

Poly[[diaquatris[μ_4 -(*p*-phenylenedioxy)-diacetato]dipraseodymium(III) dihydrate]

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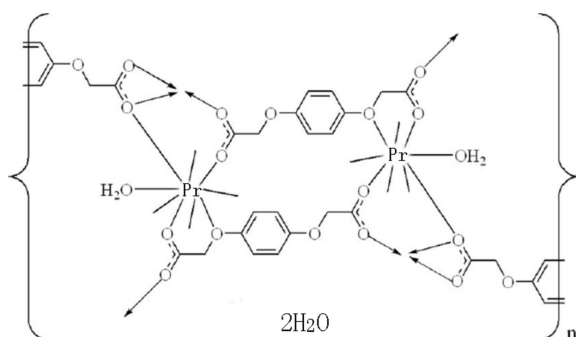
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.006$ Å; R factor = 0.030; wR factor = 0.073; data-to-parameter ratio = 17.1.

The title praseodymium coordination polymer, $\{[\text{Pr}_2(\text{C}_{10}\text{H}_8\text{O}_6)_3(\text{H}_2\text{O})_2] \cdot 2\text{H}_2\text{O}\}_n$, was obtained by the hydrothermal reaction of $\text{Pr}(\text{NO}_3)_3$ with (*p*-phenylenedioxy)diacetic acid in alkaline aqueous solution. Each Pr^{III} atom is coordinated by nine O atoms, eight from four (*p*-phenylenedioxy)diacetate ligands and one from a water molecule, displaying a tricapped trigonal prismatic geometry. There is a centre of symmetry at the mid-point of the $\text{Pr} \cdots \text{Pr}$ vector. The bridging ligands crosslink the metal ions to form a three-dimensional network, with channels running along the c axis in which the uncoordinated water molecules are located. The crystal structure is stabilized by intermolecular $\text{O}-\text{H} \cdots \text{O}$ hydrogen-bonding interactions.

Related literature

For related literature, see: Choi & Jeon (2003); Qiu *et al.* (2006); Tao *et al.* (2000).



Experimental

Crystal data

$[\text{Pr}_2(\text{C}_{10}\text{H}_8\text{O}_6)_3(\text{H}_2\text{O})_2] \cdot 2\text{H}_2\text{O}$

$M_r = 1026.38$

Monoclinic, $P2_1/c$

$a = 12.1685$ (3) Å

$b = 16.9339$ (4) Å

$c = 8.9299$ (2) Å

$\beta = 108.956$ (1)°

$V = 1740.30$ (7) Å³

$Z = 2$

Mo $K\alpha$ radiation

$\mu = 2.86$ mm⁻¹

$T = 293$ (2) K

$0.18 \times 0.15 \times 0.12$ mm

Data collection

Bruker APEXII area-detector diffractometer

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

$T_{\text{min}} = 0.607$, $T_{\text{max}} = 0.715$

14677 measured reflections

4182 independent reflections

3381 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.036$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.030$

$wR(F^2) = 0.073$

$S = 1.03$

4182 reflections

244 parameters

6 restraints

H-atom parameters constrained

$\Delta\rho_{\text{max}} = 0.62$ e Å⁻³

$\Delta\rho_{\text{min}} = -0.81$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$\text{O1W}-\text{H1W} \cdots \text{O2W}^i$	0.84	2.40	3.149 (5)	149
$\text{O1W}-\text{H2W} \cdots \text{O1}$	0.81	2.47	3.064 (5)	131
$\text{O2W}-\text{H3W} \cdots \text{O4}^{ii}$	0.83	2.59	2.992 (5)	111
$\text{O2W}-\text{H4W} \cdots \text{O1W}^{iii}$	0.86	2.10	2.778 (5)	135

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

Data collection: APEX2 (Bruker, 2004); cell refinement: SAINT (Bruker, 2004); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 2004); software used to prepare material for publication: SHELXTL.

The authors acknowledge South China Normal University for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2137).

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supplementary materials

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Poly[[diaquatrakis(μ_4 -(*p*-phenylenedioxy)diacetato)dipraseodymium(III)] dihydrate]

R.-H. Zeng, Y.-C. Qiu, Y.-P. Cai, J.-Z. Wu and H. Deng

Comment

Molecular self-assembly of supramolecular architectures has received much attention during recent decades (Tao *et al.*, 2000; Choi & Jeon, 2003). The structures and properties of such systems depend on the coordination and geometric preferences of both the central metal ions and the bridging building blocks, as well as on the influence of weaker non-covalent interactions, such as hydrogen bonds and π - π stacking interactions. As a building block, (*p*-phenylenedioxy)diacetic acid (1,4-BDOA) is an excellent candidate for the construction of supramolecular complexes (Qiu *et al.*, 2006). Recently, we obtained the title novel coordination polymer, (I), by the reaction of praseodymium nitrate, (*p*-phenylenedioxy)diacetic acid in alkaline aqueous solution, and its crystal structure is reported here.

In (I), each Pr^{III} ion is coordinated by nine oxygen atoms, eight from four 1,4-BDOA²⁻ ligands and one from a water molecule (Fig. 1). The coordination environment around the Pr^{III} ion can be described as a tri-capped-trigonal prismatic geometry with O—Pr—O bond angles ranging from 47.76 (8) to 149.67 (8) Å. Pairs of Pr ions are bridged by the dianionic ligands at a distance of 4.188 (3) Å to form helical chains which are further cross-linked by the ligands into a three-dimensional supramolecular network (Fig. 2) with channels running along the *c* axis hosting the uncoordinated water molecules. The crystal structure is stabilized by intermolecular O—H \cdots O hydrogen bonding interactions.

Experimental

A mixture of Pr(NO₃)₃ (0.5 mmol), (*p*-phenylenedioxy)diacetic acid (0.75 mmol), NaOH (1.5 mmol) and H₂O (10 ml) was placed in a 20 ml Teflon reactor, which was heated at 433 K for three days and then cooled to room temperature at a rate of 10 K h⁻¹. Crystals were obtained after washing with water and drying in air.

Refinement

Carbon-bound H atoms were placed at calculated positions and were treated as riding on the parent C atoms with C—H = 0.93 Å, and with $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$. Water H atoms were tentatively located in difference Fourier maps and were refined with distance restraints of O—H = 0.82 or 0.85 Å and H \cdots H = 1.29 or 1.39 Å, each within a standard deviation of 0.01 Å.

Figures

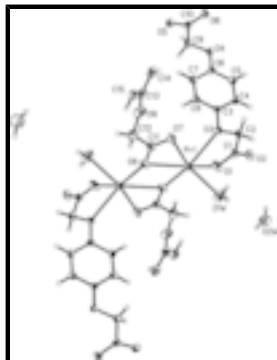


Fig. 1. The molecular structure of (I), showing the atomic-numbering scheme and displacement ellipsoids drawn at the 50% probability level. Unlabelled atoms are related to the labelled atoms by the symmetry operator $(1 - x, -y, 2 - z)$.

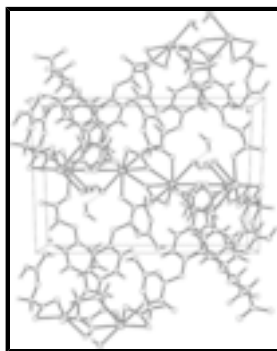


Fig. 2. The molecular packing of (I), showing the intermolecular hydrogen bonding interactions as the broken lines.

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Crystal data

$[\text{Pr}_2(\text{C}_{10}\text{H}_8\text{O}_6)_3(\text{H}_2\text{O})_2] \cdot 2\text{H}_2\text{O}$

$M_r = 1026.38$

Monoclinic, $P2_1/c$

Hall symbol: $-P\ 2ybc$

$a = 12.1685\ (3)\ \text{\AA}$

$b = 16.9339\ (4)\ \text{\AA}$

$c = 8.9299\ (2)\ \text{\AA}$

$\beta = 108.9560\ (10)^\circ$

$V = 1740.30\ (7)\ \text{\AA}^3$

$Z = 2$

$F_{000} = 1012$

$D_x = 1.959\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation

$\lambda = 0.71073\ \text{\AA}$

Cell parameters from 3500 reflections

$\theta = 1.7\text{--}28.0^\circ$

$\mu = 2.86\ \text{mm}^{-1}$

$T = 293\ (2)\ \text{K}$

Block, colourless

$0.18 \times 0.15 \times 0.12\ \text{mm}$

Data collection

Bruker APEXII area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 293\ (2)\ \text{K}$

φ and ω scans

4182 independent reflections

3381 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.036$

$\theta_{\text{max}} = 28.0^\circ$

$\theta_{\text{min}} = 2.1^\circ$

Absorption correction: multi-scan
(SADABS; Sheldrick, 1996) $h = -16 \rightarrow 16$
 $T_{\min} = 0.607$, $T_{\max} = 0.715$ $k = -17 \rightarrow 22$
 14677 measured reflections $l = -11 \rightarrow 11$

Refinement

Refinement on F^2 Secondary atom site location: difference Fourier map
 Least-squares matrix: full Hydrogen site location: inferred from neighbouring sites
 $R[F^2 > 2\sigma(F^2)] = 0.030$ H-atom parameters constrained
 $wR(F^2) = 0.073$ $w = 1/[\sigma^2(F_o^2) + (0.0304P)^2 + 2.8471P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $S = 1.03$ $(\Delta/\sigma)_{\max} = 0.001$
 4182 reflections $\Delta\rho_{\max} = 0.62 \text{ e } \text{\AA}^{-3}$
 244 parameters $\Delta\rho_{\min} = -0.81 \text{ e } \text{\AA}^{-3}$
 6 restraints Extinction correction: none
 Primary atom site location: structure-invariant direct methods

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	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.3882 (3)	0.2982 (2)	1.0544 (4)	0.0214 (7)
C2	0.2921 (3)	0.2998 (2)	0.8969 (4)	0.0230 (8)
H2A	0.2219	0.3214	0.9097	0.028*
H2B	0.3144	0.3329	0.8229	0.028*
C3	0.1633 (3)	0.2069 (2)	0.7228 (4)	0.0198 (7)
C4	0.1125 (3)	0.2595 (2)	0.6019 (5)	0.0274 (8)
H4	0.1479	0.3077	0.5967	0.033*
C5	0.0081 (3)	0.2397 (2)	0.4888 (5)	0.0289 (9)
H5	-0.0268	0.2749	0.4075	0.035*
C6	-0.0447 (3)	0.1683 (2)	0.4949 (4)	0.0218 (8)
C7	0.0062 (3)	0.1167 (2)	0.6184 (4)	0.0262 (8)
H7	-0.0295	0.0687	0.6244	0.031*
C8	0.1099 (3)	0.1363 (2)	0.7325 (4)	0.0240 (8)

supplementary materials

H8	0.1437	0.1019	0.8159	0.029*
C9	-0.1944 (3)	0.0758 (2)	0.3755 (4)	0.0270 (8)
H9A	-0.2151	0.0695	0.4709	0.032*
H9B	-0.1353	0.0369	0.3781	0.032*
C10	-0.3006 (3)	0.0605 (2)	0.2326 (4)	0.0227 (8)
C11	0.3538 (3)	0.0272 (2)	1.1574 (4)	0.0254 (8)
C12	0.3027 (4)	-0.0132 (3)	1.2703 (5)	0.0414 (11)
H12A	0.2934	-0.0690	1.2443	0.050*
H12B	0.3569	-0.0086	1.3770	0.050*
C13	0.1003 (4)	0.0075 (3)	1.1304 (5)	0.0352 (10)
C14	0.0010 (4)	0.0502 (3)	1.1204 (5)	0.0368 (10)
H14	0.0016	0.0842	1.2024	0.044*
C15	0.0980 (4)	-0.0433 (3)	1.0079 (5)	0.0377 (10)
H15	0.1636	-0.0727	1.0126	0.045*
O1	0.4518 (3)	0.23847 (17)	1.0882 (3)	0.0385 (8)
O2	0.3992 (2)	0.35833 (16)	1.1385 (3)	0.0284 (6)
O3	0.2716 (2)	0.22057 (15)	0.8373 (3)	0.0241 (6)
O4	-0.1475 (2)	0.15296 (16)	0.3742 (3)	0.0272 (6)
O5	-0.3176 (2)	-0.01103 (16)	0.2027 (3)	0.0281 (6)
O6	-0.3610 (2)	0.11699 (16)	0.1607 (3)	0.0312 (6)
O7	0.3150 (2)	0.09148 (16)	1.0965 (3)	0.0318 (6)
O8	0.4394 (2)	-0.00571 (16)	1.1333 (3)	0.0282 (6)
O9	0.1936 (3)	0.0180 (2)	1.2671 (3)	0.0414 (8)
O1W	0.6001 (3)	0.2096 (2)	0.8741 (4)	0.0525 (10)
O2W	0.7480 (3)	0.2822 (2)	0.1433 (4)	0.0648 (11)
Pr1	0.451486 (16)	0.116370 (11)	0.92970 (2)	0.01832 (7)
H1W	0.6202	0.2263	0.7986	0.022*
H2W	0.5562	0.2409	0.8926	0.022*
H3W	0.7894	0.2456	0.1300	0.022*
H4W	0.6805	0.2807	0.0727	0.022*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0247 (19)	0.019 (2)	0.0184 (16)	0.0007 (15)	0.0038 (14)	0.0004 (15)
C2	0.027 (2)	0.0151 (19)	0.0206 (17)	-0.0004 (15)	-0.0008 (15)	-0.0047 (14)
C3	0.0137 (16)	0.0204 (19)	0.0200 (16)	0.0001 (14)	-0.0021 (13)	-0.0060 (14)
C4	0.023 (2)	0.021 (2)	0.031 (2)	-0.0068 (16)	-0.0009 (16)	0.0024 (16)
C5	0.023 (2)	0.026 (2)	0.0268 (19)	-0.0029 (17)	-0.0073 (16)	0.0071 (16)
C6	0.0156 (17)	0.022 (2)	0.0199 (16)	-0.0023 (15)	-0.0047 (13)	-0.0043 (15)
C7	0.0225 (19)	0.023 (2)	0.0248 (18)	-0.0062 (16)	-0.0034 (15)	0.0009 (16)
C8	0.0203 (18)	0.022 (2)	0.0217 (17)	-0.0001 (15)	-0.0038 (14)	0.0033 (15)
C9	0.0236 (19)	0.020 (2)	0.0262 (19)	-0.0056 (16)	-0.0076 (15)	0.0021 (16)
C10	0.0204 (18)	0.025 (2)	0.0185 (17)	-0.0065 (16)	0.0009 (14)	0.0007 (15)
C11	0.0240 (19)	0.027 (2)	0.0238 (18)	-0.0021 (16)	0.0052 (15)	-0.0027 (16)
C12	0.040 (3)	0.044 (3)	0.042 (2)	0.001 (2)	0.016 (2)	0.018 (2)
C13	0.037 (2)	0.033 (3)	0.043 (2)	-0.007 (2)	0.024 (2)	0.005 (2)
C14	0.042 (3)	0.031 (2)	0.047 (3)	-0.007 (2)	0.028 (2)	-0.007 (2)

C15	0.036 (2)	0.031 (3)	0.056 (3)	0.0017 (19)	0.028 (2)	0.002 (2)
O1	0.0356 (17)	0.0254 (17)	0.0343 (16)	0.0095 (13)	-0.0166 (13)	-0.0140 (13)
O2	0.0379 (16)	0.0199 (15)	0.0197 (12)	0.0014 (12)	-0.0012 (11)	-0.0079 (11)
O3	0.0192 (13)	0.0168 (14)	0.0249 (13)	-0.0007 (10)	-0.0084 (10)	-0.0051 (10)
O4	0.0201 (13)	0.0207 (15)	0.0271 (13)	-0.0082 (11)	-0.0110 (11)	0.0041 (11)
O5	0.0237 (14)	0.0196 (15)	0.0321 (14)	-0.0063 (11)	-0.0032 (12)	-0.0030 (11)
O6	0.0239 (14)	0.0246 (16)	0.0300 (14)	-0.0006 (12)	-0.0122 (12)	0.0044 (12)
O7	0.0388 (16)	0.0234 (15)	0.0392 (16)	0.0103 (13)	0.0208 (13)	0.0093 (13)
O8	0.0252 (14)	0.0282 (16)	0.0279 (14)	0.0072 (12)	0.0039 (12)	0.0005 (12)
O9	0.0360 (17)	0.055 (2)	0.0406 (17)	-0.0066 (15)	0.0231 (15)	0.0001 (15)
O1W	0.050 (2)	0.065 (3)	0.0345 (17)	-0.0256 (18)	0.0027 (15)	0.0144 (16)
O2W	0.053 (2)	0.067 (3)	0.056 (2)	-0.012 (2)	-0.0079 (18)	0.011 (2)
Pr1	0.01760 (11)	0.01524 (11)	0.01758 (10)	-0.00029 (8)	-0.00054 (7)	0.00020 (8)

Geometric parameters (Å, °)

C1—O2	1.246 (4)	C12—H12A	0.9700
C1—O1	1.250 (4)	C12—H12B	0.9700
C1—C2	1.509 (5)	C13—O9	1.383 (5)
C2—O3	1.435 (4)	C13—C15	1.385 (6)
C2—H2A	0.9700	C13—C14	1.385 (6)
C2—H2B	0.9700	C14—C15 ⁱ	1.372 (6)
C3—C8	1.377 (5)	C14—H14	0.9300
C3—C4	1.382 (5)	C15—C14 ⁱ	1.372 (6)
C3—O3	1.400 (4)	C15—H15	0.9300
C4—C5	1.382 (5)	O1—Pr1	2.505 (3)
C4—H4	0.9300	O2—Pr1 ⁱⁱ	2.505 (2)
C5—C6	1.378 (5)	O3—Pr1	2.723 (2)
C5—H5	0.9300	O5—Pr1 ⁱⁱⁱ	2.446 (3)
C6—O4	1.385 (4)	O6—Pr1 ^{iv}	2.531 (3)
C6—C7	1.386 (5)	O7—Pr1	2.600 (3)
C7—C8	1.380 (5)	O8—Pr1 ^v	2.465 (3)
C7—H7	0.9300	O8—Pr1	2.788 (3)
C8—H8	0.9300	O1W—Pr1	2.568 (3)
C9—O4	1.427 (4)	O1W—H1W	0.8374
C9—C10	1.514 (5)	O1W—H2W	0.8059
C9—H9A	0.9700	O2W—H3W	0.8319
C9—H9B	0.9700	O2W—H4W	0.8582
C10—O5	1.244 (4)	Pr1—O5 ⁱⁱⁱ	2.446 (3)
C10—O6	1.249 (4)	Pr1—O8 ^v	2.465 (3)
C11—O7	1.241 (5)	Pr1—O2 ^{vi}	2.505 (2)
C11—O8	1.260 (4)	Pr1—O6 ^{vii}	2.531 (3)
C11—C12	1.510 (5)	Pr1—H2W	2.5404
C12—O9	1.420 (5)		
O2—C1—O1	125.3 (3)	C2—O3—Pr1	117.86 (19)
O2—C1—C2	116.5 (3)	C6—O4—C9	115.3 (3)
O1—C1—C2	118.1 (3)	C10—O5—Pr1 ⁱⁱⁱ	148.5 (2)

supplementary materials

O3—C2—C1	108.5 (3)	C10—O6—Pr1 ^{iv}	129.8 (2)
O3—C2—H2A	110.0	C11—O7—Pr1	99.8 (2)
C1—C2—H2A	110.0	C11—O8—Pr1 ^v	155.7 (3)
O3—C2—H2B	110.0	C11—O8—Pr1	90.3 (2)
C1—C2—H2B	110.0	Pr1 ^v —O8—Pr1	105.58 (9)
H2A—C2—H2B	108.4	C13—O9—C12	117.6 (3)
C8—C3—C4	120.6 (3)	Pr1—O1W—H1W	140.5
C8—C3—O3	116.7 (3)	Pr1—O1W—H2W	79.0
C4—C3—O3	122.7 (3)	H1W—O1W—H2W	109.3
C3—C4—C5	119.0 (4)	H3W—O2W—H4W	110.7
C3—C4—H4	120.5	O5 ⁱⁱⁱ —Pr1—O8 ^v	70.05 (9)
C5—C4—H4	120.5	O5 ⁱⁱⁱ —Pr1—O1	138.91 (10)
C6—C5—C4	120.9 (3)	O8 ^v —Pr1—O1	148.69 (9)
C6—C5—H5	119.5	O5 ⁱⁱⁱ —Pr1—O2 ^{vi}	73.65 (9)
C4—C5—H5	119.5	O8 ^v —Pr1—O2 ^{vi}	82.36 (9)
C5—C6—O4	116.7 (3)	O1—Pr1—O2 ^{vi}	113.49 (9)
C5—C6—C7	119.4 (3)	O5 ⁱⁱⁱ —Pr1—O6 ^{vii}	132.82 (9)
O4—C6—C7	123.9 (3)	O8 ^v —Pr1—O6 ^{vii}	77.26 (9)
C8—C7—C6	120.0 (4)	O1—Pr1—O6 ^{vii}	72.56 (9)
C8—C7—H7	120.0	O2 ^{vi} —Pr1—O6 ^{vii}	134.67 (10)
C6—C7—H7	120.0	O5 ⁱⁱⁱ —Pr1—O1W	139.07 (10)
C3—C8—C7	120.0 (3)	O8 ^v —Pr1—O1W	87.60 (11)
C3—C8—H8	120.0	O1—Pr1—O1W	74.31 (12)
C7—C8—H8	120.0	O2 ^{vi} —Pr1—O1W	69.60 (9)
O4—C9—C10	112.6 (3)	O6 ^{vii} —Pr1—O1W	69.51 (10)
O4—C9—H9A	109.1	O5 ⁱⁱⁱ —Pr1—O7	73.11 (9)
C10—C9—H9A	109.1	O8 ^v —Pr1—O7	119.94 (9)
O4—C9—H9B	109.1	O1—Pr1—O7	72.20 (10)
C10—C9—H9B	109.1	O2 ^{vi} —Pr1—O7	128.92 (9)
H9A—C9—H9B	107.8	O6 ^{vii} —Pr1—O7	96.22 (9)
O5—C10—O6	127.3 (3)	O1W—Pr1—O7	146.24 (11)
O5—C10—C9	112.6 (3)	O5 ⁱⁱⁱ —Pr1—O3	88.99 (8)
O6—C10—C9	120.0 (3)	O8 ^v —Pr1—O3	149.67 (8)
O7—C11—O8	122.1 (4)	O1—Pr1—O3	59.33 (8)
O7—C11—C12	120.6 (4)	O2 ^{vi} —Pr1—O3	70.52 (8)
O8—C11—C12	117.2 (4)	O6 ^{vii} —Pr1—O3	131.89 (8)
O9—C12—C11	113.8 (4)	O1W—Pr1—O3	95.18 (10)
O9—C12—H12A	108.8	O7—Pr1—O3	71.23 (8)
C11—C12—H12A	108.8	O5 ⁱⁱⁱ —Pr1—O8	66.83 (8)
O9—C12—H12B	108.8	O8 ^v —Pr1—O8	74.42 (9)
C11—C12—H12B	108.8	O1—Pr1—O8	103.55 (9)
H12A—C12—H12B	107.7	O2 ^{vi} —Pr1—O8	138.96 (8)
O9—C13—C15	125.3 (4)	O6 ^{vii} —Pr1—O8	72.30 (8)

O9—C13—C14	116.0 (4)	O1W—Pr1—O8	140.50 (9)
C15—C13—C14	118.7 (4)	O7—Pr1—O8	47.76 (8)
C15 ⁱ —C14—C13	121.4 (4)	O3—Pr1—O8	118.08 (8)
C15 ⁱ —C14—H14	119.3	O5 ⁱⁱⁱ —Pr1—H2W	145.7
C13—C14—H14	119.3	O8 ^v —Pr1—H2W	105.7
C14 ⁱ —C15—C13	119.9 (4)	O1—Pr1—H2W	58.7
C14 ⁱ —C15—H15	120.1	O2 ^{vi} —Pr1—H2W	72.0
C13—C15—H15	120.1	O6 ^{vii} —Pr1—H2W	75.2
C1—O1—Pr1	130.1 (2)	O1W—Pr1—H2W	18.1
C1—O2—Pr1 ⁱⁱ	135.0 (2)	O7—Pr1—H2W	130.5
C3—O3—C2	115.8 (3)	O3—Pr1—H2W	79.1
C3—O3—Pr1	126.0 (2)	O8—Pr1—H2W	146.6

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1W—H1W \cdots O2W ⁱⁱ	0.84	2.40	3.149 (5)	149
O1W—H2W \cdots O1	0.81	2.47	3.064 (5)	131
O2W—H3W \cdots O4 ^{viii}	0.83	2.59	2.992 (5)	111
O2W—H4W \cdots O1W ^{ix}	0.86	2.10	2.778 (5)	135

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

Fig. 1

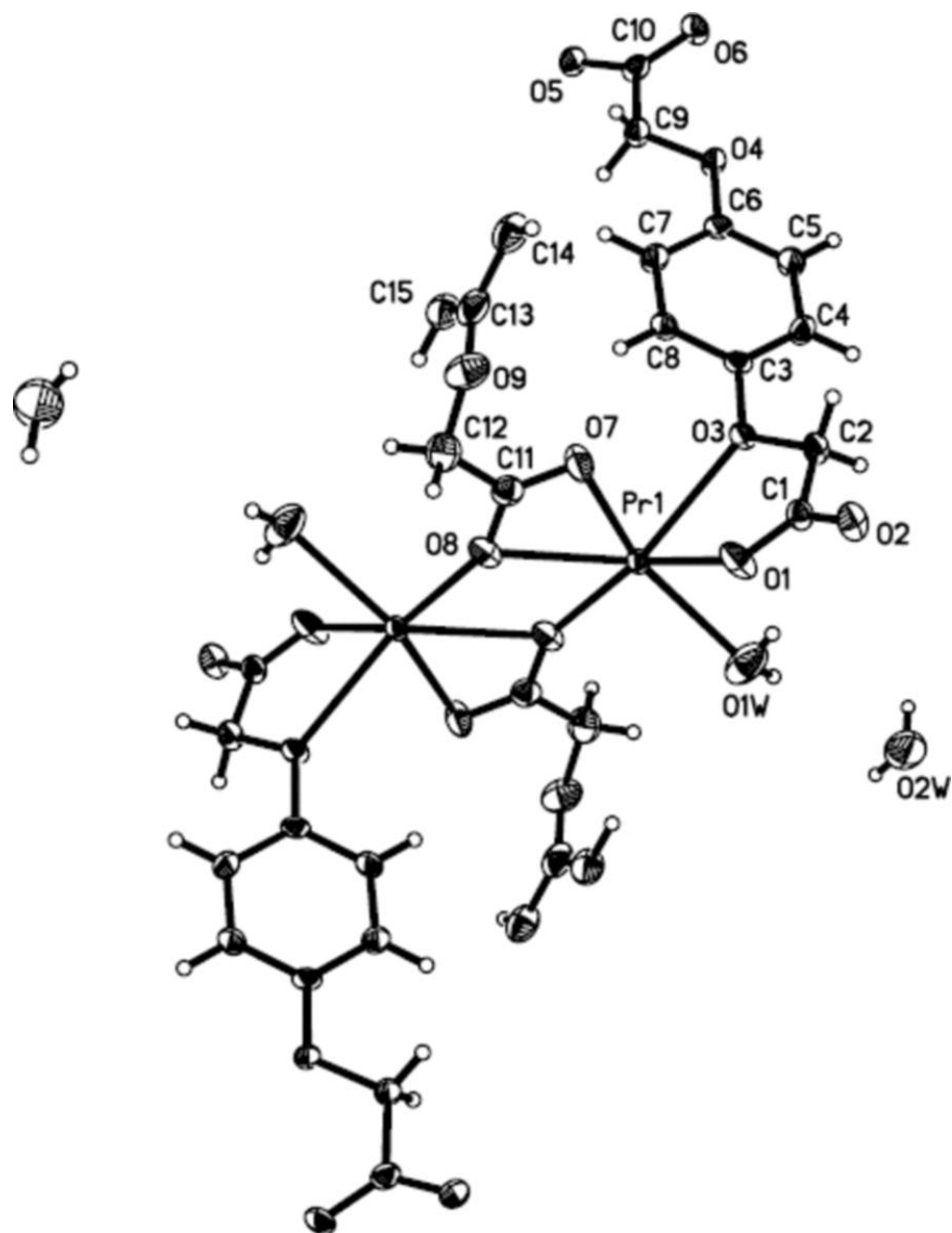


Fig. 2

