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Poly[[tris(μ_2-4,4′-bipyridine *N*,*N*′-dioxide)hexanitratodigadolinium(III)] dichloromethane disolvate]

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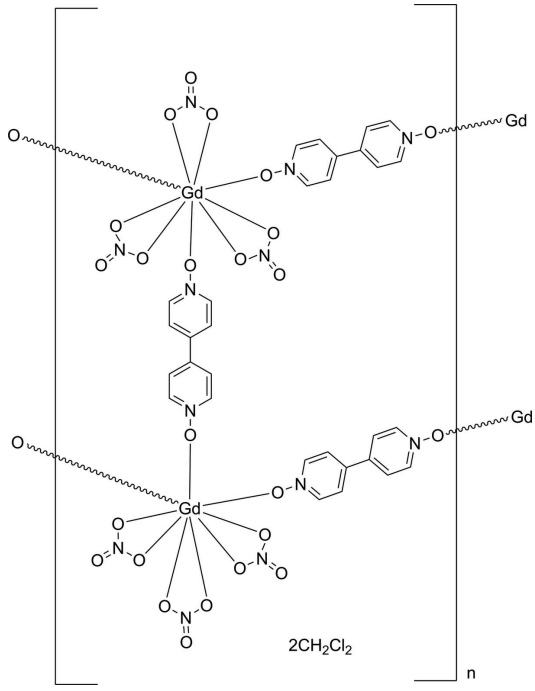
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.020; wR factor = 0.051; data-to-parameter ratio = 20.9.

The title one-dimensional coordination network, $\{[Gd_2(NO_3)_6(C_{10}H_8N_2O_2)_3]\cdot 2CH_2Cl_2\}_n$, is isostructural with the previously reported Tb and Tl coordination networks and to its Eu analog. The Gd^{III} cation is coordinated in a distorted tricapped trigonal-prismatic fashion by nine O atoms from three bridging 4,4′-bipyridine *N*,*N*′-dioxide ligands and three chelating nitrate anions. None of the atoms lie on a special position, but there is an inversion center located between the rings of one of the ligands. The network topology is ladder-like, and each ladder interacts with six neighboring ladders through C—H···O hydrogen bonds. The packing motif of the ladders allows for the formation of channels that run parallel to the *a* axis; these channels are filled with CH_2Cl_2 solvent molecules that interact with the ladders through C—H···O hydrogen bonds

Related literature

For the isostructural Tb and Tl, coordination networks, see: Long *et al.* (2002); Moitsheki *et al.* (2006). For the isostructural Eu coordination network and detailed background to this study, see: Dillner *et al.* (2010).



Experimental

Crystal data

$[Gd_2(NO_3)_6(C_{10}H_8N_2O_2)_3]\cdot 2CH_2Cl_2$
M_r = 1420.96
Triclinic, $P\overline{1}$
a = 7.9917 (5) Å
b = 11.5668 (7) Å
c = 13.0347 (8) Å
α = 86.059 (1)°
β = 80.134 (1)°
γ = 78.255 (1)°
V = 1161.52 (12) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 3.16 mm^{-1}
T = 100 K
0.51 × 0.48 × 0.25 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.529, T_{max} = 0.746
13791 measured reflections
6990 independent reflections
6776 reflections with $I > 2\sigma(I)$
R_{int} = 0.019

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.020
$wR(F^2)$ = 0.051
S = 1.06
6990 reflections
334 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.34 e Å^{-3}
$\Delta\rho_{min}$ = −1.26 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5···O7^{i}	0.95	2.41	3.082 (2)	127
C9—H9···O9^{ii}	0.95	2.57	3.287 (2)	132
C12—H12···O2^{iii}	0.95	2.43	3.300 (2)	152
C16—H16*B*···O12^{ii}	0.99	2.43	3.246 (3)	139
C16—H16*A*···O8	0.99	2.56	3.302 (3)	132
C16—H16*A*···O9	0.99	2.50	3.084 (3)	117

Symmetry codes: (i) $x+1, y, z$; (ii) $-x+1, -y+2, -z+2$; (iii) $-x+2, -y+2, -z+1$.

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *X-SEED*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZL2303).

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supplementary materials

Acta Cryst. (2010). E**66**, m1158-m1159 [**doi:10.1107/S1600536810033258**]

Poly[[tris(μ_2-4,4'-bipyridine *N*,*N*'-dioxide)hexanitratodigadolinium(III)] dichloromethane disolvate]

A. J. Dillner, C. P. Lilly and J. M. Knaust

Comment

The description of the structure of the title compound is part of a set of consecutive papers on one-dimensional ladder-like coordination networks of the type $[Ln_2(NO_3)_6(C_{10}H_8N_2O_2)_3]_n$, with Ln = Eu (Dillner *et al.*, 2010) and Gd (this publication), respectively. Both compounds are also isostructural to the previously reported Tb and Tl, coordination networks (Long *et al.*, 2002 and Moitsheki *et al.*, 2006). The background to this study is given in Dillner *et al.* (2010).

Experimental

$Gd(NO_3)_3$ (0.051 g 0.15 mmol) was placed in the bottom of a test tube and covered with CH_2Cl_2 (5 ml). *4,4*'-bipyridine-*N,N*'-dioxide·H_2O (0.0376 g, 0.182 mmol) was dissolved in methanol (8 ml), and this solution was layered over the CH_2Cl_2. The two solutions were allowed to slowly mix. Over a period of several weeks the $Gd(NO_3)_3$ dissolved, and yellow plate-like crystals of the title compound formed.

Refinement

All H atoms were positioned geometrically and refined using a riding model with C—H = 0.95 Å and with U_{iso}(H) = 1.2 times U_{eq}(C).

Figures

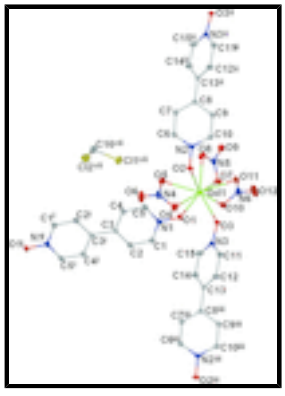


Fig. 1. The coordination environment of the Gd^{+3} cation in the title compound with atom labels and 50% probability displacement ellipsoids. Hydrogen atoms have been omitted for clarity. Color scheme: Gd: green, C: grey, N: blue, O: red, Cl: yellow. Symmetry codes: (i) -x+3, -y+1, -z+1; (ii) x, y, z+1; (iii) x, y, z-1; (vii) -x+2, -y+1, z+2.

Poly[[tris(μ$_2$-4,4'-bipyridine *N*,*N*'-dioxide)hexanitratodigadolinium(III)] dichloromethane disolvate]

Crystal data

$[Gd_2(NO_3)_6(C_{10}H_8N_2O_2)_3]\cdot 2CH_2Cl_2$	$Z = 1$
$M_r = 1420.96$	$F(000) = 692$
Triclinic, $P\overline{1}$	$D_x = 2.031$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 7.9917$ (5) Å	Cell parameters from 9995 reflections
$b = 11.5668$ (7) Å	$\theta = 2.4$–$31.4°$
$c = 13.0347$ (8) Å	$\mu = 3.16$ mm^{-1}
$\alpha = 86.059$ (1)°	$T = 100$ K
$\beta = 80.134$ (1)°	Plate, yellow
$\gamma = 78.255$ (1)°	0.51 × 0.48 × 0.25 mm
$V = 1161.52$ (12) Å^3	

Data collection

Bruker SMART APEX CCD diffractometer	6990 independent reflections
Radiation source: fine-focus sealed tube	6776 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.019$
ω scans	$\theta_{max} = 31.5°$, $\theta_{min} = 1.6°$
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)	$h = -11\rightarrow 11$
$T_{min} = 0.529$, $T_{max} = 0.746$	$k = -16\rightarrow 16$
13791 measured reflections	$l = -19\rightarrow 19$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.020$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.051$	H-atom parameters constrained
$S = 1.06$	$w = 1/[\sigma^2(F_o^2) + (0.0269P)^2 + 0.7108P]$ where $P = (F_o^2 + 2F_c^2)/3$
6990 reflections	$(\Delta/\sigma)_{max} = 0.003$
334 parameters	$\Delta\rho_{max} = 1.34$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -1.26$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds

in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ 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	0.777386 (9)	0.833312 (7)	0.717678 (6)	0.01052 (3)
O1	1.02444 (16)	0.82720 (11)	0.59321 (10)	0.0154 (2)
O2	0.95666 (17)	0.87415 (12)	0.83066 (9)	0.0156 (2)
O3	0.62864 (17)	0.87372 (12)	0.57713 (9)	0.0165 (2)
O4	0.80192 (19)	0.63739 (12)	0.64108 (12)	0.0228 (3)
O5	0.95223 (19)	0.63785 (12)	0.76314 (11)	0.0215 (3)
O6	0.9729 (2)	0.47510 (14)	0.68376 (16)	0.0329 (4)
O7	0.48223 (18)	0.79088 (13)	0.77573 (10)	0.0200 (3)
O8	0.64333 (17)	0.77345 (13)	0.89476 (11)	0.0200 (3)
O9	0.37413 (18)	0.75493 (13)	0.93691 (11)	0.0224 (3)
O10	0.80809 (18)	1.04012 (12)	0.66218 (10)	0.0186 (3)
O11	0.59902 (18)	1.01912 (12)	0.78729 (11)	0.0191 (3)
O12	0.6429 (3)	1.19502 (15)	0.73675 (17)	0.0438 (5)
N1	1.15539 (19)	0.73739 (13)	0.56764 (11)	0.0133 (3)
N2	0.91991 (19)	0.86889 (13)	0.93448 (11)	0.0126 (3)
N3	0.69504 (19)	0.86834 (13)	0.47630 (11)	0.0132 (3)
N4	0.9111 (2)	0.57955 (14)	0.69595 (14)	0.0191 (3)
N5	0.49582 (19)	0.77173 (13)	0.87144 (12)	0.0149 (3)
N6	0.6826 (2)	1.08859 (15)	0.72846 (13)	0.0201 (3)
C1	1.1729 (3)	0.68680 (17)	0.47533 (15)	0.0200 (4)
H1	1.0924	0.7154	0.4293	0.024*
C2	1.3074 (3)	0.59355 (18)	0.44774 (15)	0.0204 (4)
H2	1.3185	0.5581	0.3827	0.024*
C3	1.4277 (2)	0.55043 (15)	0.51390 (13)	0.0129 (3)
C4	1.4065 (2)	0.60763 (17)	0.60766 (14)	0.0177 (3)
H4	1.4869	0.5823	0.6544	0.021*
C5	1.2700 (2)	0.70055 (17)	0.63297 (14)	0.0179 (3)
H5	1.2569	0.7387	0.6969	0.021*
C6	0.9834 (2)	0.76999 (16)	0.98742 (14)	0.0154 (3)
H6	1.0519	0.7040	0.9506	0.018*
C7	0.9492 (2)	0.76424 (15)	1.09522 (14)	0.0153 (3)
H7	0.9932	0.6941	1.1322	0.018*
C8	0.8502 (2)	0.86129 (15)	1.14956 (13)	0.0126 (3)
C9	0.7879 (2)	0.96209 (15)	1.09168 (13)	0.0147 (3)
H9	0.7208	1.0298	1.1266	0.018*
C10	0.8227 (2)	0.96446 (15)	0.98455 (13)	0.0149 (3)
H10	0.7785	1.0331	0.9458	0.018*
C11	0.7464 (2)	0.96300 (15)	0.42487 (14)	0.0158 (3)

H11	0.7456	1.0312	0.4617	0.019*
C12	0.8003 (2)	0.96117 (16)	0.31859 (13)	0.0158 (3)
H12	0.8341	1.0289	0.2822	0.019*
C13	0.8053 (2)	0.86070 (15)	0.26447 (13)	0.0125 (3)
C14	0.7610 (3)	0.76171 (16)	0.32125 (14)	0.0182 (3)
H14	0.7694	0.6903	0.2871	0.022*
C15	0.7051 (3)	0.76792 (17)	0.42680 (14)	0.0192 (3)
H15	0.6733	0.7008	0.4653	0.023*
C16	0.5603 (3)	0.60138 (19)	1.10231 (18)	0.0274 (4)
H16A	0.5816	0.6058	1.0252	0.033*
H16B	0.5414	0.6826	1.1273	0.033*
Cl1	0.74334 (7)	0.51440 (4)	1.14775 (4)	0.02581 (10)
Cl2	0.37217 (7)	0.54128 (6)	1.14632 (5)	0.03300 (12)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Gd1	0.01086 (4)	0.01200 (4)	0.00842 (4)	−0.00199 (3)	−0.00084 (3)	−0.00099 (3)
O1	0.0135 (6)	0.0135 (5)	0.0165 (6)	0.0004 (4)	0.0023 (4)	−0.0032 (4)
O2	0.0171 (6)	0.0228 (6)	0.0077 (5)	−0.0069 (5)	−0.0002 (4)	−0.0010 (4)
O3	0.0157 (6)	0.0253 (6)	0.0072 (5)	−0.0025 (5)	−0.0004 (4)	−0.0001 (4)
O4	0.0244 (7)	0.0162 (6)	0.0299 (8)	−0.0021 (5)	−0.0116 (6)	−0.0034 (5)
O5	0.0256 (7)	0.0168 (6)	0.0221 (7)	−0.0001 (5)	−0.0081 (5)	−0.0025 (5)
O6	0.0301 (8)	0.0153 (7)	0.0541 (11)	0.0024 (6)	−0.0136 (8)	−0.0090 (7)
O7	0.0187 (6)	0.0300 (7)	0.0136 (6)	−0.0096 (5)	−0.0040 (5)	0.0010 (5)
O8	0.0145 (6)	0.0303 (7)	0.0169 (6)	−0.0085 (5)	−0.0045 (5)	0.0055 (5)
O9	0.0146 (6)	0.0271 (7)	0.0223 (7)	−0.0042 (5)	0.0027 (5)	0.0063 (5)
O10	0.0202 (6)	0.0169 (6)	0.0166 (6)	−0.0025 (5)	0.0012 (5)	−0.0002 (5)
O11	0.0180 (6)	0.0176 (6)	0.0190 (6)	−0.0021 (5)	0.0025 (5)	−0.0009 (5)
O12	0.0555 (12)	0.0136 (7)	0.0512 (12)	−0.0006 (7)	0.0156 (9)	−0.0018 (7)
N1	0.0120 (6)	0.0130 (6)	0.0139 (6)	−0.0021 (5)	0.0007 (5)	−0.0016 (5)
N2	0.0129 (6)	0.0171 (7)	0.0090 (6)	−0.0055 (5)	−0.0011 (5)	−0.0020 (5)
N3	0.0130 (6)	0.0172 (7)	0.0094 (6)	−0.0027 (5)	−0.0020 (5)	0.0000 (5)
N4	0.0162 (7)	0.0153 (7)	0.0253 (8)	−0.0028 (6)	−0.0022 (6)	−0.0017 (6)
N5	0.0131 (6)	0.0137 (6)	0.0175 (7)	−0.0027 (5)	−0.0018 (5)	0.0012 (5)
N6	0.0220 (8)	0.0162 (7)	0.0195 (8)	−0.0003 (6)	−0.0005 (6)	−0.0008 (6)
C1	0.0214 (9)	0.0221 (9)	0.0145 (8)	0.0037 (7)	−0.0051 (7)	−0.0047 (7)
C2	0.0222 (9)	0.0225 (9)	0.0153 (8)	0.0028 (7)	−0.0057 (7)	−0.0082 (7)
C3	0.0124 (7)	0.0140 (7)	0.0124 (7)	−0.0043 (6)	0.0002 (6)	−0.0025 (6)
C4	0.0143 (8)	0.0231 (9)	0.0152 (8)	0.0008 (6)	−0.0030 (6)	−0.0071 (6)
C5	0.0151 (8)	0.0233 (9)	0.0154 (8)	−0.0016 (6)	−0.0025 (6)	−0.0085 (6)
C6	0.0155 (8)	0.0158 (7)	0.0139 (8)	−0.0013 (6)	−0.0008 (6)	−0.0032 (6)
C7	0.0167 (8)	0.0142 (7)	0.0141 (8)	−0.0004 (6)	−0.0024 (6)	−0.0009 (6)
C8	0.0120 (7)	0.0153 (7)	0.0105 (7)	−0.0027 (6)	−0.0016 (5)	−0.0007 (5)
C9	0.0157 (8)	0.0148 (7)	0.0121 (7)	−0.0007 (6)	−0.0007 (6)	−0.0016 (6)
C10	0.0163 (8)	0.0153 (7)	0.0124 (7)	−0.0021 (6)	−0.0020 (6)	0.0002 (6)
C11	0.0205 (8)	0.0136 (7)	0.0138 (8)	−0.0039 (6)	−0.0028 (6)	−0.0014 (6)
C12	0.0211 (8)	0.0146 (7)	0.0125 (7)	−0.0064 (6)	−0.0017 (6)	0.0001 (6)

C13	0.0118 (7)	0.0146 (7)	0.0105 (7)	−0.0013 (5)	−0.0017 (5)	0.0000 (5)
C14	0.0278 (9)	0.0140 (8)	0.0134 (8)	−0.0051 (7)	−0.0033 (7)	−0.0012 (6)
C15	0.0295 (10)	0.0168 (8)	0.0133 (8)	−0.0095 (7)	−0.0039 (7)	0.0015 (6)
C16	0.0267 (10)	0.0235 (10)	0.0293 (11)	−0.0009 (8)	−0.0048 (8)	0.0068 (8)
Cl1	0.0292 (2)	0.0199 (2)	0.0288 (2)	−0.00077 (18)	−0.01067 (19)	−0.00114 (17)
Cl2	0.0267 (3)	0.0391 (3)	0.0304 (3)	−0.0049 (2)	−0.0016 (2)	0.0060 (2)

Geometric parameters (Å, °)

Gd1—O3	2.3216 (13)	C1—H1	0.9500
Gd1—O1	2.3230 (13)	C2—C3	1.395 (2)
Gd1—O2	2.3534 (13)	C2—H2	0.9500
Gd1—O11	2.4601 (13)	C3—C4	1.398 (2)
Gd1—O8	2.4879 (14)	C3—C3^{i}	1.481 (3)
Gd1—O7	2.4872 (14)	C4—C5	1.379 (2)
Gd1—O5	2.4958 (14)	C4—H4	0.9500
Gd1—O4	2.4967 (14)	C5—H5	0.9500
Gd1—O10	2.4992 (14)	C6—C7	1.384 (2)
Gd1—N6	2.9021 (17)	C6—H6	0.9500
Gd1—N5	2.9152 (15)	C7—C8	1.394 (2)
Gd1—N4	2.9277 (16)	C7—H7	0.9500
O1—N1	1.3308 (18)	C8—C9	1.396 (2)
O2—N2	1.3346 (18)	C8—C13^{ii}	1.479 (2)
O3—N3	1.3310 (18)	C9—C10	1.376 (2)
O4—N4	1.277 (2)	C9—H9	0.9500
O5—N4	1.265 (2)	C10—H10	0.9500
O6—N4	1.219 (2)	C11—C12	1.379 (2)
O7—N5	1.271 (2)	C11—H11	0.9500
O8—N5	1.271 (2)	C12—C13	1.391 (2)
O9—N5	1.217 (2)	C12—H12	0.9500
O10—N6	1.268 (2)	C13—C14	1.394 (2)
O11—N6	1.280 (2)	C13—C8^{iii}	1.479 (2)
O12—N6	1.215 (2)	C14—C15	1.374 (3)
N1—C5	1.343 (2)	C14—H14	0.9500
N1—C1	1.347 (2)	C15—H15	0.9500
N2—C6	1.348 (2)	C16—Cl1	1.766 (2)
N2—C10	1.352 (2)	C16—Cl2	1.774 (2)
N3—C11	1.343 (2)	C16—H16A	0.9900
N3—C15	1.349 (2)	C16—H16B	0.9900
C1—C2	1.378 (3)		
O3—Gd1—O1	85.06 (5)	C5—N1—C1	121.14 (15)
O3—Gd1—O2	154.22 (5)	O2—N2—C6	119.65 (14)
O1—Gd1—O2	83.54 (5)	O2—N2—C10	119.01 (14)
O3—Gd1—O11	85.96 (5)	C6—N2—C10	121.33 (15)
O1—Gd1—O11	122.79 (4)	O3—N3—C11	120.02 (15)
O2—Gd1—O11	80.97 (5)	O3—N3—C15	118.90 (15)
O3—Gd1—O8	123.47 (4)	C11—N3—C15	121.06 (15)
O1—Gd1—O8	148.53 (5)	O6—N4—O5	122.12 (18)

O2—Gd1—O8	74.82 (4)	O6—N4—O4	122.15 (18)
O11—Gd1—O8	76.46 (5)	O5—N4—O4	115.72 (15)
O3—Gd1—O7	72.31 (4)	O6—N4—Gd1	177.12 (15)
O1—Gd1—O7	150.94 (5)	O5—N4—Gd1	57.84 (9)
O2—Gd1—O7	124.33 (4)	O4—N4—Gd1	57.95 (9)
O11—Gd1—O7	74.51 (5)	O9—N5—O8	122.12 (16)
O8—Gd1—O7	51.32 (4)	O9—N5—O7	122.00 (16)
O3—Gd1—O5	125.67 (5)	O8—N5—O7	115.87 (15)
O1—Gd1—O5	79.17 (5)	O9—N5—Gd1	175.14 (13)
O2—Gd1—O5	74.49 (5)	O8—N5—Gd1	58.03 (9)
O11—Gd1—O5	144.96 (5)	O7—N5—Gd1	58.00 (8)
O8—Gd1—O5	73.25 (5)	O12—N6—O10	122.46 (18)
O7—Gd1—O5	99.15 (5)	O12—N6—O11	121.17 (17)
O3—Gd1—O4	75.01 (5)	O10—N6—O11	116.37 (15)
O1—Gd1—O4	78.88 (5)	O12—N6—Gd1	177.69 (16)
O2—Gd1—O4	124.87 (5)	O10—N6—Gd1	59.06 (9)
O11—Gd1—O4	150.14 (5)	O11—N6—Gd1	57.34 (8)
O8—Gd1—O4	94.89 (5)	N1—C1—C2	120.02 (17)
O7—Gd1—O4	77.84 (5)	N1—C1—H1	120.0
O5—Gd1—O4	51.08 (5)	C2—C1—H1	120.0
O3—Gd1—O10	76.63 (5)	C1—C2—C3	120.99 (16)
O1—Gd1—O10	71.20 (4)	C1—C2—H2	119.5
O2—Gd1—O10	77.83 (5)	C3—C2—H2	119.5
O11—Gd1—O10	51.76 (4)	C2—C3—C4	116.88 (16)
O8—Gd1—O10	124.27 (5)	C2—C3—C3^{i}	121.81 (19)
O7—Gd1—O10	118.86 (5)	C4—C3—C3^{i}	121.3 (2)
O5—Gd1—O10	141.26 (5)	C5—C4—C3	120.61 (17)
O4—Gd1—O10	140.09 (5)	C5—C4—H4	119.7
O3—Gd1—N6	80.79 (5)	C3—C4—H4	119.7
O1—Gd1—N6	96.87 (5)	N1—C5—C4	120.33 (16)
O2—Gd1—N6	77.73 (5)	N1—C5—H5	119.8
O11—Gd1—N6	25.98 (4)	C4—C5—H5	119.8
O8—Gd1—N6	100.45 (5)	N2—C6—C7	120.24 (16)
O7—Gd1—N6	97.21 (5)	N2—C6—H6	119.9
O5—Gd1—N6	152.20 (5)	C7—C6—H6	119.9
O4—Gd1—N6	155.69 (5)	C6—C7—C8	120.07 (16)
O10—Gd1—N6	25.79 (4)	C6—C7—H7	120.0
O3—Gd1—N5	97.81 (4)	C8—C7—H7	120.0
O1—Gd1—N5	164.46 (4)	C7—C8—C9	117.78 (15)
O2—Gd1—N5	99.36 (4)	C7—C8—C13^{ii}	123.06 (15)
O11—Gd1—N5	72.72 (4)	C9—C8—C13^{ii}	119.14 (15)
O8—Gd1—N5	25.68 (4)	C10—C9—C8	120.69 (16)
O7—Gd1—N5	25.68 (4)	C10—C9—H9	119.7
O5—Gd1—N5	86.86 (5)	C8—C9—H9	119.7
O4—Gd1—N5	87.08 (5)	N2—C10—C9	119.89 (16)
O10—Gd1—N5	124.33 (4)	N2—C10—H10	120.1
N6—Gd1—N5	98.67 (5)	C9—C10—H10	120.1
O3—Gd1—N4	100.41 (5)	N3—C11—C12	120.02 (16)

O1—Gd1—N4	77.11 (5)	N3—C11—H11	120.0
O2—Gd1—N4	99.46 (5)	C12—C11—H11	120.0
O11—Gd1—N4	159.79 (5)	C11—C12—C13	120.29 (16)
O8—Gd1—N4	84.12 (5)	C11—C12—H12	119.9
O7—Gd1—N4	89.07 (5)	C13—C12—H12	119.9
O5—Gd1—N4	25.41 (5)	C12—C13—C14	118.11 (15)
O4—Gd1—N4	25.69 (5)	C12—C13—C8^{iii}	120.50 (15)
O10—Gd1—N4	148.30 (5)	C14—C13—C8^{iii}	121.35 (15)
N6—Gd1—N4	173.67 (5)	C15—C14—C13	119.68 (16)
N5—Gd1—N4	87.36 (4)	C15—C14—H14	120.2
N1—O1—Gd1	129.39 (10)	C13—C14—H14	120.2
N2—O2—Gd1	124.82 (10)	N3—C15—C14	120.67 (17)
N3—O3—Gd1	127.48 (10)	N3—C15—H15	119.7
N4—O4—Gd1	96.36 (10)	C14—C15—H15	119.7
N4—O5—Gd1	96.75 (11)	Cl1—C16—Cl2	111.26 (12)
N5—O7—Gd1	96.32 (10)	Cl1—C16—H16A	109.4
N5—O8—Gd1	96.29 (10)	Cl2—C16—H16A	109.4
N6—O10—Gd1	95.16 (11)	Cl1—C16—H16B	109.4
N6—O11—Gd1	96.67 (10)	Cl2—C16—H16B	109.4
O1—N1—C5	119.58 (14)	H16A—C16—H16B	108.0
O1—N1—C1	119.26 (15)		

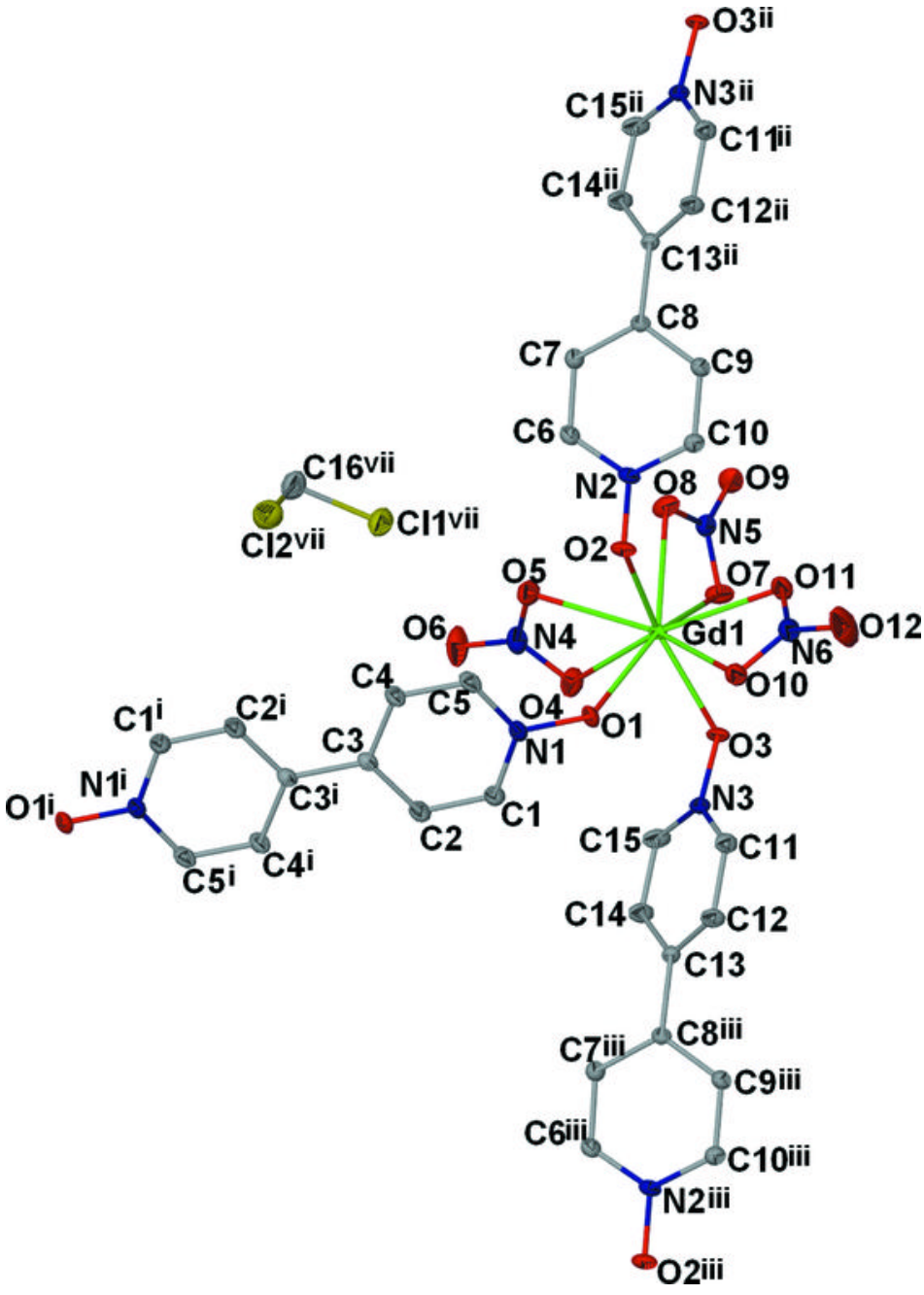
Symmetry codes: (i) −*x*+3, −*y*+1, −*z*+1; (ii) *x*, *y*, *z*+1; (iii) *x*, *y*, *z*−1.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···O7^{iv}	0.95	2.41	3.082 (2)	127.
C9—H9···O9^{v}	0.95	2.57	3.287 (2)	132.
C12—H12···O2^{vi}	0.95	2.43	3.300 (2)	152.
C16—H16B···O12^{v}	0.99	2.43	3.246 (3)	139.
C16—H16A···O8	0.99	2.56	3.302 (3)	132.
C16—H16A···O9	0.99	2.50	3.084 (3)	117.

Symmetry codes: (iv) *x*+1, *y*, *z*; (v) −*x*+1, −*y*+2, −*z*+2; (vi) −*x*+2, −*y*+2, −*z*+1.

Fig. 1


O3ii
N3ii
C15ii
C11ii
C14ii
C12ii
C13ii
C8
C7
C9
C6
C10
N2
O8
O9
N5
O2
O5
O7
O11
O6
N4
Gd1
N6
O12
O10
C4
C5
O4
O1
C1i
C2i
C3
N1
O3
N1i
O1i
C3i
C1
N3
C2
C15
C11
C5i
C4i
C14
C12
C13
C8iii
C7iii
C9iii
C6iii
C10iii
N2iii
O2iii
C16vii
Cl1vii
Cl2vii