

Poly[tetraaquabis(μ_3 -oxalato- $\kappa^5 O^1, O^2:O^1':O^1', O^2'$)(μ_2 -oxalato- $\kappa^4 O^1, O^2:O^1', O^2'$)dipraseodymium(III)]

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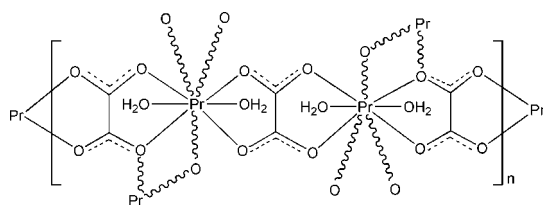
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(C-C) = 0.007$ Å; R factor = 0.029; wR factor = 0.072; data-to-parameter ratio = 14.7.

In the title complex, $[Pr_2(C_2O_4)_3(H_2O)_4]_n$, the two independent Pr^{III} ions are both nine-coordinated in a distorted monocapped square-antiprismatic geometry by seven O atoms from four oxalate ligands and two water molecules. The Pr^{III} ions are bridged by the oxalate ligands, forming a layer parallel to (001). O—H...O hydrogen bonds connect the layers.

Related literature

For the structures and potential applications of lanthanide complexes, see: Ma *et al.* (2001); Shibasaki & Yoshikawa (2002); Song *et al.* (2012).



Experimental

Crystal data

$[Pr_2(C_2O_4)_3(H_2O)_4]$ $V = 1390.4 (5) \text{ \AA}^3$
 $M_r = 617.94$ $Z = 4$
 Orthorhombic, $P2_12_12_1$ $Mo K\alpha$ radiation
 $a = 8.6358 (17) \text{ \AA}$ $\mu = 7.02 \text{ mm}^{-1}$
 $b = 9.5356 (19) \text{ \AA}$ $T = 293 \text{ K}$
 $c = 16.885 (3) \text{ \AA}$ $0.23 \times 0.22 \times 0.20 \text{ mm}$

Data collection

Rigaku Mercury CCD 13654 measured reflections
 diffractometer 3181 independent reflections
 Absorption correction: multi-scan 2826 reflections with $I > 2\sigma(I)$
 (*CrystalClear*; Rigaku, 2002) $R_{int} = 0.047$
 $T_{min} = 0.295, T_{max} = 0.334$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.029$ $\Delta\rho_{max} = 1.34 \text{ e \AA}^{-3}$
 $wR(F^2) = 0.072$ $\Delta\rho_{min} = -1.44 \text{ e \AA}^{-3}$
 $S = 1.04$ Absolute structure: Flack (1983),
 3181 reflections 1344 Friedel pairs
 217 parameters Flack parameter: 0.49 (3)
 H-atom parameters constrained

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$O1W-H1W\cdots O2^i$	0.85	2.02	2.852 (6)	166
$O1W-H2W\cdots O8^{ii}$	0.85	2.15	2.998 (6)	173
$O2W-H3W\cdots O4^{iii}$	0.85	2.40	2.998 (6)	128
$O2W-H4W\cdots O6^{iv}$	0.85	2.01	2.792 (6)	152
$O3W-H5W\cdots O12^v$	0.85	1.97	2.780 (6)	158
$O3W-H6W\cdots O3^v$	0.85	2.60	3.379 (7)	154
$O4W-H7W\cdots O1^{vi}$	0.85	2.16	2.865 (6)	140
$O4W-H8W\cdots O9^v$	0.85	2.04	2.882 (6)	169

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

Data collection: *CrystalClear* (Rigaku, 2002); cell refinement: *CrystalClear*; data reduction: *CrystalStructure* (Rigaku/MS, 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: HY2521).

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supporting information

Acta Cryst. (2012). E68, m444 [https://doi.org/10.1107/S1600536812011014]

Poly[tetraaquabis(μ_3 -oxalato- $\kappa^5 O^1, O^2:O^1':O^1', O^2'$)(μ_2 -oxalato- $\kappa^4 O^1, O^2:O^1', O^2'$)dipraseodymium(III)]

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S1. Comment

During the past decade, considerable efforts have been devoted to the design and construction of new lanthanide coordination polymers due to their intriguing structural diversity and potential applications in many areas (Ma *et al.*, 2001; Shibasaki & Yoshikawa, 2002; Song *et al.*, 2012). Oxalate owning four carboxylate O atoms is highly accessible to lanthanide ions to form novel structures.

As shown in Fig. 1, in the asymmetric unit of the title complex, there are two independent Pr^{III} ions with a similar coordination environment. Each Pr^{III} ion is nine-coordinated by seven O atoms from four oxalate ligands and two O atoms from two terminal water molecules. The Pr1 and Pr2 atoms are bridged by two carboxylate O atoms, forming a Pr₂O₂ subunit with a Pr...Pr distance of 4.2893 (7) Å. Such subunits are connected by the oxalate ligands, generating a layer parallel to (0 0 1). It is noted that the oxalate ligands exhibit two kinds of coordination modes: one adopts a bis-dentate coordination mode bridging two Pr^{III} ions; the other adopts a chelating and bridging coordination mode connecting three Pr^{III} ions. The adjacent layers are further linked into a three-dimensional network *via* intermolecular O—H...O hydrogen bonds (Table 1).

S2. Experimental

A mixture of Pr(NO₃)₃·6H₂O (0.5 mmol, 0.217 g) and oxalic acid (1 mmol, 0.09 g) in 10 ml of H₂O was sealed in an autoclave equipped with a Teflon liner (30 ml) and then heated to 453 K for 4 days. After gradual cooling to room temperature, crystals were obtained and collected by filtration with a yield of 31% based on Pr.

S3. Refinement

H atoms of water molecules were located in a difference Fourier map and refined as riding, with O—H = 0.85 Å and with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$. The highest residual electron density was found at 0.82 Å from Pr1 atom and the deepest hole at 0.80 Å from Pr2 atom.

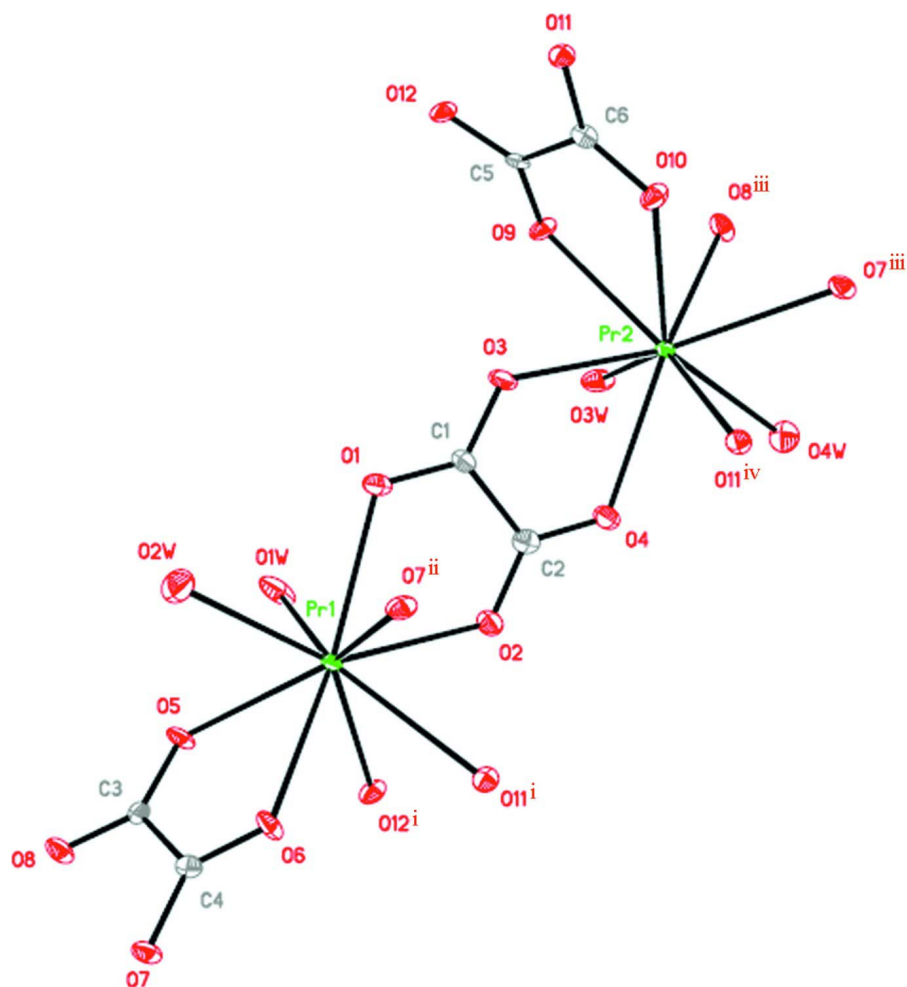


Figure 1

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

Poly[tetraaquabis(μ_3 -oxalato- $\kappa^5O^1, O^2:O^1':O^2'$)(μ_2 -oxalato- $\kappa^4O^1, O^2:O^1', O^2'$)dipraseodymium(III)]

Crystal data

$[\text{Pr}_2(\text{C}_2\text{O}_4)_3(\text{H}_2\text{O})_4]$

$M_r = 617.94$

Orthorhombic, $P2_12_12_1$

Hall symbol: P 2ac 2ab

$a = 8.6358 (17) \text{ \AA}$

$b = 9.5356 (19) \text{ \AA}$

$c = 16.885 (3) \text{ \AA}$

$V = 1390.4 (5) \text{ \AA}^3$

$Z = 4$

$F(000) = 1160$

$D_x = 2.952 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 3600 reflections

$\theta = 1.4\text{--}28.0^\circ$

$\mu = 7.02 \text{ mm}^{-1}$

$T = 293 \text{ K}$

Block, green

$0.23 \times 0.22 \times 0.20 \text{ mm}$

Data collection

Rigaku Mercury CCD
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator
 ω scans

Absorption correction: multi-scan

(CrystalClear; Rigaku, 2002) $T_{\min} = 0.295$, $T_{\max} = 0.334$

13654 measured reflections

3181 independent reflections

2826 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.047$ $\theta_{\max} = 27.4^\circ$, $\theta_{\min} = 3.2^\circ$ $h = -9 \rightarrow 11$ $k = -12 \rightarrow 12$ $l = -21 \rightarrow 21$ *Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.029$ $wR(F^2) = 0.072$ $S = 1.04$

3181 reflections

217 parameters

0 restraints

Primary atom site location: structure-invariant
direct methodsSecondary atom site location: difference Fourier
mapHydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0284P)^2 + 3.201P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} = 0.001$ $\Delta\rho_{\max} = 1.34 \text{ e } \text{\AA}^{-3}$ $\Delta\rho_{\min} = -1.44 \text{ e } \text{\AA}^{-3}$ Absolute structure: Flack (1983), 1344 Friedel
pairs

Absolute structure parameter: 0.49 (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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Pr1	0.37510 (4)	0.75389 (2)	0.143154 (14)	0.01214 (9)
Pr2	-0.12589 (4)	0.26126 (3)	0.137142 (14)	0.01185 (8)
O1	0.3263 (5)	0.4984 (4)	0.1336 (3)	0.0245 (10)
O2	0.1023 (5)	0.6852 (4)	0.1081 (2)	0.0220 (9)
O3	0.1479 (5)	0.3304 (5)	0.1473 (3)	0.0383 (12)
O4	-0.0761 (5)	0.5159 (5)	0.1102 (3)	0.0236 (10)
O5	0.5734 (5)	0.8913 (4)	0.0744 (2)	0.0220 (9)
O6	0.4832 (5)	0.9677 (5)	0.2184 (2)	0.0221 (9)
O7	0.6490 (5)	1.1490 (4)	0.2172 (2)	0.0209 (9)
O8	0.7467 (5)	1.0643 (5)	0.0716 (3)	0.0255 (10)
O9	0.0572 (5)	0.0999 (5)	0.0683 (2)	0.0205 (9)
O10	-0.0198 (5)	0.0560 (4)	0.2191 (2)	0.0230 (9)
O11	0.1596 (4)	-0.1155 (4)	0.2289 (2)	0.0186 (9)
O12	0.2521 (5)	-0.0484 (4)	0.0791 (2)	0.0219 (9)
O1W	0.4097 (7)	0.6778 (5)	0.0052 (2)	0.0361 (14)
H1W	0.4747	0.7253	-0.0215	0.054*
H2W	0.3561	0.6140	-0.0168	0.054*

O2W	0.6418 (6)	0.6597 (5)	0.1743 (3)	0.0357 (11)
H3W	0.7010	0.6599	0.1341	0.053*
H4W	0.6369	0.5950	0.2088	0.053*
O3W	-0.1196 (7)	0.3125 (5)	-0.0081 (2)	0.0296 (10)
H5W	-0.1447	0.3960	-0.0200	0.044*
H6W	-0.1567	0.2530	-0.0404	0.044*
O4W	-0.3828 (6)	0.3679 (5)	0.0986 (2)	0.0303 (10)
H7W	-0.4443	0.4093	0.1304	0.045*
H8W	-0.4120	0.3834	0.0513	0.045*
C1	0.1907 (7)	0.4536 (6)	0.1341 (4)	0.0214 (13)
C2	0.0597 (7)	0.5610 (6)	0.1160 (3)	0.0196 (12)
C3	0.6393 (7)	0.9949 (6)	0.1035 (3)	0.0160 (12)
C4	0.5861 (6)	1.0398 (6)	0.1870 (3)	0.0169 (12)
C5	0.1355 (7)	0.0127 (5)	0.1057 (3)	0.0164 (11)
C6	0.0863 (6)	-0.0190 (6)	0.1925 (3)	0.0166 (12)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pr1	0.01379 (15)	0.00894 (14)	0.01370 (14)	-0.00143 (13)	0.00092 (11)	0.00098 (9)
Pr2	0.01324 (15)	0.00861 (13)	0.01371 (14)	-0.00137 (13)	0.00076 (12)	-0.00112 (9)
O1	0.025 (2)	0.013 (2)	0.035 (2)	-0.0023 (16)	-0.001 (2)	0.0004 (18)
O2	0.019 (2)	0.019 (2)	0.028 (2)	-0.0007 (18)	-0.0038 (19)	0.0043 (16)
O3	0.018 (2)	0.0103 (19)	0.086 (4)	-0.0033 (18)	-0.005 (2)	0.009 (2)
O4	0.022 (2)	0.018 (2)	0.031 (2)	-0.0029 (16)	-0.0023 (19)	0.0017 (18)
O5	0.030 (2)	0.015 (2)	0.020 (2)	-0.0103 (17)	0.0063 (18)	-0.0088 (17)
O6	0.025 (2)	0.025 (2)	0.0165 (18)	-0.0139 (18)	0.0081 (18)	-0.0051 (18)
O7	0.028 (2)	0.0162 (19)	0.0188 (18)	-0.0058 (17)	0.0033 (19)	-0.0052 (15)
O8	0.030 (2)	0.022 (3)	0.024 (2)	-0.0126 (19)	0.010 (2)	-0.0098 (19)
O9	0.025 (2)	0.020 (2)	0.0162 (19)	0.0110 (18)	0.0016 (18)	0.0036 (17)
O10	0.027 (2)	0.024 (2)	0.019 (2)	0.0093 (18)	0.0056 (19)	0.0051 (19)
O11	0.021 (2)	0.019 (2)	0.0155 (18)	0.0023 (16)	-0.0005 (17)	0.0045 (15)
O12	0.027 (2)	0.017 (2)	0.022 (2)	0.0088 (18)	0.0093 (18)	0.0092 (18)
O1W	0.056 (4)	0.027 (3)	0.025 (2)	-0.023 (2)	0.016 (2)	-0.0094 (17)
O2W	0.030 (3)	0.030 (3)	0.046 (3)	0.008 (2)	0.003 (3)	0.006 (2)
O3W	0.046 (3)	0.020 (2)	0.024 (2)	0.007 (3)	0.002 (2)	0.0062 (15)
O4W	0.027 (2)	0.038 (3)	0.027 (2)	0.008 (2)	-0.001 (2)	0.0004 (17)
C1	0.022 (3)	0.013 (3)	0.029 (3)	-0.003 (2)	0.002 (3)	0.000 (3)
C2	0.027 (3)	0.018 (3)	0.014 (3)	-0.001 (2)	0.000 (2)	-0.001 (2)
C3	0.016 (3)	0.015 (3)	0.017 (3)	0.002 (3)	0.004 (3)	-0.0010 (18)
C4	0.021 (3)	0.014 (3)	0.015 (3)	-0.001 (2)	-0.001 (2)	-0.002 (2)
C5	0.022 (3)	0.009 (3)	0.018 (3)	0.000 (3)	0.000 (3)	0.0023 (18)
C6	0.020 (3)	0.016 (3)	0.014 (2)	-0.001 (2)	-0.002 (2)	0.002 (2)

Geometric parameters (Å, °)

Pr1—O12 ⁱ	2.419 (4)	O4—C2	1.253 (7)
Pr1—O5	2.449 (4)	O5—C3	1.241 (6)

Pr1—O1W	2.458 (4)	O6—C4	1.242 (7)
Pr1—O1	2.478 (4)	O7—C4	1.281 (7)
Pr1—O2	2.516 (4)	O8—C3	1.261 (7)
Pr1—O2W	2.527 (5)	O9—C5	1.244 (7)
Pr1—O7 ⁱⁱ	2.570 (4)	O10—C6	1.247 (7)
Pr1—O6	2.578 (4)	O11—C6	1.275 (7)
Pr1—O11 ⁱ	2.666 (4)	O12—C5	1.247 (7)
Pr2—O8 ⁱⁱⁱ	2.442 (4)	O1W—H1W	0.8500
Pr2—O3	2.460 (4)	O1W—H2W	0.8501
Pr2—O9	2.494 (4)	O2W—H3W	0.8500
Pr2—O3W	2.501 (4)	O2W—H4W	0.8500
Pr2—O4	2.508 (4)	O3W—H5W	0.8500
Pr2—O4W	2.526 (5)	O3W—H6W	0.8499
Pr2—O11 ^{iv}	2.565 (4)	O4W—H7W	0.8511
Pr2—O10	2.566 (4)	O4W—H8W	0.8513
Pr2—O7 ⁱⁱⁱ	2.598 (4)	C1—C2	1.556 (9)
O1—C1	1.247 (7)	C3—C4	1.544 (7)
O2—C2	1.247 (7)	C5—C6	1.555 (8)
O3—C1	1.252 (7)		
O12 ⁱ —Pr1—O5	71.23 (15)	O9—Pr2—O10	63.55 (13)
O12 ⁱ —Pr1—O1W	81.93 (16)	O3W—Pr2—O10	132.08 (14)
O5—Pr1—O1W	67.89 (15)	O4—Pr2—O10	140.82 (14)
O12 ⁱ —Pr1—O1	131.49 (15)	O4W—Pr2—O10	139.42 (14)
O5—Pr1—O1	127.89 (14)	O11 ^{iv} —Pr2—O10	85.07 (13)
O1W—Pr1—O1	70.66 (15)	O8 ⁱⁱⁱ —Pr2—O7 ⁱⁱⁱ	65.29 (13)
O12 ⁱ —Pr1—O2	71.72 (14)	O3—Pr2—O7 ⁱⁱⁱ	142.48 (15)
O5—Pr1—O2	133.05 (13)	O9—Pr2—O7 ⁱⁱⁱ	117.55 (13)
O1W—Pr1—O2	79.30 (16)	O3W—Pr2—O7 ⁱⁱⁱ	127.34 (15)
O1—Pr1—O2	64.51 (14)	O4—Pr2—O7 ⁱⁱⁱ	128.43 (13)
O12 ⁱ —Pr1—O2W	140.37 (15)	O4W—Pr2—O7 ⁱⁱⁱ	69.05 (14)
O5—Pr1—O2W	69.61 (15)	O11 ^{iv} —Pr2—O7 ⁱⁱⁱ	69.21 (11)
O1W—Pr1—O2W	88.94 (17)	O10—Pr2—O7 ⁱⁱⁱ	70.88 (13)
O1—Pr1—O2W	79.57 (15)	C1—O1—Pr1	119.7 (4)
O2—Pr1—O2W	144.08 (15)	C2—O2—Pr1	119.9 (4)
O12 ⁱ —Pr1—O7 ⁱⁱ	132.68 (13)	C1—O3—Pr2	121.5 (4)
O5—Pr1—O7 ⁱⁱ	134.42 (14)	C2—O4—Pr2	118.6 (4)
O1W—Pr1—O7 ⁱⁱ	139.87 (15)	C3—O5—Pr1	123.9 (4)
O1—Pr1—O7 ⁱⁱ	70.32 (14)	C4—O6—Pr1	119.1 (3)
O2—Pr1—O7 ⁱⁱ	92.21 (13)	C4—O7—Pr1 ^v	130.3 (3)
O2W—Pr1—O7 ⁱⁱ	75.20 (14)	C4—O7—Pr2 ^{vi}	116.5 (3)
O12 ⁱ —Pr1—O6	76.29 (15)	Pr1 ^v —O7—Pr2 ^{vi}	112.19 (14)
O5—Pr1—O6	63.73 (12)	C3—O8—Pr2 ^{vi}	122.8 (3)
O1W—Pr1—O6	131.05 (14)	C5—O9—Pr2	121.3 (4)
O1—Pr1—O6	150.63 (14)	C6—O10—Pr2	120.4 (3)
O2—Pr1—O6	131.37 (13)	C6—O11—Pr2 ^{vii}	134.4 (3)
O2W—Pr1—O6	81.29 (14)	C6—O11—Pr1 ^{viii}	114.9 (3)
O7 ⁱⁱ —Pr1—O6	83.38 (13)	Pr2 ^{vii} —O11—Pr1 ^{viii}	110.13 (14)

O12 ⁱ —Pr1—O11 ⁱ	64.69 (12)	C5—O12—Pr1 ^{viii}	123.9 (3)
O5—Pr1—O11 ⁱ	119.72 (13)	Pr1—O1W—H1W	115.2
O1W—Pr1—O11 ⁱ	137.50 (16)	Pr1—O1W—H2W	124.0
O1—Pr1—O11 ⁱ	112.07 (13)	H1W—O1W—H2W	120.6
O2—Pr1—O11 ⁱ	66.14 (12)	Pr1—O2W—H3W	112.4
O2W—Pr1—O11 ⁱ	133.55 (12)	Pr1—O2W—H4W	110.8
O7 ⁱⁱ —Pr1—O11 ⁱ	68.09 (12)	H3W—O2W—H4W	125.4
O6—Pr1—O11 ⁱ	67.40 (12)	Pr2—O3W—H5W	114.3
O8 ⁱⁱⁱ —Pr2—O3	132.12 (15)	Pr2—O3W—H6W	119.4
O8 ⁱⁱⁱ —Pr2—O9	66.40 (15)	H5W—O3W—H6W	112.1
O3—Pr2—O9	65.72 (15)	Pr2—O4W—H7W	124.9
O8 ⁱⁱⁱ —Pr2—O3W	73.46 (15)	Pr2—O4W—H8W	124.9
O3—Pr2—O3W	89.72 (18)	H7W—O4W—H8W	109.1
O9—Pr2—O3W	69.50 (14)	O1—C1—O3	126.9 (6)
O8 ⁱⁱⁱ —Pr2—O4	137.69 (15)	O1—C1—C2	117.2 (5)
O3—Pr2—O4	65.69 (14)	O3—C1—C2	116.0 (5)
O9—Pr2—O4	113.85 (14)	O2—C2—O4	126.4 (6)
O3W—Pr2—O4	68.22 (15)	O2—C2—C1	115.6 (5)
O8 ⁱⁱⁱ —Pr2—O4W	78.30 (16)	O4—C2—C1	118.0 (5)
O3—Pr2—O4W	138.94 (15)	O5—C3—O8	125.9 (5)
O9—Pr2—O4W	133.26 (13)	O5—C3—C4	116.5 (5)
O3W—Pr2—O4W	71.82 (15)	O8—C3—C4	117.6 (5)
O4—Pr2—O4W	73.38 (14)	O6—C4—O7	125.7 (5)
O8 ⁱⁱⁱ —Pr2—O11 ^{iv}	134.49 (13)	O6—C4—C3	116.7 (5)
O3—Pr2—O11 ^{iv}	85.69 (15)	O7—C4—C3	117.6 (5)
O9—Pr2—O11 ^{iv}	139.96 (13)	O9—C5—O12	124.6 (5)
O3W—Pr2—O11 ^{iv}	141.03 (13)	O9—C5—C6	117.4 (5)
O4—Pr2—O11 ^{iv}	74.70 (14)	O12—C5—C6	118.0 (5)
O4W—Pr2—O11 ^{iv}	86.72 (13)	O10—C6—O11	127.2 (5)
O8 ⁱⁱⁱ —Pr2—O10	79.57 (15)	O10—C6—C5	115.4 (5)
O3—Pr2—O10	79.85 (14)	O11—C6—C5	117.3 (5)
O12 ⁱ —Pr1—O1—C1	-43.6 (5)	O4W—Pr2—O9—C5	-146.9 (4)
O5—Pr1—O1—C1	-141.8 (4)	O11 ^{iv} —Pr2—O9—C5	29.4 (5)
O1W—Pr1—O1—C1	-103.0 (5)	O10—Pr2—O9—C5	-12.7 (4)
O2—Pr1—O1—C1	-15.9 (4)	O7 ⁱⁱⁱ —Pr2—O9—C5	-60.5 (5)
O2W—Pr1—O1—C1	164.5 (5)	O8 ⁱⁱⁱ —Pr2—O10—C6	77.6 (4)
O7 ⁱⁱ —Pr1—O1—C1	86.6 (5)	O3—Pr2—O10—C6	-58.9 (4)
O6—Pr1—O1—C1	114.3 (5)	O9—Pr2—O10—C6	8.9 (4)
O11 ⁱ —Pr1—O1—C1	31.5 (5)	O3W—Pr2—O10—C6	21.4 (5)
O12 ⁱ —Pr1—O2—C2	171.5 (4)	O4—Pr2—O10—C6	-87.1 (5)
O5—Pr1—O2—C2	132.1 (4)	O4W—Pr2—O10—C6	135.4 (4)
O1W—Pr1—O2—C2	86.6 (4)	O11 ^{iv} —Pr2—O10—C6	-145.4 (4)
O1—Pr1—O2—C2	13.0 (4)	O7 ⁱⁱⁱ —Pr2—O10—C6	144.9 (5)
O2W—Pr1—O2—C2	13.6 (5)	Pr1—O1—C1—O3	-163.0 (6)
O7 ⁱⁱ —Pr1—O2—C2	-53.9 (4)	Pr1—O1—C1—C2	17.5 (7)
O6—Pr1—O2—C2	-137.1 (4)	Pr2—O3—C1—O1	-176.1 (5)
O11 ⁱ —Pr1—O2—C2	-118.8 (4)	Pr2—O3—C1—C2	3.5 (8)

O8 ⁱⁱⁱ —Pr2—O3—C1	132.1 (5)	Pr1—O2—C2—O4	170.7 (5)
O9—Pr2—O3—C1	132.4 (6)	Pr1—O2—C2—C1	-9.8 (7)
O3W—Pr2—O3—C1	64.9 (5)	Pr2—O4—C2—O2	-176.5 (5)
O4—Pr2—O3—C1	-1.2 (5)	Pr2—O4—C2—C1	4.0 (7)
O4W—Pr2—O3—C1	3.6 (6)	O1—C1—C2—O2	-5.0 (8)
O11 ^{iv} —Pr2—O3—C1	-76.4 (5)	O3—C1—C2—O2	175.4 (6)
O10—Pr2—O3—C1	-162.1 (5)	O1—C1—C2—O4	174.6 (5)
O7 ⁱⁱⁱ —Pr2—O3—C1	-123.3 (5)	O3—C1—C2—O4	-5.0 (9)
O8 ⁱⁱⁱ —Pr2—O4—C2	-128.4 (4)	Pr1—O5—C3—O8	176.5 (5)
O3—Pr2—O4—C2	-1.8 (4)	Pr1—O5—C3—C4	-2.1 (7)
O9—Pr2—O4—C2	-47.9 (5)	Pr2 ^{vi} —O8—C3—O5	-177.6 (5)
O3W—Pr2—O4—C2	-101.8 (5)	Pr2 ^{vi} —O8—C3—C4	1.0 (7)
O4W—Pr2—O4—C2	-178.4 (5)	Pr1—O6—C4—O7	179.3 (4)
O11 ^{iv} —Pr2—O4—C2	90.4 (4)	Pr1—O6—C4—C3	0.9 (6)
O10—Pr2—O4—C2	28.9 (5)	Pr1 ^v —O7—C4—O6	8.5 (9)
O7 ⁱⁱⁱ —Pr2—O4—C2	137.0 (4)	Pr2 ^{vi} —O7—C4—O6	175.9 (5)
O12 ⁱ —Pr1—O5—C3	85.5 (5)	Pr1 ^v —O7—C4—C3	-173.1 (3)
O1W—Pr1—O5—C3	174.2 (5)	Pr2 ^{vi} —O7—C4—C3	-5.7 (6)
O1—Pr1—O5—C3	-146.1 (4)	O5—C3—C4—O6	0.7 (8)
O2—Pr1—O5—C3	125.0 (4)	O8—C3—C4—O6	-178.0 (6)
O2W—Pr1—O5—C3	-88.3 (5)	O5—C3—C4—O7	-177.8 (6)
O7 ⁱⁱ —Pr1—O5—C3	-46.6 (5)	O8—C3—C4—O7	3.4 (8)
O6—Pr1—O5—C3	1.8 (4)	Pr2—O9—C5—O12	-163.2 (4)
O11 ⁱ —Pr1—O5—C3	41.0 (5)	Pr2—O9—C5—C6	15.3 (7)
O12 ⁱ —Pr1—O6—C4	-76.9 (4)	Pr1 ^{viii} —O12—C5—O9	-168.6 (4)
O5—Pr1—O6—C4	-1.3 (4)	Pr1 ^{viii} —O12—C5—C6	12.9 (7)
O1W—Pr1—O6—C4	-10.7 (5)	Pr2—O10—C6—O11	173.1 (4)
O1—Pr1—O6—C4	120.0 (4)	Pr2—O10—C6—C5	-5.4 (7)
O2—Pr1—O6—C4	-126.7 (4)	Pr2 ^{vii} —O11—C6—O10	9.0 (9)
O2W—Pr1—O6—C4	70.2 (4)	Pr1 ^{viii} —O11—C6—O10	179.4 (5)
O7 ⁱⁱ —Pr1—O6—C4	146.1 (4)	Pr2 ^{vii} —O11—C6—C5	-172.6 (3)
O11 ⁱ —Pr1—O6—C4	-144.9 (4)	Pr1 ^{viii} —O11—C6—C5	-2.2 (6)
O8 ⁱⁱⁱ —Pr2—O9—C5	-102.6 (5)	O9—C5—C6—O10	-6.3 (8)
O3—Pr2—O9—C5	77.7 (4)	O12—C5—C6—O10	172.3 (5)
O3W—Pr2—O9—C5	177.1 (5)	O9—C5—C6—O11	175.1 (5)
O4—Pr2—O9—C5	123.9 (4)	O12—C5—C6—O11	-6.4 (8)

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1W—H1W \cdots O2 ^{ix}	0.85	2.02	2.852 (6)	166
O1W—H2W \cdots O8 ^x	0.85	2.15	2.998 (6)	173
O2W—H3W \cdots O4 ^{xi}	0.85	2.40	2.998 (6)	128
O2W—H4W \cdots O6 ⁱⁱ	0.85	2.01	2.792 (6)	152
O3W—H5W \cdots O12 ^{xii}	0.85	1.97	2.780 (6)	158
O3W—H6W \cdots O3 ^{xii}	0.85	2.60	3.379 (7)	154

O4W—H7W···O1 ^{xiii}	0.85	2.16	2.865 (6)	140
O4W—H8W···O9 ^{xii}	0.85	2.04	2.882 (6)	169

Symmetry codes: (ii) $-x+1, y-1/2, -z+1/2$; (ix) $x+1/2, -y+3/2, -z$; (x) $x-1/2, -y+3/2, -z$; (xi) $x+1, y, z$; (xii) $x-1/2, -y+1/2, -z$; (xiii) $x-1, y, z$.