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

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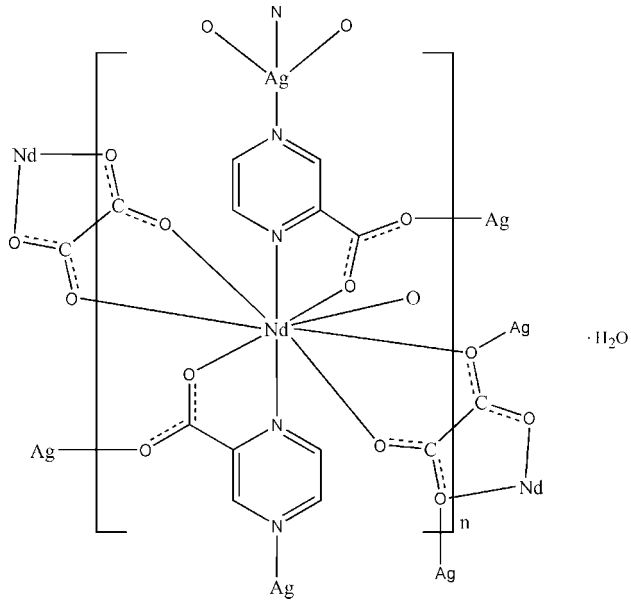
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.015 Å; R factor = 0.038; wR factor = 0.111; data-to-parameter ratio = 11.3.

In the title coordination polymer, $\{[AgNd(C_5H_3N_2O_2)_2(C_2O_4)]\cdot H_2O\}_n$, 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 $Ag(2\text{-pyz})_2$ units, forming a three-dimensional polymeric framework. Intermolecular O—H···O and C—H···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

$[AgNd(C_5H_3N_2O_2)_2(C_2O_4)]\cdot H_2O$
M_r = 604.33
Monoclinic, $P2_1/c$
a = 10.112 (2) Å
b = 18.847 (4) Å
c = 8.0359 (16) Å
β = 95.47 (3)°
V = 1524.6 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 4.72 mm^{-1}
T = 293 K
0.32 × 0.26 × 0.21 mm

Data collection

Rigaku/MSC Mercury CCD diffractometer
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_{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
$\Delta\rho_{max}$ = 1.59 e Å^{-3}
$\Delta\rho_{min}$ = −1.77 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1W···O4^{i}	0.84	2.31	2.975 (13)	137
C3—H3···O1^{ii}	0.93	2.34	3.221 (12)	158
C3—H3···O8^{ii}	0.93	2.49	3.150 (13)	128
C4—H4···O5	0.93	2.54	3.170 (13)	125
C9—H9···O2^{iii}	0.93	2.47	3.270 (15)	145
C9—H9···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: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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

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

Tian-Jun Feng and Yan-Mei Wen

S1. 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 Nd_2O_3, $AgNO_3$, 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 crystallogaphically 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···Nd separations of 6.290 (2) Å and 6.435 (3) Å. The interconnection of the Nd–oxalate chains and $Ag(2\text{-pyz})_2$ units result in the formation of a three-dimensional polymeric structure. Intermolecular O—H···O and C—H···O hydrogen bonds involving the non-coordinated water molecules are observed in the crystal structure (Table 1, Fig. 2).

S2. Experimental

A mixture of Nd_2O_3 (0.168 g, 0.5 mmol), $AgNO_3$ (0.169 g, 1 mmol), pyrazine-2-carboxylic acid (0.124 g, 1 mmol), oxalic acid (0.09 g, 1 mmol), HNO_3 (0.12 ml) and H_2O (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).

S3. 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_{iso}(H) = 1.2 U_{eq}(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_{iso}(H) = 1.5 U_{eq}(O). The hightest peak is located 1.31 Å from O1 and the deepest hole is located 0.94 Å from Nd1.

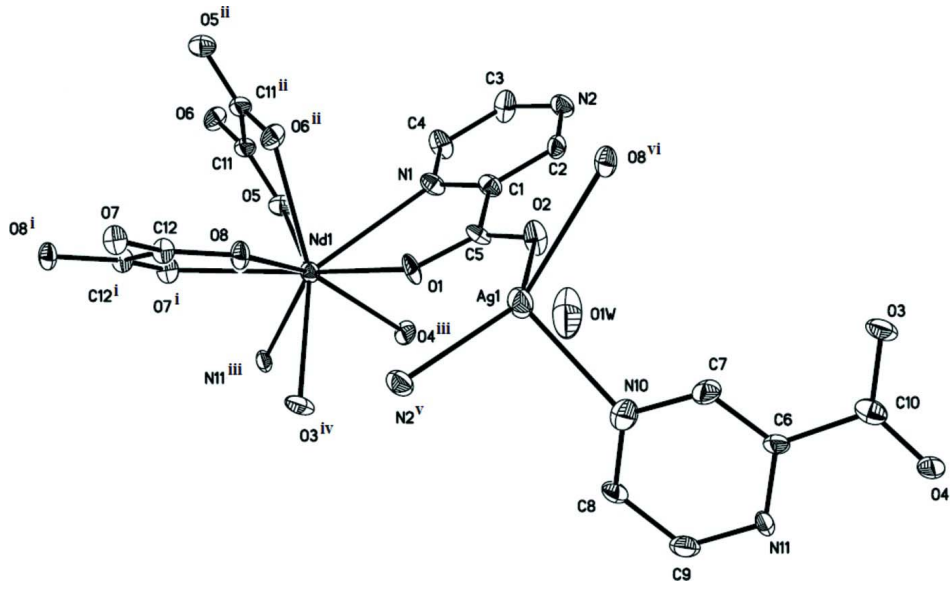

Figure 1

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*.]

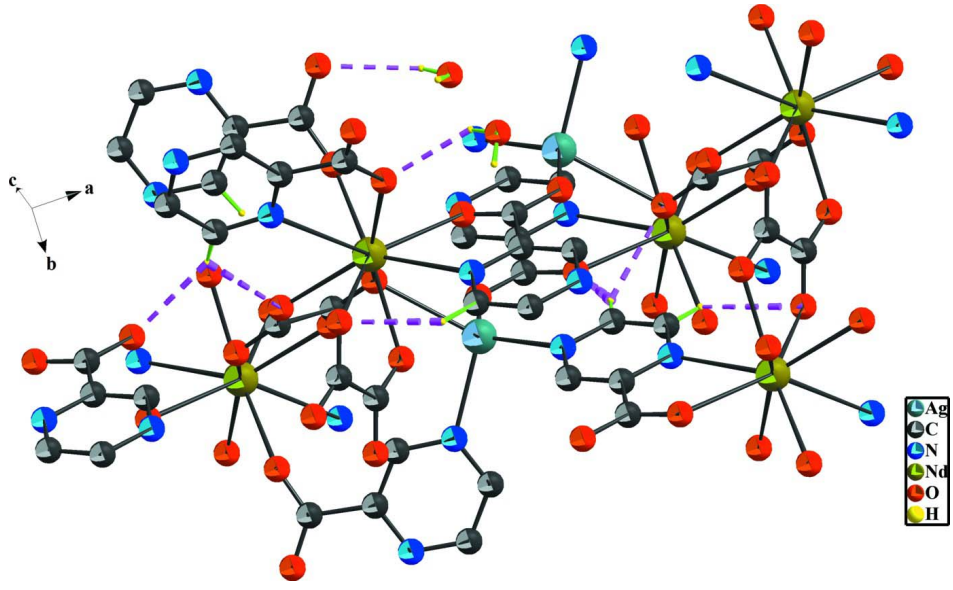

Figure 2

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.

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Crystal data

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Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc

a = 10.112 (2) Å
b = 18.847 (4) Å
c = 8.0359 (16) Å
β = 95.47 (3)°
V = 1524.6 (5) Å^3
Z = 4
F(000) = 1148
D_x = 2.633 Mg m^{-3}

Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2433 reflections
θ = 1.4–28.0°
μ = 4.72 mm^{-1}
T = 293 K
Block, colourless
0.32 × 0.26 × 0.21 mm

Data collection

Rigaku/MSC Mercury CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
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_{int} = 0.093
θ_{max} = 25.2°, θ_{min} = 3.3°
h = −12→12
k = −22→22
l = −9→9

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.111
S = 1.13
2747 reflections
244 parameters
3 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0182P)^2 + 17.3537P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.028
$\Delta\rho_{max}$ = 1.59 e Å^{-3}
$\Delta\rho_{min}$ = −1.77 e Å^{-3}

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}
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)
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 (Å²)

	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 (Å, º)

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)
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 (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*···O4^{iv}	0.84	2.31	2.975 (13)	137
C3—H3···O1^{vi}	0.93	2.34	3.221 (12)	158
C3—H3···O8^{vi}	0.93	2.49	3.150 (13)	128
C4—H4···O5	0.93	2.54	3.170 (13)	125

C9—H9···O2^{ix}	0.93	2.47	3.270 (15)	145
C9—H9···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) $-x+2, y-1/2, -z+3/2$.