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A one-dimensional ladder-like coordination polymer: poly[[hexaaquabis(μ-5-nitrobenzene-1,3-dicarboxylato-κ^3O,O',O'')(μ-oxalato-$\kappa^4O,O':O'',O'''$)-diyttrium(III)] trihydrate]

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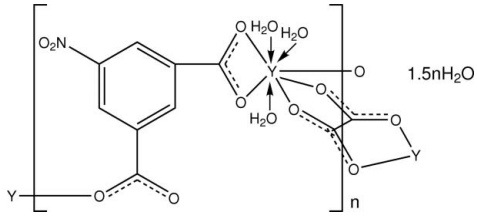
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.008 Å; disorder in solvent or counterion; R factor = 0.043; wR factor = 0.112; data-to-parameter ratio = 12.7.

In the crystal structure of the title one-dimensional coordination polymer, $[Y_2(C_8H_3NO_6)_2(C_2O_4)(H_2O)_6]\cdot 3H_2O$, each Y^{III} ion is bridged to its neighbours by two 5-nitrobenzene-1,3-dicarboxylate (nbdc) dianions and one oxalate dianion (located on an inversion centre) to form a ladder-like polymeric structure. The two carboxylate groups of nbdc assume different modes of coordination, one is chelating whereas the other is monodentate. Three water molecules coordinate to the Y^{III} ion to complete an eight-coordinate distorted dodecahedral geometry. The ladder-like polymers are assembled together by hydrogen bonding and π–π stacking [centrio–centriod distance = 3.819 (9) Å] in the crystal structure.

Related literature

For general background, see: Biradha (2003); Braga *et al.* (2005); Burrows *et al.* (2003); Kongshaug & Fjellvag (2006); Moulton & Zaworotko (2001); Ohmori *et al.* (2004); Tang *et al.* (2006); Janiak (2003). For related structures, see: Thomas *et al.* (2002); Nordell *et al.* (2003); Janiak (2000). For related literature, see: Ren *et al.* (2006); Si *et al.* (2004).



Experimental

Crystal data

$[Y_2(C_8H_3NO_6)_2(C_2O_4)(H_2O)_6]\cdot 3H_2O$
M_r = 846.21
Triclinic, $P\overline{1}$
a = 7.4270 (15) Å
b = 9.2070 (18) Å
c = 11.522 (2) Å
α = 74.16 (3)°
β = 71.76 (3)°
γ = 80.01 (2)°
V = 716.5 (3) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 4.14 mm^{-1}
T = 298 (2) K
0.20 × 0.15 × 0.12 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (*XCAD4*; Harms & Wocadlo, 1995)
T_{min} = 0.48, T_{max} = 0.60
3018 measured reflections
2785 independent reflections
2260 reflections with $I > 2\sigma(I)$
R_{int} = 0.097
3 standard reflections
every 200 reflections
intensity decay: 1.0%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.112
S = 1.05
2785 reflections
220 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.67 e Å^{-3}
$\Delta\rho_{min}$ = −0.64 e Å^{-3}

Table 1
Selected bond lengths (Å).

O1—Y	2.414 (4)	O8—Y	2.361 (3)
O2—Y	2.424 (4)	O9—Y	2.314 (4)
O3—Y^{i}	2.299 (3)	O10—Y	2.336 (4)
O7—Y^{ii}	2.365 (3)	O11—Y	2.311 (4)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O9—H9A···O2^{iii}	0.85	2.14	2.735 (5)	127
O9—H9B···O4^{iv}	0.85	2.07	2.726 (5)	134
O10—H10A···O6^{iii}	0.85	2.36	3.115 (7)	148
O10—H10B···O12^{ii}	0.85	2.30	2.778 (6)	116
O10—H10B···O12^{ii}	0.85	2.30	2.778 (6)	116
O11—H11A···O4^{v}	0.85	2.09	2.694 (5)	127
O11—H11B···O5^{vi}	0.85	2.57	2.987 (6)	111
O11—H11B···O7^{vii}	0.85	2.23	2.784 (5)	123
O12—H12A···O1	0.85	2.11	2.841 (6)	144
O12—H12B···O10^{i}	0.85	2.21	2.953 (6)	147

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

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 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: XU2377).

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supporting information

Acta Cryst. (2008). E**64**, m120–m121 [https://doi.org/10.1107/S1600536807064306]

A one-dimensional ladder-like coordination polymer: poly[[hexaaquabis(μ-5-nitrobenzene-1,3-dicarboxylato-κ^3O,O',O'')(μ-oxalato-$\kappa^4O,O':O'',O'''$)diyttrium(III)] trihydrate]

Zhong Fu, Ying Lin, Yun-You Zhou and Hong-Tao Zhang

S1. Comment

There is an intense research interest for the crystal engineering of coordination polymers owing to their intriguing molecular topologies, such as molecular grids, ladders, rings, diamondoids and honeycombs, and potential applications as functional materials (Biradha, 2003; Braga *et al.*, 2005; Janiak, 2003; Ohmori *et al.*, 2004). In order to construct the infinite structure, plentiful multidentate organic ligands are used to bridge metal ions (Moulton & Zaworotko, 2001). Among them, V-shape molecules, such as isophthalic acid and 5-amino-isophthalic acid, have received much attention because such a molecular geometry can result in unexpected structure comparing with that constructed by linear ligands (Burrows *et al.*, 2003; Tang *et al.*, 2006; Kongshaug & Fjellvag, 2006; Si *et al.*, 2004; Ren *et al.*, 2006). Herein, we present a novel ladder-like coordination polymer (I): $Y_2(C_8H_3NO_6)_2(C_2O_4)(H_2O)_6.3(H_2O)$, in which metal ions are bridged by a V-shape ligand, 5-nitrobenzene-1,3-dicarboxylate (5-nitroisophthalate, abbreviated as 5-NIP), and oxalate ligands.

As shown in Figure 1, the Y(III) ion adopts an eight-coordinate geometry which may be described as a distorted dodecahedron (Table 1): it is bounded to three water oxygen atoms (O9, O10 and O11) and five carboxylate oxygen atoms, in which O1, O2 and O3^{iii} [symmetry code: (iii) *x*, *y* - 1, *z*] are from two 5-NIP ligands and O7^{i}, O8 [symmetry code: (i) 1 - *x*, -*y*, 1 - *z*] are from one oxalate ligand. The H13A/O13/H13B water molecule has a fractional site occupancy of 0.50. The ligand 5-NIP chelates the Y(III) ion *via* its O1/C1/O2 carboxylate group, while its another O3/C8/O4 carboxylate group coordinates to a symmetry related Y(III) ion in monodentate fashion *via* the atom O3. The O5/N1/O6 nitro group is almost coplanar with the phenyl ring (C2/C3/C4/C5/C6/C7). The O1/C1/O2 carboxylate group is slightly twisted from the phenyl ring with the dihedral angel of 10.26 (41)° based on the phenyl (C2/C3/C4/C5/C6/C7) and the carboxyl (O1/C1/O2) planes. The O3/C8/O4 carboxylate group is out of the phenyl plane with the dihedral angel of 44.41 (36)° based on the phenyl (C2/C3/C4/C5/C6/C7) and the carboxyl (O3/C8/O4) planes. Both two carboxylate groups of the oxalate ligand bridge two symmetry related Y(III) ions in $\eta^1:\eta^1:\mu_2$ mode. The oxalate is almost perpendicular to the phenyl plane of 5-NIP with the dihedral angel of 87.42 (26)° based on the phenyl (C2/C3/C4/C5/C6/C7) and the oxalate (O7/C9/O8/C9^{i}/O7^{i}/O8^{i}) [symmetry code: (i) 1 - *x*, -*y*, 1 - *z*] planes. The bond distance of two sp^2 C9—C9^{i} [symmetry code: (i) 1 - *x*, -*y*, 1 - *z*] in oxalate is elongated similar with other coordination compounds containing oxalate (Thomas *et al.*, 2002; Nordell *et al.*, 2003). Thus, the ligands 5-NIP link the neighbouring Y(III) ions in the head-to-tail mode to construct an infinite zigzag chain which runs along the *b* axis direction. Two adjacent zigzag chains are connected *via* oxalate bridging in the *c* axis direction to form a ladder-like structure with a grid of 9.207 (11)Å × 6.138 (17)Å based on the intra-ladder intervals of Yttrium (III) ions.

(Burrows *et al.*, 2003; Tang *et al.*, 2006; Kongshaug & Fjellvag, 2006).

All ladders are assembled together through a number of hydrogen bonding (Table 2) between 5-NIP carboxyl O atoms (O1, O2 and O4), nitro O atoms (O5 and O6), oxalate O7 atom and coordination water O atoms (O9, O10 and O11) as well as lattice water molecules (O12 and O13). Among them, H10A and H11B atoms are involved in a three-centered hydrogen bond, respectively. Moreover, the center-center distance between two adjacent phenyl rings of the different ladders is 3.819 (9) Å. It indicates the presence of π-π staking between two adjacent inter-ladder 5-NIP (Janiak *et al.*, 2000). Therefore all ladders are packing *via* hydrogen bonding and the π-π interactions in the crystal.

S2. Experimental

Y_2O_3 (22.5 mg, 0.10 mmol), 5-nitro-isophthalic acid (42.2 mg, 0.20 mmol) and $Na_2C_2O_4$ (26.8 mg, 0.20 mmol) were dissolved in 13 ml water. The mixture was placed in a Teflon-lined stainless steel vessel (25 ml). The vessel was sealed and heated at 443 K for 1 week, then cooled to room temperature. Colorless block crystals were collected by filtration, followed by washing with water and ethanol in 45% yield (38.5 mg). The crystals becam opaque when exposed for a long time in air.

S3. Refinement

The lattice O13 water molecule was refined with a fixed site occupancy factor of 0.50. H atoms bonded to C atoms were introduced at calculated positions and refined using a riding model with C—H = 0.93 Å. All water H atoms were located in difference maps at an intermediate stage of the refinement and were then treated as riding, with O—H = 0.85 Å. U_{iso}(H) = 1.2U_{iso}(C,*O*).

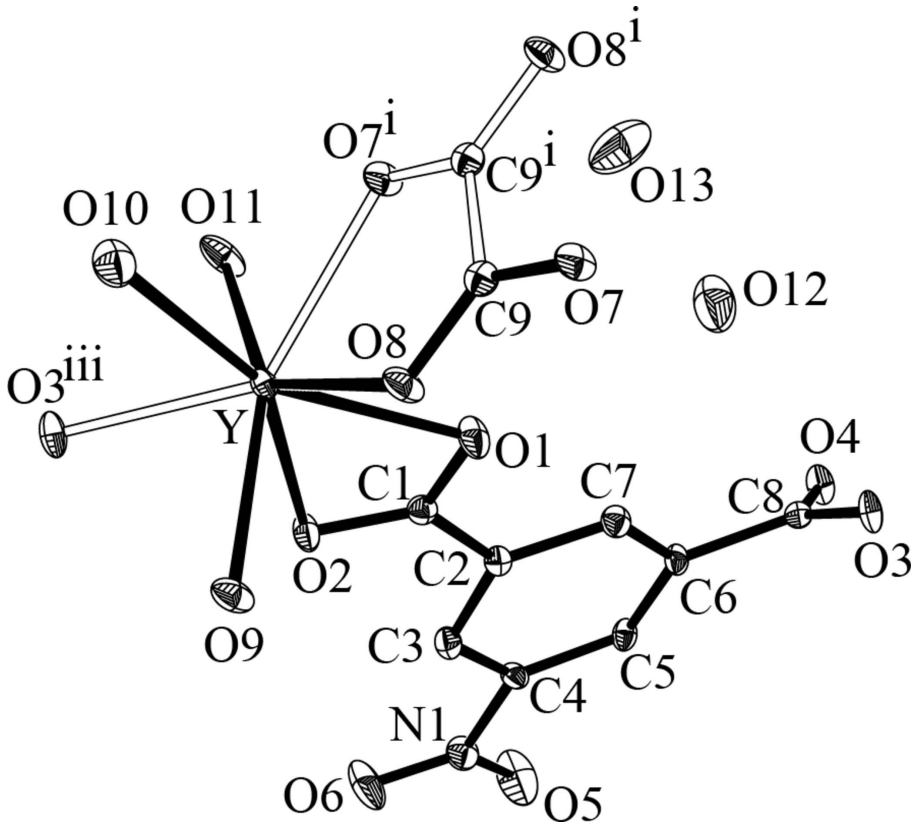

Figure 1

The molecular structure of (I), a drawing of the asymmetric unit (solid line portion) with displacement ellipsoids at the 30% probability level, H Atoms have been omitted for clarity [symmetry code: (i) 1 - *x*, -*y*, 1 - *z*; (iii) *x*, *y* - 1, *z*].

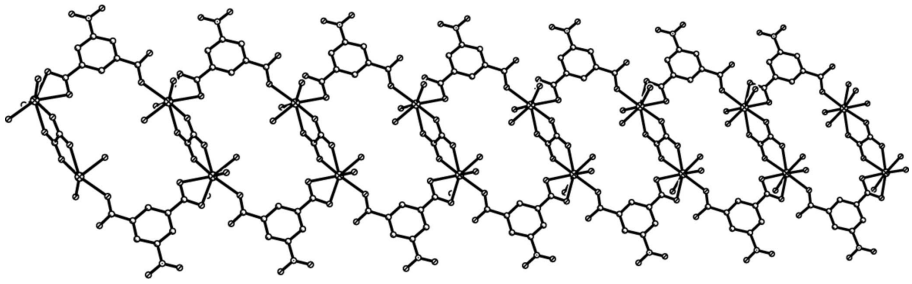

Figure 2

Two adjacent zigzag chains connected *via* oxalate bridging to generate a ladder-like structure with a grid of 9.207 (11)Å × 6.138 (17) Å. All hydrogen atoms and the lattice water molecules have been omitted for clarity.

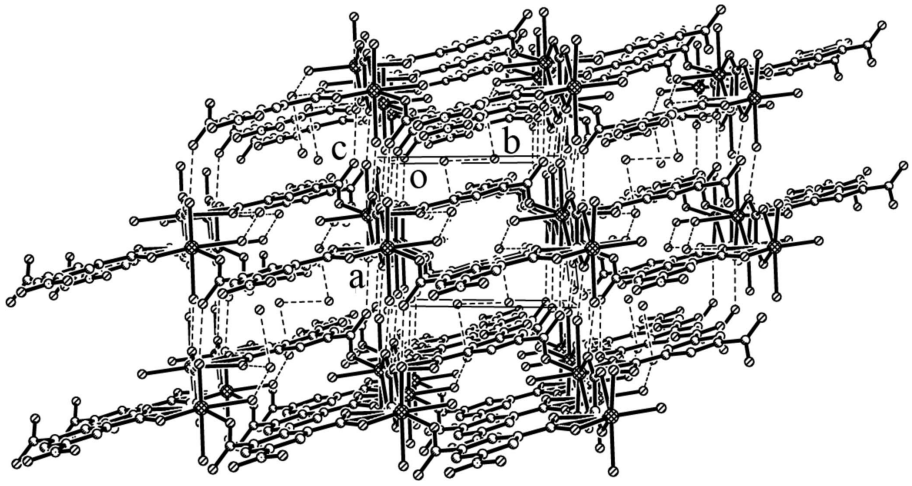

Figure 3

A packing diagram of the title compound viewed down the *c* axis. All hydrogen atoms have been omitted for clarity.

poly[[hexaaquabis(*μ*-5-nitrobenzene-1,3-dicarboxylato-κ^3O,O',O'')(*μ*- oxalato-$\kappa^4O,O':O'',O'''$)diyttrium(III)] trihydrate]

Crystal data

$[Y_2(C_8H_3NO_6)_2(C_2O_4)(H_2O)_6]\cdot 3H_2O$
M_r = 846.21
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 7.4270 (15) Å
b = 9.2070 (18) Å
c = 11.522 (2) Å
α = 74.16 (3)°
β = 71.76 (3)°
γ = 80.01 (2)°
V = 716.5 (3) Å^3
Z = 1
$F(000)$ = 424
D_x = 1.961 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 25 reflections
θ = 2.3–15.0°
μ = 4.14 mm^{-1}
T = 298 K
Block, colorless
0.20 × 0.15 × 0.12 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega/2\theta$ scans
Absorption correction: ψ scan (*XCAD4*; Harms & Wocadlo, 1995)
T_{min} = 0.48, T_{max} = 0.60

3018 measured reflections
2785 independent reflections
2260 reflections with $I > 2\sigma(I)$
$R_{int} = 0.097$
$\theta_{max} = 26.0°$, $\theta_{min} = 1.9°$
$h = 0 \rightarrow 9$
$k = -11 \rightarrow 11$
$l = -13 \rightarrow 14$
3 standard reflections every 200 reflections
intensity decay: 1.0%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.112$
$S = 1.05$
2785 reflections
220 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
$w = 1/[\sigma^2(F_o^2) + (0.0432P)^2 + 2.6078P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.67$ e Å^{-3}
$\Delta\rho_{min} = -0.64$ 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}	Occ. (<1)
C1	0.3395 (7)	0.2400 (6)	0.1373 (5)	0.0176 (10)	
C2	0.2913 (7)	0.3978 (6)	0.0685 (5)	0.0182 (10)	
C3	0.2644 (7)	0.4243 (6)	−0.0506 (5)	0.0200 (11)	
H3	0.2853	0.3461	−0.0909	0.024*	
C4	0.2095 (7)	0.5698 (6)	−0.1067 (5)	0.0188 (10)	
C5	0.1769 (7)	0.6925 (6)	−0.0509 (5)	0.0187 (10)	
H5	0.1321	0.7878	−0.0904	0.022*	
C6	0.2101 (7)	0.6653 (6)	0.0648 (5)	0.0181 (10)	
C7	0.2687 (7)	0.5187 (6)	0.1238 (5)	0.0201 (11)	
H7	0.2862	0.4994	0.2030	0.024*	
C8	0.1873 (7)	0.7916 (6)	0.1298 (5)	0.0187 (10)	
C9	0.6051 (7)	−0.0058 (6)	0.4632 (5)	0.0177 (10)	
N1	0.1769 (7)	0.5962 (5)	−0.2319 (4)	0.0265 (10)	
O1	0.3821 (6)	0.2183 (4)	0.2395 (3)	0.0261 (9)	
O2	0.3332 (5)	0.1288 (4)	0.0962 (3)	0.0228 (8)	
O3	0.3182 (5)	0.7902 (4)	0.1793 (3)	0.0223 (8)	
O4	0.0460 (5)	0.8849 (4)	0.1325 (4)	0.0251 (8)	
O5	0.1269 (9)	0.7245 (5)	−0.2819 (5)	0.0564 (15)	
O6	0.1979 (8)	0.4894 (5)	−0.2778 (4)	0.0461 (12)	
O7	0.7221 (5)	0.0136 (4)	0.5150 (3)	0.0214 (8)	

O8	0.6444 (5)	−0.0325 (4)	0.3571 (3)	0.0232 (8)	
O9	0.6774 (5)	−0.0796 (4)	0.1250 (3)	0.0244 (8)	
H9A	0.6641	−0.0316	0.0534	0.029*	
H9B	0.7642	−0.0428	0.1386	0.029*	
O10	0.4350 (6)	−0.3006 (4)	0.3988 (4)	0.0326 (10)	
H10A	0.5526	−0.3322	0.3807	0.039*	
H10B	0.3968	−0.3009	0.4765	0.039*	
O11	0.0652 (5)	−0.0383 (5)	0.3376 (4)	0.0318 (10)	
H11B	0.0191	0.0193	0.3884	0.038*	
H11A	0.0252	−0.0036	0.2728	0.038*	
O12	0.3768 (8)	0.3842 (5)	0.4156 (5)	0.0492 (13)	
H12B	0.3942	0.4764	0.3793	0.059*	
H12A	0.4299	0.3285	0.3639	0.059*	
O13	0.0067 (15)	0.3583 (14)	0.5020 (11)	0.068 (3)	0.50
H13A	0.0037	0.2670	0.5003	0.081*	0.50
H13B	−0.1035	0.3933	0.5392	0.081*	0.50
Y	0.39399 (7)	−0.05405 (6)	0.27921 (5)	0.01386 (15)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.018 (2)	0.018 (3)	0.017 (2)	−0.0018 (19)	−0.005 (2)	−0.004 (2)
C2	0.019 (3)	0.017 (3)	0.019 (3)	−0.002 (2)	−0.005 (2)	−0.005 (2)
C3	0.020 (3)	0.020 (3)	0.022 (3)	−0.002 (2)	−0.007 (2)	−0.008 (2)
C4	0.020 (3)	0.024 (3)	0.015 (2)	−0.004 (2)	−0.004 (2)	−0.007 (2)
C5	0.024 (3)	0.012 (2)	0.022 (3)	−0.002 (2)	−0.011 (2)	−0.002 (2)
C6	0.021 (3)	0.018 (3)	0.020 (3)	−0.004 (2)	−0.009 (2)	−0.006 (2)
C7	0.022 (3)	0.021 (3)	0.020 (3)	−0.002 (2)	−0.009 (2)	−0.005 (2)
C8	0.017 (2)	0.020 (3)	0.018 (2)	−0.004 (2)	−0.002 (2)	−0.006 (2)
C9	0.018 (3)	0.016 (3)	0.019 (3)	−0.0011 (19)	−0.006 (2)	−0.003 (2)
N1	0.034 (3)	0.027 (3)	0.021 (2)	−0.004 (2)	−0.013 (2)	−0.004 (2)
O1	0.044 (2)	0.0195 (19)	0.0213 (19)	−0.0005 (17)	−0.0204 (17)	−0.0047 (15)
O2	0.037 (2)	0.0142 (18)	0.0217 (19)	−0.0004 (15)	−0.0135 (16)	−0.0062 (15)
O3	0.0254 (19)	0.0190 (19)	0.033 (2)	0.0032 (15)	−0.0188 (17)	−0.0132 (16)
O4	0.0216 (19)	0.025 (2)	0.036 (2)	0.0056 (15)	−0.0149 (17)	−0.0160 (17)
O5	0.113 (5)	0.028 (3)	0.036 (3)	0.007 (3)	−0.046 (3)	0.000 (2)
O6	0.078 (4)	0.038 (3)	0.034 (2)	0.007 (2)	−0.029 (2)	−0.020 (2)
O7	0.0161 (17)	0.036 (2)	0.0171 (18)	−0.0056 (15)	−0.0082 (14)	−0.0089 (16)
O8	0.0213 (19)	0.037 (2)	0.0159 (18)	−0.0030 (16)	−0.0066 (15)	−0.0118 (16)
O9	0.0205 (19)	0.039 (2)	0.0171 (18)	−0.0029 (16)	−0.0058 (15)	−0.0124 (16)
O10	0.046 (3)	0.028 (2)	0.028 (2)	0.0010 (19)	−0.0182 (19)	−0.0061 (17)
O11	0.0196 (19)	0.057 (3)	0.028 (2)	0.0038 (18)	−0.0103 (16)	−0.027 (2)
O12	0.079 (4)	0.036 (3)	0.044 (3)	−0.008 (2)	−0.033 (3)	−0.008 (2)
O13	0.045 (6)	0.075 (8)	0.074 (8)	−0.031 (6)	−0.011 (6)	0.006 (6)
Y	0.0155 (2)	0.0154 (2)	0.0136 (2)	−0.00013 (16)	−0.00695 (17)	−0.00552 (17)

Geometric parameters (Å, º)

C1—O2	1.253 (6)	N1—O6	1.204 (6)
C1—O1	1.269 (6)	N1—O5	1.215 (6)
C1—C2	1.495 (7)	O1—Y	2.414 (4)
C1—Y	2.790 (5)	O2—Y	2.424 (4)
C2—C7	1.388 (7)	O3—Y^{ii}	2.299 (3)
C2—C3	1.398 (7)	O7—Y^{i}	2.365 (3)
C3—C4	1.372 (7)	O8—Y	2.361 (3)
C3—H3	0.9264	O9—Y	2.314 (4)
C4—C5	1.397 (7)	O9—H9A	0.8500
C4—N1	1.484 (7)	O9—H9B	0.8501
C5—C6	1.380 (7)	O10—Y	2.336 (4)
C5—H5	0.9288	O10—H10A	0.8500
C6—C7	1.398 (7)	O10—H10B	0.8501
C6—C8	1.507 (7)	O11—Y	2.311 (4)
C7—H7	0.9274	O11—H11B	0.8500
C8—O4	1.233 (6)	O11—H11A	0.8498
C8—O3	1.268 (6)	O12—H12B	0.8499
C9—O8	1.247 (6)	O12—H12A	0.8500
C9—O7	1.258 (6)	O13—H13A	0.8500
C9—C9^{i}	1.527 (9)	O13—H13B	0.8500
O2—C1—O1	119.8 (5)	H10A—O10—H10B	108.3
O2—C1—C2	120.3 (4)	Y—O11—H11B	110.1
O1—C1—C2	119.9 (4)	Y—O11—H11A	109.8
O2—C1—Y	60.2 (3)	H11B—O11—H11A	109.8
O1—C1—Y	59.8 (3)	H12B—O12—H12A	109.7
C2—C1—Y	174.6 (3)	H13A—O13—H13B	109.5
C7—C2—C3	119.5 (5)	O3^{iii}—Y—O11	74.28 (13)
C7—C2—C1	120.2 (4)	O3^{iii}—Y—O9	78.95 (13)
C3—C2—C1	120.3 (4)	O11—Y—O9	147.86 (13)
C4—C3—C2	118.1 (5)	O3^{iii}—Y—O10	74.18 (13)
C4—C3—H3	121.0	O11—Y—O10	95.62 (16)
C2—C3—H3	120.8	O9—Y—O10	93.86 (15)
C3—C4—C5	123.7 (5)	O3^{iii}—Y—O8	138.88 (13)
C3—C4—N1	117.7 (4)	O11—Y—O8	139.85 (13)
C5—C4—N1	118.6 (4)	O9—Y—O8	72.16 (12)
C6—C5—C4	117.4 (5)	O10—Y—O8	79.18 (14)
C6—C5—H5	122.0	O3^{iii}—Y—O7^{i}	133.63 (13)
C4—C5—H5	120.5	O11—Y—O7^{i}	71.41 (12)
C5—C6—C7	120.3 (5)	O9—Y—O7^{i}	140.67 (12)
C5—C6—C8	121.3 (5)	O10—Y—O7^{i}	79.12 (14)
C7—C6—C8	118.4 (4)	O8—Y—O7^{i}	68.51 (12)
C2—C7—C6	120.9 (5)	O3^{iii}—Y—O1	132.35 (12)
C2—C7—H7	118.6	O11—Y—O1	90.19 (15)
C6—C7—H7	120.4	O9—Y—O1	94.96 (14)
O4—C8—O3	125.6 (5)	O10—Y—O1	153.26 (13)

O4—C8—C6	119.0 (4)	O8—Y—O1	79.61 (13)
O3—C8—C6	115.4 (4)	O7^{i}—Y—O1	78.08 (13)
O8—C9—O7	126.2 (4)	O3^{iii}—Y—O2	79.18 (12)
O8—C9—C9^{i}	117.0 (5)	O11—Y—O2	80.27 (14)
O7—C9—C9^{i}	116.8 (5)	O9—Y—O2	77.50 (13)
O6—N1—O5	123.2 (5)	O10—Y—O2	153.13 (13)
O6—N1—C4	118.6 (5)	O8—Y—O2	120.73 (13)
O5—N1—C4	118.2 (5)	O7^{i}—Y—O2	123.38 (13)
C1—O1—Y	93.2 (3)	O1—Y—O2	53.60 (12)
C1—O2—Y	93.2 (3)	O3^{iii}—Y—C1	105.48 (14)
C8—O3—Y^{ii}	136.0 (3)	O11—Y—C1	83.57 (15)
C9—O7—Y^{i}	118.6 (3)	O9—Y—C1	86.78 (14)
C9—O8—Y	119.0 (3)	O10—Y—C1	179.19 (14)
Y—O9—H9A	109.9	O8—Y—C1	101.50 (14)
Y—O9—H9B	109.8	O7^{i}—Y—C1	100.69 (14)
H9A—O9—H9B	108.4	O1—Y—C1	27.01 (13)
Y—O10—H10A	109.3	O2—Y—C1	26.64 (13)
Y—O10—H10B	109.8		

O2—C1—C2—C7	169.7 (5)	C9—O8—Y—O3^{iii}	−134.9 (4)
O1—C1—C2—C7	−8.3 (7)	C9—O8—Y—O11	1.1 (5)
O2—C1—C2—C3	−8.9 (7)	C9—O8—Y—O9	177.5 (4)
O1—C1—C2—C3	173.0 (5)	C9—O8—Y—O10	−84.8 (4)
C7—C2—C3—C4	−2.3 (7)	C9—O8—Y—O7^{i}	−2.3 (4)
C1—C2—C3—C4	176.3 (4)	C9—O8—Y—O1	78.8 (4)
C2—C3—C4—C5	−0.8 (8)	C9—O8—Y—O2	114.6 (4)
C2—C3—C4—N1	−178.6 (4)	C9—O8—Y—C1	94.7 (4)
C3—C4—C5—C6	2.9 (8)	C1—O1—Y—O3^{iii}	−6.7 (4)
N1—C4—C5—C6	−179.3 (4)	C1—O1—Y—O11	−75.3 (3)
C4—C5—C6—C7	−1.8 (7)	C1—O1—Y—O9	72.9 (3)
C4—C5—C6—C8	177.3 (4)	C1—O1—Y—O10	−178.3 (3)
C3—C2—C7—C6	3.3 (8)	C1—O1—Y—O8	143.7 (3)
C1—C2—C7—C6	−175.3 (4)	C1—O1—Y—O7^{i}	−146.3 (3)
C5—C6—C7—C2	−1.2 (8)	C1—O1—Y—O2	2.4 (3)
C8—C6—C7—C2	179.7 (4)	C1—O2—Y—O3^{iii}	170.8 (3)
C5—C6—C8—O4	44.6 (7)	C1—O2—Y—O11	95.1 (3)
C7—C6—C8—O4	−136.2 (5)	C1—O2—Y—O9	−108.3 (3)
C5—C6—C8—O3	−136.3 (5)	C1—O2—Y—O10	178.3 (3)
C7—C6—C8—O3	42.8 (7)	C1—O2—Y—O8	−48.1 (3)
C3—C4—N1—O6	0.8 (7)	C1—O2—Y—O7^{i}	35.1 (3)
C5—C4—N1—O6	−177.1 (5)	C1—O2—Y—O1	−2.4 (3)
C3—C4—N1—O5	179.5 (5)	O2—C1—Y—O3^{iii}	−9.4 (3)
C5—C4—N1—O5	1.5 (8)	O1—C1—Y—O3^{iii}	174.9 (3)
O2—C1—O1—Y	−4.3 (5)	O2—C1—Y—O11	−81.1 (3)
C2—C1—O1—Y	173.8 (4)	O1—C1—Y—O11	103.2 (3)
O1—C1—O2—Y	4.3 (5)	O2—C1—Y—O9	68.2 (3)
C2—C1—O2—Y	−173.8 (4)	O1—C1—Y—O9	−107.5 (3)
O4—C8—O3—Y^{ii}	−6.0 (8)	O2—C1—Y—O8	139.3 (3)

C6—C8—O3—Y^{ii}	175.0 (3)	O1—C1—Y—O8	−36.4 (3)
O8—C9—O7—Y^{i}	−177.9 (4)	O2—C1—Y—O7^{i}	−150.8 (3)
C9^{i}—C9—O7—Y^{i}	2.7 (7)	O1—C1—Y—O7^{i}	33.5 (3)
O7—C9—O8—Y	−177.5 (4)	O2—C1—Y—O1	175.7 (5)
C9^{i}—C9—O8—Y	1.9 (7)	O1—C1—Y—O2	−175.7 (5)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O9—H9*A*···O2^{iv}	0.85	2.14	2.735 (5)	127
O9—H9*B*···O4^{v}	0.85	2.07	2.726 (5)	134
O10—H10*A*···O6^{iv}	0.85	2.36	3.115 (7)	148
O10—H10*B*···O12^{i}	0.85	2.30	2.778 (6)	116
O10—H10*B*···O12^{i}	0.85	2.30	2.778 (6)	116
O11—H11*A*···O4^{iii}	0.85	2.09	2.694 (5)	127
O11—H11*B*···O5^{vi}	0.85	2.57	2.987 (6)	111
O11—H11*B*···O7^{vii}	0.85	2.23	2.784 (5)	123
O12—H12*A*···O1	0.85	2.11	2.841 (6)	144
O12—H12*B*···O10^{ii}	0.85	2.21	2.953 (6)	147
C3—H3···O9^{iv}	0.93	2.54	3.432 (6)	161

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