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Poly[[diaqua-μ_3-citrato-praseodymium(III)] monohydrate]

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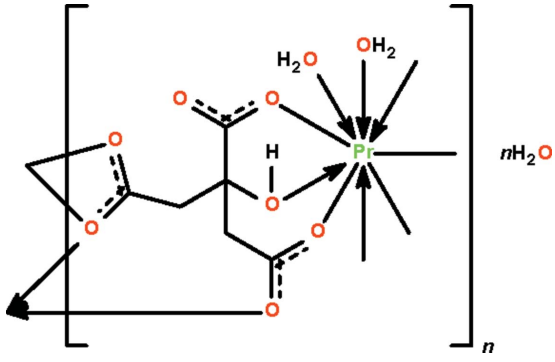
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.026; wR factor = 0.050; data-to-parameter ratio = 13.5.

In the coordination polymer, $\{[Pr(C_6H_5O_7)(H_2O)_2]\cdot H_2O\}_n$, seven of the nine coordination sites of the monocapped square-antiprismatic geometry are occupied by three O atoms of the same citrate trianion (an O atom of the hydroxy unit and the formally single-bond O atoms from two carboxyl units). Two other coordination sites are occupied by the O atoms of a chelating carboxyl unit of another citrate; one of these atoms is additionally involved in bridging. The seventh coordination site is occupied by the O atom of the formally double-bond O atom of a neighboring citrate. The remaining two coordination sites are occupied by water molecules. The citrate functions in a μ_3-bridging mode, connecting the metal atoms into a ribbon structure parallel to [010]. The structure is consolidated into a three-dimensional network by O—H···O hydrogen bonds.

Related literature

For isotypic $[Eu(C_6H_5O_7)(H_2O)_2]\cdot H_2O$, see: Tang *et al.* (2011).



Experimental

Crystal data

$[Pr(C_6H_5O_7)(H_2O)_2]\cdot H_2O$
M_r = 384.06
Monoclinic, $P2_1/n$
a = 6.2645 (3) Å
b = 9.7356 (7) Å
c = 17.0425 (10) Å
β = 91.0672 (18)°
V = 1039.22 (11) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 4.74 mm^{-1}
T = 293 K
0.30 × 0.15 × 0.10 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.331, T_{max} = 0.649
9596 measured reflections
2366 independent reflections
2182 reflections with $I > 2\sigma(I)$
R_{int} = 0.038

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.050
S = 1.18
2366 reflections
175 parameters
10 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.76 e Å^{-3}
$\Delta\rho_{min}$ = −0.81 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O7—H7···O2^{i}	0.83 (1)	1.72 (1)	2.536 (3)	167 (4)
O1w—H11···O2^{ii}	0.84 (1)	1.84 (1)	2.666 (3)	169 (4)
O1w—H12···O3^{iii}	0.84 (1)	1.89 (2)	2.692 (3)	159 (3)
O2w—H21···O1w^{iv}	0.84 (1)	2.09 (2)	2.854 (4)	151 (4)
O2w—H22···O3w	0.84 (1)	1.89 (1)	2.718 (4)	168 (4)
O3w—H31···O6^{v}	0.84 (1)	2.05 (2)	2.856 (4)	160 (6)

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SI2362).

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supplementary materials

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Poly[[diaqua-μ_3-citrato-praseodymium(III)] monohydrate]

L.-J. Han, Y.-F. Deng and S. W. Ng

Comment

A recent report describes the synthesis of $Eu(H_2O)_2(C_6H_5O_7)\cdot H_2O$, a citrate(3-) based coordination polymer that exhibits useful luminescence; the ribbon motif propagates along the *a*-axis and adjacent chains are linked by O–H···O hydrogen bonds into a three-dimensional network. The presence of manganese dichloride is crucial to the synthesis (Tang *et al.*, 2011). The present Pr analog (Scheme I) is isostructural, the two compounds crystallizing with matching cell dimensions. In the coordination polymer, $Pr(H_2O)_2(C_6H_5O_7)\cdot H_2O$ (Fig. 1), seven of the nine coordination sites a mono-capped square-anti-prismatic geometry (Fig. 2) are occupied by three O atoms of the same citrate trianion (an O atom of the hydroxy unit and the formally single-bond O atoms from two carboxyl units). Two other coordination sites are occupied by the O atoms of a chelating carboxyl unit of another citrate; one of these atoms is additionally involved in bridging. The seventh coordination site is occupied by the O atom of the formally double-bond O atom of a neighboring citrate. The remaining two coordination sites of the are occupied by water molecules. The citrate functions in a μ_3– bridging mode to connect the metal atoms into a ribbon structure. The structure is consolidated into a three-dimensional network by O–H···O hydrogen bonds (Table 1).

Experimental

Praseodymium oxide, Pr_6O_{11} (0.341 g), was suspended in water (20 ml) and to the suspension was added manganese dichloride tetrahydrate (0.395 g, 2.0 mmol) and citric acid monohydrate (0.841 g, 4.0 mmol). The mixture was placed in a 25 ml, teflon-lined, stainless-steel Parr bomb. The bomb was heated at 393 K for 72 h. It was cooled to room temperature at 30 K an hour. Green crystals were isolated in 75% yield based on Pr_6O_{11}.

Refinement

Carbon-bound H atoms treated as riding (C–H 0.97 Å) and their temperature factors were tied by a factor of 1.2 times. The hydroxy and water H atoms were located in a difference Fourier map, and were refined with distance restraints of O–H 0.84±0.01 Å and H···H 1.37±0.01 Å. Their temperature factors were tied by a factor of 1.5 times. The (5 6 3), (-6 6 1), (1 9 2), (4 10 2) and (6 7 3) reflections were omitted owing to bad disagreement.

Figures

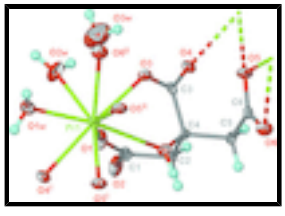

Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of a portion of polymeric $Pr(H_2O)_2(C_6H_5O_7)\cdot H_2O$ with the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

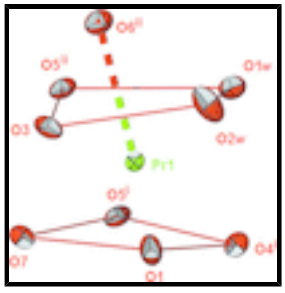

Fig. 2. Nine-coordinate geometry of Pr^{III}.

Poly[[diaqua-μ$_3$-citrato-praseodymium(III)] monohydrate]

Crystal data

$[Pr(C_6H_5O_7)(H_2O)_2]\cdot H_2O$	$F(000) = 744$
$M_r = 384.06$	$D_x = 2.455$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2yn	Cell parameters from 8369 reflections
$a = 6.2645$ (3) Å	$\theta = 3.2$–$27.4°$
$b = 9.7356$ (7) Å	$\mu = 4.74$ mm^{-1}
$c = 17.0425$ (10) Å	$T = 293$ K
$\beta = 91.0672$ (18)°	Prism, light green
$V = 1039.22$ (11) Å^3	0.30 × 0.15 × 0.10 mm
$Z = 4$	

Data collection

Rigaku R-AXIS RAPID diffractometer	2366 independent reflections
Radiation source: fine-focus sealed tube	2182 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.038$
Detector resolution: 10.000 pixels mm^{-1}	$\theta_{max} = 27.4°$, $\theta_{min} = 3.2°$
ω scans	$h = -8\rightarrow8$
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)	$k = -12\rightarrow10$
$T_{min} = 0.331$, $T_{max} = 0.649$	$l = -22\rightarrow22$
9596 measured reflections	

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.026$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.050$	H atoms treated by a mixture of independent and constrained refinement
$S = 1.18$	$w = 1/[\sigma^2(F_o^2) + (0.P)^2 + 1.4664P]$ where $P = (F_o^2 + 2F_c^2)/3$

2366 reflections	$(\Delta/\sigma)_{max} = 0.001$
175 parameters	$\Delta\rho_{max} = 0.76$ e Å^{-3}
10 restraints	$\Delta\rho_{min} = -0.81$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Pr1	0.11415 (2)	0.319324 (16)	0.566983 (9)	0.01012 (6)
O1	0.2224 (4)	0.2466 (3)	0.70094 (14)	0.0212 (5)
O2	0.3108 (4)	0.2315 (3)	0.82649 (14)	0.0245 (5)
O3	0.5035 (3)	0.2913 (2)	0.56851 (14)	0.0195 (5)
O4	0.7923 (3)	0.2852 (2)	0.64591 (13)	0.0150 (4)
O5	0.8717 (3)	0.5316 (2)	0.55742 (13)	0.0166 (4)
O6	0.7309 (4)	0.7354 (2)	0.57242 (13)	0.0185 (5)
O7	0.3381 (3)	0.5013 (2)	0.63152 (13)	0.0138 (4)
H7	0.297 (6)	0.574 (2)	0.652 (2)	0.021*
O1W	−0.1683 (3)	0.2119 (3)	0.47949 (14)	0.0192 (5)
H11	−0.172 (5)	0.219 (4)	0.4305 (6)	0.029*
H12	−0.289 (3)	0.230 (4)	0.4971 (18)	0.029*
O2W	0.1834 (4)	0.0691 (3)	0.56804 (16)	0.0277 (6)
H21	0.147 (6)	−0.001 (3)	0.543 (2)	0.042*
H22	0.300 (4)	0.054 (4)	0.591 (2)	0.042*
O3W	0.5632 (6)	−0.0132 (4)	0.6318 (2)	0.0564 (10)
H31	0.617 (8)	−0.092 (2)	0.626 (4)	0.085*
H32	0.635 (8)	0.042 (4)	0.605 (3)	0.085*
C1	0.3229 (5)	0.2872 (3)	0.76032 (18)	0.0146 (6)
C2	0.4742 (5)	0.4089 (3)	0.75574 (17)	0.0141 (6)
H2A	0.6066	0.3849	0.7829	0.017*
H2B	0.4118	0.4855	0.7836	0.017*
C3	0.6141 (5)	0.3355 (3)	0.62538 (18)	0.0125 (6)
C4	0.5269 (4)	0.4564 (3)	0.67268 (17)	0.0109 (6)
C5	0.6919 (5)	0.5734 (3)	0.67823 (17)	0.0130 (6)
H5A	0.6285	0.6513	0.7046	0.016*
H5B	0.8134	0.5429	0.7097	0.016*
C6	0.7682 (4)	0.6185 (3)	0.59874 (17)	0.0120 (6)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pr1	0.00959 (9)	0.01080 (10)	0.00997 (9)	0.00001 (6)	0.00066 (6)	0.00069 (6)
O1	0.0237 (12)	0.0235 (13)	0.0161 (12)	−0.0102 (10)	−0.0060 (9)	0.0049 (9)
O2	0.0360 (13)	0.0230 (13)	0.0142 (12)	−0.0143 (11)	−0.0037 (10)	0.0078 (10)
O3	0.0124 (11)	0.0235 (13)	0.0226 (13)	0.0015 (9)	−0.0010 (9)	−0.0123 (10)
O4	0.0116 (10)	0.0164 (11)	0.0171 (11)	0.0030 (9)	0.0016 (8)	0.0017 (9)
O5	0.0217 (11)	0.0133 (11)	0.0149 (11)	0.0037 (9)	0.0072 (8)	0.0010 (9)
O6	0.0234 (12)	0.0155 (12)	0.0167 (12)	0.0033 (9)	0.0039 (9)	0.0031 (9)
O7	0.0144 (10)	0.0114 (11)	0.0157 (11)	0.0035 (8)	−0.0022 (8)	−0.0017 (8)
O1W	0.0158 (11)	0.0267 (13)	0.0151 (12)	−0.0010 (10)	0.0013 (8)	−0.0025 (10)

O2W	0.0334 (14)	0.0158 (13)	0.0336 (15)	0.0004 (11)	−0.0102 (11)	−0.0021 (11)
O3W	0.056 (2)	0.0331 (18)	0.079 (3)	0.0182 (16)	−0.0212 (18)	−0.0082 (18)
C1	0.0145 (14)	0.0156 (16)	0.0138 (15)	−0.0021 (12)	0.0009 (11)	0.0016 (12)
C2	0.0154 (14)	0.0160 (16)	0.0110 (14)	−0.0034 (12)	0.0018 (11)	−0.0004 (12)
C3	0.0107 (14)	0.0129 (15)	0.0141 (15)	−0.0025 (11)	0.0045 (11)	0.0029 (11)
C4	0.0116 (13)	0.0104 (14)	0.0105 (14)	0.0000 (11)	0.0001 (10)	−0.0005 (11)
C5	0.0155 (14)	0.0117 (15)	0.0118 (14)	−0.0040 (12)	0.0022 (10)	−0.0006 (11)
C6	0.0092 (13)	0.0133 (16)	0.0134 (14)	−0.0026 (11)	−0.0005 (10)	−0.0009 (11)

Geometric parameters (Å, °)

Pr1—O1	2.473 (2)	O6—Pr1^{ii}	2.637 (2)
Pr1—O3	2.454 (2)	O7—C4	1.432 (3)
Pr1—O4^{i}	2.467 (2)	O7—H7	0.834 (10)
Pr1—O5^{i}	2.568 (2)	O1W—H11	0.84 (1)
Pr1—O5^{ii}	2.572 (2)	O1W—H12	0.84 (1)
Pr1—O6^{ii}	2.637 (2)	O2W—H21	0.84 (1)
Pr1—O7	2.502 (2)	O2W—H22	0.84 (1)
Pr1—O1W	2.520 (2)	O3W—H31	0.84 (1)
Pr1—O2W	2.474 (3)	O3W—H32	0.85 (1)
O1—C1	1.246 (4)	C1—C2	1.520 (4)
O2—C1	1.255 (4)	C2—C4	1.531 (4)
O3—C3	1.257 (4)	C2—H2A	0.9700
O4—C3	1.262 (4)	C2—H2B	0.9700
O4—Pr1^{iii}	2.467 (2)	C3—C4	1.533 (4)
O5—C6	1.284 (4)	C4—C5	1.540 (4)
O5—Pr1^{iii}	2.568 (2)	C5—C6	1.510 (4)
O5—Pr1^{ii}	2.572 (2)	C5—H5A	0.9700
O6—C6	1.244 (4)	C5—H5B	0.9700
O3—Pr1—O4^{i}	143.27 (8)	C6—O5—Pr1^{ii}	96.06 (18)
O3—Pr1—O1	72.72 (8)	Pr1^{iii}—O5—Pr1^{ii}	118.48 (8)
O4^{i}—Pr1—O1	70.79 (7)	C6—O6—Pr1^{ii}	94.03 (18)
O3—Pr1—O2W	73.53 (8)	C4—O7—Pr1	116.75 (17)
O4^{i}—Pr1—O2W	90.48 (8)	C4—O7—H7	108 (3)
O1—Pr1—O2W	70.50 (9)	Pr1—O7—H7	128 (3)
O3—Pr1—O7	61.63 (7)	Pr1—O1W—H11	124 (3)
O4^{i}—Pr1—O7	108.24 (7)	Pr1—O1W—H12	109 (3)
O1—Pr1—O7	69.83 (7)	H11—O1W—H12	109 (2)
O2W—Pr1—O7	126.67 (8)	Pr1—O2W—H21	139 (3)
O3—Pr1—O1W	130.32 (7)	Pr1—O2W—H22	109 (3)
O4^{i}—Pr1—O1W	72.22 (7)	H21—O2W—H22	110 (2)
O1—Pr1—O1W	127.21 (8)	H31—O3W—H32	107 (2)
O2W—Pr1—O1W	73.54 (8)	O1—C1—O2	123.7 (3)
O7—Pr1—O1W	159.37 (8)	O1—C1—C2	120.8 (3)
O3—Pr1—O5^{i}	132.58 (7)	O2—C1—C2	115.5 (3)
O4^{i}—Pr1—O5^{i}	69.79 (7)	C1—C2—C4	115.4 (2)

O1—Pr1—O5^{i}	116.15 (8)	C1—C2—H2A	108.4
O2W—Pr1—O5^{i}	153.65 (8)	C4—C2—H2A	108.4
O7—Pr1—O5^{i}	77.53 (7)	C1—C2—H2B	108.4
O1W—Pr1—O5^{i}	83.60 (7)	C4—C2—H2B	108.4
O3—Pr1—O5^{ii}	91.25 (8)	H2A—C2—H2B	107.5
O4^{i}—Pr1—O5^{ii}	124.51 (7)	O3—C3—O4	123.6 (3)
O1—Pr1—O5^{ii}	155.43 (7)	O3—C3—C4	118.1 (3)
O2W—Pr1—O5^{ii}	123.56 (8)	O4—C3—C4	118.3 (3)
O7—Pr1—O5^{ii}	86.28 (7)	O7—C4—C2	110.8 (2)
O1W—Pr1—O5^{ii}	77.36 (8)	O7—C4—C3	106.0 (2)
O5^{i}—Pr1—O5^{ii}	61.52 (8)	C2—C4—C3	109.8 (2)
O3—Pr1—O6^{ii}	66.72 (7)	O7—C4—C5	110.6 (2)
O4^{i}—Pr1—O6^{ii}	141.46 (7)	C2—C4—C5	108.8 (2)
O1—Pr1—O6^{ii}	132.42 (8)	C3—C4—C5	110.8 (2)
O2W—Pr1—O6^{ii}	74.95 (8)	C6—C5—C4	112.5 (2)
O7—Pr1—O6^{ii}	109.04 (7)	C6—C5—H5A	109.1
O1W—Pr1—O6^{ii}	69.47 (7)	C4—C5—H5A	109.1
O5^{i}—Pr1—O6^{ii}	109.42 (7)	C6—C5—H5B	109.1
O5^{ii}—Pr1—O6^{ii}	49.65 (7)	C4—C5—H5B	109.1
C1—O1—Pr1	141.7 (2)	H5A—C5—H5B	107.8
C3—O3—Pr1	120.28 (19)	O6—C6—O5	119.9 (3)
C3—O4—Pr1^{iii}	121.60 (19)	O6—C6—C5	122.0 (3)
C6—O5—Pr1^{iii}	143.1 (2)	O5—C6—C5	118.1 (3)
O3—Pr1—O1—C1	67.4 (4)	Pr1—O3—C3—O4	152.9 (2)
O4^{i}—Pr1—O1—C1	−116.8 (4)	Pr1—O3—C3—C4	−26.6 (4)
O2W—Pr1—O1—C1	145.6 (4)	Pr1^{iii}—O4—C3—O3	72.0 (4)
O7—Pr1—O1—C1	2.0 (3)	Pr1^{iii}—O4—C3—C4	−108.5 (3)
O1W—Pr1—O1—C1	−164.6 (3)	Pr1—O7—C4—C2	−83.4 (2)
O5^{i}—Pr1—O1—C1	−62.1 (4)	Pr1—O7—C4—C3	35.7 (3)
O5^{ii}—Pr1—O1—C1	16.1 (5)	Pr1—O7—C4—C5	155.86 (18)
O6^{ii}—Pr1—O1—C1	99.8 (4)	C1—C2—C4—O7	61.8 (3)
O4^{i}—Pr1—O3—C3	−49.7 (3)	C1—C2—C4—C3	−55.0 (3)
O1—Pr1—O3—C3	−43.1 (2)	C1—C2—C4—C5	−176.4 (3)
O2W—Pr1—O3—C3	−117.3 (2)	O3—C3—C4—O7	−6.7 (4)
O7—Pr1—O3—C3	32.9 (2)	O4—C3—C4—O7	173.7 (2)
O1W—Pr1—O3—C3	−167.6 (2)	O3—C3—C4—C2	113.0 (3)
O5^{i}—Pr1—O3—C3	66.8 (3)	O4—C3—C4—C2	−66.5 (3)
O5^{ii}—Pr1—O3—C3	118.0 (2)	O3—C3—C4—C5	−126.7 (3)
O6^{ii}—Pr1—O3—C3	162.4 (3)	O4—C3—C4—C5	53.7 (4)
O3—Pr1—O7—C4	−35.86 (18)	O7—C4—C5—C6	−63.2 (3)
O4^{i}—Pr1—O7—C4	105.51 (18)	C2—C4—C5—C6	175.0 (2)
O1—Pr1—O7—C4	44.86 (18)	C3—C4—C5—C6	54.1 (3)

O2W—Pr1—O7—C4	0.7 (2)	Pr1^{ii}—O6—C6—O5	6.0 (3)
O1W—Pr1—O7—C4	−166.6 (2)	Pr1^{ii}—O6—C6—C5	−173.0 (2)
O5^{i}—Pr1—O7—C4	169.07 (19)	Pr1^{iii}—O5—C6—O6	153.9 (2)
O5^{ii}—Pr1—O7—C4	−129.30 (19)	Pr1^{ii}—O5—C6—O6	−6.2 (3)
O6^{ii}—Pr1—O7—C4	−84.44 (19)	Pr1^{iii}—O5—C6—C5	−27.1 (4)
Pr1—O1—C1—O2	164.9 (2)	Pr1^{ii}—O5—C6—C5	172.8 (2)
Pr1—O1—C1—C2	−16.3 (5)	Pr1^{iii}—O5—C6—Pr1^{ii}	160.0 (3)
O1—C1—C2—C4	−11.9 (4)	C4—C5—C6—O6	114.9 (3)
O2—C1—C2—C4	167.0 (3)	C4—C5—C6—O5	−64.0 (3)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O7—H7···O2^{iv}	0.83 (1)	1.72 (1)	2.536 (3)	167 (4)
O1w—H11···O2^{v}	0.84 (1)	1.84 (1)	2.666 (3)	169 (4)
O1w—H12···O3^{i}	0.84 (1)	1.89 (2)	2.692 (3)	159 (3)
O2w—H21···O1w^{vi}	0.84 (1)	2.09 (2)	2.854 (4)	151 (4)
O2w—H22···O3w	0.84 (1)	1.89 (1)	2.718 (4)	168 (4)
O3w—H31···O6^{vii}	0.84 (1)	2.05 (2)	2.856 (4)	160 (6)

Symmetry codes: (iv) −*x*+1/2, *y*+1/2, −*z*+3/2; (v) *x*−1/2, −*y*+1/2, *z*−1/2; (i) *x*−1, *y*, *z*; (vi) −*x*, −*y*, −*z*+1; (vii) *x*, *y*−1, *z*.

Fig. 1

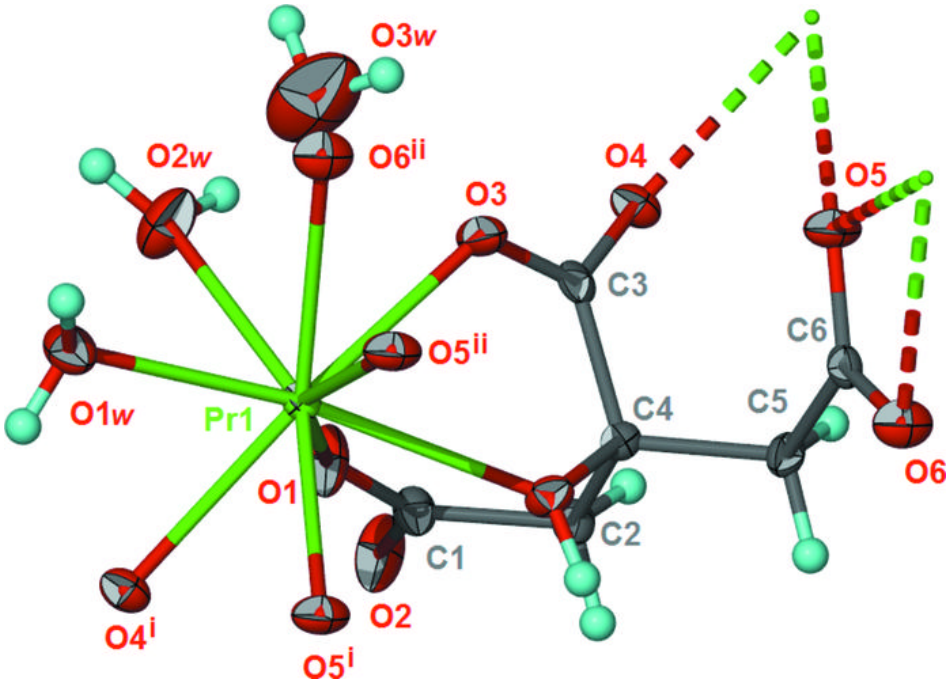
O3w
O2w
O6ii
O4
O5
O3
C3
C6
O5ii
O1w
Pr1
C4
C5
O6
O1
C2
C1
O2
O4i
O5i

Fig. 2