50	0.0442 (6)	0.8672 (5)	0.7663 (3)	0.103 (3)
H50A	0.0352	0.8331	0.8011	0.154*
H50B	−0.0151	0.8613	0.7326	0.154*
H50C	0.0538	0.9284	0.7779	0.154*
C51	0.1579 (8)	0.8747 (7)	0.6936 (4)	0.169 (5)
H51A	0.1766	0.9356	0.7022	0.254*
H51B	0.0998	0.8716	0.6589	0.254*
H51C	0.2141	0.8434	0.6839	0.254*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Gd1	0.02397 (14)	0.03787 (15)	0.04183 (15)	−0.00299 (15)	0.00883 (10)	−0.00279 (15)
N1	0.030 (3)	0.048 (3)	0.051 (3)	0.004 (2)	0.013 (2)	0.006 (2)
N2	0.035 (3)	0.057 (3)	0.058 (3)	−0.008 (3)	0.007 (2)	−0.009 (3)
N3	0.093 (5)	0.084 (5)	0.071 (5)	−0.008 (4)	0.014 (4)	−0.018 (4)

O1	0.0227 (19)	0.043 (2)	0.046 (2)	0.0017 (18)	0.0056 (16)	−0.0015 (18)
O2	0.0218 (19)	0.055 (3)	0.062 (2)	−0.0001 (19)	0.0138 (17)	0.011 (2)
O3	0.035 (2)	0.050 (2)	0.0388 (19)	−0.007 (2)	0.0123 (16)	−0.0084 (19)
O4	0.036 (2)	0.049 (2)	0.046 (2)	−0.011 (2)	0.0124 (18)	−0.0159 (18)
O5	0.058 (3)	0.046 (3)	0.065 (3)	−0.004 (2)	0.019 (2)	−0.003 (2)
O6	0.059 (3)	0.050 (3)	0.060 (3)	−0.004 (2)	0.019 (2)	0.000 (2)
O7	0.091 (5)	0.200 (8)	0.195 (7)	0.008 (5)	0.008 (5)	−0.062 (6)
C1	0.026 (3)	0.041 (4)	0.045 (3)	0.005 (3)	0.006 (3)	−0.004 (3)
C2	0.034 (4)	0.065 (4)	0.066 (4)	−0.003 (3)	0.005 (3)	0.020 (3)
C3	0.038 (4)	0.053 (4)	0.060 (4)	0.001 (3)	0.012 (3)	0.025 (3)
C4	0.057 (5)	0.072 (5)	0.075 (5)	0.008 (4)	0.002 (4)	0.025 (4)
C5	0.073 (6)	0.084 (6)	0.101 (6)	0.034 (5)	0.023 (5)	0.033 (5)
C6	0.045 (5)	0.106 (7)	0.091 (6)	0.016 (5)	0.007 (4)	0.046 (5)
C7	0.047 (4)	0.084 (6)	0.061 (5)	−0.005 (4)	−0.005 (4)	0.026 (4)
C8	0.050 (4)	0.061 (5)	0.055 (4)	−0.003 (4)	0.010 (3)	0.022 (4)
C9	0.084 (5)	0.085 (6)	0.062 (5)	0.013 (5)	−0.008 (4)	0.003 (4)
C10	0.157 (9)	0.107 (7)	0.076 (6)	0.014 (7)	−0.016 (6)	−0.011 (5)
C11	0.162 (10)	0.100 (7)	0.081 (6)	−0.023 (7)	−0.040 (6)	−0.005 (6)
C12	0.090 (6)	0.113 (8)	0.078 (6)	−0.023 (6)	−0.024 (5)	0.028 (5)
C13	0.042 (3)	0.039 (3)	0.030 (3)	0.007 (3)	0.007 (3)	−0.001 (3)
C14	0.053 (4)	0.069 (4)	0.045 (4)	−0.004 (3)	0.008 (3)	−0.018 (3)
C15	0.054 (4)	0.061 (4)	0.049 (4)	−0.006 (4)	0.018 (3)	−0.027 (3)
C16	0.096 (6)	0.080 (5)	0.062 (4)	−0.006 (4)	0.038 (4)	−0.016 (4)
C17	0.115 (8)	0.107 (8)	0.089 (6)	−0.005 (6)	0.068 (6)	−0.025 (5)
C18	0.065 (6)	0.111 (8)	0.117 (7)	−0.014 (5)	0.049 (5)	−0.057 (6)
C19	0.060 (5)	0.071 (6)	0.097 (6)	−0.005 (4)	0.030 (5)	−0.039 (5)
C20	0.049 (4)	0.059 (4)	0.063 (4)	−0.009 (4)	0.012 (3)	−0.022 (4)
C21	0.081 (5)	0.064 (5)	0.081 (5)	0.000 (4)	0.024 (4)	−0.012 (4)
C22	0.100 (7)	0.076 (6)	0.109 (7)	0.007 (5)	0.026 (6)	0.000 (5)
C23	0.097 (8)	0.081 (7)	0.134 (8)	0.013 (6)	0.006 (6)	0.001 (6)
C24	0.074 (6)	0.083 (7)	0.143 (9)	0.001 (5)	0.025 (6)	−0.033 (6)
C25	0.031 (3)	0.038 (4)	0.079 (5)	−0.007 (3)	0.005 (3)	0.005 (4)
C26	0.062 (5)	0.047 (4)	0.093 (5)	0.002 (4)	0.015 (4)	0.010 (4)
C27	0.093 (6)	0.041 (4)	0.083 (5)	−0.009 (4)	0.021 (5)	0.021 (4)
C28	0.156 (8)	0.057 (5)	0.086 (6)	−0.010 (5)	0.041 (6)	−0.009 (4)
C29	0.233 (12)	0.074 (6)	0.100 (7)	−0.041 (9)	0.054 (9)	−0.011 (5)
C30	0.188 (10)	0.093 (7)	0.103 (7)	−0.056 (9)	−0.002 (8)	0.013 (6)
C31	0.107 (6)	0.063 (5)	0.127 (7)	−0.032 (6)	−0.004 (6)	0.033 (5)
C32	0.091 (6)	0.041 (4)	0.086 (5)	−0.019 (4)	0.000 (5)	0.012 (4)
C33	0.078 (6)	0.060 (5)	0.153 (8)	−0.015 (5)	0.038 (6)	0.005 (5)
C34	0.102 (8)	0.076 (7)	0.216 (11)	−0.018 (6)	0.069 (8)	0.027 (7)
C35	0.099 (8)	0.096 (10)	0.266 (16)	−0.039 (8)	0.000 (10)	0.067 (9)
C36	0.124 (9)	0.098 (8)	0.200 (11)	−0.047 (9)	−0.028 (9)	0.051 (7)
C37	0.044 (4)	0.076 (5)	0.061 (4)	0.002 (3)	0.023 (3)	0.006 (4)
C38	0.068 (5)	0.085 (6)	0.074 (5)	0.002 (4)	0.038 (4)	0.004 (4)
C39	0.059 (5)	0.071 (5)	0.097 (6)	0.014 (4)	0.051 (4)	0.026 (4)
C40	0.041 (4)	0.064 (5)	0.081 (5)	0.011 (4)	0.032 (3)	0.028 (4)
C41	0.030 (3)	0.040 (4)	0.056 (4)	0.007 (3)	0.014 (3)	0.019 (3)
C42	0.024 (3)	0.043 (4)	0.067 (4)	−0.005 (3)	0.008 (3)	0.011 (3)

C43	0.033 (4)	0.057 (4)	0.091 (5)	−0.014 (3)	0.011 (4)	0.010 (4)
C44	0.058 (5)	0.088 (6)	0.091 (6)	−0.032 (5)	−0.010 (4)	−0.014 (5)
C45	0.063 (5)	0.116 (7)	0.076 (5)	−0.038 (5)	0.004 (4)	−0.030 (5)
C46	0.049 (4)	0.088 (5)	0.065 (4)	−0.024 (4)	0.012 (4)	−0.025 (4)
C47	0.021 (4)	0.082 (6)	0.119 (6)	−0.003 (3)	0.021 (4)	0.042 (5)
C48	0.034 (4)	0.079 (6)	0.116 (6)	−0.015 (4)	0.006 (4)	0.029 (5)
C49	0.090 (8)	0.133 (10)	0.102 (7)	0.001 (7)	0.003 (6)	−0.018 (6)
C50	0.105 (7)	0.096 (7)	0.099 (6)	0.009 (5)	0.008 (5)	−0.035 (5)
C51	0.241 (13)	0.173 (11)	0.114 (8)	−0.071 (10)	0.083 (8)	0.013 (7)

Geometric parameters (Å, °)

Gd1—O1^{i}	2.349 (3)	C19—C24	1.402 (10)
Gd1—O3	2.368 (3)	C19—C20	1.427 (8)
Gd1—O4^{i}	2.378 (3)	C20—C21	1.403 (8)
Gd1—O6	2.445 (4)	C21—C22	1.350 (9)
Gd1—O2	2.478 (3)	C21—H21	0.9300
Gd1—O5	2.480 (4)	C22—C23	1.385 (10)
Gd1—O1	2.551 (3)	C22—H22	0.9300
Gd1—N2	2.552 (4)	C23—C24	1.352 (10)
Gd1—N1	2.608 (4)	C23—H23	0.9300
Gd1—Gd1^{i}	3.9431 (7)	C24—H24	0.9300
N1—C37	1.322 (6)	C25—C26	1.533 (7)
N1—C41	1.360 (6)	C26—C27	1.484 (9)
N2—C46	1.323 (6)	C26—H26A	0.9700
N2—C42	1.349 (6)	C26—H26B	0.9700
N3—C49	1.308 (10)	C27—C28	1.349 (9)
N3—C51	1.433 (9)	C27—C32	1.424 (10)
N3—C50	1.442 (9)	C28—C29	1.408 (12)
O1—C1	1.273 (5)	C28—H28	0.9300
O1—Gd1^{i}	2.349 (3)	C29—C30	1.338 (13)
O2—C1	1.228 (6)	C29—H29	0.9300
O3—C13	1.250 (5)	C30—C31	1.395 (13)
O4—C13	1.252 (6)	C30—H30	0.9300
O4—Gd1^{i}	2.378 (3)	C31—C36	1.411 (15)
O5—C25	1.246 (7)	C31—C32	1.421 (10)
O6—C25	1.250 (7)	C32—C33	1.400 (10)
O7—C49	1.235 (10)	C33—C34	1.375 (10)
C1—C2	1.508 (7)	C33—H33	0.9300
C2—C3	1.498 (7)	C34—C35	1.388 (14)
C2—H2A	0.9700	C34—H34	0.9300
C2—H2B	0.9700	C35—C36	1.327 (15)
C3—C4	1.360 (8)	C35—H35	0.9300
C3—C8	1.414 (8)	C36—H36	0.9300
C4—C5	1.400 (8)	C37—C38	1.397 (8)
C4—H4	0.9300	C37—H37	0.9300
C5—C6	1.346 (9)	C38—C39	1.351 (8)
C5—H5	0.9300	C38—H38	0.9300

C6—C7	1.394 (9)	C39—C40	1.378 (8)
C6—H6	0.9300	C39—H39	0.9300
C7—C12	1.393 (9)	C40—C41	1.414 (7)
C7—C8	1.416 (8)	C40—C47	1.426 (8)
C8—C9	1.400 (8)	C41—C42	1.430 (7)
C9—C10	1.349 (9)	C42—C43	1.408 (7)
C9—H9	0.9300	C43—C44	1.379 (8)
C10—C11	1.395 (11)	C43—C48	1.440 (9)
C10—H10	0.9300	C44—C45	1.350 (9)
C11—C12	1.349 (11)	C44—H44	0.9300
C11—H11	0.9300	C45—C46	1.402 (8)
C12—H12	0.9300	C45—H45	0.9300
C13—C14	1.519 (7)	C46—H46	0.9300
C14—C15	1.492 (7)	C47—C48	1.325 (9)
C14—H14A	0.9700	C47—H47	0.9300
C14—H14B	0.9700	C48—H48	0.9300
C15—C16	1.373 (8)	C49—H49	0.9300
C15—C20	1.420 (8)	C50—H50A	0.9600
C16—C17	1.391 (9)	C50—H50B	0.9600
C16—H16	0.9300	C50—H50C	0.9600
C17—C18	1.345 (10)	C51—H51A	0.9600
C17—H17	0.9300	C51—H51B	0.9600
C18—C19	1.404 (10)	C51—H51C	0.9600
C18—H18	0.9300		
$O1^{i}$—Gd1—O3	74.30 (10)	C17—C16—H16	118.8
$O1^{i}$—Gd1—$O4^{i}$	76.87 (11)	C18—C17—C16	119.9 (8)
O3—Gd1—$O4^{i}$	136.41 (12)	C18—C17—H17	120.1
$O1^{i}$—Gd1—O6	86.51 (12)	C16—C17—H17	120.1
O3—Gd1—O6	125.56 (13)	C17—C18—C19	121.7 (8)
$O4^{i}$—Gd1—O6	83.91 (13)	C17—C18—H18	119.2
$O1^{i}$—Gd1—O2	123.47 (12)	C19—C18—H18	119.2
O3—Gd1—O2	77.45 (11)	C24—C19—C18	122.6 (8)
$O4^{i}$—Gd1—O2	92.41 (12)	C24—C19—C20	119.3 (8)
O6—Gd1—O2	148.21 (12)	C18—C19—C20	118.1 (8)
$O1^{i}$—Gd1—O5	75.45 (12)	C21—C20—C15	122.4 (6)
O3—Gd1—O5	73.07 (13)	C21—C20—C19	117.6 (7)
$O4^{i}$—Gd1—O5	129.15 (13)	C15—C20—C19	120.0 (7)
O6—Gd1—O5	52.75 (12)	C22—C21—C20	120.6 (7)
O2—Gd1—O5	138.38 (12)	C22—C21—H21	119.7
$O1^{i}$—Gd1—O1	72.92 (13)	C20—C21—H21	119.7
O3—Gd1—O1	68.86 (11)	C21—C22—C23	122.0 (8)
$O4^{i}$—Gd1—O1	71.83 (11)	C21—C22—H22	119.0
O6—Gd1—O1	150.99 (11)	C23—C22—H22	119.0
O2—Gd1—O1	51.34 (10)	C24—C23—C22	119.3 (9)
O5—Gd1—O1	135.55 (12)	C24—C23—H23	120.3
$O1^{i}$—Gd1—N2	142.61 (13)	C22—C23—H23	120.3

O3—Gd1—N2	78.84 (13)	C23—C24—C19	121.1 (9)
O4^{i}—Gd1—N2	139.25 (13)	C23—C24—H24	119.5
O6—Gd1—N2	88.45 (14)	C19—C24—H24	119.5
O2—Gd1—N2	73.88 (13)	O5—C25—O6	122.4 (6)
O5—Gd1—N2	72.12 (14)	O5—C25—C26	117.4 (6)
O1—Gd1—N2	120.31 (13)	O6—C25—C26	120.2 (6)
O1^{i}—Gd1—N1	148.94 (12)	C27—C26—C25	112.3 (5)
O3—Gd1—N1	136.73 (12)	C27—C26—H26A	109.1
O4^{i}—Gd1—N1	76.19 (13)	C25—C26—H26A	109.1
O6—Gd1—N1	75.55 (13)	C27—C26—H26B	109.1
O2—Gd1—N1	72.92 (12)	C25—C26—H26B	109.1
O5—Gd1—N1	110.92 (13)	H26A—C26—H26B	107.9
O1—Gd1—N1	112.36 (12)	C28—C27—C32	118.1 (8)
N2—Gd1—N1	63.16 (14)	C28—C27—C26	123.2 (8)
O1^{i}—Gd1—Gd1^{i}	38.20 (8)	C32—C27—C26	118.7 (7)
O3—Gd1—Gd1^{i}	66.76 (8)	C27—C28—C29	122.1 (10)
O4^{i}—Gd1—Gd1^{i}	70.30 (8)	C27—C28—H28	119.0
O6—Gd1—Gd1^{i}	121.98 (9)	C29—C28—H28	119.0
O2—Gd1—Gd1^{i}	85.67 (8)	C30—C29—C28	120.6 (12)
O5—Gd1—Gd1^{i}	108.19 (9)	C30—C29—H29	119.7
O1—Gd1—Gd1^{i}	34.72 (7)	C28—C29—H29	119.7
N2—Gd1—Gd1^{i}	143.12 (10)	C29—C30—C31	120.3 (12)
N1—Gd1—Gd1^{i}	139.16 (10)	C29—C30—H30	119.8
C37—N1—C41	117.3 (5)	C31—C30—H30	119.8
C37—N1—Gd1	123.7 (4)	C30—C31—C36	120.5 (12)
C41—N1—Gd1	119.0 (3)	C30—C31—C32	119.4 (10)
C46—N2—C42	118.1 (5)	C36—C31—C32	120.1 (11)
C46—N2—Gd1	120.2 (4)	C33—C32—C31	118.1 (9)
C42—N2—Gd1	121.7 (4)	C33—C32—C27	122.4 (7)
C49—N3—C51	120.8 (9)	C31—C32—C27	119.5 (9)
C49—N3—C50	120.4 (8)	C34—C33—C32	120.9 (9)
C51—N3—C50	118.8 (8)	C34—C33—H33	119.6
C1—O1—Gd1^{i}	155.1 (3)	C32—C33—H33	119.6
C1—O1—Gd1	90.3 (3)	C33—C34—C35	118.6 (11)
Gd1^{i}—O1—Gd1	107.08 (13)	C33—C34—H34	120.7
C1—O2—Gd1	94.9 (3)	C35—C34—H34	120.7
C13—O3—Gd1	138.8 (3)	C36—C35—C34	123.8 (15)
C13—O4—Gd1^{i}	134.1 (3)	C36—C35—H35	118.1
C25—O5—Gd1	91.5 (4)	C34—C35—H35	118.1
C25—O6—Gd1	93.1 (4)	C35—C36—C31	118.6 (14)
O2—C1—O1	121.3 (5)	C35—C36—H36	120.7
O2—C1—C2	122.2 (5)	C31—C36—H36	120.7
O1—C1—C2	116.5 (5)	N1—C37—C38	123.0 (6)
C3—C2—C1	115.7 (5)	N1—C37—H37	118.5
C3—C2—H2A	108.4	C38—C37—H37	118.5
C1—C2—H2A	108.4	C39—C38—C37	119.4 (6)

C3—C2—H2B	108.4	C39—C38—H38	120.3
C1—C2—H2B	108.4	C37—C38—H38	120.3
H2A—C2—H2B	107.4	C38—C39—C40	120.3 (6)
C4—C3—C8	118.6 (6)	C38—C39—H39	119.9
C4—C3—C2	119.4 (6)	C40—C39—H39	119.9
C8—C3—C2	122.0 (6)	C39—C40—C41	117.2 (6)
C3—C4—C5	121.9 (7)	C39—C40—C47	123.4 (6)
C3—C4—H4	119.0	C41—C40—C47	119.4 (6)
C5—C4—H4	119.0	N1—C41—C40	122.8 (5)
C6—C5—C4	119.9 (7)	N1—C41—C42	118.3 (5)
C6—C5—H5	120.1	C40—C41—C42	118.9 (5)
C4—C5—H5	120.1	N2—C42—C43	122.0 (6)
C5—C6—C7	120.9 (7)	N2—C42—C41	117.8 (5)
C5—C6—H6	119.5	C43—C42—C41	120.3 (5)
C7—C6—H6	119.5	C44—C43—C42	117.9 (6)
C6—C7—C12	121.9 (7)	C44—C43—C48	123.7 (7)
C6—C7—C8	119.2 (7)	C42—C43—C48	118.4 (6)
C12—C7—C8	118.9 (8)	C45—C44—C43	120.6 (6)
C9—C8—C3	122.6 (6)	C45—C44—H44	119.7
C9—C8—C7	118.0 (7)	C43—C44—H44	119.7
C3—C8—C7	119.4 (7)	C44—C45—C46	118.3 (7)
C10—C9—C8	122.0 (7)	C44—C45—H45	120.8
C10—C9—H9	119.0	C46—C45—H45	120.8
C8—C9—H9	119.0	N2—C46—C45	123.2 (6)
C9—C10—C11	119.3 (9)	N2—C46—H46	118.4
C9—C10—H10	120.3	C45—C46—H46	118.4
C11—C10—H10	120.3	C48—C47—C40	121.4 (6)
C12—C11—C10	120.7 (9)	C48—C47—H47	119.3
C12—C11—H11	119.6	C40—C47—H47	119.3
C10—C11—H11	119.6	C47—C48—C43	121.6 (7)
C11—C12—C7	121.0 (8)	C47—C48—H48	119.2
C11—C12—H12	119.5	C43—C48—H48	119.2
C7—C12—H12	119.5	O7—C49—N3	122.6 (11)
O3—C13—O4	125.9 (5)	O7—C49—H49	118.7
O3—C13—C14	116.3 (5)	N3—C49—H49	118.7
O4—C13—C14	117.7 (5)	N3—C50—H50A	109.5
C15—C14—C13	116.9 (5)	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	117.9 (6)	N3—C51—H51B	109.5
C16—C15—C14	120.2 (6)	H51A—C51—H51B	109.5
C20—C15—C14	121.8 (5)	N3—C51—H51C	109.5
C15—C16—C17	122.4 (7)	H51A—C51—H51C	109.5
C15—C16—H16	118.8	H51B—C51—H51C	109.5
$O1^{i}$—Gd1—N1—C37	27.8 (6)	C6—C7—C8—C9	179.5 (6)

O3—Gd1—N1—C37	−148.5 (4)	C12—C7—C8—C9	0.5 (9)
O4^{i}—Gd1—N1—C37	−2.8 (4)	C6—C7—C8—C3	−0.9 (9)
O6—Gd1—N1—C37	84.4 (4)	C12—C7—C8—C3	−180.0 (6)
O2—Gd1—N1—C37	−99.7 (4)	C3—C8—C9—C10	179.9 (7)
O5—Gd1—N1—C37	124.3 (4)	C7—C8—C9—C10	−0.6 (10)
O1—Gd1—N1—C37	−66.1 (4)	C8—C9—C10—C11	0.1 (13)
N2—Gd1—N1—C37	−179.9 (5)	C9—C10—C11—C12	0.4 (15)
Gd1^{i}—Gd1—N1—C37	−38.1 (5)	C10—C11—C12—C7	−0.5 (15)
O1^{i}—Gd1—N1—C41	−154.6 (3)	C6—C7—C12—C11	−178.9 (8)
O3—Gd1—N1—C41	29.1 (5)	C8—C7—C12—C11	0.1 (12)
O4^{i}—Gd1—N1—C41	174.9 (4)	Gd1—O3—C13—O4	−29.4 (9)
O6—Gd1—N1—C41	−97.9 (4)	Gd1—O3—C13—C14	152.4 (4)
O2—Gd1—N1—C41	78.0 (4)	Gd1^{i}—O4—C13—O3	9.6 (8)
O5—Gd1—N1—C41	−58.1 (4)	Gd1^{i}—O4—C13—C14	−172.3 (3)
O1—Gd1—N1—C41	111.6 (4)	O3—C13—C14—C15	−139.9 (5)
N2—Gd1—N1—C41	−2.2 (3)	O4—C13—C14—C15	41.9 (8)
Gd1^{i}—Gd1—N1—C41	139.5 (3)	C13—C14—C15—C16	−120.2 (6)
O1^{i}—Gd1—N2—C46	−23.8 (6)	C13—C14—C15—C20	63.7 (8)
O3—Gd1—N2—C46	20.8 (5)	C20—C15—C16—C17	−1.4 (10)
O4^{i}—Gd1—N2—C46	175.2 (4)	C14—C15—C16—C17	−177.7 (6)
O6—Gd1—N2—C46	−105.9 (5)	C15—C16—C17—C18	1.5 (12)
O2—Gd1—N2—C46	100.8 (5)	C16—C17—C18—C19	0.6 (13)
O5—Gd1—N2—C46	−54.8 (5)	C17—C18—C19—C24	175.9 (8)
O1—Gd1—N2—C46	78.1 (5)	C17—C18—C19—C20	−2.4 (11)
N1—Gd1—N2—C46	179.5 (5)	C16—C15—C20—C21	−177.3 (6)
Gd1^{i}—Gd1—N2—C46	41.9 (6)	C14—C15—C20—C21	−1.1 (9)
O1^{i}—Gd1—N2—C42	160.1 (4)	C16—C15—C20—C19	−0.5 (9)
O3—Gd1—N2—C42	−155.3 (4)	C14—C15—C20—C19	175.7 (5)
O4^{i}—Gd1—N2—C42	−0.9 (5)	C24—C19—C20—C21	1.0 (9)
O6—Gd1—N2—C42	77.9 (4)	C18—C19—C20—C21	179.3 (6)
O2—Gd1—N2—C42	−75.3 (4)	C24—C19—C20—C15	−176.0 (6)
O5—Gd1—N2—C42	129.1 (4)	C18—C19—C20—C15	2.4 (9)
O1—Gd1—N2—C42	−98.1 (4)	C15—C20—C21—C22	176.0 (6)
N1—Gd1—N2—C42	3.4 (4)	C19—C20—C21—C22	−0.9 (10)
Gd1^{i}—Gd1—N2—C42	−134.2 (4)	C20—C21—C22—C23	0.1 (12)
O1^{i}—Gd1—O1—C1	162.0 (3)	C21—C22—C23—C24	0.7 (13)
O3—Gd1—O1—C1	82.6 (3)	C22—C23—C24—C19	−0.6 (14)
O4^{i}—Gd1—O1—C1	−116.6 (3)	C18—C19—C24—C23	−178.5 (8)
O6—Gd1—O1—C1	−151.3 (3)	C20—C19—C24—C23	−0.2 (12)
O2—Gd1—O1—C1	−8.0 (3)	Gd1—O5—C25—O6	−5.3 (6)
O5—Gd1—O1—C1	115.5 (3)	Gd1—O5—C25—C26	173.5 (5)
N2—Gd1—O1—C1	20.4 (3)	Gd1—O6—C25—O5	5.4 (6)
N1—Gd1—O1—C1	−50.6 (3)	Gd1—O6—C25—C26	−173.4 (5)
Gd1^{i}—Gd1—O1—C1	162.0 (3)	O5—C25—C26—C27	−51.9 (8)
O1^{i}—Gd1—O1—Gd1^{i}	0.0	O6—C25—C26—C27	126.9 (7)

O3—Gd1—O1—Gd1^{i}	−79.35 (13)	C25—C26—C27—C28	106.7 (7)
O4^{i}—Gd1—O1—Gd1^{i}	81.41 (13)	C25—C26—C27—C32	−70.7 (8)
O6—Gd1—O1—Gd1^{i}	46.7 (3)	C32—C27—C28—C29	0.6 (11)
O2—Gd1—O1—Gd1^{i}	−169.97 (18)	C26—C27—C28—C29	−176.9 (7)
O5—Gd1—O1—Gd1^{i}	−46.5 (2)	C27—C28—C29—C30	1.4 (15)
N2—Gd1—O1—Gd1^{i}	−141.55 (14)	C28—C29—C30—C31	−2.1 (17)
N1—Gd1—O1—Gd1^{i}	147.41 (13)	C29—C30—C31—C36	179.3 (10)
O1^{i}—Gd1—O2—C1	−3.2 (3)	C29—C30—C31—C32	0.8 (15)
O3—Gd1—O2—C1	−64.5 (3)	C30—C31—C32—C33	179.7 (8)
O4^{i}—Gd1—O2—C1	72.7 (3)	C36—C31—C32—C33	1.3 (12)
O6—Gd1—O2—C1	155.0 (3)	C30—C31—C32—C27	1.1 (11)
O5—Gd1—O2—C1	−110.1 (3)	C36—C31—C32—C27	−177.3 (8)
O1—Gd1—O2—C1	8.3 (3)	C28—C27—C32—C33	179.7 (7)
N2—Gd1—O2—C1	−146.3 (3)	C26—C27—C32—C33	−2.7 (10)
N1—Gd1—O2—C1	147.4 (3)	C28—C27—C32—C31	−1.8 (10)
Gd1^{i}—Gd1—O2—C1	2.6 (3)	C26—C27—C32—C31	175.8 (6)
O1^{i}—Gd1—O3—C13	−17.2 (5)	C31—C32—C33—C34	−0.2 (11)
O4^{i}—Gd1—O3—C13	33.2 (6)	C27—C32—C33—C34	178.4 (7)
O6—Gd1—O3—C13	−91.0 (6)	C32—C33—C34—C35	−0.9 (13)
O2—Gd1—O3—C13	113.3 (6)	C33—C34—C35—C36	0.9 (18)
O5—Gd1—O3—C13	−96.4 (6)	C34—C35—C36—C31	0(2)
O1—Gd1—O3—C13	60.2 (5)	C30—C31—C36—C35	−179.7 (11)
N2—Gd1—O3—C13	−170.9 (6)	C32—C31—C36—C35	−1.3 (17)
N1—Gd1—O3—C13	160.8 (5)	C41—N1—C37—C38	0.7 (9)
Gd1^{i}—Gd1—O3—C13	22.6 (5)	Gd1—N1—C37—C38	178.4 (5)
O1^{i}—Gd1—O5—C25	99.7 (3)	N1—C37—C38—C39	−1.0 (10)
O3—Gd1—O5—C25	177.3 (4)	C37—C38—C39—C40	1.1 (10)
O4^{i}—Gd1—O5—C25	40.6 (4)	C38—C39—C40—C41	−0.8 (9)
O6—Gd1—O5—C25	2.9 (3)	C38—C39—C40—C47	−179.4 (6)
O2—Gd1—O5—C25	−135.9 (3)	C37—N1—C41—C40	−0.4 (8)
O1—Gd1—O5—C25	145.4 (3)	Gd1—N1—C41—C40	−178.2 (4)
N2—Gd1—O5—C25	−99.2 (4)	C37—N1—C41—C42	179.0 (5)
N1—Gd1—O5—C25	−48.4 (4)	Gd1—N1—C41—C42	1.2 (6)
Gd1^{i}—Gd1—O5—C25	119.6 (3)	C39—C40—C41—N1	0.4 (9)
O1^{i}—Gd1—O6—C25	−77.2 (3)	C47—C40—C41—N1	179.1 (5)
O3—Gd1—O6—C25	−9.4 (4)	C39—C40—C41—C42	−179.0 (5)
O4^{i}—Gd1—O6—C25	−154.4 (3)	C47—C40—C41—C42	−0.3 (8)
O2—Gd1—O6—C25	120.9 (4)	C46—N2—C42—C43	0.7 (9)
O5—Gd1—O6—C25	−2.9 (3)	Gd1—N2—C42—C43	176.9 (4)
O1—Gd1—O6—C25	−121.4 (4)	C46—N2—C42—C41	179.6 (5)
N2—Gd1—O6—C25	65.7 (3)	Gd1—N2—C42—C41	−4.2 (7)
N1—Gd1—O6—C25	128.4 (3)	N1—C41—C42—N2	1.9 (7)
Gd1^{i}—Gd1—O6—C25	−92.2 (3)	C40—C41—C42—N2	−178.7 (5)
Gd1—O2—C1—O1	−15.4 (5)	N1—C41—C42—C43	−179.2 (5)
Gd1—O2—C1—C2	162.3 (5)	C40—C41—C42—C43	0.2 (8)

Gd1^{i}—O1—C1—O2	150.2 (6)	N2—C42—C43—C44	−1.1 (9)
Gd1—O1—C1—O2	14.9 (5)	C41—C42—C43—C44	−180.0 (6)
Gd1^{i}—O1—C1—C2	−27.7 (11)	N2—C42—C43—C48	178.9 (6)
Gd1—O1—C1—C2	−163.0 (4)	C41—C42—C43—C48	0.1 (9)
O2—C1—C2—C3	−3.5 (8)	C42—C43—C44—C45	0.8 (11)
O1—C1—C2—C3	174.3 (5)	C48—C43—C44—C45	−179.2 (7)
C1—C2—C3—C4	110.7 (6)	C43—C44—C45—C46	−0.1 (12)
C1—C2—C3—C8	−70.7 (7)	C42—N2—C46—C45	0.0 (10)
C8—C3—C4—C5	0.1 (9)	Gd1—N2—C46—C45	−176.3 (5)
C2—C3—C4—C5	178.8 (6)	C44—C45—C46—N2	−0.3 (12)
C3—C4—C5—C6	0.6 (11)	C39—C40—C47—C48	178.7 (7)
C4—C5—C6—C7	−1.5 (11)	C41—C40—C47—C48	0.1 (10)
C5—C6—C7—C12	−179.3 (7)	C40—C47—C48—C43	0.2 (11)
C5—C6—C7—C8	1.7 (11)	C44—C43—C48—C47	179.7 (7)
C4—C3—C8—C9	179.6 (6)	C42—C43—C48—C47	−0.3 (10)
C2—C3—C8—C9	0.9 (9)	C51—N3—C49—O7	−2.7 (14)
C4—C3—C8—C7	0.1 (8)	C50—N3—C49—O7	179.8 (8)
C2—C3—C8—C7	−178.6 (5)		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C50—H50A···O6^{ii}	0.96	2.54	3.379 (9)	146
C47—H47···O2^{iii}	0.93	2.46	3.319 (7)	153
C6—H6···O7^{iv}	0.93	2.55	3.436 (10)	159
C51—H51C···O7	0.96	2.30	2.713 (13)	105
C46—H46···O3	0.93	2.45	3.057 (7)	123
C37—H37···O4^{i}	0.93	2.37	3.027 (7)	127
C21—H21···O5	0.93	2.59	3.412 (8)	148
C18—H18···Cg1^{v}	0.93	2.88	3.66 (2)	142
C39—H39···Cg2^{iii}	0.93	2.99	3.858 (18)	156

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

Fig. 1

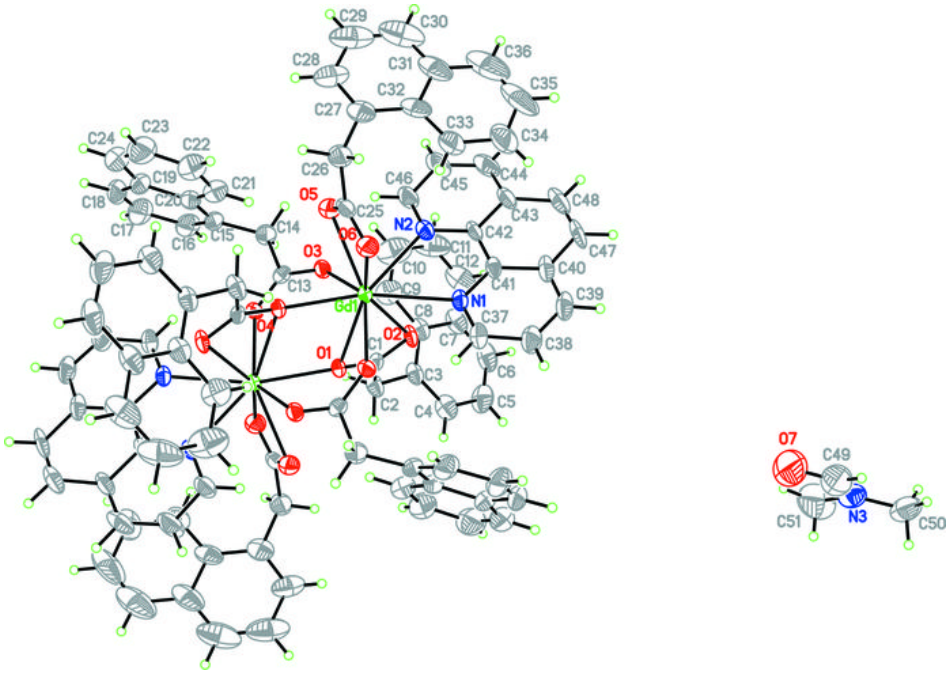
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Fig. 2

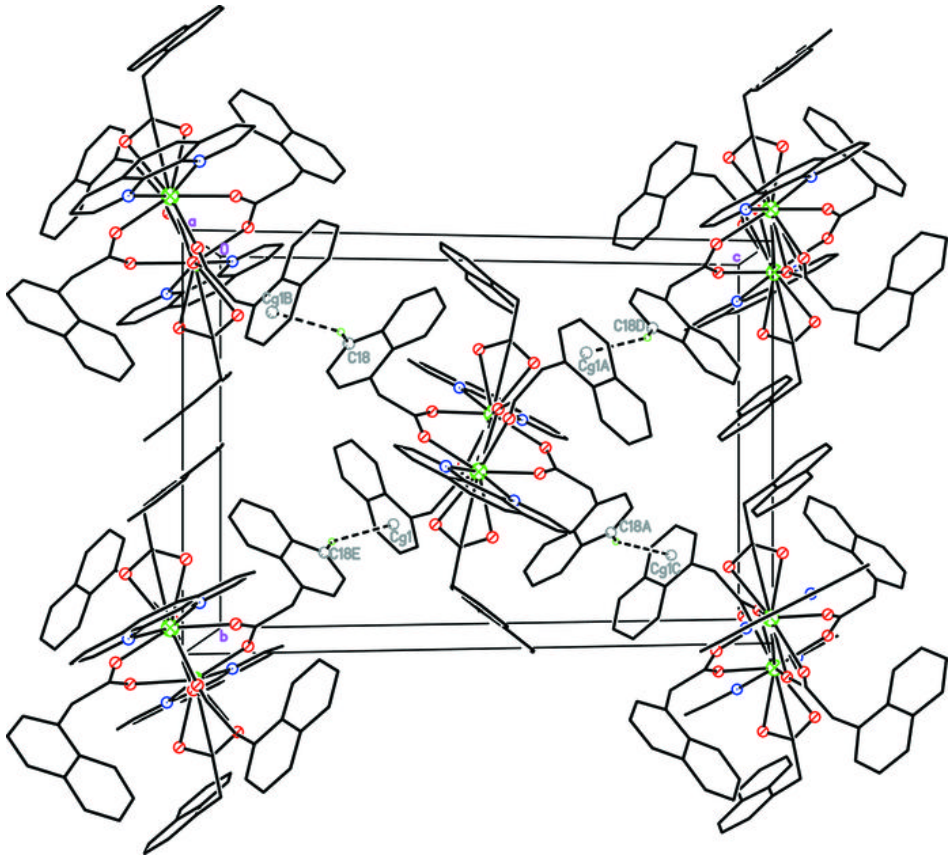

Fig. 3