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Poly[aqua(μ_3-5-azaniumylisophthalato)-(μ-oxalato)neodymium(III)]

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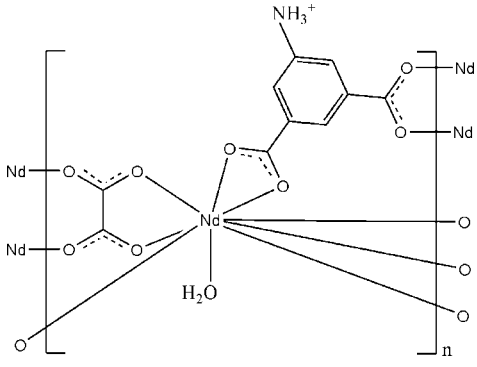
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.007 Å; R factor = 0.024; wR factor = 0.056; data-to-parameter ratio = 11.0.

The title compound, $[Nd(C_8H_6NO_4)(C_2O_4)(H_2O)]_n$, is a layer-like coordination polymer. The Nd^{III} ion is coordinated by four carboxylate O atoms from three bridging 5-azaniumylisophthalate (Haip) ligands, four carboxylate O atoms from two oxalate (ox) anions and one ligated water molecule in a tricapped trigonal–prismatic geometry. The Haip anion acts as a μ_3-bridge, connecting three Nd^{III} ions through two carboxylate groups; the ox anion adopts a bis-bidentate-bridging mode, linking two Nd^{III} ions. The layer framework is further extended to a three-dimensional supramolecular structure through N—H···O and O—H···O hydrogen bonds.

Related literature

For isotypic complexes, see: Liu *et al.* (2008); Yan *et al.* (2009).



Experimental

Crystal data

$[Nd(C_8H_6NO_4)(C_2O_4)(H_2O)]$
M_r = 430.41
Monoclinic, $C2/c$
a = 20.047 (4) Å
b = 9.592 (2) Å
c = 13.670 (3) Å
β = 117.810 (2)°
V = 2325.0 (9) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 4.52 mm^{-1}
T = 298 K
0.28 × 0.22 × 0.15 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
T_{min} = 0.364, T_{max} = 0.551
5839 measured reflections
2104 independent reflections
1792 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.056
S = 1.03
2104 reflections
191 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.71 e Å^{-3}
$\Delta\rho_{min}$ = −0.53 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1B···O5^{i}	0.89	1.91	2.795 (5)	172
N1—H1C···O8^{ii}	0.89	2.05	2.872 (5)	154
O1W—H1W···O3^{iii}	0.82	2.06	2.812 (4)	153
O1W—H2W···O1^{iv}	0.82	1.97	2.750 (4)	159

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

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: *SHELXTL* (Sheldrick, 2008); 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: NG5259).

References

Bruker (2002). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2007). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Liu, C. B., Wen, H. L., Tan, S. S. & Yi, X. G. (2008). *J. Mol. Struct.* **879**, 25–29.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Yan, L.-S., Huang, D.-H. & Liu, C.-B. (2009). *Acta Cryst.* E**65**, m750.

supplementary materials

Acta Cryst. (2012). E**68**, m537 [doi:10.1107/S1600536812013554]

Poly[aqua(μ_3-5-azaniumylisophthalato)(μ-oxalato)neodymium(III)]

Xia Yin, Tian-Tian Xiao, Jun Fan, Sheng-Run Zheng and Wei-Guang Zhang

Comment

The 5-aminoisophthalate (aip) anion adopts various coordination modes in lanthanide complexes. In this work, we present the synthesis and structure of a new neodymium coordination polymer with 5-aminoisophthalate and oxalate, [Nd(Haip)(ox)(H_2O)], which is isostructural with those reported previously (Liu *et al.*, 2008; Yan *et al.*, 2009).

In the title compound, the asymmetric unit comprises one Nd^{III} ion, one Haip ligand, one oxalate anion and one ligated water molecule (Fig. 1). The neodymium ion is nine-coordinated by four carboxylate O atoms [O1, O2, $O3^{i}$, and $O4^{ii}$, symmetry codes: (i) -*x*, 1 - *y*, -*z*; (ii) *x*, -1 + *y*, *z*] from three Haip ligands, four carboxylate O atoms [O5, O6, $O7^{iii}$, and $O8^{iii}$, symmetry codes: (iii) 1/2 - *x*, 1/2 + *y*, 1/2 - *z*] from two oxalate ions and one coordinated water molecule. The geometry is a tricapped trigonal prism configuration (Fig. 2). The Nd—O bond distances are in the range of 2.417 (3)–2.603 (3) Å.

The Haip anion acts as μ_3-bridge to connect three Nd^{III} ions through two carboxylate groups and the amino group exists as an $–NH_3^+$ unit. The oxalate anion adopts a bis-bidenatate-bridging mode to link two Nd^{III} ions with a Nd···Nd separation of 6.3821 (10) Å. The coordination of the metal ions and organic ligands (Haip and ox) results in the formation of a layer-like framework in the *ab* plane (Fig. 3).

In addition, there are O–H···O [O···O distances, 2.750 (4) and 2.812 (4) Å] and N–H···O hydrogen bonds (Table 1). The layers are further linked *via* these hydrogen bonds to form a three-dimensional supramolecular architecture (Fig. 4).

Experimental

A mixture of 5-aminoisophthalic acid (0.50 mmol, 90.6 mg), $Nd(NO_3)_3.6H_2O$ (0.30 mmol, 131.5 mg,) oxalic acid (0.50 mmol, 45.0 mg) and 10 ml H_2O was sealed in a 15 ml Teflon-lined stainless steel reactor and heated at 423 K under autogenous pressure for 72 h. After the sample had been slowly cooled to room temperature at a rate of 5 K/h, block-shaped pale-purple crystals were isolated (yield 52%). IR (KBr pellet, ν cm^{-1}): 3423 (*m*), 1631 (*s*), 1570 (*s*), 1466 (*m*), 1394 (*s*), 1326 (*m*), 1116 (*m*), 914 (*w*), 769 (*s*), 596 (*m*).

Refinement

The H atoms of water molecule were located in a difference Fourier maps and the others were placed in calculated positions and refined as riding atoms with isotropic thermal factors [C–H = 0.93 (aromatic C–H) Å; N–H = 0.89 Å; O–H = 0.83 Å; U_{iso}(H) = 1.2 U_{eq} (C), U_{iso}(H) = 1.5U_{eq}(N), and U_{iso}(H) = 1.5U_{eq}(O)].

Computing details

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

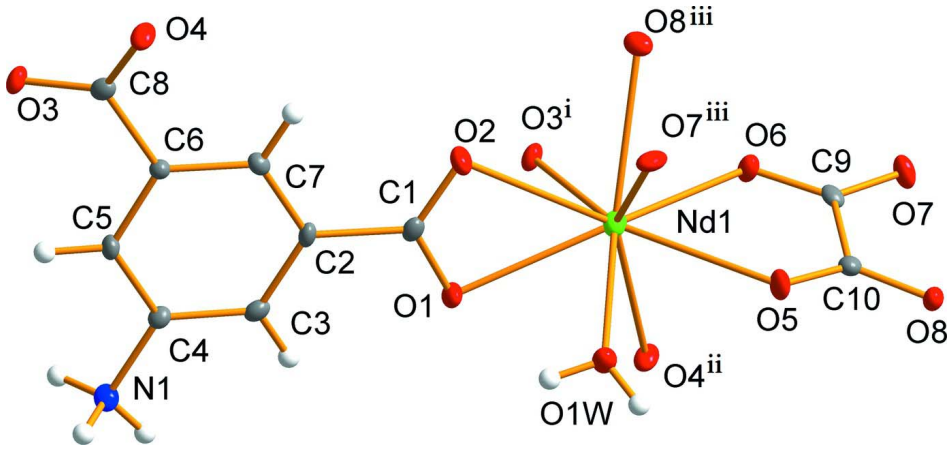

Figure 1

A fragment of the polymeric structure, with displacement ellipsoids drawn at the 30% probability level. [Symmetry codes: (i) -*x*, 1 - *y*, -*z*; (ii) *x*, -1 + *y*, *z*; (iii) 1/2 - *x*, 1/2 + *y*, 1/2 - *z*].

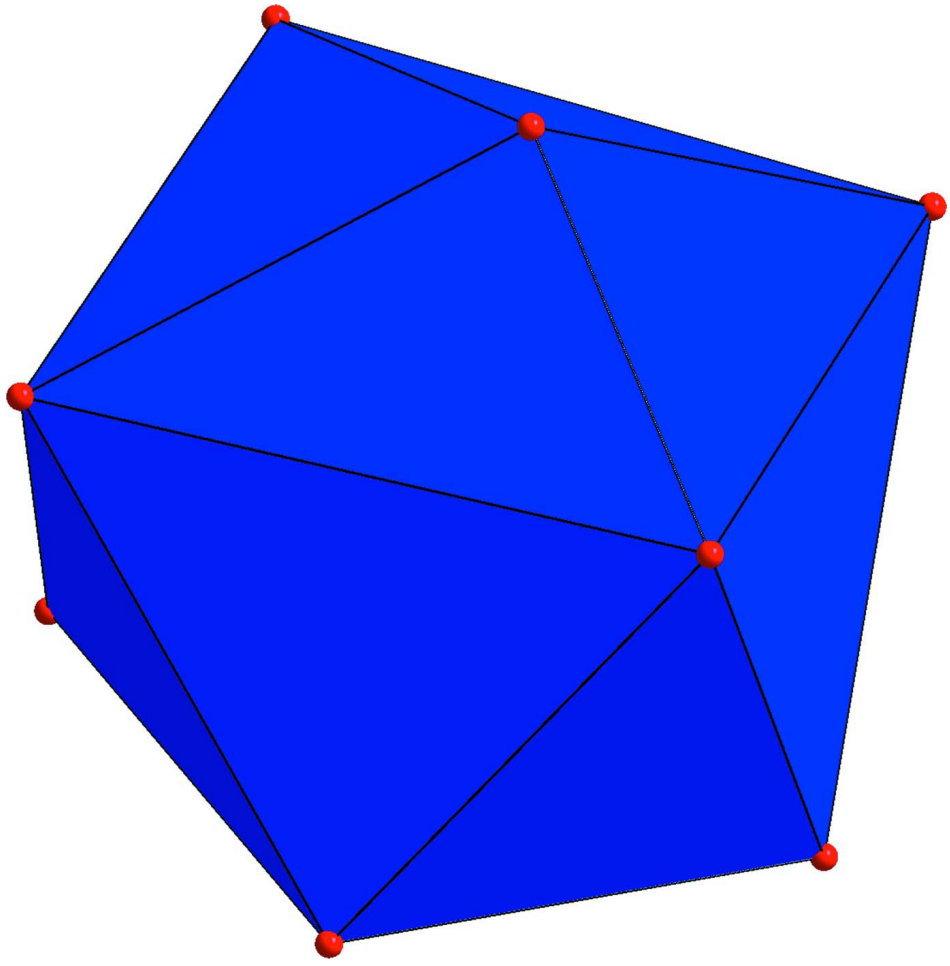

Figure 2

Geometry of the nine-coordinated Nd^{III} ion in the title compound.

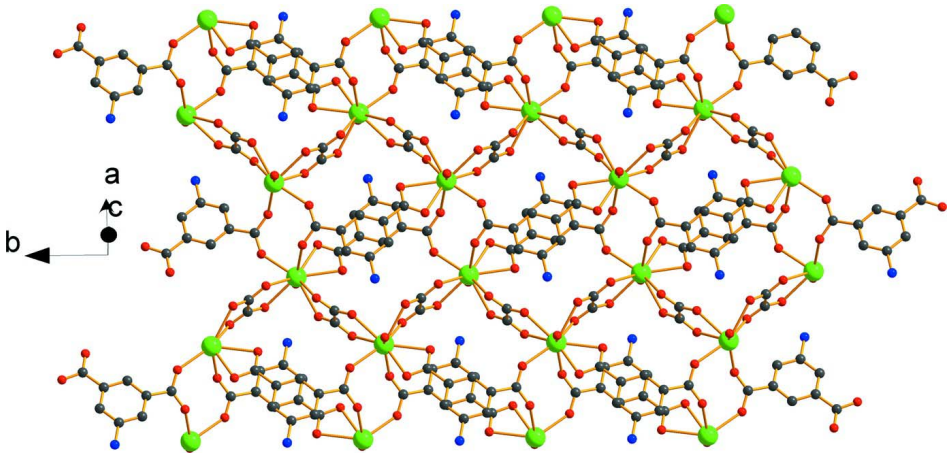

Figure 3

A packing diagram of the title compound, showing a layer-like structure in the *ab* plane.

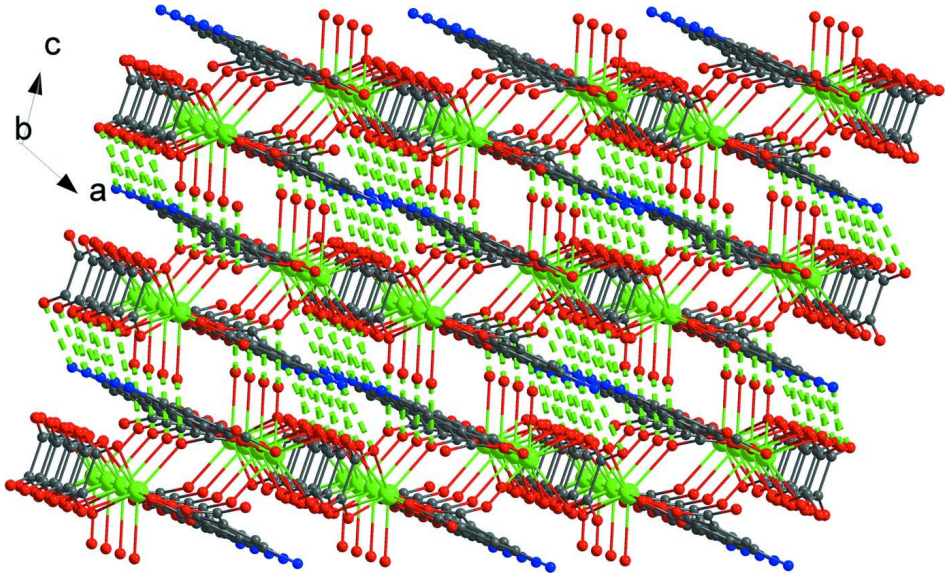

Figure 4

A packing diagram, showing a three-dimensional supramolecular network driven by hydrogen bonds (dashed lines).

Poly[aqua(μ_3-5-azaniumylisophthalato)(μ-oxalato)neodymium(III)]

Crystal data

[Nd($C_8H_6NO_4$)(C_2O_4)(H_2O)]
M_r = 430.41
Monoclinic, *C*2/*c*
Hall symbol: -c 2yc
a = 20.047 (4) Å
b = 9.592 (2) Å
c = 13.670 (3) Å
β = 117.810 (2)°
V = 2325.0 (9) Å^3
Z = 8
F(000) = 1656
D_x = 2.459 Mg m^{-3}
Mo *K*α radiation, λ = 0.71073 Å
Cell parameters from 2699 reflections
θ = 2.3–28.1°
μ = 4.52 mm^{-1}
T = 298 K
Block, pale-purple
0.28 × 0.22 × 0.15 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scan
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
T_{min} = 0.364, T_{max} = 0.551
5839 measured reflections
2104 independent reflections
1792 reflections with $I > 2\sigma(I)$
R_{int} = 0.033
θ_{max} = 25.3°, θ_{min} = 2.3°
h = −24→23
k = −6→11
l = −16→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.056
S = 1.03
2104 reflections
191 parameters
0 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
$w = 1/[\sigma^2(F_o^2) + (0.0254P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.71 e Å^{-3}
$\Delta\rho_{min}$ = −0.53 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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
C1	0.0410 (3)	0.3120 (5)	0.1508 (3)	0.0193 (10)
C2	−0.0121 (3)	0.4328 (4)	0.1225 (4)	0.0191 (10)
C3	−0.0873 (3)	0.4068 (5)	0.0894 (3)	0.0202 (10)
H3	−0.1043	0.3155	0.0846	0.024*
C4	−0.1372 (2)	0.5164 (4)	0.0632 (3)	0.0172 (10)
C5	−0.1136 (2)	0.6520 (4)	0.0653 (3)	0.0184 (10)
H5	−0.1480	0.7249	0.0465	0.022*
C6	−0.0386 (2)	0.6794 (4)	0.0956 (3)	0.0154 (9)
C7	0.0131 (2)	0.5702 (4)	0.1271 (3)	0.0181 (10)
H7	0.0639	0.5882	0.1511	0.022*
C8	−0.0168 (3)	0.8255 (5)	0.0841 (4)	0.0200 (10)
C9	0.2271 (2)	−0.2176 (5)	0.1774 (4)	0.0180 (10)
C10	0.2346 (2)	−0.2223 (5)	0.2950 (4)	0.0191 (10)
N1	−0.2164 (2)	0.4895 (4)	0.0294 (3)	0.0238 (9)
H1A	−0.2248	0.3981	0.0228	0.036*
H1B	−0.2448	0.5306	−0.0353	0.036*
H1C	−0.2282	0.5235	0.0800	0.036*

Nd1	0.131834 (12)	0.06274 (2)	0.184227 (18)	0.01456 (9)
O1	0.01407 (17)	0.1908 (3)	0.1433 (3)	0.0254 (7)
O2	0.10891 (17)	0.3304 (3)	0.1781 (2)	0.0278 (8)
O3	−0.06874 (17)	0.9033 (3)	0.0145 (2)	0.0203 (7)
O4	0.05001 (17)	0.8623 (3)	0.1427 (3)	0.0258 (8)
O5	0.20791 (17)	−0.1221 (3)	0.3242 (2)	0.0232 (7)
O6	0.19047 (18)	−0.1178 (3)	0.1175 (2)	0.0240 (7)
O7	0.25959 (17)	−0.3114 (3)	0.1530 (2)	0.0264 (8)
O8	0.26728 (17)	−0.3267 (3)	0.3532 (2)	0.0235 (7)
O1W	0.10490 (18)	0.0638 (3)	0.3446 (3)	0.0276 (8)
H1W	0.1092	0.0089	0.3930	0.041*
H2W	0.0717	0.1186	0.3396	0.041*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.026 (3)	0.018 (3)	0.015 (2)	0.004 (2)	0.011 (2)	0.0035 (19)
C2	0.023 (2)	0.017 (3)	0.019 (2)	0.008 (2)	0.010 (2)	0.0066 (19)
C3	0.025 (3)	0.018 (3)	0.018 (2)	−0.0024 (19)	0.011 (2)	0.0026 (19)
C4	0.019 (2)	0.015 (2)	0.016 (2)	−0.0019 (19)	0.0066 (19)	−0.0008 (19)
C5	0.018 (2)	0.014 (2)	0.022 (2)	0.0044 (18)	0.008 (2)	0.0010 (19)
C6	0.015 (2)	0.015 (2)	0.017 (2)	−0.0006 (18)	0.0076 (19)	0.0005 (19)
C7	0.014 (2)	0.021 (3)	0.018 (2)	0.0002 (19)	0.0065 (19)	−0.0005 (19)
C8	0.025 (3)	0.017 (3)	0.021 (2)	−0.002 (2)	0.014 (2)	−0.002 (2)
C9	0.010 (2)	0.018 (3)	0.023 (2)	−0.0036 (18)	0.007 (2)	−0.006 (2)
C10	0.016 (2)	0.019 (3)	0.023 (2)	−0.0017 (19)	0.010 (2)	0.002 (2)
N1	0.023 (2)	0.018 (2)	0.028 (2)	−0.0009 (17)	0.0108 (18)	−0.0036 (17)
Nd1	0.01452 (14)	0.01069 (14)	0.01771 (14)	0.00055 (10)	0.00688 (10)	0.00072 (10)
O1	0.0239 (18)	0.0142 (18)	0.040 (2)	0.0040 (14)	0.0170 (16)	0.0043 (15)
O2	0.0174 (18)	0.0239 (19)	0.039 (2)	0.0046 (14)	0.0104 (15)	0.0028 (15)
O3	0.0251 (18)	0.0131 (17)	0.0175 (16)	0.0024 (13)	0.0055 (14)	0.0022 (13)
O4	0.0208 (18)	0.0158 (18)	0.0324 (18)	−0.0050 (14)	0.0054 (15)	0.0014 (14)
O5	0.0280 (19)	0.0191 (17)	0.0234 (17)	0.0092 (14)	0.0128 (15)	−0.0022 (14)
O6	0.0337 (19)	0.0192 (18)	0.0240 (18)	0.0091 (15)	0.0175 (16)	0.0057 (14)
O7	0.0238 (18)	0.027 (2)	0.0259 (17)	0.0093 (15)	0.0096 (15)	−0.0052 (15)
O8	0.0238 (18)	0.0200 (19)	0.0296 (18)	0.0066 (14)	0.0149 (15)	0.0089 (14)
O1W	0.0317 (19)	0.028 (2)	0.0304 (19)	0.0082 (15)	0.0204 (16)	0.0084 (14)

Geometric parameters (Å, º)

C1—O2	1.245 (5)	C9—C10	1.544 (6)
C1—O1	1.265 (5)	C10—O5	1.253 (5)
C1—C2	1.498 (6)	C10—O8	1.256 (5)
C2—C3	1.379 (6)	N1—H1A	0.8900
C2—C7	1.402 (6)	N1—H1B	0.8900
C3—C4	1.379 (6)	N1—H1C	0.8900
C3—H3	0.9300	Nd1—O4^{i}	2.417 (3)
C4—C5	1.380 (6)	Nd1—O3^{ii}	2.425 (3)
C4—N1	1.454 (5)	Nd1—O1	2.482 (3)
C5—C6	1.387 (6)	Nd1—O1W	2.491 (3)

C5—H5	0.9300	Nd1—O6	2.492 (3)
C6—C7	1.392 (6)	Nd1—O5	2.532 (3)
C6—C8	1.497 (6)	Nd1—O8^{iii}	2.538 (3)
C7—H7	0.9300	Nd1—O7^{iii}	2.575 (3)
C8—O4	1.248 (5)	Nd1—O2	2.603 (3)
C8—O3	1.274 (5)	O1W—H1W	0.8182
C9—O7	1.244 (5)	O1W—H2W	0.8249
C9—O6	1.252 (5)		

O2—C1—O1	121.3 (4)	O4^{i}—Nd1—O6	75.26 (11)
O2—C1—C2	120.9 (4)	O3^{ii}—Nd1—O6	76.82 (10)
O1—C1—C2	117.7 (4)	O1—Nd1—O6	145.34 (10)
C3—C2—C7	120.1 (4)	O1W—Nd1—O6	131.15 (10)
C3—C2—C1	118.7 (4)	O4^{i}—Nd1—O5	73.98 (10)
C7—C2—C1	121.2 (4)	O3^{ii}—Nd1—O5	139.16 (10)
C4—C3—C2	119.8 (4)	O1—Nd1—O5	133.70 (10)
C4—C3—H3	120.1	O1W—Nd1—O5	68.83 (10)
C2—C3—H3	120.1	O6—Nd1—O5	64.51 (9)
C3—C4—C5	120.9 (4)	O4^{i}—Nd1—O8^{iii}	143.36 (10)
C3—C4—N1	120.0 (4)	O3^{ii}—Nd1—O8^{iii}	76.48 (10)
C5—C4—N1	119.1 (4)	O1—Nd1—O8^{iii}	120.75 (10)
C4—C5—C6	119.9 (4)	O1W—Nd1—O8^{iii}	134.10 (10)
C4—C5—H5	120.0	O6—Nd1—O8^{iii}	70.15 (10)
C6—C5—H5	120.0	O5—Nd1—O8^{iii}	100.92 (10)
C5—C6—C7	119.7 (4)	O4^{i}—Nd1—O7^{iii}	141.60 (10)
C5—C6—C8	118.4 (4)	O3^{ii}—Nd1—O7^{iii}	133.95 (10)
C7—C6—C8	121.7 (4)	O1—Nd1—O7^{iii}	107.11 (10)
C6—C7—C2	119.5 (4)	O1W—Nd1—O7^{iii}	71.34 (10)
C6—C7—H7	120.2	O6—Nd1—O7^{iii}	106.82 (10)
C2—C7—H7	120.2	O5—Nd1—O7^{iii}	72.95 (10)
O4—C8—O3	124.9 (4)	O8^{iii}—Nd1—O7^{iii}	63.03 (10)
O4—C8—C6	118.4 (4)	O4^{i}—Nd1—O2	133.39 (10)
O3—C8—C6	116.7 (4)	O3^{ii}—Nd1—O2	80.76 (9)
O7—C9—O6	126.7 (4)	O1—Nd1—O2	50.92 (10)
O7—C9—C10	116.8 (4)	O1W—Nd1—O2	85.21 (10)
O6—C9—C10	116.5 (4)	O6—Nd1—O2	141.25 (10)
O5—C10—O8	125.7 (4)	O5—Nd1—O2	138.60 (9)
O5—C10—C9	117.5 (4)	O8^{iii}—Nd1—O2	74.13 (10)
O8—C10—C9	116.8 (4)	O7^{iii}—Nd1—O2	68.31 (10)
C4—N1—H1A	109.5	C1—O1—Nd1	96.4 (3)
C4—N1—H1B	109.5	C1—O2—Nd1	91.2 (3)
H1A—N1—H1B	109.5	C8—O3—Nd1^{ii}	137.1 (3)
C4—N1—H1C	109.5	C8—O4—Nd1^{iv}	141.5 (3)
H1A—N1—H1C	109.5	C10—O5—Nd1	119.5 (3)
H1B—N1—H1C	109.5	C9—O6—Nd1	121.7 (3)
O4^{i}—Nd1—O3^{ii}	84.35 (10)	C9—O7—Nd1^{v}	116.4 (3)
O4^{i}—Nd1—O1	82.57 (10)	C10—O8—Nd1^{v}	115.8 (3)
O3^{ii}—Nd1—O1	74.75 (10)	Nd1—O1W—H1W	136.4
O4^{i}—Nd1—O1W	78.94 (10)	Nd1—O1W—H2W	115.3

O3^{ii}—Nd1—O1W	140.51 (11)	H1W—O1W—H2W	104.8
O1—Nd1—O1W	67.81 (10)		
O2—C1—C2—C3	178.0 (4)	O4^{i}—Nd1—O2—C1	2.9 (3)
O1—C1—C2—C3	−0.4 (6)	O3^{ii}—Nd1—O2—C1	76.0 (3)
O2—C1—C2—C7	−0.7 (7)	O1—Nd1—O2—C1	−1.9 (2)
O1—C1—C2—C7	−179.0 (4)	O1W—Nd1—O2—C1	−67.0 (3)
C7—C2—C3—C4	−1.5 (7)	O6—Nd1—O2—C1	131.1 (3)
C1—C2—C3—C4	179.8 (4)	O5—Nd1—O2—C1	−117.0 (3)
C2—C3—C4—C5	2.7 (7)	O8^{iii}—Nd1—O2—C1	154.4 (3)
C2—C3—C4—N1	−179.3 (4)	O7^{iii}—Nd1—O2—C1	−138.8 (3)
C3—C4—C5—C6	−1.0 (6)	O4—C8—O3—Nd1^{ii}	100.8 (5)
N1—C4—C5—C6	−178.9 (4)	C6—C8—O3—Nd1^{ii}	−79.5 (5)
C4—C5—C6—C7	−2.1 (6)	O3—C8—O4—Nd1^{iv}	2.2 (8)
C4—C5—C6—C8	172.9 (4)	C6—C8—O4—Nd1^{iv}	−177.5 (3)
C5—C6—C7—C2	3.3 (6)	O8—C10—O5—Nd1	−173.2 (3)
C8—C6—C7—C2	−171.5 (4)	C9—C10—O5—Nd1	7.0 (5)
C3—C2—C7—C6	−1.5 (7)	O4^{i}—Nd1—O5—C10	75.8 (3)
C1—C2—C7—C6	177.2 (4)	O3^{ii}—Nd1—O5—C10	15.1 (4)
C5—C6—C8—O4	156.3 (4)	O1—Nd1—O5—C10	138.4 (3)
C7—C6—C8—O4	−28.9 (6)	O1W—Nd1—O5—C10	159.9 (3)
C5—C6—C8—O3	−23.5 (6)	O6—Nd1—O5—C10	−5.2 (3)
C7—C6—C8—O3	151.4 (4)	O8^{iii}—Nd1—O5—C10	−66.8 (3)
O7—C9—C10—O5	173.9 (4)	O7^{iii}—Nd1—O5—C10	−124.0 (3)
O6—C9—C10—O5	−4.4 (6)	O2—Nd1—O5—C10	−145.2 (3)
O7—C9—C10—O8	−6.0 (6)	O7—C9—O6—Nd1	−178.6 (3)
O6—C9—C10—O8	175.8 (4)	C10—C9—O6—Nd1	−0.6 (5)
O2—C1—O1—Nd1	−3.5 (4)	O4^{i}—Nd1—O6—C9	−76.3 (3)
C2—C1—O1—Nd1	174.9 (3)	O3^{ii}—Nd1—O6—C9	−163.8 (3)
O4^{i}—Nd1—O1—C1	−174.7 (3)	O1—Nd1—O6—C9	−128.3 (3)
O3^{ii}—Nd1—O1—C1	−88.6 (3)	O1W—Nd1—O6—C9	−15.8 (4)
O1W—Nd1—O1—C1	104.3 (3)	O5—Nd1—O6—C9	2.7 (3)
O6—Nd1—O1—C1	−124.5 (3)	O8^{iii}—Nd1—O6—C9	116.0 (3)
O5—Nd1—O1—C1	125.9 (2)	O7^{iii}—Nd1—O6—C9	63.8 (3)
O8^{iii}—Nd1—O1—C1	−24.9 (3)	O2—Nd1—O6—C9	139.9 (3)
O7^{iii}—Nd1—O1—C1	43.4 (3)	O6—C9—O7—Nd1^{v}	156.9 (4)
O2—Nd1—O1—C1	1.8 (2)	C10—C9—O7—Nd1^{v}	−21.2 (5)
O1—C1—O2—Nd1	3.3 (4)	O5—C10—O8—Nd1^{v}	−149.6 (4)
C2—C1—O2—Nd1	−175.0 (4)	C9—C10—O8—Nd1^{v}	30.3 (5)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*B*···O5^{vi}	0.89	1.91	2.795 (5)	172
N1—H1*C*···O8^{vii}	0.89	2.05	2.872 (5)	154
O1*W*—H1*W*···O3^{viii}	0.82	2.06	2.812 (4)	153
O1*W*—H2*W*···O1^{ix}	0.82	1.97	2.750 (4)	159

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