metal-organic compounds

Poly[[diaquabis(μ_2-isonicotinato-κ^2N:O)-bis(μ_3-isonicotinato-κ^3N:O:O')-neodymium(III)disilver(I)] nitrate monohydrate]

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In the title complex, $\{[Ag_2Nd(C_6H_4NO_2)_4(H_2O)_2]NO_3 \cdot H_2O\}_n$, the Nd^{III} ion is coordinated by eight O atoms from six isonicotinate ligands and two water molecules in a distorted square antiprismatic geometry. Each Ag^I ion is coordinated by two N atoms from two different isonicotinate ligands. The crystal structure exhibits a two-dimensional heterometallic polymeric layer. O—H⋯O hydrogen bonds involving the coordinated and uncoordinated water molecules and intralayer π–π interactions between the pyridine rings [centroid–centroid distances = 3.571 (2) and 3.569 (2) Å] are observed. Each layer interacts with two neighboring ones via Ag⋯O(H_2O) contacts and interlayer π–π interactions [centroid–centroid distances = 3.479 (3) to 3.530 (3) Å], leading to a three-dimensional supramolecular network.

Related literature

For general background to metal organic frameworks, see: Batten & Robson (1998); Min & Suh (2000). For 4d–4f heterometallic coordination frameworks, see: Cai et al. (2009).
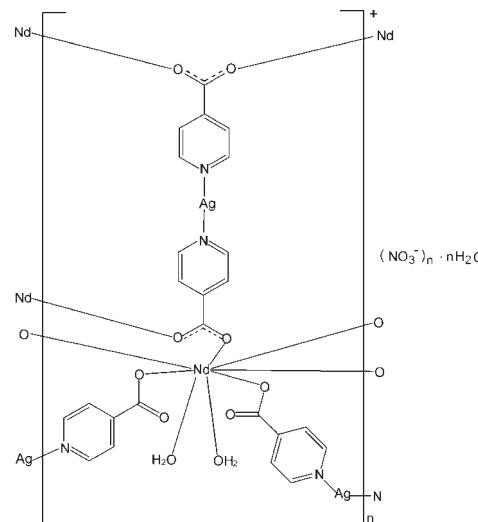
Experimental

Crystal data

$[Ag_2Nd(C_6H_4NO_2)_4(H_2O)_2]NO_3 \cdot H_2O$	β = 95.849 (1)°
M_r = 964.45	V = 2835.7 (6) Å³
Monoclinic, $P2_1/c$	Z = 4
a = 16.9618 (19) Å	Mo $K\alpha$ radiation
b = 24.793 (3) Å	μ = 3.25 mm⁻¹
c = 6.7770 (8) Å	T = 296 K
	$0.23 \times 0.20 \times 0.18$ mm

Data collection

Bruker APEXII CCD diffractometer	14629 measured reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	5092 independent reflections
T_{min} = 0.522, T_{max} = 0.592	4024 reflections with $I > 2\sigma(I)$
	R_{int} = 0.043

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.067	
S = 1.01	
5092 reflections	$\Delta\rho_{max}$ = 0.57 e Å⁻³
433 parameters	$\Delta\rho_{min}$ = −0.91 e Å⁻³
9 restraints	

Table 1
Selected bond lengths (Å).

Nd1—O1^i	2.381 (3)	Ag1—N1	2.155 (4)
Nd1—O2	2.502 (3)	Ag1—N2	2.155 (4)
Nd1—O3^{ii}	2.426 (3)	Ag1⋯O1W^i	2.888 (4)
Nd1—O4^{iii}	2.432 (3)	Ag1⋯O10	2.771 (5)
Nd1—O5	2.416 (3)	Ag2—N3^{iv}	2.200 (4)
Nd1—O7	2.406 (3)	Ag2—N4	2.184 (4)
Nd1—O2W	2.492 (4)	Ag2⋯O3W^v	2.741 (4)
Nd1—O3W	2.564 (3)	Ag2⋯O9^{vi}	2.950 (5)

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1W—H1$A\cdots$O10^{vii}	0.85 (3)	1.96 (2)	2.796 (8)	167 (7)
O1W—H1$B\cdots$O9	0.85 (4)	2.12 (5)	2.945 (8)	164 (6)
O2W—H2$A\cdots$O6	0.85 (4)	2.06 (3)	2.799 (5)	145 (5)
O2W—H2$B\cdots$O4^{iii}	0.84 (4)	2.21 (4)	3.033 (5)	166 (5)
O3W—H3$A\cdots$O8	0.85 (3)	1.87 (2)	2.653 (5)	153 (4)
O3W—H3$B\cdots$O6^{vii}	0.85 (3)	2.11 (3)	2.951 (5)	174 (5)

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXL97*.

References

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supporting information

Poly[[diaquabis(*μ*₂-isonicotinato-*κ*²*N*:*O*)bis(*μ*₃-isonicotinato-*κ*³*N*:*O*:*O*′)neodymium(III)disilver(I)] nitrate monohydrate]

Qing-Guang Zhan, Jie-Xuan Huang and Rong-Hua Zeng

S1. Comment

In recent years, assembly processes directed by metal–ligand ligation have been extensively utilized to construct metal organic frameworks with novel topologies and potentially interesting functions in magnetism, photoluminescence, sorption, catalysis (Batten & Robson, 1998; Min & Suh, 2000). However, metal-directed assembly of 4d–4f heterometallic coordination frameworks with fascinating topological networks and potential applications have been few reported (Cai *et al.*, 2009). We utilized isonicotinate as multifunctional ligand with O and N atoms on opposite sites. Here, a new metal-directed assembly of 4d–4f coordination polymer, which was synthesized under hydrothermal conditions, is reported.

  The asymmetric unit of the title complex contains one Nd^III ion, two Ag^I ions, four crystallographically unique isonicotinate ligands, one nitrate anion, two coordinated water molecules and one uncoordinated water molecule (Fig. 1). The Nd^III ion is in a distorted square antiprismatic geometry, defined by eight O atoms from six isonicotinate ligands and two water molecules. The Nd—O bond distances and O—Nd—O bond angles range from 2.381 (3) to 2.564 (3) Å and 71.79 (11) to 145.83 (12)°, respectively (Table 1). The Ag^I ion exhibits an approximatly linear or bow-like configuration, being coordinated by two N atoms from two different isonicotinate ligands. The isonicotinate ligands link Nd and Ag metal centers, forming a layer in the (010) plane, which are stabilized by O—H⋯O hydrogen bonds involving the coordinated and uncoordinated water molecules (Table 2) and intralayer *π*–*π* stacking interactions between the pyridine rings, with a centroid–centroid distances of 3.571 (2) and 3.569 (2) Å. These layers are further connected by Ag⋯O(H₂O) contacts and interlayer *π*–*π* stacking interactions [centroid–centroid distances = 3.479 (3) to 3.530 (3) Å] between the pyridine rings of two adjacent layers, assembling a three-dimensional supramolecular architecture (Fig. 2).

S2. Experimental

A mixture of Nd₂O₃ (0.183 g, 0.5 mmol), AgNO₃ (0.170 g, 1 mmol), isonicotinic acid (0.135 g, 1.5 mmol), water (10 ml) in the presence of HNO₃(0.024 g, 0.385 mmol) was stirred vigorously for 20 min and then sealed in a Teflon-lined stainless-steel autoclave (20 ml capacity). The autoclave was heated and maintained at 443 K for 3 d, and then cooled to room temperature at 5 K h⁻¹. The colorless block crystals of the title compound were obtained.

S3. Refinement

Water H atoms were tentatively located in difference Fourier maps and refined with distance restraints of O—H = 0.85 (1) Å and H⋯H = 1.35 (1) Å, and with $U_{iso}(H) = 1.5U_{eq}(O)$. H atoms attached to C atoms were placed at calculated positions and treated as riding on their parent atoms, with C—H = 0.93 Å and with $U_{iso}(H) = 1.2U_{eq}(C)$.
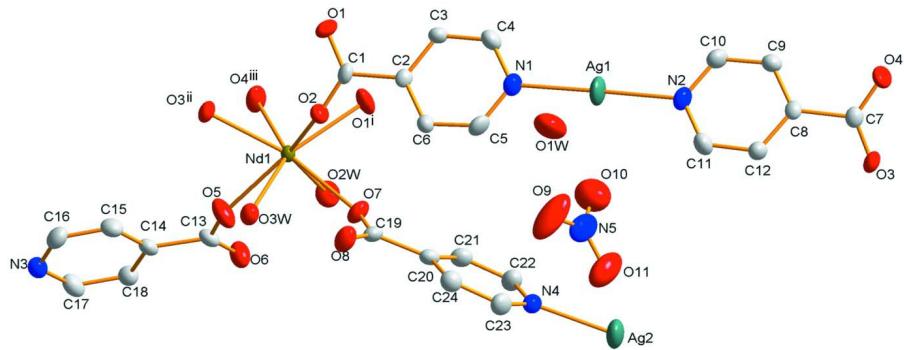
Figure 1

The asymmetric unit of the title compound. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity. [Symmetry codes: (i) x, 3/2-y, -1/2+z; (ii) -1+x, y, z; (iii) -1+x, 3/2-y, -1/2+z.]
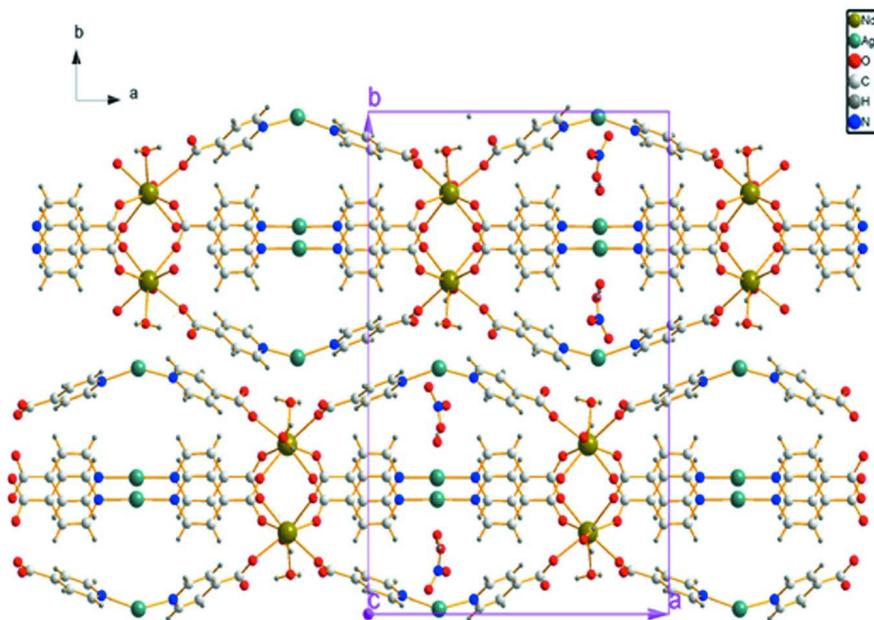
Figure 2

A view of the layered networks in the title compound.

Poly[[diaquabis(μ_2-isonicotinato-$\kappa^2N:O$)bis(μ_3- isonicotinato-$\kappa^3N:O:O′$)neodymium(III)disilver(I)] nitrate monohydrate]

Crystal data
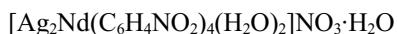
[Ag$_2$Nd(C$_6$H$_4$NO$_2$)$_4$(H$_2$O)$_2$]NO$_3$·H$_2$O	$V = 2835.7$ (6) Å^3
$M_r = 964.45$	$Z = 4$
Monoclinic, $P2_1/c$	$F(000) = 1868$
Hall symbol: -P 2ybc	$D_x = 2.259$ Mg m^{-3}
$a = 16.9648$ (19) Å	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$b = 24.793$ (3) Å	Cell parameters from 3327 reflections
$c = 6.7770$ (8) Å	$\theta = 2.4–25.9°$
$\beta = 95.849$ (1)°	$\mu = 3.25$ mm^{-1}

$T = 296$ K

$0.23 \times 0.20 \times 0.18$ mm

Block, colorless

Data collection

Bruker APEXII CCD diffractometer	14629 measured reflections
Radiation source: fine-focus sealed tube	5092 independent reflections
Graphite monochromator	4024 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.043$
Absorption correction: multi-scan	$\theta_{max} = 25.2°$, $\theta_{min} = 1.6°$
($SADABS$; Sheldrick, 1996)	$h = -17 \rightarrow 20$
$T_{min} = 0.522$, $T_{max} = 0.592$	$k = -29 \rightarrow 29$
	$l = -8 \rightarrow 5$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.032$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.067$	
$S = 1.01$	H atoms treated by a mixture of independent and constrained refinement
5092 reflections	
433 parameters	$w = 1/[\sigma^2(F_o^2) + (0.0268P)^2]$
9 restraints	where $P = (F_o^2 + 2F_c^2)/3$
Primary atom site location: structure-invariant direct methods	$(\Delta/\sigma)_{max} = 0.001$
	$\Delta\rho_{max} = 0.57$ e Å^{-3}
	$\Delta\rho_{min} = -0.91$ e Å^{-3}

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

	x	y	z	U_{iso}*/U_{eq}
Nd1	0.269306 (14)	0.662399 (10)	0.11749 (4)	0.01959 (8)
Ag1	0.77067 (2)	0.728604 (19)	0.49039 (7)	0.04705 (14)
Ag2	0.76495 (3)	0.510435 (19)	−0.09689 (7)	0.05046 (14)
O7	0.38451 (19)	0.60656 (13)	0.1017 (5)	0.0338 (9)
O2	0.35364 (18)	0.68568 (12)	0.4305 (5)	0.0289 (8)
O5	0.1656 (2)	0.60334 (15)	−0.0262 (5)	0.0456 (10)
C3	0.5223 (3)	0.77468 (17)	0.5011 (7)	0.0242 (11)
H3	0.4958	0.8074	0.5054	0.029*
C1	0.3912 (3)	0.72711 (19)	0.4857 (7)	0.0229 (11)
C2	0.4801 (3)	0.72666 (17)	0.4924 (6)	0.0197 (10)
N2	0.8974 (2)	0.72776 (16)	0.4834 (6)	0.0341 (10)
N1	0.6441 (2)	0.72777 (16)	0.4996 (6)	0.0327 (10)
C6	0.5224 (3)	0.67929 (18)	0.4894 (7)	0.0246 (11)
H6	0.4963	0.6462	0.4835	0.030*
C10	0.9388 (3)	0.77404 (19)	0.4767 (7)	0.0308 (12)
H10	0.9122	0.8067	0.4841	0.037*
C9	1.0183 (3)	0.77478 (18)	0.4595 (7)	0.0275 (12)
H9	1.0448	0.8076	0.4563	0.033*
C20	0.5069 (3)	0.56100 (17)	0.1414 (7)	0.0258 (11)
C19	0.4289 (3)	0.57592 (18)	0.2152 (8)	0.0259 (11)
O8	0.4127 (2)	0.55701 (14)	0.3746 (5)	0.0371 (9)
N4	0.6493 (2)	0.52916 (15)	0.0010 (6)	0.0316 (10)

C22	0.5972 (3)	0.56051 (19)	−0.1083 (8)	0.0337 (13)
H22	0.6094	0.5719	−0.2323	0.040*
C23	0.6300 (3)	0.5135 (2)	0.1793 (8)	0.0341 (13)
H23	0.6649	0.4912	0.2561	0.041*
C5	0.6032 (3)	0.6814 (2)	0.4951 (8)	0.0334 (13)
H5	0.6312	0.6491	0.4959	0.040*
C8	1.0594 (3)	0.72707 (18)	0.4469 (6)	0.0218 (11)
C12	1.0174 (3)	0.67961 (19)	0.4565 (7)	0.0279 (12)
H12	1.0430	0.6466	0.4493	0.033*
C14	0.0414 (3)	0.57066 (17)	−0.1642 (7)	0.0242 (11)
C15	0.0089 (3)	0.57587 (18)	0.0129 (7)	0.0308 (12)
H15	0.0389	0.5904	0.1228	0.037*
C13	0.1266 (3)	0.58696 (18)	−0.1849 (8)	0.0277 (12)
C18	−0.0059 (3)	0.54950 (18)	−0.3233 (7)	0.0291 (12)
H18	0.0130	0.5466	−0.4469	0.035*
O6	0.1513 (2)	0.58320 (14)	−0.3490 (5)	0.0413 (10)
C24	0.5615 (3)	0.52881 (19)	0.2536 (8)	0.0319 (12)
H24	0.5514	0.5176	0.3796	0.038*
C21	0.5267 (3)	0.57646 (18)	−0.0447 (8)	0.0299 (12)
H21	0.4919	0.5977	−0.1263	0.036*
C16	−0.0679 (3)	0.55962 (19)	0.0274 (8)	0.0348 (13)
H16	−0.0895	0.5645	0.1469	0.042*
C17	−0.0811 (3)	0.53274 (19)	−0.2966 (8)	0.0341 (13)
H17	−0.1117	0.5176	−0.4043	0.041*
C4	0.6027 (3)	0.77385 (19)	0.5035 (7)	0.0316 (12)
H4	0.6299	0.8064	0.5080	0.038*
C11	0.9378 (3)	0.6811 (2)	0.4766 (7)	0.0323 (12)
H11	0.9107	0.6487	0.4859	0.039*
O1	0.3610 (2)	0.76974 (13)	0.5428 (5)	0.0410 (10)
C7	1.1467 (3)	0.72688 (19)	0.4130 (7)	0.0249 (11)
O3	1.17260 (19)	0.68473 (13)	0.3448 (5)	0.0321 (8)
O4	1.1839 (2)	0.76939 (14)	0.4499 (6)	0.0419 (10)
O3W	0.2587 (2)	0.57863 (14)	0.3352 (5)	0.0308 (8)
H3B	0.2294 (19)	0.578 (2)	0.429 (4)	0.046*
H3A	0.3050 (10)	0.571 (2)	0.387 (6)	0.046*
O2W	0.2838 (2)	0.64789 (16)	−0.2408 (6)	0.0436 (10)
H2A	0.257 (2)	0.6245 (15)	−0.310 (7)	0.065*
H2B	0.251 (2)	0.6703 (17)	−0.205 (8)	0.065*
N5	0.7673 (3)	0.5865 (2)	0.3990 (10)	0.0570 (15)
O11	0.7991 (3)	0.5483 (2)	0.3274 (7)	0.0789 (15)
O9	0.7419 (3)	0.5845 (2)	0.5614 (7)	0.094 (2)
O10	0.7590 (3)	0.6295 (2)	0.3006 (8)	0.0892 (17)
N3	−0.1129 (2)	0.53684 (16)	−0.1258 (7)	0.0326 (10)
O1W	0.7704 (3)	0.65730 (16)	0.9046 (8)	0.0724 (14)
H1A	0.769 (5)	0.644 (2)	1.019 (4)	0.109*
H1B	0.763 (5)	0.6313 (17)	0.824 (7)	0.109*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Nd1	0.01421 (13)	0.02069 (13)	0.02424 (15)	−0.00081 (11)	0.00374 (10)	0.00027 (11)
Ag1	0.0152 (2)	0.0632 (3)	0.0635 (3)	0.0000 (2)	0.00745 (19)	−0.0005 (2)
Ag2	0.0231 (2)	0.0605 (3)	0.0700 (4)	0.0006 (2)	0.0150 (2)	0.0039 (2)
O7	0.028 (2)	0.037 (2)	0.037 (2)	0.0145 (16)	0.0071 (16)	0.0030 (16)
O2	0.0205 (18)	0.0311 (18)	0.035 (2)	−0.0041 (15)	0.0004 (15)	−0.0064 (15)
O5	0.041 (2)	0.062 (2)	0.033 (2)	−0.028 (2)	0.0013 (18)	−0.0006 (19)
C3	0.024 (3)	0.019 (2)	0.030 (3)	0.001 (2)	0.002 (2)	−0.001 (2)
C1	0.017 (3)	0.032 (3)	0.021 (3)	0.003 (2)	0.006 (2)	0.003 (2)
C2	0.017 (2)	0.027 (2)	0.015 (3)	0.002 (2)	−0.0024 (19)	−0.0007 (19)
N2	0.021 (2)	0.040 (3)	0.042 (3)	0.005 (2)	0.0059 (19)	0.000 (2)
N1	0.022 (2)	0.036 (3)	0.040 (3)	0.003 (2)	0.0046 (19)	0.002 (2)
C6	0.020 (3)	0.025 (3)	0.029 (3)	−0.003 (2)	0.004 (2)	−0.003 (2)
C10	0.025 (3)	0.028 (3)	0.039 (3)	0.006 (2)	0.000 (2)	−0.001 (2)
C9	0.027 (3)	0.023 (3)	0.033 (3)	−0.002 (2)	0.003 (2)	−0.002 (2)
C20	0.025 (3)	0.018 (2)	0.034 (3)	0.000 (2)	0.001 (2)	−0.002 (2)
C19	0.024 (3)	0.020 (2)	0.034 (3)	0.003 (2)	0.003 (2)	−0.005 (2)
O8	0.035 (2)	0.046 (2)	0.032 (2)	0.0109 (18)	0.0120 (17)	0.0124 (18)
N4	0.024 (2)	0.028 (2)	0.044 (3)	−0.0003 (19)	0.007 (2)	−0.004 (2)
C22	0.031 (3)	0.030 (3)	0.042 (4)	0.003 (2)	0.010 (2)	0.005 (2)
C23	0.023 (3)	0.034 (3)	0.045 (4)	0.005 (2)	−0.001 (2)	0.002 (3)
C5	0.024 (3)	0.031 (3)	0.044 (4)	0.012 (2)	0.003 (2)	0.000 (2)
C8	0.019 (3)	0.029 (3)	0.017 (3)	−0.001 (2)	0.0016 (19)	−0.003 (2)
C12	0.022 (3)	0.025 (3)	0.037 (3)	0.002 (2)	0.003 (2)	−0.001 (2)
C14	0.024 (3)	0.019 (2)	0.029 (3)	−0.004 (2)	0.000 (2)	0.000 (2)
C15	0.035 (3)	0.028 (3)	0.029 (3)	−0.005 (2)	0.003 (2)	−0.006 (2)
C13	0.028 (3)	0.023 (3)	0.031 (3)	−0.008 (2)	0.000 (2)	−0.002 (2)
C18	0.029 (3)	0.030 (3)	0.029 (3)	−0.003 (2)	0.006 (2)	−0.002 (2)
O6	0.035 (2)	0.057 (3)	0.033 (2)	−0.0149 (19)	0.0110 (17)	−0.0100 (18)
C24	0.029 (3)	0.033 (3)	0.034 (3)	−0.001 (2)	0.001 (2)	0.001 (2)
C21	0.032 (3)	0.025 (3)	0.033 (3)	0.002 (2)	0.003 (2)	0.002 (2)
C16	0.032 (3)	0.038 (3)	0.035 (3)	0.006 (3)	0.012 (2)	−0.001 (2)
C17	0.030 (3)	0.035 (3)	0.036 (3)	−0.009 (2)	−0.005 (3)	0.003 (2)
C4	0.027 (3)	0.028 (3)	0.040 (3)	−0.007 (2)	0.002 (2)	0.000 (2)
C11	0.026 (3)	0.032 (3)	0.040 (3)	−0.006 (2)	0.004 (2)	0.004 (2)
O1	0.022 (2)	0.034 (2)	0.067 (3)	0.0073 (16)	0.0020 (17)	−0.0206 (19)
C7	0.020 (3)	0.032 (3)	0.022 (3)	0.001 (2)	0.000 (2)	0.003 (2)
O3	0.0211 (19)	0.037 (2)	0.040 (2)	0.0038 (16)	0.0118 (15)	−0.0043 (17)
O4	0.022 (2)	0.043 (2)	0.061 (3)	−0.0105 (17)	0.0040 (17)	−0.0183 (19)
O3W	0.026 (2)	0.034 (2)	0.033 (2)	0.0006 (17)	0.0093 (15)	0.0029 (16)
O2W	0.043 (2)	0.058 (3)	0.030 (2)	−0.010 (2)	0.0055 (18)	−0.0101 (18)
N5	0.033 (3)	0.068 (4)	0.066 (5)	0.011 (3)	−0.011 (3)	−0.016 (4)
O11	0.052 (3)	0.109 (4)	0.073 (4)	0.026 (3)	−0.003 (2)	−0.027 (3)
O9	0.082 (4)	0.167 (6)	0.035 (3)	0.062 (4)	0.013 (3)	0.004 (3)
O10	0.096 (5)	0.084 (4)	0.090 (4)	−0.013 (3)	0.021 (3)	−0.014 (3)
N3	0.027 (2)	0.030 (2)	0.041 (3)	−0.0025 (19)	0.006 (2)	0.002 (2)

O1W	0.071 (3)	0.041 (3)	0.106 (4)	−0.009 (3)	0.010 (3)	0.001 (2)

Geometric parameters (Å, º)

Nd1—O1[i]	2.381 (3)	N4—C23	1.341 (6)
Nd1—O2	2.502 (3)	N4—C22	1.342 (6)
Nd1—O3[ii]	2.426 (3)	C22—C21	1.370 (7)
Nd1—O4[iii]	2.432 (3)	C22—H22	0.9300
Nd1—O5	2.416 (3)	C23—C24	1.366 (7)
Nd1—O7	2.406 (3)	C23—H23	0.9300
Nd1—O2W	2.492 (4)	C5—H5	0.9300
Nd1—O3W	2.564 (3)	C8—C12	1.381 (6)
Ag1—N1	2.155 (4)	C8—C7	1.521 (6)
Ag1—N2	2.155 (4)	C12—C11	1.372 (6)
Ag1—O1W[i]	2.888 (4)	C12—H12	0.9300
Ag1—O10	2.771 (5)	C14—C15	1.377 (7)
Ag2—N3[iv]	2.200 (4)	C14—C18	1.380 (6)
Ag2—N4	2.184 (4)	C14—C13	1.521 (7)
Ag2—O3W[v]	2.741 (4)	C15—C16	1.378 (7)
Ag2—O9[vi]	2.950 (5)	C15—H15	0.9300
O7—C19	1.272 (5)	C13—O6	1.232 (6)
O2—C1	1.246 (5)	C18—C17	1.372 (7)
O5—C13	1.271 (5)	C18—H18	0.9300
C3—C4	1.361 (6)	C24—H24	0.9300
C3—C2	1.387 (6)	C21—H21	0.9300
C3—H3	0.9300	C16—N3	1.348 (6)
C1—O1	1.253 (5)	C16—H16	0.9300
C1—C2	1.505 (6)	C17—N3	1.330 (7)
C2—C6	1.378 (6)	C17—H17	0.9300
N2—C11	1.348 (6)	C4—H4	0.9300
N2—C10	1.349 (6)	C11—H11	0.9300
N1—C5	1.342 (6)	C7—O4	1.241 (5)
N1—C4	1.343 (6)	C7—O3	1.241 (5)
C6—C5	1.369 (6)	O3W—H3B	0.85 (3)
C6—H6	0.9300	O3W—H3A	0.85 (3)
C10—C9	1.365 (7)	O2W—H2A	0.85 (4)
C10—H10	0.9300	O2W—H2B	0.84 (4)
C9—C8	1.381 (6)	N5—O11	1.215 (6)
C9—H9	0.9300	N5—O9	1.223 (7)
C20—C24	1.390 (6)	N5—O10	1.260 (7)
C20—C21	1.392 (7)	O1W—H1A	0.85 (3)
C20—C19	1.507 (7)	O1W—H1B	0.85 (4)
C19—O8	1.234 (6)		
O1[i]—Nd1—O7	81.12 (12)	O8—C19—C20	118.6 (4)
O1[i]—Nd1—O5	143.84 (12)	O7—C19—C20	115.6 (5)
O7—Nd1—O5	101.23 (13)	C23—N4—C22	117.1 (5)
O1[i]—Nd1—O3[ii]	118.20 (12)	C23—N4—Ag2	121.5 (3)

O7—Nd1—O3ⁱⁱ	139.85 (11)	C22—N4—Ag2	121.2 (4)
O5—Nd1—O3ⁱⁱ	83.25 (12)	N4—C22—C21	122.8 (5)
O1ⁱ—Nd1—O4ⁱⁱⁱ	77.33 (11)	N4—C22—H22	118.6
O7—Nd1—O4ⁱⁱⁱ	145.83 (12)	C21—C22—H22	118.6
O5—Nd1—O4ⁱⁱⁱ	81.87 (13)	N4—C23—C24	123.2 (5)
O3ⁱⁱ—Nd1—O4ⁱⁱⁱ	74.25 (12)	N4—C23—H23	118.4
O1ⁱ—Nd1—O2W	76.30 (13)	C24—C23—H23	118.4
O7—Nd1—O2W	73.28 (12)	N1—C5—C6	123.1 (4)
O5—Nd1—O2W	70.13 (12)	N1—C5—H5	118.4
O3ⁱⁱ—Nd1—O2W	142.39 (11)	C6—C5—H5	118.4
O4ⁱⁱⁱ—Nd1—O2W	76.03 (13)	C9—C8—C12	117.4 (4)
O1ⁱ—Nd1—O2	71.79 (11)	C9—C8—C7	121.2 (4)
O7—Nd1—O2	76.91 (11)	C12—C8—C7	121.3 (4)
O5—Nd1—O2	144.23 (11)	C11—C12—C8	120.0 (4)
O3ⁱⁱ—Nd1—O2	76.96 (11)	C11—C12—H12	120.0
O4ⁱⁱⁱ—Nd1—O2	119.84 (11)	C8—C12—H12	120.0
O2W—Nd1—O2	138.99 (12)	C15—C14—C18	117.7 (5)
O1ⁱ—Nd1—O3W	141.28 (11)	C15—C14—C13	121.5 (4)
O7—Nd1—O3W	70.39 (11)	C18—C14—C13	120.7 (5)
O5—Nd1—O3W	69.53 (11)	C14—C15—C16	120.0 (5)
O3ⁱⁱ—Nd1—O3W	74.22 (11)	C14—C15—H15	120.0
O4ⁱⁱⁱ—Nd1—O3W	139.34 (12)	C16—C15—H15	120.0
O2W—Nd1—O3W	117.61 (12)	O6—C13—O5	126.3 (5)
O2—Nd1—O3W	76.51 (10)	O6—C13—C14	118.5 (4)
O1ⁱ—Nd1—H2B	75.9 (13)	O5—C13—C14	115.2 (5)
O7—Nd1—H2B	92.3 (10)	C17—C18—C14	119.1 (5)
O5—Nd1—H2B	68.0 (13)	C17—C18—H18	120.4
O3ⁱⁱ—Nd1—H2B	125.2 (6)	C14—C18—H18	120.4
O4ⁱⁱⁱ—Nd1—H2B	56.7 (5)	C23—C24—C20	120.2 (5)
O2W—Nd1—H2B	19.3 (10)	C23—C24—H24	119.9
O2—Nd1—H2B	147.1 (13)	C20—C24—H24	119.9
O3W—Nd1—H2B	129.5 (12)	C22—C21—C20	120.3 (5)
N2—Ag1—N1	178.82 (16)	C22—C21—H21	119.9
N4—Ag2—N3ⁱᵛ	147.86 (15)	C20—C21—H21	119.9
C19—O7—Nd1	138.6 (3)	N3—C16—C15	122.2 (5)
C1—O2—Nd1	132.5 (3)	N3—C16—H16	118.9
C13—O5—Nd1	146.1 (3)	C15—C16—H16	118.9
C4—C3—C2	119.9 (4)	N3—C17—C18	123.8 (5)
C4—C3—H3	120.0	N3—C17—H17	118.1
C2—C3—H3	120.0	C18—C17—H17	118.1
O2—C1—O1	125.1 (4)	N1—C4—C3	122.5 (4)
O2—C1—C2	118.9 (4)	N1—C4—H4	118.7
O1—C1—C2	115.9 (4)	C3—C4—H4	118.7
C6—C2—C3	117.7 (4)	N2—C11—C12	122.4 (5)
C6—C2—C1	121.9 (4)	N2—C11—H11	118.8
C3—C2—C1	120.4 (4)	C12—C11—H11	118.8
C11—N2—C10	117.4 (4)	C1—O1—Nd1ᵛⁱⁱ	163.4 (3)
C11—N2—Ag1	121.4 (3)	O4—C7—O3	126.7 (5)

C10—N2—Ag1	121.1 (3)	O4—C7—C8	116.7 (4)
C5—N1—C4	117.4 (4)	O3—C7—C8	116.5 (4)
C5—N1—Ag1	121.4 (3)	C7—O3—Nd1^{iv}	135.8 (3)
C4—N1—Ag1	121.2 (3)	C7—O4—Nd1^{viii}	162.1 (3)
C5—C6—C2	119.3 (4)	Nd1—O3W—H3B	122 (3)
C5—C6—H6	120.4	Nd1—O3W—H3A	108 (3)
C2—C6—H6	120.4	H3B—O3W—H3A	105.7 (17)
N2—C10—C9	122.5 (4)	Nd1—O2W—H2A	122 (4)
N2—C10—H10	118.8	Nd1—O2W—H2B	59 (4)
C9—C10—H10	118.8	H2A—O2W—H2B	106 (4)
C10—C9—C8	120.3 (4)	O11—N5—O9	122.7 (7)
C10—C9—H9	119.9	O11—N5—O10	118.7 (7)
C8—C9—H9	119.9	O9—N5—O10	118.6 (6)
C24—C20—C21	116.4 (5)	C17—N3—C16	117.0 (5)
C24—C20—C19	121.2 (5)	C17—N3—Ag2ⁱⁱ	121.6 (3)
C21—C20—C19	122.3 (4)	C16—N3—Ag2ⁱⁱ	121.4 (4)
O8—C19—O7	125.8 (5)	H1A—O1W—H1B	106 (5)

Symmetry codes: (i) x, $-y+3/2$, $z-1/2$; (ii) $x-1$, y, z; (iii) $x-1$, $-y+3/2$, $z-1/2$; (iv) $x+1$, y, z; (v) $-x+1$, $-y+1$, $-z$; (vi) x, y, $z-1$; (vii) x, $-y+3/2$, $z+1/2$; (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
O1W—H1A···O10^{ix}	0.85 (3)	1.96 (2)	2.796 (8)	167 (7)
O1W—H1B···O9	0.85 (4)	2.12 (5)	2.945 (8)	164 (6)
O2W—H2A···O6	0.85 (4)	2.06 (3)	2.799 (5)	145 (5)
O2W—H2B···O4ⁱⁱⁱ	0.84 (4)	2.21 (4)	3.033 (5)	166 (5)
O3W—H3A···O8	0.85 (3)	1.87 (2)	2.653 (5)	153 (4)
O3W—H3B···O6^{ix}	0.85 (3)	2.11 (3)	2.951 (5)	174 (5)

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