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catena-Poly[[diaqua(isonicotinato-κ^2O,O')gadolinium(III)]-di-μ-isonicotinato-$\kappa^4O:O'$]

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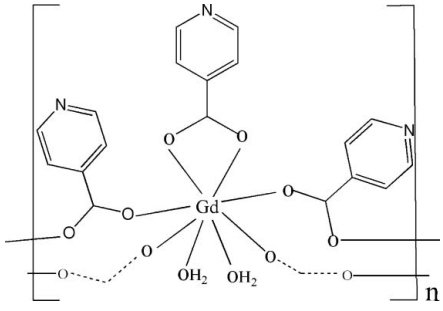
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.020; wR factor = 0.044; data-to-parameter ratio = 11.9.

Single crystals of the title compound, $[Gd(C_6H_4NO_2)_3(H_2O)_2]_n$, were obtained by evaporation of an aqueous solution of isonicotinic acid and gadolinium(III) nitrate. The Gd^{III} cation is eight-coordinated by four carboxylate O atoms of bridging isonicotinate anions, two carboxylate O atoms of a chelating isonicotinate anion and two water molecules. The coordination environment around the rare earth cation might be described as a distorted bicapped trigonal prism. As a result of the two coordination modes of the isonicotinate ligands (with one as a bidentate chelate ligand and the others as bridging ligands), an infinite chain along the a axis is formed. Medium-strength hydrogen bonds of the types O—H···O and O—H···N between the water molecules and adjacent chains generate a three-dimensional framework.

Related literature

Potential applications and different structures and topologies of coordination polymers in general are given by Yaghi *et al.* (1998, 2003), Eddaoudi *et al.* (2001) and Moulton & Zaworotko (2001). For isonicotinate ligands in particular, see Aakeroy *et al.* (1999) and Burrows *et al.* (1998). The use of isonicotinate metal complexes as drugs is discussed by Sorenson (1976).



Experimental

Crystal data

$[Gd(C_6H_4NO_2)_3(H_2O)_2]$
M_r = 559.59
Monoclinic, $P2_1/c$
a = 9.4786 (6) Å
b = 18.9589 (11) Å
c = 10.7557 (6) Å
β = 92.3130 (10)°
V = 1931.3 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 3.49 mm^{-1}
T = 293 (2) K
0.39 × 0.31 × 0.26 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.286, T_{max} = 0.404
9640 measured reflections
3435 independent reflections
3102 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.020
$wR(F^2)$ = 0.044
S = 1.06
3435 reflections
288 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.61 e Å^{-3}
$\Delta\rho_{min}$ = −0.62 e Å^{-3}

Table 1
Selected bond lengths (Å).

Gd1—O5	2.326 (2)	Gd1—O8	2.426 (2)
Gd1—O3	2.348 (2)	Gd1—O7	2.442 (2)
Gd1—O4^{i}	2.349 (2)	Gd1—O2	2.451 (2)
Gd1—O6^{ii}	2.391 (2)	Gd1—O1	2.576 (2)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O8—H8B···N2^{iii}	0.822 (10)	1.986 (12)	2.805 (4)	175 (4)
O7—H7A···N3^{iv}	0.820 (10)	1.989 (11)	2.807 (4)	176 (4)
O7—H7B···O1^{i}	0.819 (10)	2.001 (16)	2.788 (3)	161 (4)
O8—H8A···O2^{ii}	0.818 (10)	1.968 (16)	2.759 (3)	162 (4)

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

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); 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: WM2123).

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supplementary materials

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catena-Poly[[diaqua(isonicotinato-κ^2O,O')gadolinium(III)]-di-μ-isonicotinato-$\kappa^4O:O'$]

F.-Y. Chen, W.-T. Wu, F. Liu, L. Yao and S.-Y. He

Comment

The interest in crystal engineering of coordination polymers originates from their potential applications as materials for molecular selection, ion exchange, catalysis, and because of their intriguing variety of architectures and topologies (Yaghi *et al.*, 1998, 2003; Eddaoudi *et al.*, 2001; Moulton & Zaworotko, 2001). In particular, isonicotinate metal complexes are of considerable interest because isonicotinic acid plays an important role in the metabolism of all living cells (Sorenson, 1976), and acts as a versatile ligand to construct supramolecular architectures (Aakeroy *et al.*, 1999; Burrows *et al.*, 1998). Moreover, isonicotinate metal complexes find also use as drugs (Sorenson, 1976). In this article we report on the crystal structure of the title complex (I), a new coordination polymer of isonicotinic acid with Gd^{III}.

A part of the monomeric structure of (I) is shown in Fig. 1 and selected geometric parameters are gathered in Table 1. The Gd^{III} cation is coordinated by eight O atoms in a distorted bicapped trigonal-prismatic environment. The [GdO_8] polyhedron is built by two O atoms from two water molecules, by four carboxylate O atoms of bridging isonicotinate anions and by two carboxylate O atoms of chelating isonicotinate anions. Each adjacent Gd^{III} is bridged by two O atoms of two isonicotinate ligands to form an infinite chain along the *a* axis. The bond lengths of C7—O3, C7—O4 and C13—O5, C13—O6 are 1.251 (4), 1.250 (4) Å and 1.258 (3), 1.242 (4) Å, respectively, indicating that a delocalized π-bond is present.

Adjacent chains are linked into a framework structure by hydrogen bond interactions. Two types of hydrogen bonds are present in (I) (Table 2): One type is formed between O atoms of the coordinating water molecules and the N atoms of the isonicotinate ligands (O7—H7A···N3 and O8—H8B···N2), whereas the other type consists of O atoms of the coordinating water molecules and the carboxylate O atoms of the isonicotinate ligands (O7—H7B···O1, O8—H8A···O2).

Experimental

A solution of isonicotinic acid (0.3693 g, 3 mmol) in 30 ml hot water was added under stirring to a solution of $Gd(NO_3)_3{\cdot}5H_2O$ (0.4333 g, 1 mmol) in 10 ml water and the pH of the mixture was adjusted to about 5.4 using aqueous ammonia. $Gd(NO_3)_3{\cdot}5H_2O$ was prepared by dissolving Gd_2O_3 (99.95%) in diluted HNO_3, and then crystallizing the products. After stirring for 2 h and cooling to room temperature, the mixture was filtered. Light-yellow single crystals of (I) were obtained from the filtrate after two weeks.

Refinement

The H atoms attached to C atoms were treated as riding with C—H = 0.93 Å and U_{iso}(H) = 1.5U_{eq}(C) of the parent atom. The H atoms of the water molecules were refined with U_{iso}(H) = 1.2U_{eq}(O) and distance restraints of 0.82 (1) Å.

Figures

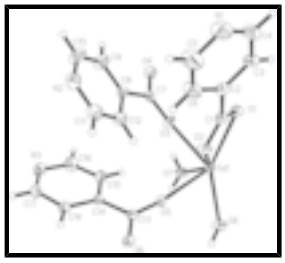


Fig. 1. Part of the monomeric molecular structure of (I) with the atom-numbering scheme and with displacement ellipsoids drawn at the 30% probability level. H atoms are displayed as spheres of arbitrary radius.

catena-Poly[[diaqua(isonicotinato-κ^2*O*,*O*')gadolinium(III)]-di-μ- isonicotinato-κ^4*O*:*O*']

Crystal data

$[Gd(C_6H_4NO_2)_3(H_2O)_2]$	F_{000} = 1092
M_r = 559.59	D_x = 1.925 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 3435 reflections
a = 9.4786 (6) Å	θ = 2.2–25.1º
b = 18.9589 (11) Å	μ = 3.49 mm^{-1}
c = 10.7557 (6) Å	T = 293 (2) K
β = 92.3130 (10)º	Prism, light yellow
V = 1931.3 (2) Å^3	0.39 × 0.31 × 0.26 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	3435 independent reflections
Radiation source: fine-focus sealed tube	3102 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.023
T = 293(2) K	θ_{max} = 25.1º
φ and ω scans	θ_{min} = 2.2º
Absorption correction: multi-scan (SADABS; Bruker, 2000)	h = −11→9
T_{min} = 0.286, T_{max} = 0.404	k = −22→21
9640 measured reflections	l = −12→12

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.020	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.044	$w = 1/[\sigma^2(F_o^2) + (0.015P)^2 + 1.4397P]$

	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{max} = 0.013$
3435 reflections	$\Delta\rho_{max} = 0.61$ e Å^{-3}
288 parameters	$\Delta\rho_{min} = -0.62$ e Å^{-3}
4 restraints	Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.00020 (8)

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}
O4	0.4038 (2)	0.44208 (12)	0.1958 (2)	0.0356 (5)
Gd1	0.752460 (15)	0.509995 (7)	−0.043256 (12)	0.02074 (6)
C1	0.7433 (3)	0.60647 (16)	0.1627 (3)	0.0289 (7)
C2	0.7397 (3)	0.64748 (17)	0.2816 (3)	0.0338 (8)
O8	0.8820 (3)	0.47313 (14)	−0.2220 (2)	0.0363 (5)
O3	0.6058 (2)	0.46285 (12)	0.10665 (18)	0.0352 (5)
O5	0.9145 (2)	0.42758 (11)	0.0353 (2)	0.0336 (5)
O7	0.6381 (2)	0.40567 (12)	−0.1344 (2)	0.0332 (5)
C3	0.6672 (4)	0.71045 (18)	0.2911 (3)	0.0397 (8)
H3	0.6153	0.7285	0.2232	0.048*
N1	0.7408 (4)	0.7220 (2)	0.5057 (3)	0.0650 (10)
C4	0.6733 (4)	0.7460 (2)	0.4033 (4)	0.0505 (10)
H4	0.6275	0.7893	0.4076	0.061*
C7	0.5354 (3)	0.44658 (15)	0.1983 (3)	0.0262 (7)
N2	0.7527 (4)	0.42460 (18)	0.5549 (3)	0.0529 (9)
C12	0.7578 (4)	0.43956 (18)	0.3345 (3)	0.0384 (8)
H12	0.8117	0.4467	0.2652	0.046*
C8	0.6130 (3)	0.43428 (16)	0.3216 (3)	0.0291 (7)
C11	0.8212 (4)	0.4342 (2)	0.4511 (3)	0.0500 (10)
H11	0.9191	0.4374	0.4578	0.060*
C6	0.8133 (4)	0.6229 (2)	0.3861 (3)	0.0544 (11)
H6	0.8658	0.5816	0.3833	0.065*
C5	0.8074 (5)	0.6613 (3)	0.4954 (4)	0.0729 (14)
H5	0.8534	0.6430	0.5663	0.087*

O6	1.1211 (2)	0.38840 (11)	0.1093 (2)	0.0342 (5)
C14	0.9197 (3)	0.31977 (15)	0.1482 (3)	0.0248 (7)
C13	0.9910 (3)	0.38314 (15)	0.0928 (3)	0.0253 (7)
C9	0.5393 (4)	0.4215 (2)	0.4275 (3)	0.0508 (10)
H9	0.4419	0.4153	0.4225	0.061*
C10	0.6130 (5)	0.4179 (2)	0.5414 (3)	0.0611 (12)
H10	0.5620	0.4105	0.6123	0.073*
O1	0.6452 (2)	0.61156 (11)	0.08095 (19)	0.0298 (5)
O2	0.8464 (2)	0.56526 (11)	0.14872 (19)	0.0325 (5)
N3	0.7840 (3)	0.20752 (15)	0.2622 (3)	0.0466 (8)
C18	0.9898 (3)	0.27771 (17)	0.2350 (3)	0.0346 (8)
H18	1.0844	0.2859	0.2565	0.042*
C15	0.7804 (4)	0.30338 (18)	0.1172 (3)	0.0406 (9)
H15	0.7292	0.3298	0.0581	0.049*
C17	0.9179 (4)	0.22308 (18)	0.2898 (3)	0.0437 (9)
H17	0.9663	0.1958	0.3493	0.052*
C16	0.7191 (4)	0.24716 (19)	0.1757 (4)	0.0531 (11)
H16	0.6260	0.2362	0.1530	0.064*
H8B	0.846 (4)	0.456 (2)	−0.286 (2)	0.068 (14)*
H7B	0.561 (2)	0.3912 (19)	−0.114 (3)	0.051 (12)*
H8A	0.962 (2)	0.458 (2)	−0.215 (4)	0.072 (15)*
H7A	0.677 (4)	0.3713 (14)	−0.164 (3)	0.060 (13)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O4	0.0236 (13)	0.0500 (14)	0.0325 (13)	0.0001 (10)	−0.0065 (10)	0.0056 (10)
Gd1	0.01908 (9)	0.02429 (9)	0.01873 (9)	−0.00065 (6)	−0.00063 (6)	0.00041 (6)
C1	0.0265 (18)	0.0293 (17)	0.0312 (18)	−0.0064 (14)	0.0031 (14)	−0.0061 (13)
C2	0.0285 (19)	0.0401 (19)	0.0329 (18)	−0.0074 (15)	0.0037 (14)	−0.0097 (15)
O8	0.0247 (14)	0.0577 (16)	0.0265 (13)	0.0039 (12)	−0.0011 (10)	−0.0086 (11)
O3	0.0396 (14)	0.0452 (13)	0.0211 (11)	−0.0065 (11)	0.0049 (10)	0.0059 (10)
O5	0.0330 (13)	0.0316 (12)	0.0365 (13)	0.0050 (10)	0.0034 (10)	0.0110 (10)
O7	0.0241 (13)	0.0315 (13)	0.0443 (14)	−0.0043 (11)	0.0060 (11)	−0.0117 (11)
C3	0.034 (2)	0.044 (2)	0.041 (2)	−0.0027 (16)	0.0047 (16)	−0.0115 (16)
N1	0.081 (3)	0.069 (2)	0.045 (2)	0.005 (2)	−0.0005 (19)	−0.0261 (18)
C4	0.051 (3)	0.046 (2)	0.055 (2)	−0.0013 (19)	0.006 (2)	−0.0177 (19)
C7	0.0306 (19)	0.0223 (15)	0.0255 (16)	0.0002 (13)	−0.0013 (14)	−0.0015 (12)
N2	0.055 (2)	0.069 (2)	0.0329 (18)	0.0093 (18)	−0.0135 (16)	0.0028 (15)
C12	0.031 (2)	0.053 (2)	0.0309 (18)	0.0014 (16)	−0.0019 (15)	0.0007 (15)
C8	0.0297 (18)	0.0334 (17)	0.0240 (16)	0.0024 (14)	0.0004 (13)	0.0019 (13)
C11	0.037 (2)	0.068 (3)	0.043 (2)	0.003 (2)	−0.0134 (18)	0.0041 (19)
C6	0.064 (3)	0.057 (2)	0.041 (2)	0.015 (2)	−0.009 (2)	−0.0164 (18)
C5	0.096 (4)	0.079 (3)	0.042 (2)	0.023 (3)	−0.017 (2)	−0.021 (2)
O6	0.0230 (13)	0.0344 (12)	0.0452 (14)	−0.0059 (10)	0.0006 (10)	0.0064 (10)
C14	0.0225 (17)	0.0227 (15)	0.0292 (16)	−0.0012 (12)	0.0007 (13)	0.0012 (12)
C13	0.0284 (19)	0.0234 (15)	0.0243 (16)	−0.0019 (13)	0.0022 (13)	−0.0020 (12)
C9	0.037 (2)	0.081 (3)	0.034 (2)	−0.002 (2)	−0.0031 (17)	0.0075 (19)

C10	0.058 (3)	0.098 (3)	0.028 (2)	0.005 (3)	0.0020 (19)	0.011 (2)
O1	0.0229 (12)	0.0337 (12)	0.0327 (12)	−0.0012 (9)	−0.0016 (10)	−0.0029 (9)
O2	0.0234 (12)	0.0436 (13)	0.0303 (12)	0.0047 (10)	−0.0004 (9)	−0.0121 (10)
N3	0.0411 (19)	0.0375 (17)	0.062 (2)	−0.0076 (14)	0.0088 (16)	0.0150 (15)
C18	0.0269 (19)	0.0366 (18)	0.040 (2)	−0.0009 (14)	0.0018 (15)	0.0075 (15)
C15	0.032 (2)	0.0389 (19)	0.050 (2)	−0.0056 (15)	−0.0069 (17)	0.0153 (16)
C17	0.045 (2)	0.039 (2)	0.046 (2)	0.0038 (17)	0.0003 (18)	0.0166 (16)
C16	0.031 (2)	0.051 (2)	0.076 (3)	−0.0139 (18)	−0.007 (2)	0.017 (2)

Geometric parameters (Å, °)

O4—C7	1.250 (4)	C7—C8	1.508 (4)
O4—Gd1^{i}	2.349 (2)	N2—C11	1.327 (5)
Gd1—O5	2.326 (2)	N2—C10	1.332 (5)
Gd1—O3	2.348 (2)	C12—C11	1.373 (5)
Gd1—O4^{i}	2.349 (2)	C12—C8	1.377 (4)
Gd1—O6^{ii}	2.391 (2)	C12—H12	0.9300
Gd1—O8	2.426 (2)	C8—C9	1.382 (5)
Gd1—O7	2.442 (2)	C11—H11	0.9300
Gd1—O2	2.451 (2)	C6—C5	1.385 (5)
Gd1—O1	2.576 (2)	C6—H6	0.9300
Gd1—C1	2.877 (3)	C5—H5	0.9300
C1—O1	1.258 (4)	O6—C13	1.242 (4)
C1—O2	1.265 (4)	O6—Gd1^{ii}	2.391 (2)
C1—C2	1.497 (4)	C14—C18	1.378 (4)
C2—C6	1.380 (5)	C14—C15	1.384 (4)
C2—C3	1.383 (5)	C14—C13	1.513 (4)
O8—H8B	0.822 (10)	C9—C10	1.387 (5)
O8—H8A	0.818 (10)	C9—H9	0.9300
O3—C7	1.251 (4)	C10—H10	0.9300
O5—C13	1.258 (3)	N3—C17	1.325 (5)
O7—H7B	0.819 (10)	N3—C16	1.328 (5)
O7—H7A	0.820 (10)	C18—C17	1.385 (5)
C3—C4	1.382 (5)	C18—H18	0.9300
C3—H3	0.9300	C15—C16	1.378 (5)
N1—C5	1.319 (5)	C15—H15	0.9300
N1—C4	1.332 (5)	C17—H17	0.9300
C4—H4	0.9300	C16—H16	0.9300
C7—O4—Gd1^{i}	126.1 (2)	C4—C3—C2	118.8 (3)
O5—Gd1—O3	83.99 (8)	C4—C3—H3	120.6
O5—Gd1—O4^{i}	154.48 (8)	C2—C3—H3	120.6
O3—Gd1—O4^{i}	104.65 (8)	C5—N1—C4	116.4 (3)
O5—Gd1—O6^{ii}	108.51 (7)	N1—C4—C3	123.8 (4)
O3—Gd1—O6^{ii}	145.91 (8)	N1—C4—H4	118.1
O4^{i}—Gd1—O6^{ii}	77.91 (7)	C3—C4—H4	118.1
O5—Gd1—O8	75.31 (8)	O4—C7—O3	124.3 (3)
O3—Gd1—O8	140.12 (9)	O4—C7—C8	117.3 (3)

O4^{i}—Gd1—O8	83.28 (8)	O3—C7—C8	118.3 (3)
O6^{ii}—Gd1—O8	73.80 (8)	C11—N2—C10	116.1 (3)
O5—Gd1—O7	82.98 (8)	C11—C12—C8	119.0 (3)
O3—Gd1—O7	72.64 (8)	C11—C12—H12	120.5
O4^{i}—Gd1—O7	77.04 (8)	C8—C12—H12	120.5
O6^{ii}—Gd1—O7	138.85 (8)	C12—C8—C9	117.7 (3)
O8—Gd1—O7	71.30 (8)	C12—C8—C7	121.7 (3)
O5—Gd1—O2	76.63 (7)	C9—C8—C7	120.5 (3)
O3—Gd1—O2	77.83 (7)	N2—C11—C12	124.6 (4)
O4^{i}—Gd1—O2	128.37 (8)	N2—C11—H11	117.7
O6^{ii}—Gd1—O2	74.71 (7)	C12—C11—H11	117.7
O8—Gd1—O2	127.78 (8)	C2—C6—C5	118.6 (4)
O7—Gd1—O2	145.57 (8)	C2—C6—H6	120.7
O5—Gd1—O1	125.61 (7)	C5—C6—H6	120.7
O3—Gd1—O1	70.81 (7)	N1—C5—C6	124.4 (4)
O4^{i}—Gd1—O1	79.75 (7)	N1—C5—H5	117.8
O6^{ii}—Gd1—O1	76.40 (7)	C6—C5—H5	117.8
O8—Gd1—O1	148.16 (8)	C13—O6—Gd1^{ii}	121.92 (19)
O7—Gd1—O1	129.45 (7)	C18—C14—C15	117.6 (3)
O2—Gd1—O1	51.76 (7)	C18—C14—C13	121.0 (3)
O5—Gd1—C1	100.79 (8)	C15—C14—C13	121.4 (3)
O3—Gd1—C1	71.09 (8)	O6—C13—O5	124.4 (3)
O4^{i}—Gd1—C1	104.73 (8)	O6—C13—C14	117.7 (3)
O6^{ii}—Gd1—C1	75.38 (8)	O5—C13—C14	117.9 (3)
O8—Gd1—C1	145.64 (9)	C8—C9—C10	118.9 (4)
O7—Gd1—C1	142.88 (8)	C8—C9—H9	120.5
O2—Gd1—C1	25.92 (8)	C10—C9—H9	120.5
O1—Gd1—C1	25.92 (7)	N2—C10—C9	123.7 (4)
O1—C1—O2	121.1 (3)	N2—C10—H10	118.2
O1—C1—C2	121.0 (3)	C9—C10—H10	118.2
O2—C1—C2	117.8 (3)	C1—O1—Gd1	90.52 (18)
O1—C1—Gd1	63.55 (15)	C1—O2—Gd1	96.22 (17)
O2—C1—Gd1	57.86 (15)	C17—N3—C16	116.3 (3)
C2—C1—Gd1	171.8 (2)	C14—C18—C17	119.3 (3)
C6—C2—C3	117.8 (3)	C14—C18—H18	120.4
C6—C2—C1	119.5 (3)	C17—C18—H18	120.4
C3—C2—C1	122.7 (3)	C16—C15—C14	118.6 (3)
Gd1—O8—H8B	125 (3)	C16—C15—H15	120.7
Gd1—O8—H8A	122 (3)	C14—C15—H15	120.7
H8B—O8—H8A	107 (4)	N3—C17—C18	123.7 (3)
C7—O3—Gd1	169.9 (2)	N3—C17—H17	118.2
C13—O5—Gd1	171.0 (2)	C18—C17—H17	118.2
Gd1—O7—H7B	123 (3)	N3—C16—C15	124.5 (3)
Gd1—O7—H7A	127 (3)	N3—C16—H16	117.8
H7B—O7—H7A	105 (4)	C15—C16—H16	117.8
O5—Gd1—C1—O1	−164.59 (17)	C8—C12—C11—N2	−0.6 (6)

O3—Gd1—C1—O1	−84.84 (18)	C3—C2—C6—C5	1.9 (6)
O4^{i}—Gd1—C1—O1	15.90 (19)	C1—C2—C6—C5	−179.3 (4)
O6^{ii}—Gd1—C1—O1	88.90 (18)	C4—N1—C5—C6	1.4 (8)
O8—Gd1—C1—O1	115.70 (19)	C2—C6—C5—N1	−3.2 (8)
O7—Gd1—C1—O1	−72.0 (2)	Gd1^{ii}—O6—C13—O5	4.0 (4)
O2—Gd1—C1—O1	173.9 (3)	Gd1^{ii}—O6—C13—C14	−174.64 (18)
O5—Gd1—C1—O2	21.48 (19)	C18—C14—C13—O6	13.5 (4)
O3—Gd1—C1—O2	101.23 (19)	C15—C14—C13—O6	−168.9 (3)
O4^{i}—Gd1—C1—O2	−158.03 (17)	C18—C14—C13—O5	−165.2 (3)
O6^{ii}—Gd1—C1—O2	−85.03 (18)	C15—C14—C13—O5	12.4 (4)
O8—Gd1—C1—O2	−58.2 (3)	C12—C8—C9—C10	3.0 (6)
O7—Gd1—C1—O2	114.1 (2)	C7—C8—C9—C10	−173.1 (3)
O1—Gd1—C1—O2	−173.9 (3)	C11—N2—C10—C9	−0.9 (7)
O1—C1—C2—C6	155.2 (3)	C8—C9—C10—N2	−1.6 (7)
O2—C1—C2—C6	−23.0 (5)	O2—C1—O1—Gd1	6.0 (3)
O1—C1—C2—C3	−26.1 (5)	C2—C1—O1—Gd1	−172.2 (3)
O2—C1—C2—C3	155.7 (3)	O5—Gd1—O1—C1	18.7 (2)
O5—Gd1—O3—C7	95.4 (12)	O3—Gd1—O1—C1	86.05 (18)
O4^{i}—Gd1—O3—C7	−109.1 (12)	O4^{i}—Gd1—O1—C1	−164.38 (18)
O6^{ii}—Gd1—O3—C7	−19.1 (13)	O6^{ii}—Gd1—O1—C1	−84.47 (18)
O8—Gd1—O3—C7	153.8 (12)	O8—Gd1—O1—C1	−105.5 (2)
O7—Gd1—O3—C7	179.9 (11),	O7—Gd1—O1—C1	131.98 (17)
O2—Gd1—O3—C7	17.8 (12)	O2—Gd1—O1—C1	−3.37 (17)
O1—Gd1—O3—C7	−35.7 (12)	O1—C1—O2—Gd1	−6.3 (3)
C1—Gd1—O3—C7	−8.2 (12)	C2—C1—O2—Gd1	171.9 (2)
C6—C2—C3—C4	0.8 (5)	O5—Gd1—O2—C1	−158.30 (19)
C1—C2—C3—C4	−177.9 (3)	O3—Gd1—O2—C1	−71.67 (18)
C5—N1—C4—C3	1.6 (6)	O4^{i}—Gd1—O2—C1	27.5 (2)
C2—C3—C4—N1	−2.7 (6)	O6^{ii}—Gd1—O2—C1	87.92 (19)
Gd1^{i}—O4—C7—O3	−17.4 (4)	O8—Gd1—O2—C1	142.63 (18)
Gd1^{i}—O4—C7—C8	160.10 (19)	O7—Gd1—O2—C1	−103.0 (2)
Gd1—O3—C7—O4	120.9 (11)	O1—Gd1—O2—C1	3.37 (17)
Gd1—O3—C7—C8	−56.5 (13)	C15—C14—C18—C17	−2.1 (5)
C11—C12—C8—C9	−2.0 (5)	C13—C14—C18—C17	175.6 (3)
C11—C12—C8—C7	174.1 (3)	C18—C14—C15—C16	1.1 (5)
O4—C7—C8—C12	−178.6 (3)	C13—C14—C15—C16	−176.6 (3)
O3—C7—C8—C12	−1.0 (4)	C16—N3—C17—C18	0.8 (6)
O4—C7—C8—C9	−2.6 (5)	C14—C18—C17—N3	1.2 (6)
O3—C7—C8—C9	175.1 (3)	C17—N3—C16—C15	−1.9 (6)
C10—N2—C11—C12	2.1 (6)	C14—C15—C16—N3	1.0 (6)

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

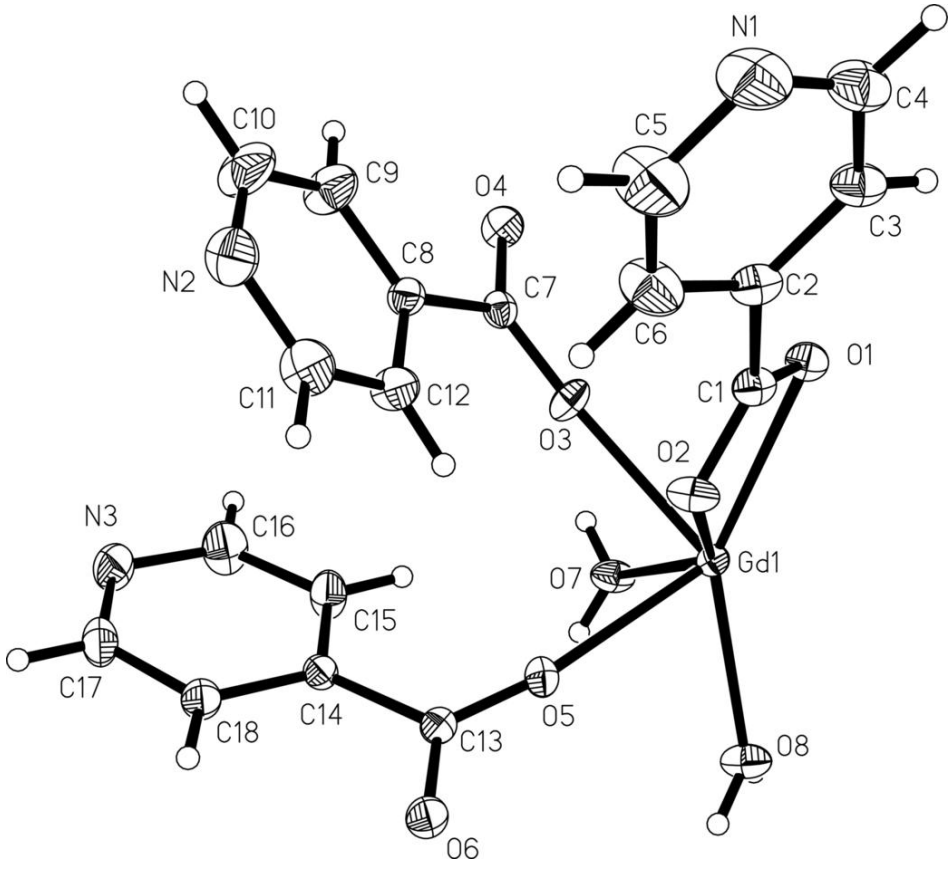
Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O8—H8B···N2^{iii}	0.822 (10)	1.986 (12)	2.805 (4)	175 (4)

O7—H7A···N3^{iv}	0.820 (10)	1.989 (11)	2.807 (4)	176 (4)
O7—H7B···O1^{i}	0.819 (10)	2.001 (16)	2.788 (3)	161 (4)
O8—H8A···O2^{ii}	0.818 (10)	1.968 (16)	2.759 (3)	162 (4)

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

Fig. 1


N1
C4
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C10
C9
O4
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C7
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O1
C11
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C1
O3
O2
N3
C16
O7
Gd1
C15
C17
C14
O5
C18
C13
O8
O6