

Poly[[hemi- μ_4 -oxalato-hemi- μ_2 -oxalato-bis(μ_3 -pyrazine-2-carboxylato)-neodymium(III)silver(I)] monohydrate]

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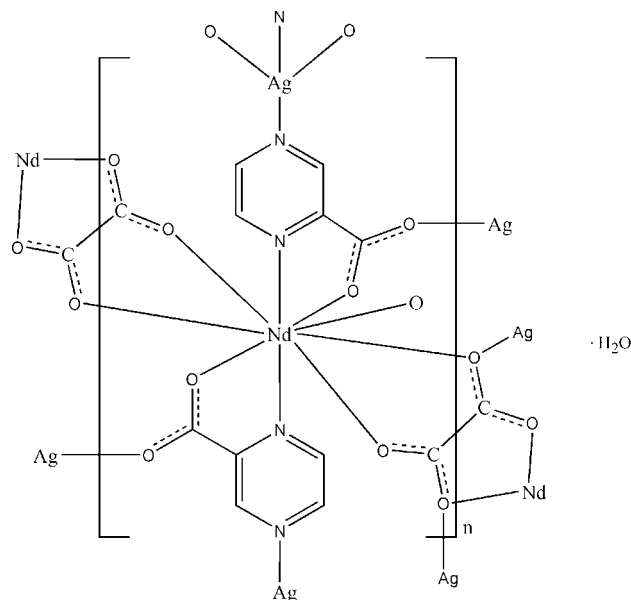
Received 28 May 2009; accepted 4 June 2009

Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.015$ Å; R factor = 0.038; wR factor = 0.111; data-to-parameter ratio = 11.3.

In the title coordination polymer, $[\{\text{AgNd}(\text{C}_5\text{H}_3\text{N}_2\text{O}_2)_2(\text{C}_2\text{O}_4)\}_m \cdot \text{H}_2\text{O}]_n$, the Nd^{III} atom is coordinated in a distorted monocapped square-antiprismatic geometry by two O and two N atoms of two *N,O*-bidentate pyrazine-2-carboxylate (2-pzc) ligands, four O atoms of two bidentate oxalate ligands, and one O atom of a monodentate carboxylate group of a 2-pzc ligand. The Ag^{I} ion is coordinated in a distorted tetrahedral geometry by two N atoms from two monodentate 2-pzc ligands, one O atom from one monodentate oxalate ligand and one O atom of a bridging carboxylate group of a 2-pzc ligand. The oxalate anions link neighbouring neodymium(III) metal centres into Nd–oxalate chains, which are interconnected by $\text{Ag}(2\text{-pyz})_2$ units, forming a three-dimensional polymeric framework. Intermolecular $\text{O}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds are observed in the crystal structure.

Related literature

For general background to coordination polymers and open-framework materials, see: Barbour (2006); Kepert (2006); Kong *et al.* (2008); Zhang *et al.* (2005); Gheorghe *et al.* (2002). For the synthesis and crystal structure of heterometallic complexes of pyrazine-2-carboxylic acid, see: Ciurtin *et al.* (2002); Dong *et al.* (2000).



Experimental

Crystal data

$[\text{AgNd}(\text{C}_5\text{H}_3\text{N}_2\text{O}_2)_2(\text{C}_2\text{O}_4)] \cdot \text{H}_2\text{O}$
 $M_r = 604.33$
 Monoclinic, $P2_1/c$
 $a = 10.112$ (2) Å
 $b = 18.847$ (4) Å
 $c = 8.0359$ (16) Å
 $\beta = 95.47$ (3)°

$V = 1524.6$ (5) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 4.72$ mm⁻¹
 $T = 293$ K
 $0.32 \times 0.26 \times 0.21$ mm

Data collection

Rigaku/MSC Mercury CCD diffractometer
 Absorption correction: multi-scan (*REQAB*; Jacobson, 1998)
 $T_{\text{min}} = 0.241$, $T_{\text{max}} = 0.370$

12072 measured reflections
 2747 independent reflections
 1946 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.093$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.038$
 $wR(F^2) = 0.111$
 $S = 1.13$
 2747 reflections
 244 parameters

3 restraints
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 1.59$ e Å⁻³
 $\Delta\rho_{\text{min}} = -1.77$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
O1W—H1W \cdots O4 ⁱ	0.84	2.31	2.975 (13)	137
C3—H3 \cdots O1 ⁱⁱ	0.93	2.34	3.221 (12)	158
C3—H3 \cdots O8 ⁱⁱ	0.93	2.49	3.150 (13)	128
C4—H4 \cdots O5	0.93	2.54	3.170 (13)	125
C9—H9 \cdots O2 ⁱⁱⁱ	0.93	2.47	3.270 (15)	145
C9—H9 \cdots O7 ^{iv}	0.93	2.35	2.971 (15)	124

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick,

2008); molecular graphics: *ORTEP II* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

The authors acknowledge Lanzhou Jiaotong University for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2330).

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supplementary materials

Acta Cryst. (2009). E65, m833-m834 [doi:10.1107/S160053680902128X]

Poly[[hemi- μ_4 -oxalato-hemi- μ_2 -oxalato-bis(μ_3 -pyrazine-2-carboxylato)neodymium(III)silver(I)] monohydrate]

T.-J. Feng and Y.-M. Wen

Comment

In recent years, much research work has been focused on the design and synthesis of new potentially multifunctional heterometallic materials with useful structural properties, such as porosity, gas storage abilities and ion exchange capabilities (Barbour, 2006; Kepert, 2006; Kong *et al.*, 2008; Zhang *et al.*, 2005; Gheorghe *et al.*, 2002). Pyrazine-2-carboxylate (2-pzc) is such a potential multidentate ligand, which can be used to generate high-dimensional heterometallic frameworks (Ciurtin *et al.*, 2002; Dong *et al.*, 2000). On the basis of above considerations, we chose pyrazine-2-carboxylic acid, mixed 4d-4f metal ions and nitric acid as our building blocks. A new three-dimensional 4d-4f coordination framework resulted from the hydrothermal treatment of Nd₂O₃, AgNO₃, oxalic acid, pyrazine-2-carboxylic acid and nitric acid in water.

As depicted in Fig. 1, the asymmetric unit of the title compound contains one neodymium(III) atom, one silver(I) atom, two crystallographically independent 2-pzc ligands, two halves of oxalate anions and one lattice water molecule. The neodymium(III) atom is nine-coordinated in a distorted monocapped square-antiprismatic geometry by two O and two N atoms of two N,O-bidentate pyrazine-2-carboxylate (2-pzc) ligands, four O atoms of two bidentate oxalate ligands, and one O atom of a monodentate carboxylate group of a 2-pzc ligand. Each silver(I) ion can be described as having a distorted tetrahedral coordination geometry provided by two N atoms from two monodentate 2-pzc ligands, one O atom from one monodentate oxalate ligand and one O atom of a bridging carboxylate group of a 2-pzc ligand. In the crystal structure, zigzag Nd–oxalate chains are formed *via* the oxalate ligands, with Nd \cdots Nd separations of 6.290 (2) Å and 6.435 (3) Å. The interconnection of the Nd–oxalate chains and Ag(2-pyz)₂ units result in the formation of a three-dimensional polymeric structure. Intermolecular O—H \cdots O and C—H \cdots O hydrogen bonds involving the non-coordinated water molecules are observed in the crystal structure (Table 1, Fig. 2).

Experimental

A mixture of Nd₂O₃ (0.168 g, 0.5 mmol), AgNO₃ (0.169 g, 1 mmol), pyrazine-2-carboxylic acid (0.124 g, 1 mmol), oxalic acid (0.09 g, 1 mmol), HNO₃ (0.12 ml) and H₂O (10 ml) was placed in a 23 ml Teflon-lined reactor, which was heated to 433 K for 3 d and then cooled to room temperature at a rate of 10 K h⁻¹. The colourless crystals obtained were washed with water and dried in air (yield 46% based on Nd).

Refinement

C-bound H atoms were placed at calculated positions and were treated as riding on their parent atoms, with C—H = 0.93 Å and with $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$. The water H-atoms were located in a difference map, and were refined with a distance restraint of O—H = 0.84 Å and with $U_{\text{iso}}(\text{H}) = 1.5 U_{\text{eq}}(\text{O})$. The highest peak is located 1.31 Å from O1 and the deepest hole is located 0.94 Å from Nd1.

Figures

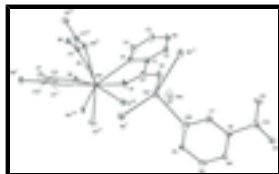


Fig. 1. The asymmetric unit of the title compound. Displacement ellipsoids are drawn at the 50% probability level. H atoms are omitted for clarity. [Symmetry codes: (i) $1 - x, 2 - y, 1 - z$; (ii) $1 - x, 2 - y, -z$; (iii) $-1 + x, 1.5 - y, -1/2 + z$; (iv) $-1 + x, y, z$; (v) $x, y, 1 + z$; (vi) $2 - x, 2 - y, 1 - z$.]

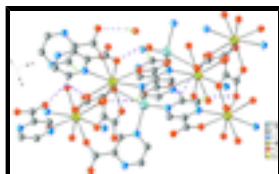


Fig. 2. A partial packing diagram of the title compound showing the intermolecular hydrogen bonds as dashed lines. Hydrogen atoms not involved in hydrogen bonds are omitted.

Poly[[hemi- μ_4 -oxalato-hemi- μ_2 -oxalato-bis(μ_3 -pyrazine-2-carboxylato)neodymium(III)silver(I)] monohydrate]

Crystal data

[AgNd(C₅H₃N₂O₂)₂(C₂O₄)₂] \cdot H₂O

$M_r = 604.33$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 10.112$ (2) Å

$b = 18.847$ (4) Å

$c = 8.0359$ (16) Å

$\beta = 95.47$ (3)°

$V = 1524.6$ (5) Å³

$Z = 4$

$F_{000} = 1148$

$D_x = 2.633$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 2433 reflections

$\theta = 1.4$ – 28.0 °

$\mu = 4.72$ mm⁻¹

$T = 293$ K

Block, colourless

$0.32 \times 0.26 \times 0.21$ mm

Data collection

Rigaku/MSM Mercury CCD diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 293$ K

ω scans

Absorption correction: multi-scan (REQAB; Jacobson, 1998)

$T_{\min} = 0.241$, $T_{\max} = 0.370$

12072 measured reflections

2747 independent reflections

1946 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.093$

$\theta_{\max} = 25.2$ °

$\theta_{\min} = 3.3$ °

$h = -12 \rightarrow 12$

$k = -22 \rightarrow 22$

$l = -9 \rightarrow 9$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.038$

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$wR(F^2) = 0.111$	$w = 1/[\sigma^2(F_o^2) + (0.0182P)^2 + 17.3537P]$
$S = 1.13$	where $P = (F_o^2 + 2F_c^2)/3$
2747 reflections	$(\Delta/\sigma)_{\max} = 0.028$
244 parameters	$\Delta\rho_{\max} = 1.59 \text{ e } \text{\AA}^{-3}$
3 restraints	$\Delta\rho_{\min} = -1.77 \text{ e } \text{\AA}^{-3}$
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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Ag1	1.15900 (9)	0.92327 (6)	0.60684 (11)	0.0369 (3)
C1	0.9481 (10)	0.9114 (6)	0.0822 (13)	0.026 (3)
N1	0.8209 (8)	0.9101 (5)	0.0274 (10)	0.027 (2)
Nd1	0.64656 (5)	0.89514 (3)	0.26047 (7)	0.02128 (18)
O1	0.8807 (6)	0.9057 (5)	0.3541 (8)	0.0298 (19)
O1W	0.9655 (10)	0.7408 (7)	0.0126 (18)	0.099 (5)
H1W	0.9199	0.7431	0.0945	0.149*
H2W	0.9262	0.7594	-0.0734	0.149*
C2	1.0449 (10)	0.9146 (6)	-0.0258 (13)	0.029 (3)
H2	1.1337	0.9136	0.0168	0.035*
N2	1.0149 (9)	0.9190 (5)	-0.1900 (11)	0.030 (2)
O2	1.0988 (7)	0.9106 (5)	0.3253 (8)	0.035 (2)
C3	0.8869 (11)	0.9176 (7)	-0.2454 (13)	0.037 (3)
H3	0.8622	0.9195	-0.3598	0.045*
O3	1.6618 (7)	0.8233 (4)	0.5173 (9)	0.034 (2)
C4	0.7896 (11)	0.9134 (7)	-0.1356 (12)	0.034 (3)
H4	0.7006	0.9130	-0.1775	0.041*
O4	1.7098 (7)	0.7193 (4)	0.6421 (10)	0.0317 (18)
C5	0.9806 (10)	0.9093 (6)	0.2720 (13)	0.027 (3)
O5	0.5044 (7)	0.9079 (4)	-0.0030 (9)	0.0309 (18)
O6	0.3693 (7)	0.9833 (4)	-0.1510 (9)	0.0304 (19)
O7	0.5658 (7)	1.0571 (4)	0.6552 (9)	0.0274 (18)
O8	0.6685 (7)	0.9827 (4)	0.4928 (8)	0.0270 (18)
N10	1.2894 (9)	0.8232 (6)	0.6898 (12)	0.039 (3)

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C11	0.4622 (10)	0.9689 (6)	-0.0439 (13)	0.026 (3)
N11	1.4588 (8)	0.7064 (5)	0.7235 (10)	0.024 (2)
C12	0.5689 (10)	1.0120 (6)	0.5441 (11)	0.022 (2)
C6	1.4972 (10)	0.7674 (6)	0.6640 (13)	0.027 (3)
C7	1.4155 (11)	0.8253 (6)	0.6552 (14)	0.031 (3)
H7	1.4498	0.8685	0.6234	0.037*
C8	1.2491 (11)	0.7609 (6)	0.7402 (15)	0.034 (3)
H8	1.1617	0.7560	0.7654	0.041*
C9	1.3340 (11)	0.7018 (7)	0.7569 (14)	0.033 (3)
H9	1.3016	0.6587	0.7922	0.040*
C10	1.6348 (11)	0.7698 (7)	0.6033 (13)	0.030 (3)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.0338 (5)	0.0520 (7)	0.0262 (4)	0.0081 (4)	0.0096 (4)	0.0043 (4)
C1	0.028 (6)	0.024 (7)	0.026 (6)	-0.007 (5)	0.006 (5)	-0.004 (5)
N1	0.028 (5)	0.035 (6)	0.018 (4)	-0.008 (4)	0.002 (4)	0.001 (4)
Nd1	0.0222 (3)	0.0239 (3)	0.0182 (3)	0.0008 (3)	0.0041 (2)	-0.0008 (3)
O1	0.009 (3)	0.063 (6)	0.017 (3)	-0.001 (4)	0.001 (3)	0.002 (4)
O1W	0.052 (7)	0.092 (11)	0.155 (12)	0.000 (6)	0.020 (7)	-0.042 (9)
C2	0.019 (5)	0.040 (8)	0.028 (6)	0.009 (5)	0.003 (4)	0.009 (5)
N2	0.032 (5)	0.037 (6)	0.022 (5)	-0.001 (4)	0.008 (4)	0.004 (4)
O2	0.021 (4)	0.066 (7)	0.017 (4)	0.004 (4)	-0.004 (3)	-0.006 (4)
C3	0.033 (7)	0.064 (10)	0.014 (5)	0.016 (6)	-0.003 (5)	-0.007 (5)
O3	0.036 (5)	0.040 (6)	0.027 (4)	-0.009 (4)	0.005 (3)	0.015 (4)
C4	0.036 (7)	0.055 (9)	0.012 (5)	-0.002 (6)	0.007 (5)	-0.007 (5)
O4	0.034 (4)	0.015 (4)	0.048 (5)	-0.001 (3)	0.013 (4)	0.008 (4)
C5	0.027 (6)	0.029 (7)	0.025 (5)	-0.008 (5)	0.010 (5)	0.006 (5)
O5	0.039 (5)	0.029 (5)	0.025 (4)	-0.004 (4)	0.000 (3)	0.003 (4)
O6	0.022 (4)	0.033 (5)	0.035 (4)	0.005 (3)	-0.007 (3)	0.002 (4)
O7	0.024 (4)	0.033 (5)	0.024 (4)	-0.001 (3)	0.000 (3)	-0.008 (4)
O8	0.026 (4)	0.034 (5)	0.021 (4)	0.007 (3)	0.006 (3)	-0.007 (3)
N10	0.029 (5)	0.043 (7)	0.043 (6)	0.004 (5)	-0.001 (5)	0.004 (5)
C11	0.024 (6)	0.028 (7)	0.027 (6)	0.002 (5)	0.003 (5)	0.008 (5)
N11	0.018 (4)	0.027 (6)	0.029 (5)	0.000 (4)	0.010 (4)	0.001 (4)
C12	0.034 (6)	0.020 (6)	0.012 (5)	0.000 (5)	0.003 (4)	-0.012 (4)
C6	0.026 (6)	0.032 (7)	0.023 (5)	0.000 (5)	0.002 (4)	0.013 (5)
C7	0.034 (7)	0.016 (7)	0.043 (7)	-0.001 (5)	0.003 (5)	0.002 (5)
C8	0.033 (6)	0.022 (7)	0.050 (7)	-0.004 (5)	0.019 (6)	0.011 (6)
C9	0.038 (7)	0.029 (7)	0.032 (6)	-0.004 (5)	0.006 (5)	0.011 (5)
C10	0.044 (7)	0.029 (8)	0.019 (5)	-0.007 (6)	0.010 (5)	-0.004 (5)

Geometric parameters (\AA , $^\circ$)

Ag1—N2 ⁱ	2.291 (9)	C3—H3	0.9300
Ag1—O2	2.299 (7)	O3—C10	1.267 (13)
Ag1—N10	2.360 (10)	O3—Nd1 ^{vii}	2.461 (7)

C1—N1	1.320 (13)	C4—H4	0.9300
C1—C2	1.370 (14)	O4—C10	1.240 (14)
C1—C5	1.530 (14)	O4—Nd1 ^{viii}	2.465 (7)
N1—C4	1.319 (13)	O5—C11	1.259 (13)
N1—Nd1	2.707 (8)	O6—C11	1.242 (12)
Nd1—O1	2.423 (6)	O6—Nd1 ⁱⁱ	2.455 (8)
Nd1—O6 ⁱⁱ	2.455 (8)	O7—C12	1.235 (11)
Nd1—O5	2.456 (7)	O7—Nd1 ^v	2.482 (7)
Nd1—O3 ⁱⁱⁱ	2.461 (7)	O8—C12	1.252 (12)
Nd1—O4 ^{iv}	2.465 (8)	N10—C8	1.319 (15)
Nd1—O7 ^v	2.482 (7)	N10—C7	1.332 (14)
Nd1—O8	2.486 (7)	C11—C11 ⁱⁱ	1.53 (2)
Nd1—N11 ^{iv}	2.692 (9)	N11—C9	1.317 (13)
O1—C5	1.260 (12)	N11—C6	1.318 (14)
O1W—H1W	0.8400	N11—Nd1 ^{viii}	2.692 (9)
O1W—H2W	0.8405	C12—C12 ^v	1.57 (2)
C2—N2	1.328 (13)	C6—C7	1.367 (15)
C2—H2	0.9300	C6—C10	1.517 (15)
N2—C3	1.329 (13)	C7—H7	0.9300
N2—Ag1 ^{vi}	2.291 (9)	C8—C9	1.406 (16)
O2—C5	1.231 (12)	C8—H8	0.9300
C3—C4	1.385 (15)	C9—H9	0.9300
N2 ⁱ —Ag1—O2	124.8 (3)	N2—C2—H2	119.2
N2 ⁱ —Ag1—N10	98.4 (3)	C1—C2—H2	119.2
O2—Ag1—N10	106.5 (3)	C2—N2—C3	117.0 (9)
N1—C1—C2	121.5 (10)	C2—N2—Ag1 ^{vi}	127.6 (7)
N1—C1—C5	116.3 (9)	C3—N2—Ag1 ^{vi}	115.3 (7)
C2—C1—C5	122.3 (9)	C5—O2—Ag1	120.1 (7)
C1—N1—C4	117.7 (9)	N2—C3—C4	121.1 (10)
C1—N1—Nd1	116.7 (6)	N2—C3—H3	119.5
C4—N1—Nd1	125.5 (7)	C4—C3—H3	119.5
O1—Nd1—O6 ⁱⁱ	93.6 (3)	C10—O3—Nd1 ^{vii}	153.6 (7)
O1—Nd1—O5	137.2 (2)	N1—C4—C3	121.1 (10)
O6 ⁱⁱ —Nd1—O5	65.6 (2)	N1—C4—H4	119.4
O1—Nd1—O3 ⁱⁱⁱ	78.7 (2)	C3—C4—H4	119.4
O6 ⁱⁱ —Nd1—O3 ⁱⁱⁱ	144.2 (3)	C10—O4—Nd1 ^{viii}	126.5 (7)
O5—Nd1—O3 ⁱⁱⁱ	139.7 (3)	O2—C5—O1	128.3 (10)
O1—Nd1—O4 ^{iv}	84.8 (3)	O2—C5—C1	117.1 (9)
O6 ⁱⁱ —Nd1—O4 ^{iv}	133.5 (3)	O1—C5—C1	114.6 (9)
O5—Nd1—O4 ^{iv}	84.6 (3)	C11—O5—Nd1	118.1 (7)
O3 ⁱⁱⁱ —Nd1—O4 ^{iv}	81.1 (3)	C11—O6—Nd1 ⁱⁱ	118.1 (7)
O1—Nd1—O7 ^v	136.9 (2)	C12—O7—Nd1 ^v	122.0 (6)
O6 ⁱⁱ —Nd1—O7 ^v	74.4 (2)	C12—O8—Nd1	121.6 (6)

supplementary materials

O5—Nd1—O7 ^v	75.5 (2)	C8—N10—C7	114.8 (10)
O3 ⁱⁱⁱ —Nd1—O7 ^v	87.6 (3)	C8—N10—Ag1	128.1 (8)
O4 ^{iv} —Nd1—O7 ^v	133.3 (2)	C7—N10—Ag1	116.0 (8)
O1—Nd1—O8	72.4 (2)	O6—C11—O5	126.5 (10)
O6 ⁱⁱ —Nd1—O8	69.4 (2)	O6—C11—C11 ⁱⁱ	117.6 (13)
O5—Nd1—O8	125.8 (3)	O5—C11—C11 ⁱⁱ	115.8 (11)
O3 ⁱⁱⁱ —Nd1—O8	75.0 (3)	C9—N11—C6	116.9 (9)
O4 ^{iv} —Nd1—O8	149.6 (2)	C9—N11—Nd1 ^{viii}	127.6 (7)
O7 ^v —Nd1—O8	64.6 (2)	C6—N11—Nd1 ^{viii}	115.5 (6)
O1—Nd1—N11 ^{iv}	138.7 (3)	O7—C12—O8	128.2 (10)
O6 ⁱⁱ —Nd1—N11 ^{iv}	127.1 (2)	O7—C12—C12 ^v	116.3 (11)
O5—Nd1—N11 ^{iv}	68.0 (3)	O8—C12—C12 ^v	115.5 (10)
O3 ⁱⁱⁱ —Nd1—N11 ^{iv}	71.9 (3)	N11—C6—C7	121.2 (10)
O4 ^{iv} —Nd1—N11 ^{iv}	62.7 (3)	N11—C6—C10	117.0 (10)
O7 ^v —Nd1—N11 ^{iv}	70.6 (3)	C7—C6—C10	121.9 (10)
O8—Nd1—N11 ^{iv}	124.5 (2)	N10—C7—C6	123.6 (11)
O1—Nd1—N1	61.6 (2)	N10—C7—H7	118.2
O6 ⁱⁱ —Nd1—N1	71.3 (3)	C6—C7—H7	118.2
O5—Nd1—N1	76.1 (2)	N10—C8—C9	122.1 (11)
O3 ⁱⁱⁱ —Nd1—N1	130.2 (3)	N10—C8—H8	118.9
O4 ^{iv} —Nd1—N1	67.3 (3)	C9—C8—H8	118.9
O7 ^v —Nd1—N1	142.1 (3)	N11—C9—C8	121.1 (11)
O8—Nd1—N1	115.7 (3)	N11—C9—H9	119.5
N11 ^{iv} —Nd1—N1	119.8 (3)	C8—C9—H9	119.5
C5—O1—Nd1	130.6 (6)	O4—C10—O3	126.2 (11)
H1W—O1W—H2W	111.8	O4—C10—C6	117.0 (10)
N2—C2—C1	121.5 (10)	O3—C10—C6	116.8 (10)

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

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1W—H1W \cdots O4 ^{iv}	0.84	2.31	2.975 (13)	137
C3—H3 \cdots O1 ^{vi}	0.93	2.34	3.221 (12)	158
C3—H3 \cdots O8 ^{vi}	0.93	2.49	3.150 (13)	128
C4—H4 \cdots O5	0.93	2.54	3.170 (13)	125
C9—H9 \cdots O2 ^{ix}	0.93	2.47	3.270 (15)	145
C9—H9 \cdots O7 ^x	0.93	2.35	2.971 (15)	124

Symmetry codes: (iv) $x-1, -y+3/2, z-1/2$; (vi) $x, y, z-1$; (ix) $x, -y+3/2, z+1/2$; (x) $-x+2, y-1/2, -z+3/2$.

Fig. 2

