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catena-Poly[[[diaqua(6-carboxypyridine-2-carboxylato-κ^3O,N,O')gadolinium(III)]-μ-pyridine-2,6-dicarboxylato-$\kappa^4N,O,O':O''$] tetrahydrate]

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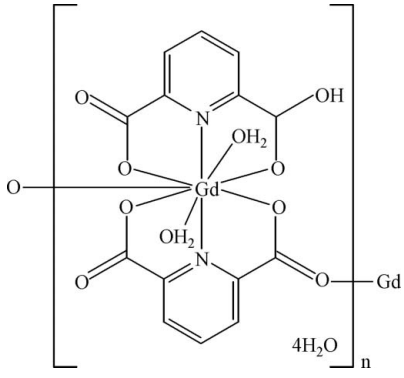
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.015 Å; R factor = 0.037; wR factor = 0.134; data-to-parameter ratio = 12.4.

The title compound, $[Gd(C_7H_3NO_4)(C_7H_4NO_4)(H_2O)_2]\cdot 4H_2O$, is isostructural with its La^{III}, Ce^{III}, Pr^{III}, Nd^{III}, Sm^{III} and Eu^{III} analogues. The Gd^{III} ion is nine-coordinated by two O and one N atoms from a tridentate 6-carboxypyridine-2-carboxylate ligand, two O and one N atoms from a tridentate pyridine-2,6-dicarboxylate ligand, one O atom belonging to a neighboring pyridine-2,6-dicarboxylate ligand, and two water molecules. The bridging pyridine-2,6-dicarboxylate ligand gives rise to infinite chains.

Related literature

The isostructural lanthanide compounds are those with La^{III} (Guerriero *et al.*, 1987; Ghosh & Bharadwaj, 2005), Ce^{III} (Okabe *et al.*, 2002; Ghosh & Bharadwaj, 2003; Rafizadeh *et al.*, 2005; Ramezanipour *et al.*, 2005), Pr^{III} (Ghosh & Bharadwaj, 2003; Zhao *et al.*, 2005), Nd^{III} (Miao *et al.*, 1992), Sm^{III} (Liu *et al.*, 2005, 2006; Rafizadeh *et al.*, 2005; Song *et al.*, 2005) and Eu^{III} (Brayshaw *et al.*, 2005).



Experimental

Crystal data

$[Gd(C_7H_3NO_4)(C_7H_4NO_4)(H_2O)_2]\cdot 4H_2O$
M_r = 596.56
Monoclinic, $P2_1/c$
a = 14.1267 (3) Å
b = 11.2787 (2) Å
c = 13.0162 (2) Å
β = 101.728 (1)°
V = 2030.59 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 3.34 mm^{-1}
T = 293 (2) K
0.10 × 0.10 × 0.10 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.731, T_{max} = 0.731
7168 measured reflections
3925 independent reflections
3237 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.134
S = 1.00
3925 reflections
317 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.05 e Å^{-3}
$\Delta\rho_{min}$ = −1.13 e Å^{-3}

Data collection: *SMART* (Bruker 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BI2197).

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supplementary materials

Acta Cryst. (2007). E**63**, m1967 [**doi:10.1107/S1600536807029789**]

catena-Poly[[[diaqua(6-carboxypyridine-2-carboxylato-κ^3O,N,O')gadolinium(III)]-μ-pyridine-2,6-dicarboxylato-$\kappa^4N,O,O':O''$] tetrahydrate]

L.-J. Hao and T.-L. Yu

Comment

The title compound is isostructural with its La^{III} (Guerriero *et al.*, 1987; Ghosh & Bharadwaj, 2005), Ce^{III} (Okabe *et al.*, 2002; Ghosh & Bharadwaj, 2003; Rafizadeh *et al.*, 2005; Ramezanipour *et al.*, 2005), Pr^{III} (Ghosh & Bharadwaj, 2003; Zhao *et al.*, 2005), Nd^{III} (Miao *et al.*, 1992), Sm^{III} (Liu *et al.*, 2005; Liu *et al.*, 2006; Rafizadeh *et al.*, 2005; Song *et al.*, 2005) and Eu^{III} (Brayshaw *et al.*, 2005) analogues.

The Gd^{III} ion is nine-coordinated by four O and two N atoms from two independent tridentate pyridine-2,6-dicarboxylate ligands, one O atom belonging to a neighboring pyridine-2,6-dicarboxylate ligand and two water molecules (Fig. 1). The bridging pyridine-2,6-dicarboxylate ligand gives rise to infinite chains along the *c*-axis (Fig. 2). An extensive network of hydrogen bonds exists between the water molecules.

Experimental

A mixture of $GdCl_3$ (0.5 mmol), NaOH (0.5 mmol), pyridine-2,6-dicarboxylic acid (0.5 mmol), H_2O (8 ml) and ethanol (8 ml) in a 25 ml Teflon-lined stainless steel autoclave was kept at 433 K for three days. Colourless crystals were obtained after cooling to room temperature with a yield of 36%. Elemental analysis calculated: C 28.16, H 3.18, N 4.69%; found: C 28.50, H 3.22, N 4.76%.

Refinement

The H atoms of the water molecule were located from difference Fourier maps and were refined with distance restraints of H···H = 1.38 (2)Å and O—H = 0.82 (2) Å. All other H atoms were placed in calculated positions with: a C—H bond distance of 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

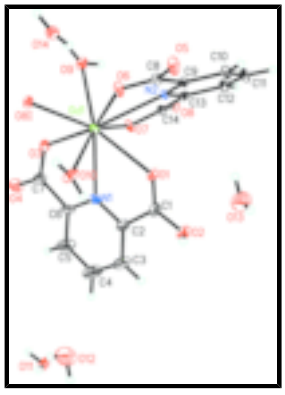

Fig. 1. The asymmetric unit of the title compound showing 30% probability displacement ellipsoids for non-H atoms. Atom O8I is generated by the symmetry code: x, 1/2 − y, 1/2 + z.

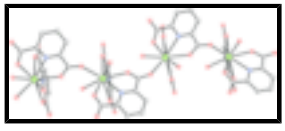

Fig. 2. Part of an infinite chain running along the *c*-axis.

catena-Poly[[[diaqua(6-carboxypyridine-2-carboxylato- κ^3O,N,O')gadolinium(III)]-μ-pyridine- 2,6-dicarboxylato-$\kappa^4N,O,O':O''$] tetrahydrate]

Crystal data

$[Gd(C_7H_3N_1O_4)(C_7H_4N_1O_4)(H_2O_1)_2]\cdot 4H_2O$	F_{000} = 1172
M_r = 596.56	D_x = 1.951 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 3925 reflections
a = 14.1267 (3) Å	θ = 1.5–26.0º
b = 11.2787 (2) Å	μ = 3.34 mm^{-1}
c = 13.0162 (2) Å	T = 293 (2) K
β = 101.728 (1)º	Cubic, colourless
V = 2030.59 (6) Å^3	0.10 × 0.10 × 0.10 mm
Z = 4	

Data collection

Bruker SMART CCD diffractometer	3925 independent reflections
Radiation source: fine-focus sealed tube	3237 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.033
T = 293(2) K	θ_{max} = 26.0º
φ and ω scans	θ_{min} = 1.5º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −16→16
T_{min} = 0.731, T_{max} = 0.731	k = −13→13
7168 measured reflections	l = −7→15

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.037$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.134$	$w = 1/[\sigma^2(F_o^2) + (0.1152P)^2 + 2.6596P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{max} < 0.001$
3925 reflections	$\Delta\rho_{max} = 1.05$ e Å^{-3}
317 parameters	$\Delta\rho_{min} = -1.12$ 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}
Gd1	0.26984 (3)	0.29481 (3)	0.64844 (3)	0.0182 (3)
C1	0.4427 (8)	0.5000 (9)	0.6318 (8)	0.031 (2)
C2	0.5030 (7)	0.3903 (10)	0.6329 (8)	0.032 (2)
C3	0.6014 (9)	0.3898 (13)	0.6353 (11)	0.052 (3)
H3	0.6354	0.4605	0.6362	0.063*
C4	0.6477 (11)	0.2826 (13)	0.6365 (17)	0.041 (3)
H4	0.7141	0.2801	0.6399	0.084*
C5	0.5952 (9)	0.1780 (13)	0.6325 (13)	0.055 (4)
H5	0.6253	0.1049	0.6313	0.066*
C6	0.4975 (7)	0.1849 (9)	0.6305 (8)	0.027 (2)
C7	0.4325 (7)	0.0764 (9)	0.6274 (8)	0.026 (2)
C8	0.1194 (6)	0.5248 (8)	0.6735 (7)	0.0199 (18)
C9	0.1269 (6)	0.5389 (7)	0.5597 (6)	0.0150 (15)
C10	0.0915 (7)	0.6395 (8)	0.5001 (7)	0.0239 (19)
H10	0.0641	0.7026	0.5298	0.029*
C11	0.0990 (7)	0.6412 (8)	0.3934 (7)	0.026 (2)
H11	0.0772	0.7068	0.3520	0.031*

C12	0.1382 (6)	0.5472 (7)	0.3510 (6)	0.0206 (17)
H12	0.1411	0.5463	0.2803	0.025*
C13	0.1740 (6)	0.4515 (7)	0.4171 (6)	0.0163 (16)
C14	0.2257 (6)	0.3477 (7)	0.3807 (7)	0.0167 (17)
N1	0.4519 (6)	0.2884 (6)	0.6323 (6)	0.0227 (18)
N2	0.1687 (5)	0.4485 (6)	0.5185 (5)	0.0140 (13)
O1	0.3562 (5)	0.4925 (6)	0.6348 (5)	0.0286 (15)
O2	0.4846 (6)	0.5978 (7)	0.6261 (7)	0.049 (2)
H2	0.4491	0.6558	0.6226	0.073*
O3	0.3440 (5)	0.0970 (6)	0.6299 (5)	0.0265 (14)
O4	0.4693 (5)	−0.0207 (6)	0.6241 (7)	0.0424 (19)
O5	0.0799 (6)	0.6041 (6)	0.7145 (5)	0.0329 (16)
O6	0.1550 (5)	0.4297 (5)	0.7180 (4)	0.0245 (14)
O7	0.2736 (5)	0.2815 (5)	0.4534 (5)	0.0202 (14)
O8	0.2190 (5)	0.3336 (6)	0.2838 (4)	0.0216 (13)
O9	0.1254 (5)	0.1838 (6)	0.5631 (5)	0.0284 (15)
O10	0.3672 (6)	0.3476 (7)	0.8247 (5)	0.0405 (19)
O11	0.9704 (6)	0.0577 (6)	0.5986 (6)	0.0370 (18)
O12	0.7979 (9)	0.4016 (10)	0.9161 (12)	0.090 (4)
O13	0.3766 (9)	0.7743 (10)	0.6153 (14)	0.092 (4)
O14	0.0414 (5)	0.3081 (6)	0.8505 (6)	0.0277 (16)
H21	0.125 (12)	0.205 (12)	0.503 (5)	0.080*
H22	0.085 (9)	0.134 (11)	0.573 (10)	0.080*
H23	0.407 (8)	0.401 (11)	0.839 (10)	0.080*
H24	0.335 (10)	0.333 (15)	0.868 (9)	0.080*
H25	0.968 (12)	0.086 (10)	0.655 (6)	0.080*
H26	0.954 (12)	−0.014 (6)	0.588 (10)	0.080*
H27	0.855 (4)	0.419 (16)	0.918 (10)	0.080*
H28	0.786 (10)	0.398 (17)	0.978 (6)	0.080*
H29	0.383 (11)	0.828 (12)	0.660 (11)	0.080*
H30	0.323 (6)	0.744 (14)	0.603 (13)	0.080*
H31	0.005 (11)	0.252 (10)	0.843 (11)	0.080*
H32	0.067 (11)	0.324 (13)	0.802 (8)	0.080*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Gd1	0.0194 (4)	0.0192 (4)	0.0153 (4)	0.00107 (14)	0.0021 (2)	0.00124 (13)
C1	0.039 (6)	0.023 (5)	0.032 (5)	−0.006 (4)	0.006 (4)	0.004 (4)
C2	0.026 (5)	0.036 (6)	0.032 (5)	−0.012 (4)	0.004 (4)	0.002 (4)
C3	0.031 (6)	0.054 (8)	0.075 (9)	−0.016 (6)	0.019 (6)	−0.006 (6)
C4	0.038 (5)	0.037 (5)	0.046 (5)	−0.001 (5)	0.007 (5)	−0.001 (5)
C5	0.024 (6)	0.051 (7)	0.093 (11)	−0.001 (6)	0.019 (7)	−0.015 (8)
C6	0.014 (5)	0.033 (5)	0.033 (5)	−0.002 (4)	0.001 (4)	−0.003 (4)
C7	0.016 (5)	0.032 (5)	0.030 (5)	−0.001 (4)	0.003 (4)	0.001 (4)
C8	0.019 (4)	0.022 (4)	0.018 (4)	0.001 (3)	0.004 (3)	−0.001 (3)
C9	0.015 (4)	0.012 (4)	0.017 (4)	0.002 (3)	0.003 (3)	−0.001 (3)
C10	0.031 (5)	0.020 (4)	0.021 (4)	0.008 (4)	0.006 (4)	0.001 (3)

C11	0.033 (5)	0.024 (5)	0.018 (4)	0.007 (4)	−0.003 (4)	0.006 (3)
C12	0.027 (5)	0.021 (4)	0.012 (4)	0.006 (3)	0.001 (3)	0.002 (3)
C13	0.016 (4)	0.017 (4)	0.015 (4)	−0.003 (3)	0.001 (3)	−0.002 (3)
C14	0.017 (4)	0.017 (4)	0.015 (4)	0.001 (3)	0.002 (3)	−0.001 (3)
N1	0.020 (4)	0.028 (4)	0.019 (4)	0.000 (3)	0.002 (3)	0.000 (3)
N2	0.014 (3)	0.014 (3)	0.013 (3)	0.003 (3)	0.001 (3)	0.002 (3)
O1	0.028 (4)	0.020 (3)	0.036 (4)	−0.008 (3)	0.001 (3)	0.003 (3)
O2	0.049 (5)	0.037 (4)	0.052 (5)	−0.022 (4)	−0.009 (4)	0.008 (4)
O3	0.027 (4)	0.018 (3)	0.034 (4)	0.001 (3)	0.004 (3)	0.002 (3)
O4	0.033 (4)	0.023 (4)	0.069 (5)	0.013 (3)	0.005 (4)	−0.002 (4)
O5	0.052 (5)	0.024 (3)	0.027 (3)	0.016 (3)	0.018 (3)	0.002 (3)
O6	0.038 (4)	0.023 (3)	0.015 (3)	0.012 (3)	0.010 (3)	0.004 (2)
O7	0.027 (4)	0.022 (3)	0.012 (3)	0.011 (2)	0.003 (3)	0.002 (2)
O8	0.029 (4)	0.021 (3)	0.013 (3)	0.006 (3)	0.001 (3)	−0.002 (2)
O9	0.032 (4)	0.037 (4)	0.015 (3)	−0.010 (3)	0.002 (3)	0.005 (3)
O10	0.046 (5)	0.056 (5)	0.017 (3)	−0.032 (4)	0.000 (3)	−0.001 (3)
O11	0.051 (5)	0.034 (4)	0.032 (4)	−0.014 (3)	0.025 (4)	−0.002 (3)
O12	0.062 (7)	0.047 (6)	0.148 (12)	0.013 (5)	−0.011 (7)	−0.004 (7)
O13	0.066 (8)	0.043 (6)	0.163 (14)	0.000 (5)	0.013 (9)	−0.004 (7)
O14	0.026 (4)	0.033 (4)	0.023 (4)	−0.002 (3)	0.002 (3)	0.001 (3)

Geometric parameters (Å, °)

Gd1—O9	2.458 (7)	C9—N2	1.343 (10)
Gd1—O3	2.497 (6)	C9—C10	1.408 (11)
Gd1—O8^{i}	2.496 (6)	C10—C11	1.414 (12)
Gd1—O10	2.496 (6)	C10—H10	0.930
Gd1—O6	2.523 (6)	C11—C12	1.363 (13)
Gd1—O7	2.554 (6)	C11—H11	0.930
Gd1—O1	2.566 (6)	C12—C13	1.409 (11)
Gd1—N1	2.624 (9)	C12—H12	0.930
Gd1—N2	2.631 (6)	C13—N2	1.338 (10)
C1—O1	1.232 (13)	C13—C14	1.506 (11)
C1—O2	1.261 (13)	C14—O8	1.256 (10)
C1—C2	1.501 (15)	C14—O7	1.285 (10)
C2—N1	1.356 (12)	O2—H2	0.820
C2—C3	1.383 (16)	O8—Gd1^{ii}	2.496 (6)
C3—C4	1.37 (2)	O9—H21	0.82 (9)
C3—H3	0.930	O9—H22	0.83 (12)
C4—C5	1.39 (2)	O10—H23	0.82 (13)
C4—H4	0.930	O10—H24	0.81 (13)
C5—C6	1.377 (16)	O11—H25	0.81 (9)
C5—H5	0.930	O11—H26	0.85 (7)
C6—N1	1.335 (13)	O12—H27	0.83 (9)
C6—C7	1.526 (13)	O12—H28	0.86 (9)
C7—O4	1.216 (12)	O13—H29	0.83 (15)
C7—O3	1.278 (12)	O13—H30	0.82 (10)
C8—O5	1.232 (11)	O14—H31	0.81 (12)
C8—O6	1.273 (10)	O14—H32	0.81 (14)

C8—C9	1.515 (11)		
O9—Gd1—O3	80.1 (2)	C6—C5—H5	120.7
O9—Gd1—O8^{i}	72.1 (2)	N1—C6—C5	122.2 (11)
O3—Gd1—O8^{i}	74.7 (2)	N1—C6—C7	114.4 (9)
O9—Gd1—O10	142.0 (2)	C5—C6—C7	123.4 (10)
O3—Gd1—O10	98.0 (3)	O4—C7—O3	126.3 (9)
O8^{i}—Gd1—O10	70.9 (2)	O4—C7—C6	117.6 (9)
O9—Gd1—O6	86.2 (2)	O3—C7—C6	116.0 (8)
O3—Gd1—O6	152.5 (2)	O5—C8—O6	125.9 (8)
O8^{i}—Gd1—O6	78.4 (2)	O5—C8—C9	118.4 (8)
O10—Gd1—O6	78.5 (3)	O6—C8—C9	115.7 (7)
O9—Gd1—O7	72.8 (2)	N2—C9—C10	121.9 (7)
O3—Gd1—O7	76.0 (2)	N2—C9—C8	115.7 (7)
O8^{i}—Gd1—O7	137.3 (2)	C10—C9—C8	122.3 (7)
O10—Gd1—O7	144.0 (2)	C11—C10—C9	117.5 (8)
O6—Gd1—O7	122.46 (19)	C11—C10—H10	121.2
O9—Gd1—O1	140.7 (2)	C9—C10—H10	121.3
O3—Gd1—O1	123.7 (2)	C12—C11—C10	120.3 (8)
O8^{i}—Gd1—O1	139.7 (2)	C12—C11—H11	119.9
O10—Gd1—O1	71.0 (2)	C10—C11—H11	119.8
O6—Gd1—O1	81.4 (2)	C11—C12—C13	118.3 (8)
O7—Gd1—O1	82.9 (2)	C11—C12—H12	120.8
O9—Gd1—N1	133.4 (2)	C13—C12—H12	120.9
O3—Gd1—N1	62.0 (2)	N2—C13—C12	122.4 (7)
O8^{i}—Gd1—N1	117.9 (2)	N2—C13—C14	114.8 (7)
O10—Gd1—N1	73.4 (3)	C12—C13—C14	122.7 (7)
O6—Gd1—N1	139.3 (2)	O8—C14—O7	125.9 (7)
O7—Gd1—N1	72.5 (2)	O8—C14—C13	118.2 (7)
O1—Gd1—N1	62.0 (2)	O7—C14—C13	115.9 (7)
O9—Gd1—N2	75.7 (2)	C6—N1—C2	118.9 (9)
O3—Gd1—N2	135.2 (2)	C6—N1—Gd1	120.6 (6)
O8^{i}—Gd1—N2	129.7 (2)	C2—N1—Gd1	120.4 (6)
O10—Gd1—N2	124.0 (3)	C9—N2—C13	119.4 (7)
O6—Gd1—N2	61.85 (19)	C9—N2—Gd1	118.0 (5)
O7—Gd1—N2	61.20 (19)	C13—N2—Gd1	121.2 (5)
O1—Gd1—N2	65.6 (2)	C1—O1—Gd1	123.4 (6)
N1—Gd1—N2	112.3 (2)	C1—O2—H2	114.00
O1—C1—O2	122.8 (10)	C7—O3—Gd1	126.7 (6)
O1—C1—C2	120.5 (9)	C8—O6—Gd1	124.6 (5)
O2—C1—C2	116.7 (10)	C14—O7—Gd1	125.7 (5)
N1—C2—C3	121.8 (11)	C14—O8—Gd1^{ii}	144.0 (5)
N1—C2—C1	113.4 (8)	Gd1—O9—H21	98 (10)
C3—C2—C1	124.7 (10)	Gd1—O9—H22	144 (9)
C2—C3—C4	118.6 (12)	H21—O9—H22	118 (13)
C2—C3—H3	120.8	Gd1—O10—H23	127 (10)
C4—C3—H3	120.6	Gd1—O10—H24	108 (10)
C5—C4—C3	119.8 (14)	H23—O10—H24	117 (7)

C5—C4—H4	120.1	H25—O11—H26	118 (6)
C3—C4—H4	120.1	H27—O12—H28	111 (13)
C4—C5—C6	118.6 (13)	H29—O13—H30	114 (16)
C4—C5—H5	120.7	H31—O14—H32	118 (7)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O13	0.82	1.68	2.495 (9)	180
O9—H21···O14^{ii}	0.82 (9)	2.09 (10)	2.782 (10)	141 (13)
O9—H22···O11^{iii}	0.83 (12)	1.92 (13)	2.728 (10)	165 (16)
O10—H23···O4^{iv}	0.82 (13)	1.93 (12)	2.713 (10)	160 (17)
O10—H24···O7^{i}	0.81 (13)	2.01 (8)	2.752 (9)	152 (17)
O11—H25···O5^{v}	0.81 (9)	1.96 (7)	2.719 (9)	156 (14)
O11—H26···O14^{v}	0.85 (7)	2.15 (9)	2.905 (10)	147 (13)
O12—H27···O11^{i}	0.83 (9)	2.59 (12)	3.072 (15)	119 (11)
O12—H28···O13^{v}	0.86 (9)	2.75 (15)	2.810 (18)	85 (10)
O13—H29···O4^{vi}	0.83 (15)	2.20 (14)	2.649 (14)	114 (13)
O13—H30···O12^{iv}	0.82 (10)	2.44 (16)	2.810 (18)	108 (14)
O14—H31···O5^{vii}	0.81 (12)	2.10 (13)	2.891 (10)	165 (13)

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

Fig. 1

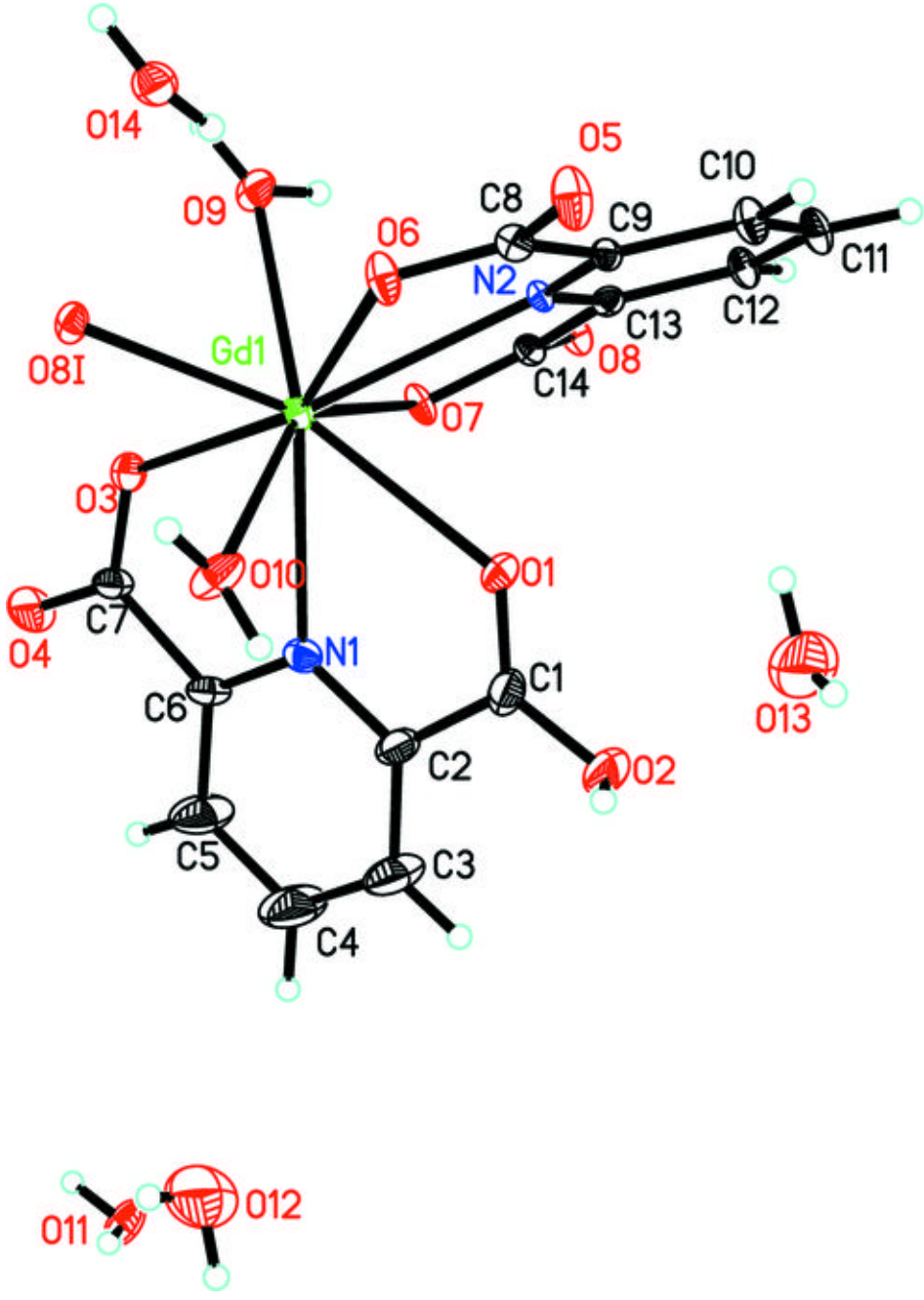
O14
O9
O5
C10
C8
C9
O6
C11
N2
C12
C13
O8I
Gd1
O8
C14
O7
O3
O10
O1
C7
O4
N1
C1
O13
C6
C2
O2
C5
C3
C4
O11
O12

Fig. 2