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Poly[[diaquahemi-μ_4-oxalato-μ_2-oxalato-praseodymium(III)] monohydrate]

Ting-Hai Yang,* Qiang Chen, Wei Zhuang, Zhe Wang and Bang-Yi Yue

High-Tech Institute of Nanjing University, Changzhou 213164, People's Republic of China
Correspondence e-mail: tinghaiyang@gmail.com

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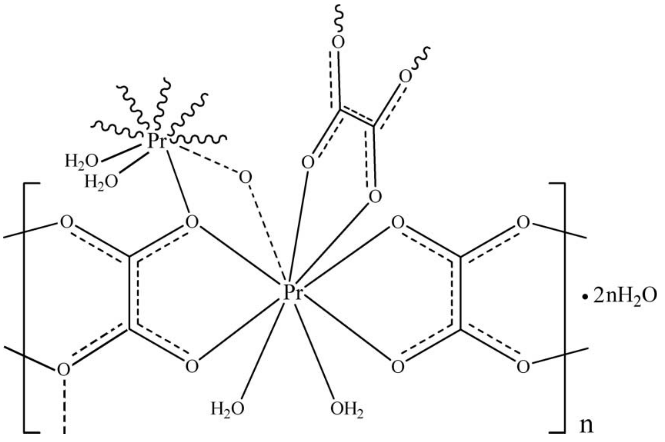
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.008 Å; R factor = 0.029; wR factor = 0.075; data-to-parameter ratio = 12.9.

In the title complex, $\{[Pr(C_2O_4)_{1.5}(H_2O)_2]\cdot H_2O\}_n$, the Pr^{III} ion, which lies on a crystallographic inversion centre, is coordinated by seven O atoms from four oxalate ligands and two O atoms from two water ligands; further Pr—O coordination from tetradentate oxalate ligands forms a three-dimensional structure. The compound crystallized as a monohydrate, the water molecule occupying space in small voids and being secured by O—H···O hydrogen bonding as an acceptor from ligand water H atoms and as a donor to oxalate O-acceptor sites.

Related literature

For background to lanthanide oxalates and their preparation, see: Hansson (1970, 1972, 1973*a*, 1973*b*); Michaelides *et al.* (1988); Ollendorf & Weigel (1969); Steinfink & Brunton (1970); Trollet *et al.* (1998); Trombe (2003); Unaleroglu *et al.* (1997). For related structures, see: Trombe *et al.* (2004); Barrett Adams *et al.* (1998); Beagley *et al.* (1988).



Experimental

Crystal data

$[Pr(C_2O_4)_{1.5}(H_2O)_2]\cdot H_2O$
M_r = 326.99
Triclinic, $P\overline{1}$
a = 6.0367 (12) Å
b = 7.6222 (15) Å
c = 8.9353 (18) Å
α = 98.330 (4)°
β = 99.814 (3)°
γ = 96.734 (4)°
V = 396.58 (14) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 6.17 mm^{-1}
T = 273 K
0.18 × 0.16 × 0.10 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.341, T_{max} = 0.542
2140 measured reflections
1521 independent reflections
1450 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.075
S = 1.00
1521 reflections
118 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.80 e Å^{-3}
$\Delta\rho_{min}$ = −1.50 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2W—H2WB···O1W	0.84	2.55	2.858 (7)	103
O1W—H1WA···O2^{i}	0.84	1.96	2.694 (6)	146
O1W—H1WA···O3^{ii}	0.84	2.60	3.235 (6)	133
O1W—H1WB···O3W^{iii}	0.84	2.00	2.833 (6)	169
O2W—H2WA···O3W^{iv}	0.84	1.98	2.807 (7)	166
O2W—H2WB···O3^{v}	0.84	2.20	2.919 (6)	144
O3W—H3WA···O6^{vi}	0.84	2.08	2.829 (7)	149
O3W—H3WB···O4^{vii}	0.84	2.03	2.833 (6)	159

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

Data collection: *SMART* (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: *SHELXTL* (Sheldrick, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NK2001).

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Poly[[diaquahemi-μ_4-oxalato-μ_2-oxalato-praseodymium(III)] monohydrate]

Ting-Hai Yang, Qiang Chen, Wei Zhuang, Zhe Wang and Bang-Yi Yue

S1. Comment

In the last decade considerable attention has been afforded to the structures and properties of lanthanide oxalates due to their ability to act as precursors of lanthanide oxides. Some single crystals of lanthanide oxalates, such as[Ln(C_2O_4)$_3$(H_2O)$_4$].(H_2O) (Ln = Sc or Yb), [Ln_2(C_2O_4)$_3$(H_2O)$_6$].4H_2O (Ln = La, Ce, Pr or Nd) and [Nd_2(C_2O_4)$_3$(H_2O)$_6$] have been obtained either in silica gel (Ollendorff & Weigel, 1969), by hydrothermal reaction (Michaelides *et al.*, 1988) or by other methods (Hansson, 1970, 1972, 1973*a*,b; Unaleroglu *et al.*, 1997; Trollet *et al.*, 1998; Trombe, 2003). Crystals of [Ln(C_2O_4)(HC_2O_4)].4H_2O (Ln = Er or Tm) were prepared by saturating a boiling solution of oxalic acid in 3 *M* H_2SO_4 with the lanthanide oxide and then slowly cooling to 273 K (Steinfink & Brunton, 1970). However, a few praseodymium oxalate complex has been reported. The present paper is concerned with a new crystal structure of praseodymium oxalate complex with a three-dimensional network structure.

The asymmetric unit of the title compound, [Pr(C_2O_4)$_{1.5}$(H_2O)$_2$].(H_2O), (I), is shown in Fig. 1. The Pr atom lies on an inversion centre and is coordinated by seven O atoms [O1, O1^{iv}, O2^{ii}, O3, O4^{iii}, O5 and O6^{i}] from four oxlate ligands, and two O atoms from two aqua ligands, thereby forming a slightly distorted PrO_9 polyhedral coordination geometry. The Pr—O bond distances range from 2.451 (4) Å to 2.608 (3) Å, in agreement with those in compounds (Trombe *et al.* (2004); Barrett Adams *et al.* (1998)).

In the complex, the equivalent Pr atom are connected is coordinated by seven O atoms from four oxalate ligands and two O atoms from water ligands. Further Pr–O coordination from the tetradentate oxalate ligands forms a three-dimensional structure (Fig.2). The compound crystallized as a monohydrate; this water molecule occupies space in small voids and is secured by O–H···O hydrogen bonding as an acceptor from ligand water H-atoms and as a donor to oxalate O acceptor sites.

S2. Experimental

All solvents and chemicals were of analytical grade and were used without further purification. $Pr(NO_3)_3 \cdot 6H_2O$ (0.05 mmol, 0.023 g), $Na_2C_2O_4$(0.075 mmol, 0.011 g), and deionized water (10 ml) were mixed together. The mixture was sealed in a Teflon-line autoclave and then heated at 443 K for 5 d under autogenous pressure and then cooled to room temperature. Green crystals were obtained.

S3. Refinement

All non-hydrogen atoms were refined anisotropically. The water H atoms were located in a difference Fourier map and refined with a distance restraint of O-H = 0.83-0.85 Å, and with $U_{iso}(H) = 1.5U_{iso}(O)$.

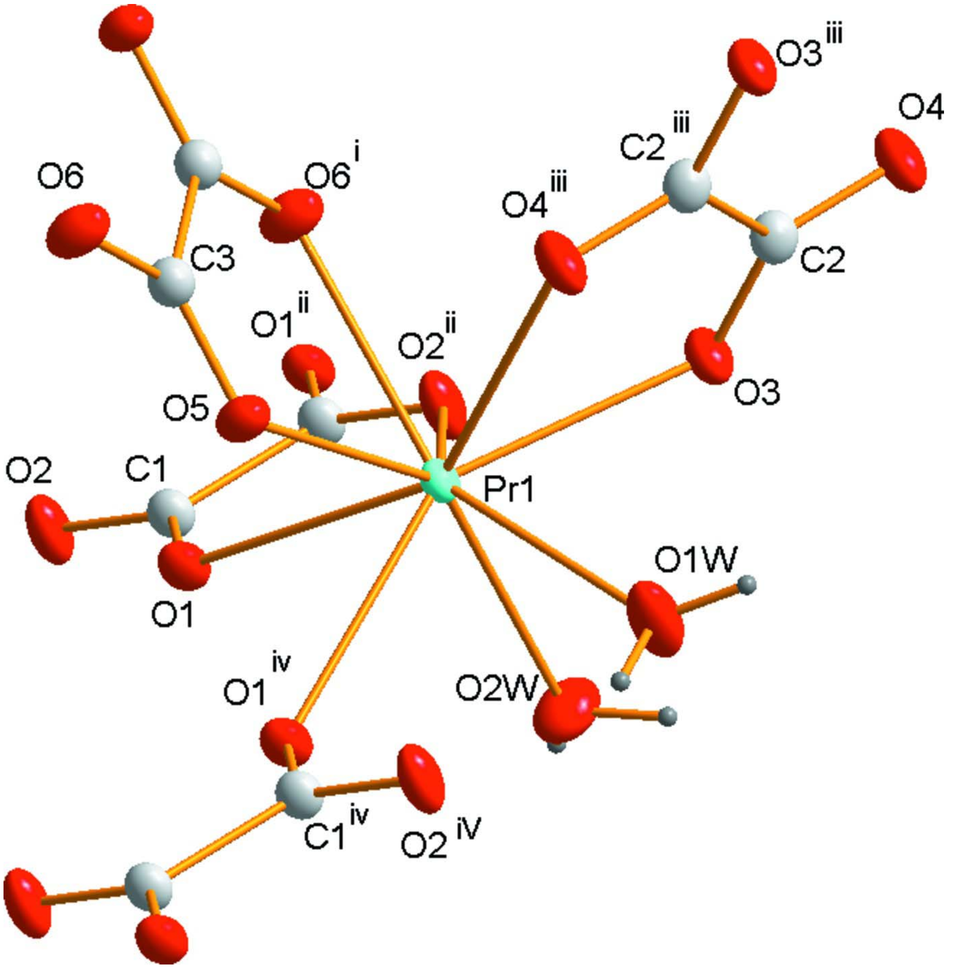

Figure 1

Molecular structure of (I), showing 50% probability displacement ellipsoids. [symmetry codes:(i) -*x* + 2,-*y* + 1,-*z* + 1; (ii) -*x* + 3,-*y* + 2,-*z* + 1; (iii) -*x* + 2,-*y* + 1,-*z*; (iv) -*x* + 2,-*y* + 2,-*z* + 1.

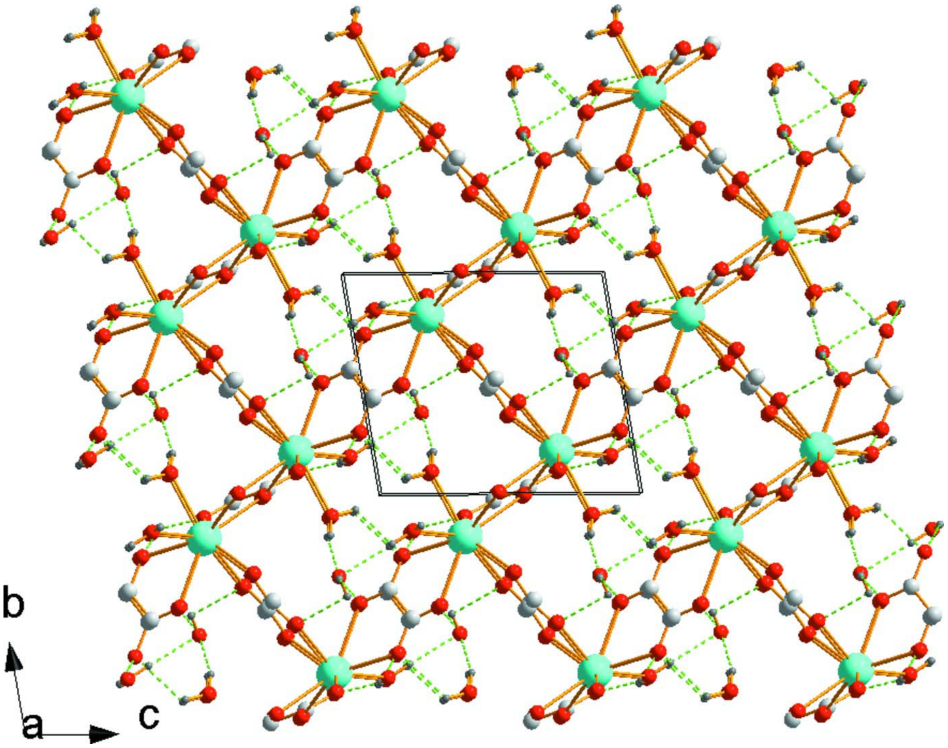

Figure 2

The unit cell packing diagram of (I).

Poly[[diaquahemi-μ_4-oxalato-μ_2-oxalato-praseodymium(III)] monohydrate]

Crystal data

$[Pr(C_2O_4)_{1.5}(H_2O)_2]\cdot H_2O$
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Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 6.0367$ (12) Å
$b = 7.6222$ (15) Å
$c = 8.9353$ (18) Å
$\alpha = 98.330$ (4)°
$\beta = 99.814$ (3)°
$\gamma = 96.734$ (4)°
$V = 396.58$ (14) Å^3

$Z = 2$
$F(000) = 310$
$D_x = 2.738$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 905 reflections
$\theta = 3.3$–28.3°
$\mu = 6.17$ mm^{-1}
$T = 273$ K
Block, green
0.18 × 0.16 × 0.10 mm

Data collection

Bruker SMART APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min} = 0.341$, $T_{max} = 0.542$

2140 measured reflections
1521 independent reflections
1450 reflections with $I > 2\sigma(I)$
$R_{int} = 0.020$
$\theta_{max} = 26.0°$, $\theta_{min} = 2.4°$
$h = -7\rightarrow7$
$k = -9\rightarrow8$
$l = -10\rightarrow11$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.029$
$wR(F^2) = 0.075$
$S = 1.00$
1521 reflections
118 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
$w = 1/[\sigma^2(F_o^2) + (0.049P)^2 + 1.09P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.80$ e Å^{-3}
$\Delta\rho_{min} = -1.50$ 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}
Pr1	1.00780 (5)	0.80762 (4)	0.29489 (3)	0.01182 (13)
C1	1.4452 (9)	1.0278 (7)	0.5703 (6)	0.0155 (11)
C2	1.0808 (10)	0.5659 (7)	−0.0322 (7)	0.0163 (12)
C3	0.8789 (9)	0.5155 (7)	0.5109 (6)	0.0157 (11)
O1	1.2322 (6)	0.9964 (5)	0.5514 (4)	0.0156 (8)
O2	1.5785 (7)	1.1009 (6)	0.6910 (5)	0.0220 (9)
O3	1.1296 (7)	0.7232 (5)	0.0431 (5)	0.0195 (9)
O4	1.1455 (7)	0.5077 (5)	−0.1515 (5)	0.0217 (9)
O5	0.8004 (7)	0.6413 (5)	0.4552 (5)	0.0195 (9)
O6	0.7818 (7)	0.4116 (6)	0.5849 (5)	0.0230 (9)
O1W	0.6751 (7)	0.8292 (7)	0.0928 (5)	0.0310 (11)
H1WA	0.5581	0.8534	0.1260	0.046*
H1WB	0.6299	0.7771	0.0011	0.046*
O2W	1.0612 (8)	1.0993 (6)	0.2071 (5)	0.0288 (10)
H2WA	1.1653	1.1872	0.2227	0.043*
H2WB	0.9752	1.1029	0.1239	0.043*
O3W	0.4213 (9)	0.3694 (7)	0.2101 (6)	0.0420 (13)
H3WA	0.4103	0.4339	0.2922	0.063*
H3WB	0.5590	0.3823	0.2031	0.063*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pr1	0.01064 (19)	0.01179 (18)	0.01243 (18)	0.00024 (12)	0.00360 (12)	−0.00045 (12)
C1	0.012 (3)	0.016 (3)	0.019 (3)	0.001 (2)	0.005 (2)	0.001 (2)

C2	0.015 (3)	0.016 (3)	0.018 (3)	0.002 (2)	0.005 (2)	0.002 (2)
C3	0.016 (3)	0.016 (3)	0.014 (3)	0.002 (2)	0.004 (2)	0.000 (2)
O1	0.0075 (19)	0.019 (2)	0.020 (2)	0.0013 (15)	0.0047 (15)	−0.0003 (16)
O2	0.013 (2)	0.032 (2)	0.016 (2)	−0.0027 (17)	0.0036 (16)	−0.0062 (18)
O3	0.023 (2)	0.016 (2)	0.017 (2)	−0.0029 (16)	0.0072 (17)	−0.0033 (16)
O4	0.025 (2)	0.018 (2)	0.020 (2)	−0.0062 (17)	0.0118 (17)	−0.0028 (17)
O5	0.021 (2)	0.019 (2)	0.023 (2)	0.0084 (17)	0.0089 (17)	0.0085 (17)
O6	0.017 (2)	0.026 (2)	0.031 (2)	0.0070 (18)	0.0095 (18)	0.0138 (19)
O1W	0.015 (2)	0.053 (3)	0.023 (2)	0.010 (2)	0.0049 (18)	−0.005 (2)
O2W	0.029 (3)	0.021 (2)	0.035 (3)	−0.0021 (19)	0.001 (2)	0.013 (2)
O3W	0.029 (3)	0.050 (3)	0.038 (3)	−0.013 (2)	0.013 (2)	−0.017 (2)

Geometric parameters (Å, º)

Pr1—O5	2.448 (4)	C2—C2$^{\mathrm{iii}}$	1.555 (11)
Pr1—O2W	2.466 (4)	C3—O5	1.248 (7)
Pr1—O6$^{\mathrm{i}}$	2.472 (4)	C3—O6	1.258 (7)
Pr1—O2$^{\mathrm{ii}}$	2.490 (4)	C3—C3$^{\mathrm{i}}$	1.548 (11)
Pr1—O1W	2.500 (4)	O1—Pr1$^{\mathrm{iv}}$	2.609 (4)
Pr1—O3	2.504 (4)	O2—Pr1$^{\mathrm{ii}}$	2.490 (4)
Pr1—O4$^{\mathrm{iii}}$	2.541 (4)	O4—Pr1$^{\mathrm{iii}}$	2.541 (4)
Pr1—O1	2.586 (4)	O6—Pr1$^{\mathrm{i}}$	2.472 (4)
Pr1—O1$^{\mathrm{iv}}$	2.609 (4)	O1W—H1WA	0.8413
C1—O2	1.243 (7)	O1W—H1WB	0.8417
C1—O1	1.258 (7)	O2W—H2WA	0.8412
C1—C1$^{\mathrm{ii}}$	1.546 (11)	O2W—H2WB	0.8372
C2—O4	1.238 (7)	O3W—H3WA	0.8386
C2—O3	1.263 (7)	O3W—H3WB	0.8400

O5—Pr1—O2W	142.99 (15)	O6$^{\mathrm{i}}$—Pr1—O1$^{\mathrm{iv}}$	120.77 (14)
O5—Pr1—O6$^{\mathrm{i}}$	65.89 (14)	O2$^{\mathrm{ii}}$—Pr1—O1$^{\mathrm{iv}}$	121.99 (13)
O2W—Pr1—O6$^{\mathrm{i}}$	142.54 (15)	O1W—Pr1—O1$^{\mathrm{iv}}$	77.27 (13)
O5—Pr1—O2$^{\mathrm{ii}}$	131.79 (14)	O3—Pr1—O1$^{\mathrm{iv}}$	146.78 (13)
O2W—Pr1—O2$^{\mathrm{ii}}$	71.54 (15)	O4$^{\mathrm{iii}}$—Pr1—O1$^{\mathrm{iv}}$	122.88 (13)
O6$^{\mathrm{i}}$—Pr1—O2$^{\mathrm{ii}}$	71.37 (14)	O1—Pr1—O1$^{\mathrm{iv}}$	65.40 (14)
O5—Pr1—O1W	97.65 (15)	O2—C1—O1	126.7 (5)
O2W—Pr1—O1W	70.26 (16)	O2—C1—C1$^{\mathrm{ii}}$	116.0 (6)
O6$^{\mathrm{i}}$—Pr1—O1W	142.27 (16)	O1—C1—C1$^{\mathrm{ii}}$	117.3 (6)
O2$^{\mathrm{ii}}$—Pr1—O1W	130.26 (15)	O4—C2—O3	126.8 (5)
O5—Pr1—O3	133.93 (13)	O4—C2—C2$^{\mathrm{iii}}$	117.5 (6)
O2W—Pr1—O3	78.07 (15)	O3—C2—C2$^{\mathrm{iii}}$	115.7 (6)
O6$^{\mathrm{i}}$—Pr1—O3	92.40 (14)	O5—C3—O6	126.5 (5)
O2$^{\mathrm{ii}}$—Pr1—O3	67.24 (13)	O5—C3—C3$^{\mathrm{i}}$	117.1 (6)
O1W—Pr1—O3	74.66 (14)	O6—C3—C3$^{\mathrm{i}}$	116.4 (6)
O5—Pr1—O4$^{\mathrm{iii}}$	70.30 (13)	C1—O1—Pr1	118.7 (3)
O2W—Pr1—O4$^{\mathrm{iii}}$	132.32 (15)	C1—O1—Pr1$^{\mathrm{iv}}$	123.3 (3)
O6$^{\mathrm{i}}$—Pr1—O4$^{\mathrm{iii}}$	69.96 (15)	Pr1—O1—Pr1$^{\mathrm{iv}}$	114.60 (14)
O2$^{\mathrm{ii}}$—Pr1—O4$^{\mathrm{iii}}$	114.58 (14)	C1—O2—Pr1$^{\mathrm{ii}}$	123.5 (4)

O1W—Pr1—O4^{iii}	72.53 (15)	C2—O3—Pr1	121.8 (4)
O3—Pr1—O4^{iii}	64.03 (13)	C2—O4—Pr1^{iii}	120.5 (4)
O5—Pr1—O1	85.86 (13)	C3—O5—Pr1	120.4 (4)
O2W—Pr1—O1	81.79 (14)	C3—O6—Pr1^{i}	119.7 (4)
O6^{i}—Pr1—O1	77.20 (14)	Pr1—O1W—H1WA	115.2
O2^{ii}—Pr1—O1	63.42 (12)	Pr1—O1W—H1WB	132.7
O1W—Pr1—O1	137.77 (14)	H1WA—O1W—H1WB	106.2
O3—Pr1—O1	130.36 (13)	Pr1—O2W—H2WA	136.4
O4^{iii}—Pr1—O1	145.06 (13)	Pr1—O2W—H2WB	113.6
O5—Pr1—O1^{iv}	67.14 (13)	H2WA—O2W—H2WB	107.3
O2W—Pr1—O1^{iv}	76.00 (14)	H3WA—O3W—H3WB	107.4

O2—C1—O1—Pr1	−172.7 (5)	C2^{iii}—C2—O3—Pr1	6.3 (8)
C1^{ii}—C1—O1—Pr1	8.0 (8)	O5—Pr1—O3—C2	1.9 (5)
O2—C1—O1—Pr1^{iv}	29.2 (8)	O2W—Pr1—O3—C2	−156.5 (4)
C1^{ii}—C1—O1—Pr1^{iv}	−150.1 (5)	O6^{i}—Pr1—O3—C2	60.1 (4)
O5—Pr1—O1—C1	133.4 (4)	O2^{ii}—Pr1—O3—C2	128.7 (5)
O2W—Pr1—O1—C1	−81.6 (4)	O1W—Pr1—O3—C2	−83.9 (4)
O6^{i}—Pr1—O1—C1	67.2 (4)	O4^{iii}—Pr1—O3—C2	−6.2 (4)
O2^{ii}—Pr1—O1—C1	−8.2 (4)	O1—Pr1—O3—C2	135.3 (4)
O1W—Pr1—O1—C1	−129.8 (4)	O1^{iv}—Pr1—O3—C2	−117.2 (4)
O3—Pr1—O1—C1	−15.0 (5)	O3—C2—O4—Pr1^{iii}	−174.2 (5)
O4^{iii}—Pr1—O1—C1	87.3 (4)	C2^{iii}—C2—O4—Pr1^{iii}	4.8 (9)
O1^{iv}—Pr1—O1—C1	−159.9 (5)	O6—C3—O5—Pr1	−174.3 (5)
O5—Pr1—O1—Pr1^{iv}	−66.72 (16)	C3^{i}—C3—O5—Pr1	6.5 (8)
O2W—Pr1—O1—Pr1^{iv}	78.30 (17)	O2W—Pr1—O5—C3	−154.9 (4)
O6^{i}—Pr1—O1—Pr1^{iv}	−132.92 (18)	O6^{i}—Pr1—O5—C3	−6.5 (4)
O2^{ii}—Pr1—O1—Pr1^{iv}	151.7 (2)	O2^{ii}—Pr1—O5—C3	−36.2 (5)
O1W—Pr1—O1—Pr1^{iv}	30.1 (3)	O1W—Pr1—O5—C3	138.0 (4)
O3—Pr1—O1—Pr1^{iv}	144.93 (15)	O3—Pr1—O5—C3	61.9 (5)
O4^{iii}—Pr1—O1—Pr1^{iv}	−112.8 (2)	O4^{iii}—Pr1—O5—C3	69.7 (4)
O1^{iv}—Pr1—O1—Pr1^{iv}	0.0	O1—Pr1—O5—C3	−84.4 (4)
O1—C1—O2—Pr1^{ii}	−171.6 (4)	O1^{iv}—Pr1—O5—C3	−149.4 (4)
C1^{ii}—C1—O2—Pr1^{ii}	7.8 (9)	O5—C3—O6—Pr1^{i}	−173.9 (4)
O4—C2—O3—Pr1	−174.7 (5)	C3^{i}—C3—O6—Pr1^{i}	5.3 (8)

Symmetry codes: (i) $-x+2, -y+1, -z+1$; (ii) $-x+3, -y+2, -z+1$; (iii) $-x+2, -y+1, -z$; (iv) $-x+2, -y+2, -z+1$.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2*W*—H2*WB*···O1*W*	0.84	2.55	2.858 (7)	103
O1*W*—H1*WA*···O2^{iv}	0.84	1.96	2.694 (6)	146
O1*W*—H1*WA*···O3^{v}	0.84	2.60	3.235 (6)	133
O1*W*—H1*WB*···O3*W*^{vi}	0.84	2.00	2.833 (6)	169
O2*W*—H2*WA*···O3*W*^{vii}	0.84	1.98	2.807 (7)	166
O2*W*—H2*WB*···O3^{viii}	0.84	2.20	2.919 (6)	144

O3*W*—H3*WA*···O6^{ix}	0.84	2.08	2.829 (7)	149
O3*W*—H3*WB*···O4^{iii}	0.84	2.03	2.833 (6)	159

Symmetry codes: (iii) −*x*+2, −*y*+1, −*z*; (iv) −*x*+2, −*y*+2, −*z*+1; (v) *x*−1, *y*, *z*; (vi) −*x*+1, −*y*+1, −*z*; (vii) *x*+1, *y*+1, *z*; (viii) −*x*+2, −*y*+2, −*z*; (ix) −*x*+1, −*y*+1, −*z*+1.