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[13,27-Dimethyl-3,6,9,17,20,23-hexaazatricyclo[23.3.1.1^{11,15}]triaconta-1(29),2,9,11,13,15(30),16,23,25,27-decaene-29,30-diol-$\kappa^5N^3,N^6,N^9,O^{29},O^{30}$]bis(nitrato-$\kappa^2O,O'$)gadolinium(III) nitrate monohydrate

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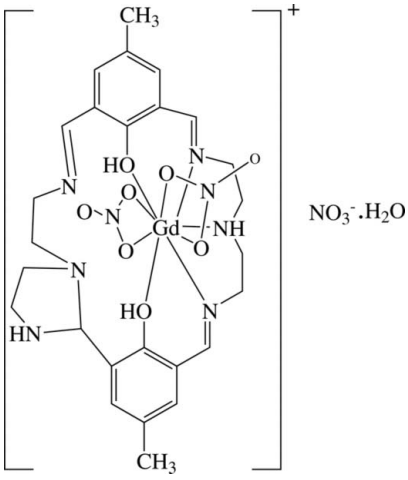
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.008 Å; disorder in solvent or counterion; R factor = 0.049; wR factor = 0.107; data-to-parameter ratio = 15.0.

The Gd atom in the title title complex, $[Gd(NO_3)_2(C_{26}H_{34}N_6O_2)]NO_3{\cdot}H_2O$, exhibits a nine-coordinate distorted tricapped trigonal prismatic coordination geometry. The water molecule is disordered, with restrained occupancy factors of 0.4 and 0.6, with one component lying on a twofold rotation axis.

Related literature

For related literature, see: Alexander (1995); Bunzli & Moret (1988); Guerriero *et al.* (1987); Hu *et al.* (2003, 2004).



Experimental

Crystal data

$[Gd(NO_3)_2(C_{26}H_{34}N_6O_2)]NO_3{\cdot}H_2O$
M_r = 823.89
Monoclinic, $C2/c$
a = 23.764 (3) Å
b = 14.298 (3) Å
c = 19.804 (2) Å
β = 91.769 (2)°
V = 6724.5 (13) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 2.05 mm^{-1}
T = 291 (2) K
0.30 × 0.26 × 0.24 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.55, T_{max} = 0.61
19136 measured reflections
6596 independent reflections
4171 reflections with $I > 2\sigma(I)$
R_{int} = 0.046

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.107
S = 0.98
6596 reflections
440 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −1.38 e Å^{-3}

Table 1
Selected bond lengths (Å).

Gd1—O1	2.263 (4)	Gd1—O7	2.553 (4)
Gd1—O2	2.281 (3)	Gd1—N2	2.554 (4)
Gd1—O6	2.483 (4)	Gd1—N3	2.555 (5)
Gd1—O3	2.485 (4)	Gd1—N1	2.558 (5)
Gd1—O4	2.527 (4)		

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; 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: BQ2010).

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supplementary materials

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[13,27-Dimethyl-3,6,9,17,20,23-hexaazatricyclo[23.3.1.1^{11,15}]triaconta-1(29),2,9,11,13,15(30),16,23,25,27-decaene-29,30-diol-$\kappa^5N^3,N^6,N^9,O^{29},O^{30}$]bis(nitrato-$\kappa^2O,O'$)gadolinium(III) nitrate monohydrate

X.-L. Hu, L. Qiu, J. Yuan and Z.-Q. Pan

Comment

Lanthanide macrocyclic complexes have been received extensive attention, owing to their many possible applications in biological systems, material science and chemical processes (Alexander, 1995;Hu *et al.*, 2003; Hu *et al.*, 2004). A series of lanthanide(III) complexes with macrocyclic Schiff bases have synthesized by one step template condensation of 2,6-di-formyl- 4-chlorophenol with 1,5-diamino-3-azapentane in the presence of lanthanide ions (Alexander, 1995). Guerriero *et al.* (1987) and Bunzli *et al.* (1988) have reported the crystal structures of the Tb(III) and Eu(III) complexes in which the central ion is nine-coordinate, being bound to five donor atoms from the cyclic polydentate ligand and to four O atoms of two bidentae nitrates.

The title complex (I) (Fig. 1), which is synthesized by template reaction of 2,6-diformyl-4-methylphenol with 1,5-diamino-3-azapentane in the presence of gadolinium(III) nitrate, exhibits a similar coordinate geometry (Fig. 2). Gd1 is encaptured with in the macrocyclic ligand which provided five donor atoms (the two O atoms O1, O2 from the phenolates and the three N atoms N1, N2, N3 from one end of the macrocycle). The ninefold coordination is completed around Gd1 by two bidentate nitrates which locate on the opposite sides of the bisphenoidal positions. The third nitrate is ionic. At the free end of the macrocycle, a further five-membered imidazoling rings is formed by contraction, this makes the ligand more compact hence allowing a more appropriate spatial arrangement of the donor atoms of the macrocyclic ligand around the lanthanide ions. The coordination polyhedron can be described as a distorted tricapped trigonal prism in which N2, O4 and O7 are the caps, as show in Fig.2.

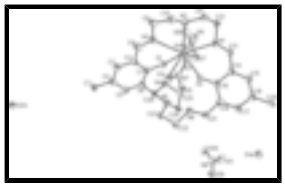
Experimental

To a methanolic solution (20 ml) of 2,6-diformyl-4-methylphenol(1 mmol) and $Gd(NO_3)_3{\cdot}6H_2O$ (0.5 mmol), 1,5-diamino-3-azapentane (1 mmol) was added dropwise. After refluxing 3 h, the solvent was removed. Yellow solid was recrystallized in acetonitrile and then yellow block crystals suitable for X-ray analysis were obtained.

Refinement

The carbon-bound H atoms were generated geometrically (C–H 0.93 to 0.97 Å) and were included in the refinement in the riding model approximation, with U(H) set to 1.2U_{eq}(C). The water H atom was located in a difference Fourier map, and was refined with an O–H distance restraint of 0.85±0.01 Å; its temperature factor was refined.

Figures



(I).

Figure 1. Thermal ellipsoid plot of (I). Displacement ellipsoids are drawn at the 30% probability level.

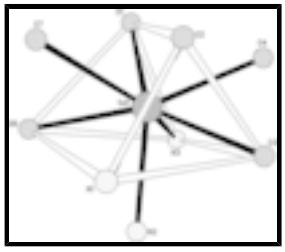


Figure 2. Coordination polyhedron in (I).

(13,27-Dimethyl-3,6,9,17,20,23-hexaazatricyclo[23.3.1.1^{11,15}]triaconta- 1(29),2,9,11,13,15 (30),16,23,25,27-decaene-29,30-diol- N^3,N^6,N^9,O^{29},O^{30})bis(nitrato-κ^2O,O')gadolinium(III) nitrate hydrate

Crystal data

$[Gd(NO_3)_2(C_{26}H_{34}N_6O_2)]NO_3{\cdot}H_2O$	F_{000} = 3320
M_r = 823.89	D_x = 1.628 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 5110 reflections
a = 23.764 (3) Å	θ = 2.6–25.0º
b = 14.298 (3) Å	μ = 2.05 mm^{-1}
c = 19.804 (2) Å	*T* = 291 (2) K
β = 91.769 (2)º	Block, yellow
V = 6724.5 (13) Å^3	0.30 × 0.26 × 0.24 mm
Z = 8	

Data collection

Bruker SMART CCD area-detector diffractometer	6596 independent reflections
Radiation source: sealed tube	4171 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.046
T = 291(2) K	θ_{max} = 26.0º
φ and ω scans	θ_{min} = 2.6º
Absorption correction: multi-scan (SADABS; Bruker, 2000)	*h* = −29→22
T_{min} = 0.55, T_{max} = 0.61	*k* = −16→17
19136 measured reflections	*l* = −23→24

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.049$	H-atom parameters constrained
$wR(F^2) = 0.107$	$w = 1/[\sigma^2(F_o^2) + (0.052P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.98$	$(\Delta/\sigma)_{max} < 0.001$
6596 reflections	$\Delta\rho_{max} = 0.41$ e Å^{-3}
440 parameters	$\Delta\rho_{min} = -1.38$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1	0.2695 (2)	0.9536 (4)	0.1213 (3)	0.0501 (13)	
C2	0.2875 (2)	1.0154 (4)	0.0702 (3)	0.0563 (14)	
C3	0.3425 (3)	1.0095 (4)	0.0459 (3)	0.0585 (14)	
H3	0.3543	1.0526	0.0142	0.070*	
C4	0.3791 (3)	0.9403 (4)	0.0685 (3)	0.0570 (14)	
C5	0.3604 (3)	0.8761 (4)	0.1157 (3)	0.0589 (15)	
H5	0.3843	0.8279	0.1298	0.071*	
C6	0.3075 (3)	0.8820 (4)	0.1422 (3)	0.0563 (14)	
C7	0.4394 (2)	0.9327 (5)	0.0409 (3)	0.0607 (15)	
H7A	0.4659	0.9601	0.0727	0.091*	
H7B	0.4409	0.9652	−0.0014	0.091*	
H7C	0.4487	0.8680	0.0344	0.091*	
C8	0.2520 (3)	1.0863 (4)	0.0406 (3)	0.0652 (16)	
H8	0.2692	1.1261	0.0103	0.078*	
C9	0.1757 (3)	1.1865 (4)	0.0145 (3)	0.0593 (15)	
H9A	0.1914	1.1923	−0.0299	0.071*	
H9B	0.1851	1.2426	0.0400	0.071*	
C10	0.1122 (3)	1.1764 (4)	0.0078 (3)	0.0611 (16)	

H10A	0.0958	1.2350	−0.0076	0.073*
H10B	0.1028	1.1286	−0.0254	0.073*
C11	0.0258 (3)	1.1483 (4)	0.0724 (3)	0.0575 (15)
H11A	0.0110	1.2113	0.0686	0.069*
H11B	0.0114	1.1124	0.0341	0.069*
C12	0.0074 (3)	1.1057 (4)	0.1351 (3)	0.0569 (15)
H12A	−0.0334	1.1062	0.1361	0.068*
H12B	0.0220	1.1411	0.1735	0.068*
C13	−0.0081 (2)	0.9434 (4)	0.1513 (3)	0.0542 (14)
H13	−0.0445	0.9626	0.1602	0.065*
C14	0.0023 (2)	0.8441 (4)	0.1526 (3)	0.0537 (13)
C15	−0.0424 (3)	0.7853 (4)	0.1679 (3)	0.0626 (15)
H15	−0.0763	0.8134	0.1786	0.075*
C16	−0.0405 (2)	0.6898 (4)	0.1684 (3)	0.0536 (13)
C17	0.0090 (3)	0.6498 (4)	0.1495 (3)	0.0586 (15)
H17	0.0111	0.5849	0.1472	0.070*
C18	0.0560 (3)	0.7014 (4)	0.1337 (3)	0.0570 (14)
C19	0.0547 (2)	0.8007 (4)	0.1346 (3)	0.0504 (13)
C20	−0.0906 (3)	0.6320 (4)	0.1876 (3)	0.0613 (16)
H20A	−0.1194	0.6724	0.2039	0.092*
H20B	−0.0794	0.5885	0.2223	0.092*
H20C	−0.1048	0.5984	0.1487	0.092*
C21	0.1067 (3)	0.6533 (4)	0.1148 (3)	0.0512 (13)
H21	0.1063	0.5882	0.1161	0.061*
C22	0.2031 (2)	0.6402 (4)	0.0824 (3)	0.0548 (14)
H22A	0.2052	0.6290	0.0342	0.066*
H22B	0.2023	0.5802	0.1052	0.066*
C23	0.2554 (2)	0.6978 (4)	0.1079 (3)	0.0516 (13)
H23A	0.2868	0.6556	0.1166	0.062*
H23B	0.2661	0.7412	0.0730	0.062*
C24	0.2306 (3)	0.6971 (4)	0.2291 (3)	0.0546 (14)
H24A	0.2590	0.6506	0.2405	0.065*
H24B	0.1942	0.6666	0.2241	0.065*
C25	0.2295 (3)	0.7747 (4)	0.2825 (3)	0.0647 (16)
H25A	0.1912	0.7939	0.2910	0.078*
H25B	0.2476	0.7545	0.3246	0.078*
C26	0.2897 (2)	0.8117 (4)	0.1911 (3)	0.0499 (13)
H26	0.3224	0.7748	0.2064	0.060*
Gd1	0.132602 (11)	0.996866 (19)	0.112967 (14)	0.04773 (10)
N1	0.0281 (2)	1.0091 (3)	0.1389 (2)	0.0551 (11)
N2	0.0895 (2)	1.1511 (3)	0.0718 (3)	0.0590 (13)
H2	0.1009	1.1958	0.1020	0.071*
N3	0.2000 (2)	1.1025 (3)	0.0500 (2)	0.0542 (12)
N4	0.2619 (2)	0.8522 (3)	0.2508 (2)	0.0554 (11)
H4A	0.2385	0.8989	0.2379	0.067*
H4B	0.2878	0.8752	0.2805	0.067*
N5	0.2444 (2)	0.7482 (4)	0.1676 (3)	0.0641 (13)
N6	0.1521 (2)	0.6931 (3)	0.0965 (2)	0.0584 (12)
H6A	0.1527	0.7530	0.0924	0.070*

N7	0.1260 (2)	0.8939 (3)	−0.0123 (2)	0.0533 (11)	
N8	0.1368 (2)	1.0475 (4)	0.2570 (3)	0.0598 (12)	
N9	0.1283 (2)	0.3947 (4)	0.1408 (3)	0.0589 (13)	
O1	0.22107 (16)	0.9625 (3)	0.15061 (18)	0.0525 (9)	
O2	0.09826 (15)	0.8486 (2)	0.12235 (18)	0.0485 (8)	
O3	0.09112 (17)	0.9594 (3)	−0.00056 (19)	0.0583 (10)	
O4	0.17109 (19)	0.8926 (3)	0.0223 (2)	0.0637 (11)	
O5	0.11340 (17)	0.8315 (3)	−0.0522 (2)	0.0648 (11)	
O6	0.13705 (18)	1.1068 (3)	0.2101 (2)	0.0640 (11)	
O7	0.13078 (17)	0.9602 (3)	0.2391 (2)	0.0616 (10)	
O8	0.1408 (2)	1.0668 (3)	0.3166 (3)	0.0853 (14)	
O9	0.14265 (19)	0.3210 (3)	0.1536 (2)	0.0661 (12)	
O10	0.15358 (18)	0.4520 (3)	0.1704 (2)	0.0627 (11)	
O11	0.0879 (2)	0.4096 (3)	0.1042 (2)	0.0685 (12)	
O1W	0.0000	0.3603 (5)	0.2500	0.069 (2)	0.80
H1WA	0.0081	0.3026	0.2474	0.083*	0.40
H1WB	0.0145	0.3896	0.2175	0.083*	0.40
O2W	0.8107 (3)	0.9370 (5)	0.1122 (3)	0.0629 (17)	0.60
H2WD	0.8465	0.9383	0.1129	0.075*	0.60
H2WB	0.7981	0.9918	0.1189	0.075*	0.60

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.048 (3)	0.049 (3)	0.053 (3)	0.013 (2)	−0.006 (2)	0.011 (2)
C2	0.040 (3)	0.055 (4)	0.074 (4)	0.009 (2)	0.002 (3)	0.003 (3)
C3	0.057 (3)	0.052 (3)	0.067 (3)	0.007 (3)	−0.001 (3)	−0.003 (3)
C4	0.050 (3)	0.062 (4)	0.058 (3)	0.010 (3)	−0.004 (3)	0.013 (3)
C5	0.054 (4)	0.057 (3)	0.065 (3)	0.007 (3)	−0.004 (3)	0.010 (3)
C6	0.050 (3)	0.057 (3)	0.062 (3)	0.007 (3)	0.005 (3)	−0.004 (3)
C7	0.035 (3)	0.074 (4)	0.073 (4)	0.013 (3)	0.007 (3)	0.010 (3)
C8	0.072 (5)	0.064 (4)	0.059 (3)	0.009 (3)	−0.007 (3)	−0.009 (3)
C9	0.059 (4)	0.061 (4)	0.056 (3)	0.013 (3)	−0.010 (3)	−0.007 (3)
C10	0.066 (4)	0.053 (3)	0.063 (4)	−0.004 (3)	−0.016 (3)	−0.014 (3)
C11	0.060 (4)	0.052 (3)	0.059 (3)	−0.007 (3)	−0.019 (3)	0.000 (3)
C12	0.049 (3)	0.054 (3)	0.067 (4)	−0.007 (3)	−0.008 (3)	0.024 (3)
C13	0.035 (3)	0.060 (3)	0.067 (3)	−0.004 (3)	0.001 (2)	0.014 (3)
C14	0.037 (3)	0.064 (4)	0.061 (3)	0.003 (3)	0.005 (2)	0.011 (3)
C15	0.054 (4)	0.066 (4)	0.068 (4)	0.002 (3)	0.008 (3)	0.026 (3)
C16	0.046 (3)	0.060 (3)	0.055 (3)	0.014 (3)	0.010 (2)	0.013 (3)
C17	0.055 (4)	0.062 (4)	0.059 (3)	0.005 (3)	0.005 (3)	0.006 (3)
C18	0.063 (4)	0.053 (3)	0.055 (3)	−0.002 (3)	0.000 (3)	0.006 (2)
C19	0.036 (3)	0.046 (3)	0.069 (3)	−0.002 (2)	0.003 (2)	0.005 (2)
C20	0.061 (4)	0.053 (3)	0.071 (4)	0.025 (3)	0.027 (3)	0.018 (3)
C21	0.061 (4)	0.033 (3)	0.059 (3)	0.001 (2)	−0.006 (3)	0.008 (2)
C22	0.052 (4)	0.057 (3)	0.056 (3)	−0.008 (3)	0.017 (3)	0.007 (3)
C23	0.039 (3)	0.059 (3)	0.057 (3)	−0.009 (2)	0.013 (2)	0.003 (3)
C24	0.046 (3)	0.063 (4)	0.056 (3)	0.001 (3)	0.004 (3)	−0.018 (3)

C25	0.056 (4)	0.069 (4)	0.069 (4)	0.020 (3)	0.009 (3)	−0.005 (3)
C26	0.030 (3)	0.064 (3)	0.055 (3)	−0.003 (2)	−0.003 (2)	−0.006 (2)
Gd1	0.03673 (14)	0.04502 (15)	0.06105 (16)	0.00045 (12)	−0.00490 (10)	0.00840 (13)
N1	0.048 (3)	0.050 (3)	0.067 (3)	−0.009 (2)	−0.005 (2)	0.020 (2)
N2	0.057 (3)	0.047 (3)	0.071 (3)	−0.004 (2)	−0.028 (2)	0.007 (2)
N3	0.043 (3)	0.060 (3)	0.059 (3)	0.007 (2)	−0.007 (2)	−0.014 (2)
N4	0.046 (3)	0.060 (3)	0.060 (3)	−0.001 (2)	−0.006 (2)	0.009 (2)
N5	0.061 (3)	0.065 (3)	0.066 (3)	0.000 (3)	0.000 (3)	0.001 (2)
N6	0.066 (3)	0.046 (3)	0.063 (3)	−0.002 (2)	0.004 (3)	0.004 (2)
N7	0.048 (3)	0.050 (3)	0.063 (3)	0.002 (2)	0.011 (2)	0.002 (2)
N8	0.049 (3)	0.067 (3)	0.064 (3)	0.009 (3)	0.012 (2)	0.008 (3)
N9	0.054 (3)	0.057 (3)	0.065 (3)	−0.001 (2)	−0.022 (2)	0.026 (2)
O1	0.048 (2)	0.053 (2)	0.057 (2)	0.0023 (17)	0.0058 (18)	0.0030 (17)
O2	0.047 (2)	0.0388 (18)	0.061 (2)	0.0012 (16)	0.0111 (17)	0.0042 (15)
O3	0.055 (2)	0.062 (2)	0.057 (2)	−0.008 (2)	−0.0115 (18)	0.0004 (18)
O4	0.062 (3)	0.064 (3)	0.065 (2)	0.006 (2)	0.004 (2)	0.0013 (19)
O5	0.061 (3)	0.067 (3)	0.066 (3)	−0.004 (2)	0.003 (2)	0.036 (2)
O6	0.063 (3)	0.065 (3)	0.064 (2)	0.008 (2)	−0.005 (2)	0.014 (2)
O7	0.054 (3)	0.067 (3)	0.065 (2)	0.010 (2)	0.0086 (19)	0.026 (2)
O8	0.064 (3)	0.075 (3)	0.118 (4)	0.006 (2)	0.019 (3)	0.005 (3)
O9	0.066 (3)	0.069 (3)	0.062 (2)	0.021 (2)	−0.018 (2)	−0.014 (2)
O10	0.062 (3)	0.058 (2)	0.066 (2)	−0.015 (2)	−0.022 (2)	0.021 (2)
O11	0.067 (3)	0.070 (3)	0.067 (3)	−0.011 (2)	−0.017 (2)	0.017 (2)
O1W	0.067 (5)	0.072 (5)	0.071 (5)	0.000	0.016 (4)	0.000
O2W	0.047 (4)	0.067 (4)	0.074 (4)	0.005 (3)	0.002 (3)	0.005 (3)

Geometric parameters (Å, °)

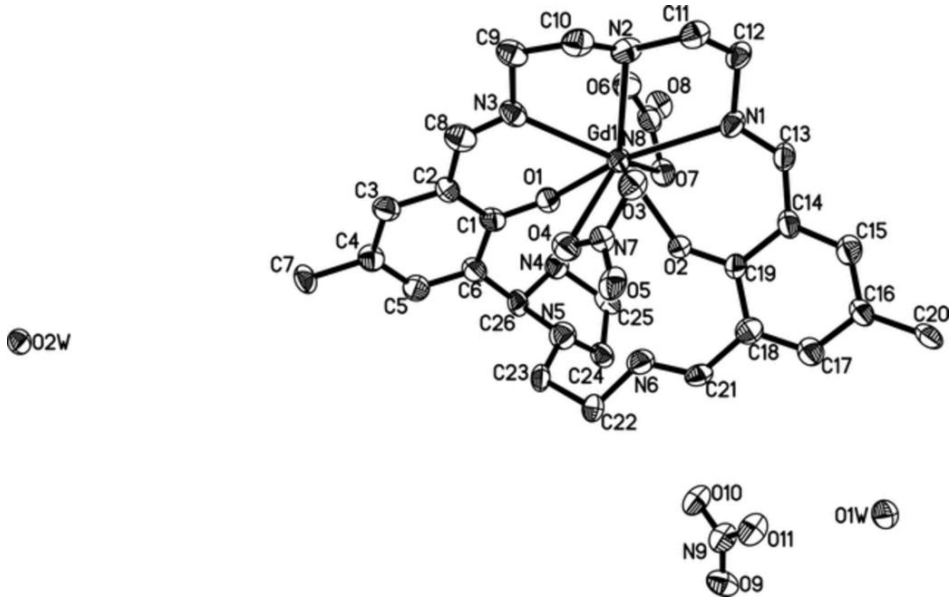
C1—O1	1.311 (6)	C21—N6	1.284 (8)
C1—C6	1.417 (7)	C21—H21	0.9300
C1—C2	1.421 (8)	C22—N6	1.462 (8)
C2—C3	1.408 (8)	C22—C23	1.563 (8)
C2—C8	1.433 (8)	C22—H22A	0.9700
C3—C4	1.383 (8)	C22—H22B	0.9700
C3—H3	0.9300	C23—N5	1.415 (7)
C4—C5	1.392 (8)	C23—H23A	0.9700
C4—C7	1.552 (8)	C23—H23B	0.9700
C5—C6	1.380 (8)	C24—N5	1.465 (8)
C5—H5	0.9300	C24—C25	1.533 (8)
C6—C26	1.467 (8)	C24—H24A	0.9700
C7—H7A	0.9600	C24—H24B	0.9700
C7—H7B	0.9600	C25—N4	1.497 (8)
C7—H7C	0.9600	C25—H25A	0.9700
C8—N3	1.275 (8)	C25—H25B	0.9700
C8—H8	0.9300	C26—N5	1.473 (7)
C9—N3	1.499 (7)	C26—N4	1.490 (7)
C9—C10	1.516 (8)	C26—H26	0.9800
C9—H9A	0.9700	Gd1—O1	2.263 (4)
C9—H9B	0.9700	Gd1—O2	2.281 (3)

C10—N2	1.439 (8)	Gd1—O6	2.483 (4)
C10—H10A	0.9700	Gd1—O3	2.485 (4)
C10—H10B	0.9700	Gd1—O4	2.527 (4)
C11—C12	1.462 (8)	Gd1—O7	2.553 (4)
C11—N2	1.515 (8)	Gd1—N2	2.554 (4)
C11—H11A	0.9700	Gd1—N3	2.555 (5)
C11—H11B	0.9700	Gd1—N1	2.558 (5)
C12—N1	1.467 (7)	Gd1—N7	2.884 (5)
C12—H12A	0.9700	Gd1—N8	2.941 (6)
C12—H12B	0.9700	N2—H2	0.9100
C13—N1	1.302 (7)	N4—H4A	0.9000
C13—C14	1.442 (8)	N4—H4B	0.9000
C13—H13	0.9300	N6—H6A	0.8600
C14—C15	1.394 (8)	N7—O5	1.223 (6)
C14—C19	1.446 (8)	N7—O4	1.254 (6)
C15—C16	1.365 (8)	N7—O3	1.277 (6)
C15—H15	0.9300	N8—O8	1.213 (7)
C16—C17	1.371 (8)	N8—O6	1.258 (6)
C16—C20	1.507 (8)	N8—O7	1.304 (7)
C17—C18	1.383 (9)	N9—O9	1.133 (6)
C17—H17	0.9300	N9—O10	1.164 (6)
C18—C19	1.420 (8)	N9—O11	1.204 (6)
C18—C21	1.445 (9)	N9—O1W	3.824 (6)
C19—O2	1.271 (6)	O1W—H1WA	0.8499
C20—H20A	0.9600	O1W—H1WB	0.8501
C20—H20B	0.9600	O2W—H2WD	0.8499
C20—H20C	0.9600	O2W—H2WB	0.8500
O1—C1—C6	120.1 (5)	N5—C26—H26	109.3
O1—C1—C2	122.9 (5)	N4—C26—H26	109.3
C6—C1—C2	117.0 (5)	O1—Gd1—O2	95.90 (13)
C3—C2—C1	120.6 (5)	O1—Gd1—O6	82.25 (13)
C3—C2—C8	116.4 (6)	O2—Gd1—O6	122.13 (13)
C1—C2—C8	123.0 (6)	O1—Gd1—O3	126.15 (14)
C4—C3—C2	120.9 (6)	O2—Gd1—O3	74.96 (13)
C4—C3—H3	119.5	O6—Gd1—O3	147.48 (13)
C2—C3—H3	119.5	O1—Gd1—O4	75.71 (14)
C3—C4—C5	118.5 (6)	O2—Gd1—O4	69.41 (13)
C3—C4—C7	120.9 (5)	O6—Gd1—O4	156.35 (14)
C5—C4—C7	120.5 (5)	O3—Gd1—O4	51.10 (14)
C6—C5—C4	121.9 (5)	O1—Gd1—O7	71.15 (13)
C6—C5—H5	119.0	O2—Gd1—O7	73.31 (14)
C4—C5—H5	119.0	O6—Gd1—O7	51.25 (14)
C5—C6—C1	120.9 (5)	O3—Gd1—O7	145.32 (14)
C5—C6—C26	119.6 (5)	O4—Gd1—O7	126.28 (14)
C1—C6—C26	119.5 (5)	O1—Gd1—N2	130.66 (15)
C4—C7—H7A	109.5	O2—Gd1—N2	133.42 (14)
C4—C7—H7B	109.5	O6—Gd1—N2	73.01 (14)
H7A—C7—H7B	109.5	O3—Gd1—N2	75.73 (15)
C4—C7—H7C	109.5	O4—Gd1—N2	115.63 (16)

H7A—C7—H7C	109.5	O7—Gd1—N2	118.06 (16)
H7B—C7—H7C	109.5	O1—Gd1—N3	72.45 (14)
N3—C8—C2	129.1 (7)	O2—Gd1—N3	145.13 (14)
N3—C8—H8	115.5	O6—Gd1—N3	89.51 (14)
C2—C8—H8	115.5	O3—Gd1—N3	85.59 (14)
N3—C9—C10	109.5 (5)	O4—Gd1—N3	75.83 (14)
N3—C9—H9A	109.8	O7—Gd1—N3	128.93 (14)
C10—C9—H9A	109.8	N2—Gd1—N3	65.50 (16)
N3—C9—H9B	109.8	O1—Gd1—N1	147.86 (14)
C10—C9—H9B	109.8	O2—Gd1—N1	72.23 (13)
H9A—C9—H9B	108.2	O6—Gd1—N1	79.62 (15)
N2—C10—C9	110.2 (5)	O3—Gd1—N1	80.55 (15)
N2—C10—H10A	109.6	O4—Gd1—N1	123.92 (15)
C9—C10—H10A	109.6	O7—Gd1—N1	76.80 (14)
N2—C10—H10B	109.6	N2—Gd1—N1	67.85 (15)
C9—C10—H10B	109.6	N3—Gd1—N1	133.27 (14)
H10A—C10—H10B	108.1	O1—Gd1—N7	101.41 (14)
C12—C11—N2	110.1 (5)	O2—Gd1—N7	65.53 (13)
C12—C11—H11A	109.6	O6—Gd1—N7	171.41 (12)
N2—C11—H11A	109.6	O3—Gd1—N7	26.18 (13)
C12—C11—H11B	109.6	O4—Gd1—N7	25.71 (13)
N2—C11—H11B	109.6	O7—Gd1—N7	137.25 (14)
H11A—C11—H11B	108.2	N2—Gd1—N7	98.95 (15)
C11—C12—N1	109.1 (5)	N3—Gd1—N7	84.27 (14)
C11—C12—H12A	109.9	N1—Gd1—N7	100.38 (15)
N1—C12—H12A	109.9	O1—Gd1—N8	74.39 (14)
C11—C12—H12B	109.9	O2—Gd1—N8	98.69 (14)
N1—C12—H12B	109.9	O6—Gd1—N8	25.03 (13)
H12A—C12—H12B	108.3	O3—Gd1—N8	158.56 (14)
N1—C13—C14	126.9 (6)	O4—Gd1—N8	146.35 (14)
N1—C13—H13	116.6	O7—Gd1—N8	26.26 (14)
C14—C13—H13	116.6	N2—Gd1—N8	95.62 (16)
C15—C14—C13	117.8 (5)	N3—Gd1—N8	108.96 (14)
C15—C14—C19	117.5 (6)	N1—Gd1—N8	78.01 (15)
C13—C14—C19	124.5 (5)	N7—Gd1—N8	163.50 (15)
C16—C15—C14	125.4 (6)	C13—N1—C12	117.8 (5)
C16—C15—H15	117.3	C13—N1—Gd1	129.8 (4)
C14—C15—H15	117.3	C12—N1—Gd1	112.3 (3)
C15—C16—C17	116.3 (6)	C10—N2—C11	114.6 (4)
C15—C16—C20	121.6 (5)	C10—N2—Gd1	109.9 (4)
C17—C16—C20	122.1 (5)	C11—N2—Gd1	111.4 (3)
C16—C17—C18	123.0 (6)	C10—N2—H2	106.8
C16—C17—H17	118.5	C11—N2—H2	106.8
C18—C17—H17	118.5	Gd1—N2—H2	106.8
C17—C18—C19	120.8 (6)	C8—N3—C9	116.0 (6)
C17—C18—C21	119.3 (5)	C8—N3—Gd1	126.1 (4)
C19—C18—C21	119.9 (5)	C9—N3—Gd1	117.6 (4)
O2—C19—C18	121.2 (5)	C26—N4—C25	107.0 (4)
O2—C19—C14	122.0 (5)	C26—N4—H4A	110.3

C18—C19—C14	116.8 (5)	C25—N4—H4A	110.3
C16—C20—H20A	109.5	C26—N4—H4B	110.3
C16—C20—H20B	109.5	C25—N4—H4B	110.3
H20A—C20—H20B	109.5	H4A—N4—H4B	108.6
C16—C20—H20C	109.5	C23—N5—C24	119.5 (5)
H20A—C20—H20C	109.5	C23—N5—C26	115.2 (5)
H20B—C20—H20C	109.5	C24—N5—C26	103.0 (4)
N6—C21—C18	125.2 (5)	C21—N6—C22	122.3 (5)
N6—C21—H21	117.4	C21—N6—H6A	118.9
C18—C21—H21	117.4	C22—N6—H6A	118.9
N6—C22—C23	108.7 (5)	O5—N7—O4	122.1 (5)
N6—C22—H22A	110.0	O5—N7—O3	120.3 (5)
C23—C22—H22A	110.0	O4—N7—O3	117.4 (5)
N6—C22—H22B	110.0	O5—N7—Gd1	159.1 (4)
C23—C22—H22B	110.0	O4—N7—Gd1	61.0 (3)
H22A—C22—H22B	108.3	O3—N7—Gd1	59.2 (3)
N5—C23—C22	111.9 (5)	O8—N8—O6	124.3 (6)
N5—C23—H23A	109.2	O8—N8—O7	119.2 (5)
C22—C23—H23A	109.2	O6—N8—O7	116.5 (5)
N5—C23—H23B	109.2	O8—N8—Gd1	177.1 (4)
C22—C23—H23B	109.2	O6—N8—Gd1	56.7 (3)
H23A—C23—H23B	107.9	O7—N8—Gd1	60.0 (3)
N5—C24—C25	102.8 (5)	O9—N9—O10	113.2 (5)
N5—C24—H24A	111.2	O9—N9—O11	121.9 (6)
C25—C24—H24A	111.2	O10—N9—O11	124.6 (5)
N5—C24—H24B	111.2	O9—N9—O1W	89.7 (4)
C25—C24—H24B	111.2	O10—N9—O1W	102.3 (4)
H24A—C24—H24B	109.1	O11—N9—O1W	74.2 (3)
N4—C25—C24	103.1 (5)	C1—O1—Gd1	134.0 (3)
N4—C25—H25A	111.1	C19—O2—Gd1	144.3 (3)
C24—C25—H25A	111.1	N7—O3—Gd1	94.6 (3)
N4—C25—H25B	111.1	N7—O4—Gd1	93.3 (3)
C24—C25—H25B	111.1	N8—O6—Gd1	98.3 (4)
H25A—C25—H25B	109.1	N8—O7—Gd1	93.7 (3)
C6—C26—N5	115.8 (5)	N9—O1W—H1WA	84.5
C6—C26—N4	113.7 (5)	H1WA—O1W—H1WB	109.5
N5—C26—N4	98.7 (4)	H2WD—O2W—H2WB	109.5
C6—C26—H26	109.3		

Fig. 1


C10
N2
C11
C9
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O6
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N1
C8
Gd1
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C13
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C3
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C26
O2W
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C23
C24
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C21
C22
O10
O1W
O11
N9
O9

Fig. 2