



Crystal structure and characterization of a new lanthanide coordination polymer, $[\text{Pr}_2(\text{pydc})(\text{phth})_2(\text{H}_2\text{O})_3] \cdot \text{H}_2\text{O}$

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Keywords: crystal structure; coordination polymer; lanthanide; pyridine-2,5-dicarboxylate; phthalate.

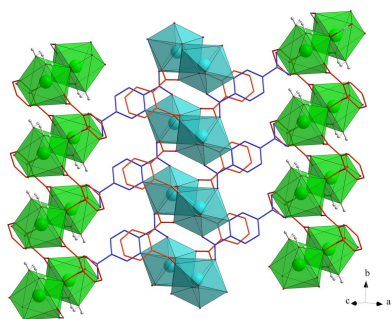
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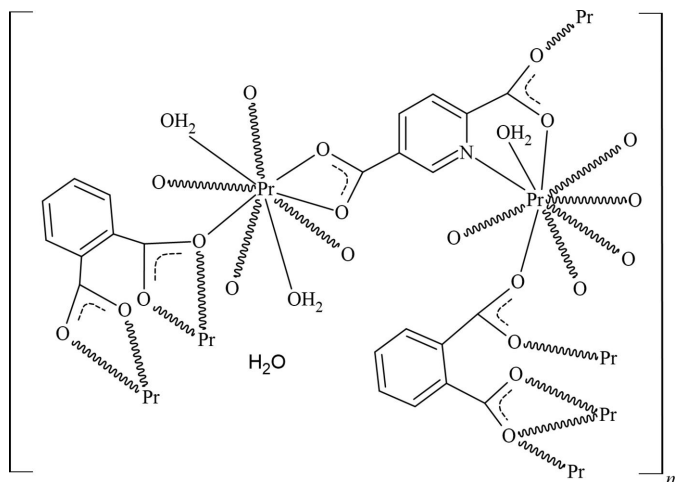
A new lanthanide coordination polymer, poly[[triquabis(μ_4 -phthalato)(μ_3 -pyridine-2,5-dicarboxylato)dipraseodymium] monohydrate], $\{[\text{Pr}_2(\text{C}_7\text{H}_3\text{NO}_4)_2(\text{C}_8\text{H}_4\text{O}_4)(\text{H}_2\text{O})_3] \cdot \text{H}_2\text{O}\}_n$ or $\{[\text{Pr}_2(\text{phth})_2(\text{pydc})(\text{H}_2\text{O})_3] \cdot \text{H}_2\text{O}\}_n$, (pydc^{2-} = pyridine-2,5-dicarboxylate and phth^{2-} = phthalate) was synthesized and characterized, revealing the structure to be an assembly of di-periodic $\{\text{Pr}_2(\text{pydc})(\text{phth})_2(\text{H}_2\text{O})_3\}_n$ layers. Each layer is built up by edge-sharing $\{\text{Pr}_2\text{N}_2\text{O}_{14}\}$ and $\{\text{Pr}_2\text{O}_{16}\}$ dimers, which are connected through a new coordination mode of pydc^{2-} and phth^{2-} . These layers are stabilized by internal hydrogen bonds and π - π interactions. In addition, a three-dimensional supramolecular framework is built by interlayer hydrogen-bonding interactions involving the non-coordinated water molecule. Thermogravimetric analysis shows that the title compound is thermally stable up to 400°C.

1. Chemical context

Lanthanide coordination polymers (LnCPs) have attracted widespread interest because of their unique properties and wide range of potential applications, such as in luminescent temperature sensing (Rocha *et al.*, 2016), catalysis (Sinchow *et al.*, 2022), gas detection (Thammakan *et al.*, 2023) and drug delivery (Wei *et al.*, 2020). However, the high coordination numbers of the trivalent lanthanides (Ln^{III}) and the versatility in their coordination geometries complicates the control of intermolecular interactions and the prediction of coordination polymer frameworks. In addition, the synthesis of these frameworks is also influenced considerably by differences in synthetic procedures and conditions such as solvents, pH, reaction temperature and time, among other factors (Sinchow *et al.*, 2019). Organic ligands are utilized as a template for the structural design, to direct the framework architecture. Among the organic ligands available, polycarboxylic acids are notably the most used because they are hard base ligands and can facilitate diverse coordination modes. In this work, pyridine-2,5-dicarboxylic acid (H_2pydc) and phthalic acid (H_2phth) were chosen to be the structure-directing ligands. Relevant structures include, for example, $[\text{Pr}_3(\text{phen})_2(\text{phth})_4(\text{NO}_3)] \cdot \text{H}_2\text{O}$ (phen = 1,10-phenanthroline) (refcode: LAXWOX; Thirumurugan & Natarajan, 2005), $[\text{Eu}(\text{phth})(\text{OAc})(\text{H}_2\text{O})]$ (OAc = acetate) (refcode: TAZDAD; Jittipiboonwat *et al.*, 2022), $[\text{Pr}(\text{pydc})(\text{pip})_{1/2}(\text{H}_2\text{O})]$ (pip = 2,5-piperazinedicarboxylate) (refcode: WUWBIB; Ay *et al.*, 2016) and $[\text{Pr}(\text{pydc})(\text{NA})\text{H}_2\text{O}]_n$ (NA = nicotinic acid) (refcode: MEJNEY; Hu *et al.*, 2022).



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2. Structural commentary

The asymmetric unit of $[\text{Pr}_2(\text{pydc})(\text{phth})_2(\text{H}_2\text{O})_3]\cdot\text{H}_2\text{O}$ is composed of two Pr^{III} metal centers, one molecule of pydc^{2-} , two molecules of phth^{2-} , three coordinated water molecules and a non-ligated water molecule (Fig. 1). The Pr1 ion is ninefold coordinated to one N atom from pydc^{2-} and eight O atoms from four phth^{2-} , two pydc^{2-} and one water molecule to form a $\{\text{Pr}(1)\text{NO}_8\}$ motif that can be described as a distorted tricapped trigonal prism. The Pr2 ion is also ninefold coordinated, being surrounded by nine O atoms from three phth^{2-} , one pydc^{2-} and two water molecules in a distorted tricapped trigonal-prismatic $\{\text{Pr}(2)\text{O}_9\}$ motif. The Pr–O bond lengths are in the range 2.413 (3)–2.691 (3) Å and the Pr–N bond is 2.696 (3) Å (Table 1), in accordance with a previous report for Pr^{III} frameworks of pydc^{2-} [2.390 (2)–2.717 (3) Å; Sinchow *et al.*, 2019] and phth^{2-} [2.456 (4)–2.696 (4) Å; Thirumurugan & Natarajan, 2005]. The $\{\text{Pr}(1)\text{NO}_8\}$ motif is linked to the adjacent Pr1, forming edge-sharing $\{\text{Pr}(1)_2\text{N}_2\text{O}_{14}\}$

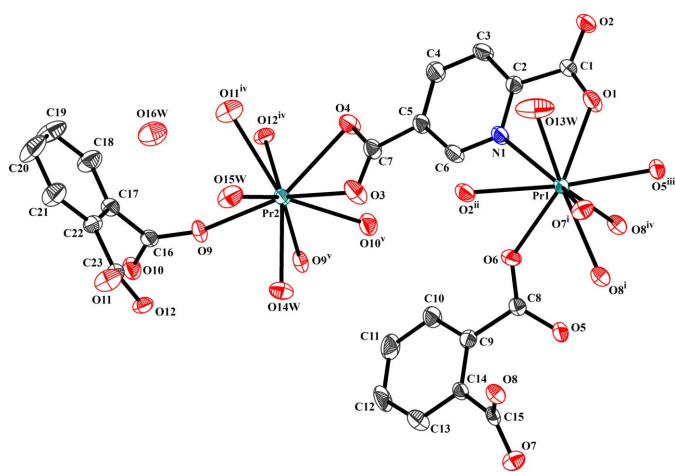


Figure 1

Extended asymmetric unit of $[\text{Pr}_2(\text{pydc})(\text{phth})_2(\text{H}_2\text{O})_3]\cdot\text{H}_2\text{O}$ drawn using 50% probability for ellipsoids (hydrogen atoms are omitted for clarity). Symmetry codes: (i) $-x + 1, -y + 2, -z + 1$; (ii) $x, y + 1, z$; (iii) $-x + 1, -y + 1, -z + 1$; (iv) $x, y - 1, z$; (v) $-x + \frac{3}{2}, -y + \frac{3}{2}, -z + \frac{1}{2}$.

Table 1

Selected bond lengths (Å).

Pr1–O7 ⁱ	2.536 (3)	Pr2–O12 ^{iv}	2.514 (2)
Pr1–O2 ⁱⁱ	2.580 (2)	Pr2–O15W	2.413 (3)
Pr1–O5 ⁱⁱⁱ	2.473 (2)	Pr2–O9 ^v	2.691 (3)
Pr1–O8 ⁱ	2.689 (2)	Pr2–O9	2.469 (2)
Pr1–O8 ^{iv}	2.473 (3)	Pr2–O4	2.526 (2)
Pr1–O6	2.446 (3)	Pr2–O10 ^v	2.510 (3)
Pr1–O1	2.439 (2)	Pr2–O3	2.575 (3)
Pr1–N1	2.696 (3)	Pr2–O14W	2.460 (2)
Pr1–O13W	2.571 (4)	Pr2–O11 ^{iv}	2.529 (3)

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

dimers, and two neighboring $\{\text{Pr}(1)_2\text{N}_2\text{O}_{14}\}$ dimers are fused through the $\mu_4\text{-}\eta^2\text{:}\eta^1\text{:}\eta^1\text{:}\eta^1$ carboxyl group of phth^{2-} to form an infinite chain in the b -axis direction. In a similar fashion, two $\{\text{Pr}(2)\text{O}_9\}$ motifs are linked to produce $\{\text{Pr}(2)_2\text{O}_{16}\}$ dimers. These dimers are then connected by the carboxyl groups of phth^{2-} in a $\mu_3\text{-}\eta^2\text{:}\eta^1\text{:}\eta^1\text{:}\eta^1$ fashion to form a mono-periodic chain also extending in the b -axis direction. These chains are connected through a novel coordination mode for pydc^{2-} involving a $\mu_1\text{-}\eta^1\text{:}\eta^1\text{:}\eta^1$ carboxyl group at one side and a $\mu_2\text{-}\eta^1\text{:}\eta^1$ carboxyl group together with the pyridyl N atom coordinated on the other side to form a $\{[\text{Pr}_2(\text{pydc})(\text{phth})_2(\text{H}_2\text{O})_3]\}_n$ layer extending in the (101) plane (Fig. 2a).

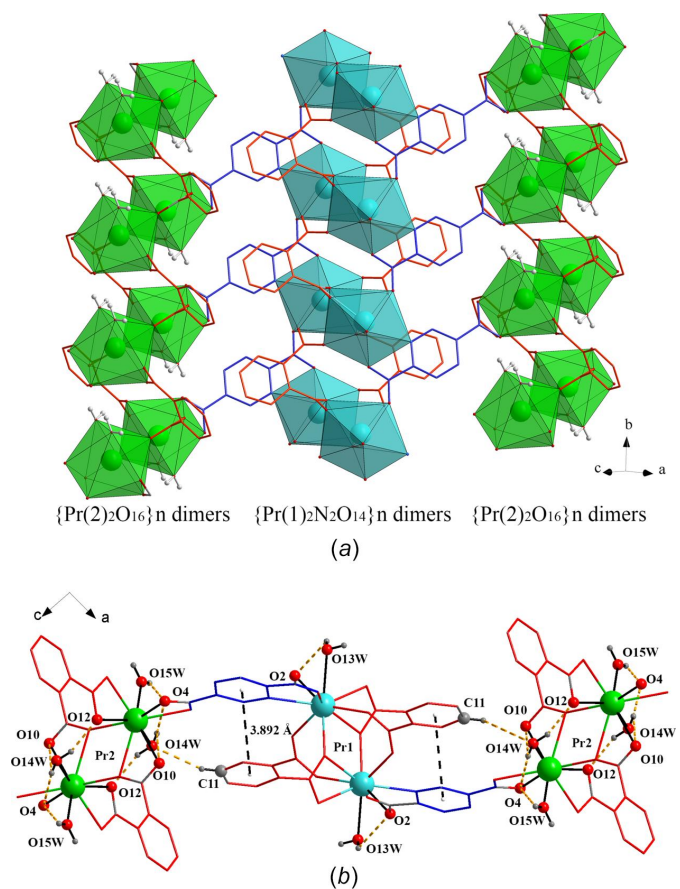


Figure 2

View of (a) the $\{\text{Pr}(1)_2\text{N}_2\text{O}_{14}\}$ and $\{\text{Pr}(2)_2\text{O}_{16}\}$ dimers in the (101) plane and (b) the hydrogen bonding and π – π interactions in the dimers.

Table 2

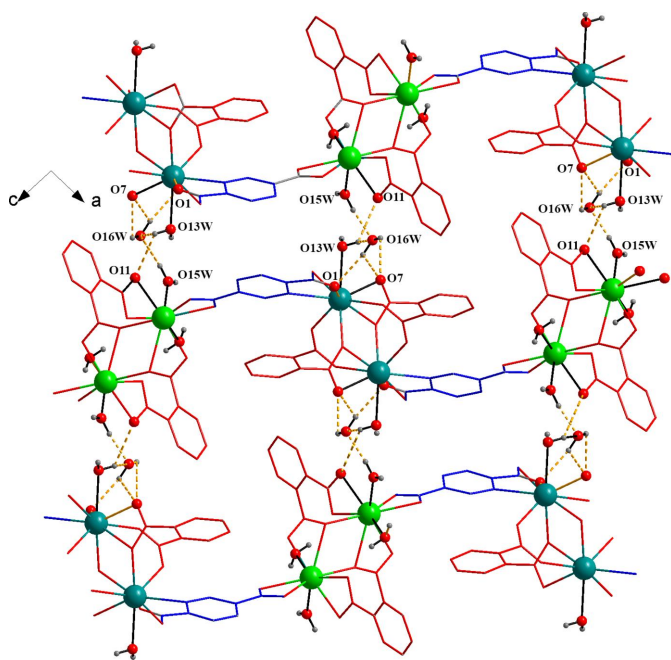
Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O13W–H13A \cdots O11 ^{vi}	0.85	2.57	3.003 (5)	113
O13W–H13A \cdots O16W ^{vi}	0.85	2.26	2.881 (5)	130
O13W–H13B \cdots O2 ⁱⁱ	0.86	2.52	2.820 (4)	102
O14W–H14A \cdots O12 ^{vii}	0.85	1.95	2.766 (4)	160
O14W–H14B \cdots O4 ⁱⁱ	0.85	2.04	2.887 (4)	174
O14W–H14B \cdots O10 ^{vii}	0.85	2.58	2.912 (4)	104
O15W–H15A \cdots O16W	0.85	1.75	2.595 (4)	170
O15W–H15B \cdots O4 ⁱⁱ	0.85	1.92	2.725 (3)	158
O16W–H16B \cdots O7 ^{viii}	0.85	2.31	2.709 (4)	109
O16W–H16B \cdots O1 ^{ix}	0.85	2.13	2.938 (5)	158
C11–H11 \cdots O14W	0.93	2.51	3.375 (5)	156

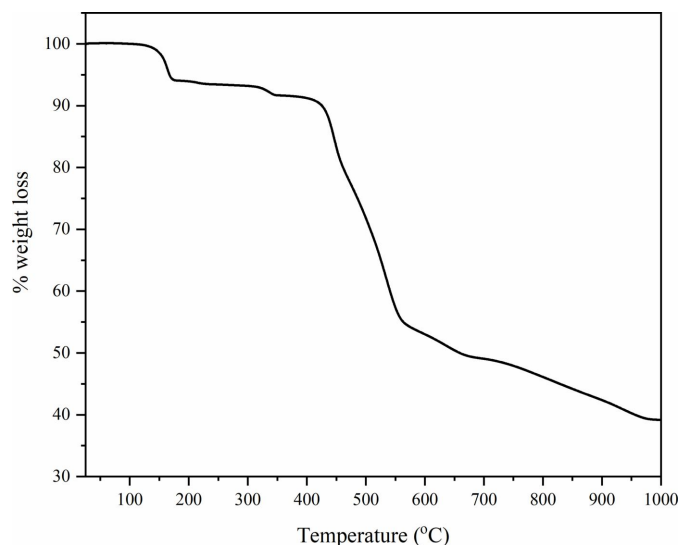
Symmetry codes: (ii) $x, y + 1, z$; (vi) $-x + \frac{3}{2}, y - 1, -z + 1$; (vii) $-x + \frac{3}{2}, -y + \frac{5}{2}, -z + \frac{1}{2}$; (viii) $x + \frac{1}{2}, -y + 2, z$; (ix) $-x + \frac{3}{2}, y + 1, -z + 1$.

3. Supramolecular features

The di-periodic supramolecular framework of the $\{[\text{Pr}_2(\text{pydc})(\text{pht})_2(\text{H}_2\text{O})_3]\}_n$ layers is further connected by intralayer hydrogen bonding, *i.e.* O13W–H13B \cdots O2, O14W–H14A \cdots O12, O14W–H14B \cdots O4, O14W–H14B \cdots O10, O15W–H15B \cdots O4 and C11–H11 \cdots O14W interactions and π – π interactions (Fig. 2*b* and Table 2). The π – π interaction between two aromatic rings (pydc²⁻ and pht²⁻) is classified as a parallel stacked geometry (Banerjee *et al.*, 2019), with an offset of 1.250 Å, interplanar angle of 5.96° and centroid-to-centroid distance of 3.892 (2) Å. In addition, the interlayer hydrogen-bonding interactions involve the coordinated water (O13W) and the hydrogen-bonded water (O16W). These interactions are O13W–H13A \cdots O11, O13W–H13A \cdots O16W, O15W–H15A \cdots O16W, O16W–


Figure 3

Three-dimensional supramolecular framework of $[\text{Pr}_2(\text{pydc})(\text{pht})_2(\text{H}_2\text{O})_3]\cdot\text{H}_2\text{O}$.


Figure 4

Thermogravimetric analysis of $[\text{Pr}_2(\text{pydc})(\text{pht})_2(\text{H}_2\text{O})_3]\cdot\text{H}_2\text{O}$.

H16A \cdots O7, O16W–H16B \cdots O1 and O16W–H16B \cdots O7 interactions (Fig. 3 and Table 2).

4. Thermogravimetric analysis

The thermogravimetric curve of the title compound shows four steps of weight loss in the temperature range 30°C to 1000°C (Fig. 4). The first step occurs at 100–185°C with a 6.0% weight loss attributed to the removal of one hydrogen-bonded water and two coordinated water molecules (calc. 6.4%). The second step observed at 300–350°C is due to the loss of the other coordinated water molecule (exp. 2.5%, calc. 2.1%). This step is possibly due to the removal of O14W, which is held by both strong and weak hydrogen-bonding interactions. The next step of weight loss occurs in the temperature range 400–580°C and represents a higher weight loss of 37.3%. This step can be attributed to the pyrolysis of the organic ligands (two pht²⁻ ligands, calc. 38.7%). The last step of weight loss, from 580 to 1000°C, could be due to the elimination of the bridging pydc²⁻ ligand to form praseodymium oxide residues (exp. 14.7%, calc. 19.5%).

5. Database survey

A search for the title compound in the Cambridge Structural Database (CSD version 5.44, April 2023; Groom *et al.*, 2016) using CONQUEST software (version 2023.2.0; Bruno *et al.*, 2002) did not match with any reported structures. Regarding organic ligands, there were 123 structures of lanthanide coordination polymers that included pydc²⁻. Among these structures, interestingly, there were none in which pydc²⁻ adopts the same coordination mode as in the title compound (Sinchow *et al.*, 2019). This new mode of coordination acts as a μ_3 -bridge to link three Pr^{III} ions and facilitates the formation of a di-periodic coordination framework. Regarding pht²⁻, there were 118 structures deposited in the CSD, none of which

contains pydc^{2-} in the structure. However, there is a structure including both pydc^{2-} and phth^{2-} ligands that incorporates a first-row transition metal: $[\text{Gd}_2(\text{H}_2\text{O})_2\text{Ni}(\text{H}_2\text{O})_2(\text{phth})_2(\text{pydc})_2]_3 \cdot 8\text{H}_2\text{O}$ (refcode: XOZYER; Mahata *et al.*, 2009).

6. Synthesis and crystallization

All chemicals were used as received without further purification: Pr_6O_{11} (TJTM, 99.9%), pyridine-2,5-dicarboxylic acid (H_2pydc ; Sigma-Aldrich, 98%), 1,2-benzenedicarboxylic acid (H_2phth ; Sigma-Aldrich, 98%) and NaOH (QReC, 99%). The $\text{Pr}(\text{NO}_3)_3 \cdot 6\text{H}_2\text{O}$ precursor was prepared by crystallization from solution of the lanthanide oxide in nitric acid (RCI Labscan, 65%).

To synthesize $[\text{Pr}_2(\text{pydc})(\text{phth})_2(\text{H}_2\text{O})_3] \cdot \text{H}_2\text{O}$, a solution of H_2pydc (0.125 mmol, 20.8 mg) and H_2phth (0.25 mmol, 41.5 mg) was prepared in 8 mL of deionized water, then 1.35 mL of 0.5 M NaOH were added and the pH adjusted to 5. $\text{Pr}(\text{NO}_3)_3 \cdot 6\text{H}_2\text{O}$ (0.25 mmol, 146.6 mg) was dissolved in 2 mL of deionized water and mixed with the ligand solution. The reaction mixture was then transferred into a 23 mL Teflon-lined hydrothermal reactor and held at 423 K for 72 h. Green block-shaped crystals were collected and dried at room temperature. The crystals were characterized using FT-IR spectroscopy (Nicolet iS5 FTIR Spectrometer; iD5 ATR mode; cm^{-1}): 3243(*br*), 1615(*w*), 1575(*m*), 1543(*m*), 1517(*m*), 1481(*m*), 1450(*w*), 1391(*m*), 1354(*m*), 1283(*w*), 1143(*w*), 1088(*w*), 1028(*w*), 870(*w*), 840(*m*), 762(*m*), 670(*m*), 648(*w*). The FT-IR spectrum shows a broad band at 3243 cm^{-1} attributed to the $\nu(\text{O}-\text{H})$ stretching from the water molecules. The characteristic peak at 1615 cm^{-1} corresponds to the $\text{C}=\text{O}$ stretching vibrational mode of the carboxylate group. The peak at 1283 cm^{-1} is due to the $\text{C}-\text{N}$ stretching of the pydc^{2-} ligand.

Thermogravimetric analyses (TGA) were carried out using a Mettler Toledo TGA/DSC 3+, with a heating rate of 20 °C min^{-1} , ramping from 30 to 1100 °C under a nitrogen gas flow.

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. All hydrogen atoms of aromatic rings and water molecules were positioned geometrically and refined using a riding model with $U_{\text{iso}}(\text{H}) = 1.2-1.5U_{\text{eq}}(\text{C}, \text{O})$.

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Table 3
Experimental details.

Crystal data	
Chemical formula	$[\text{Pr}_2(\text{C}_7\text{H}_3\text{NO}_4)_2(\text{C}_8\text{H}_4\text{O}_4)(\text{H}_2\text{O})_3] \cdot \text{H}_2\text{O}$
M_r	847.21
Crystal system, space group	Monoclinic, <i>I2/a</i>
Temperature (K)	293
a, b, c (Å)	27.4898 (4), 5.9436 (1), 32.0473 (5)
β (°)	93.854 (1)
V (Å ³)	5224.31 (14)
Z	8
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	3.77
Crystal size (mm)	0.3 × 0.2 × 0.08
Data collection	
Diffractometer	SuperNova, Single source at offset/far, HyPix3000
Absorption correction	Multi-scan (<i>CrysAlis PRO</i> ; Rigaku OD, 2019)
$T_{\text{min}}, T_{\text{max}}$	0.448, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	26747, 5561, 5004
R_{int}	0.062
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.648
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.031, 0.081, 1.05
No. of reflections	5561
No. of parameters	387
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³)	1.03, -1.08

Computer programs: *CrysAlis PRO* (Rigaku OD, 2019), *SHELXT2018/2* (Sheldrick, 2015a), *SHELXL2018/3* (Sheldrick, 2015b) and *OLEX2* (Dolomanov *et al.*, 2009).

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supporting information

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Computing details

Poly[[triquabis(μ_4 -phthalato)(μ_3 -pyridine-2,5-dicarboxylato)dipraseodymium] monohydrate]

Crystal data

$[\text{Pr}_2(\text{C}_7\text{H}_3\text{NO}_4)_2(\text{C}_8\text{H}_4\text{O}_4)(\text{H}_2\text{O})_3]\cdot\text{H}_2\text{O}$

$M_r = 847.21$

Monoclinic, $I2/a$

$a = 27.4898$ (4) Å

$b = 5.9436$ (1) Å

$c = 32.0473$ (5) Å

$\beta = 93.854$ (1)°

$V = 5224.31$ (14) Å³

$Z = 8$

$F(000) = 3280$

$D_x = 2.154$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 20454 reflections

$\theta = 2.0\text{--}27.3^\circ$

$\mu = 3.77$ mm⁻¹

$T = 293$ K

Block, clear light green

$0.3 \times 0.2 \times 0.08$ mm

Data collection

SuperNova, Single source at offset/far,

HyPix3000

diffractometer

Radiation source: micro-focus sealed X-ray

tube, SuperNova (Mo) X-ray Source

Mirror monochromator

Detector resolution: 10.0000 pixels mm⁻¹

ω scans

Absorption correction: multi-scan

(CrysAlisPro; Rigaku OD, 2019)

$T_{\min} = 0.448$, $T_{\max} = 1.000$

26747 measured reflections

5561 independent reflections

5004 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.062$

$\theta_{\max} = 27.4^\circ$, $\theta_{\min} = 1.9^\circ$

$h = -32 \rightarrow 34$

$k = -7 \rightarrow 7$

$l = -40 \rightarrow 40$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.031$

$wR(F^2) = 0.081$

$S = 1.05$

5561 reflections

387 parameters

0 restraints

Primary atom site location: dual

Hydrogen site location: mixed

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0445P)^2]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.003$

$\Delta\rho_{\max} = 1.03$ e Å⁻³

$\Delta\rho_{\min} = -1.08$ e Å⁻³

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. The crystal structure was solved using the dual-space algorithm with the SHELXT program (Sheldrick, 2015a) and refined on F^2 by the full-matrix least-squares technique using the SHELXL program (Sheldrick, 2015b) via the Olex2 interface (Dolomanov *et al.*, 2009).

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Pr1	0.57085 (2)	0.43694 (3)	0.52003 (2)	0.01775 (8)
Pr2	0.75715 (2)	0.65833 (3)	0.31515 (2)	0.01807 (8)
O7	0.45283 (10)	1.3428 (4)	0.41664 (9)	0.0278 (6)
O2	0.63896 (9)	−0.2639 (4)	0.52143 (8)	0.0258 (6)
O12	0.80011 (9)	1.3574 (4)	0.27660 (8)	0.0233 (6)
O5	0.48823 (9)	0.7809 (4)	0.44133 (8)	0.0245 (6)
O8	0.50558 (9)	1.2895 (4)	0.47057 (8)	0.0225 (6)
O15W	0.79900 (10)	0.9333 (4)	0.35981 (10)	0.0348 (7)
H15A	0.828906	0.931811	0.368452	0.052*
H15B	0.788865	1.062225	0.366759	0.052*
O9	0.79607 (10)	0.8562 (4)	0.25842 (8)	0.0247 (6)
O4	0.74925 (10)	0.3284 (4)	0.36394 (9)	0.0288 (7)
O10	0.82266 (10)	1.0318 (4)	0.20438 (9)	0.0285 (6)
O6	0.56535 (10)	0.6744 (4)	0.45754 (9)	0.0270 (6)
O3	0.71029 (11)	0.6308 (4)	0.38190 (9)	0.0332 (7)
O14W	0.70712 (9)	1.0001 (4)	0.30575 (9)	0.0272 (6)
H14A	0.711517	1.058376	0.282044	0.041*
H14B	0.717297	1.099306	0.323394	0.041*
O11	0.84297 (10)	1.5114 (5)	0.32951 (9)	0.0328 (7)
O1	0.59351 (10)	0.0418 (4)	0.52815 (9)	0.0314 (7)
N1	0.63969 (11)	0.2702 (5)	0.47251 (10)	0.0237 (7)
O16W	0.89141 (13)	0.9700 (6)	0.38119 (11)	0.0511 (9)
H16A	0.898260	0.843887	0.370560	0.077*
H16B	0.898930	0.954362	0.407190	0.077*
O13W	0.63638 (14)	0.3845 (6)	0.58034 (11)	0.0575 (10)
H13A	0.623288	0.331315	0.601685	0.086*
H13B	0.647446	0.512964	0.588387	0.086*
C15	0.49303 (14)	1.2686 (5)	0.43171 (12)	0.0201 (8)
C22	0.88149 (13)	1.2236 (6)	0.29160 (12)	0.0224 (8)
C17	0.87562 (14)	1.0344 (6)	0.26623 (12)	0.0226 (8)
C23	0.83927 (13)	1.3731 (6)	0.29984 (12)	0.0214 (8)
C6	0.66161 (14)	0.3836 (6)	0.44322 (12)	0.0236 (8)
H6	0.650321	0.527214	0.436258	0.028*
C16	0.82826 (14)	0.9752 (6)	0.24196 (12)	0.0209 (8)
C2	0.65666 (13)	0.0621 (5)	0.48235 (12)	0.0200 (8)
C8	0.53344 (13)	0.7948 (5)	0.43889 (12)	0.0192 (8)

C5	0.70056 (13)	0.2984 (6)	0.42248 (12)	0.0229 (8)
C1	0.62796 (14)	-0.0633 (5)	0.51323 (12)	0.0196 (8)
C14	0.52822 (13)	1.1759 (5)	0.40244 (12)	0.0194 (8)
C7	0.72085 (14)	0.4317 (6)	0.38760 (12)	0.0236 (9)
C18	0.91496 (15)	0.8966 (7)	0.26096 (15)	0.0364 (11)
H18	0.911010	0.769656	0.244119	0.044*
C21	0.92728 (15)	1.2708 (7)	0.31040 (14)	0.0347 (10)
H21	0.931630	1.397619	0.327226	0.042*
C4	0.71830 (15)	0.0895 (6)	0.43396 (13)	0.0299 (10)
H4	0.744967	0.029575	0.421450	0.036*
C11	0.59980 (15)	1.0454 (7)	0.35039 (14)	0.0355 (11)
H11	0.623695	1.001566	0.332856	0.043*
C3	0.69586 (14)	-0.0308 (6)	0.46450 (12)	0.0266 (9)
H3	0.707294	-0.172427	0.472697	0.032*
C10	0.58662 (14)	0.9040 (6)	0.38164 (13)	0.0271 (9)
H10	0.602064	0.765556	0.385436	0.033*
C9	0.55037 (13)	0.9663 (6)	0.40764 (12)	0.0213 (8)
C13	0.54177 (15)	1.3151 (6)	0.37105 (13)	0.0300 (10)
H13	0.526545	1.453984	0.367252	0.036*
C12	0.57745 (16)	1.2535 (7)	0.34501 (14)	0.0377 (11)
H12	0.586413	1.350458	0.324088	0.045*
C19	0.96019 (16)	0.9438 (8)	0.28028 (16)	0.0454 (13)
H19	0.986346	0.847910	0.276856	0.054*
C20	0.96632 (17)	1.1326 (8)	0.30449 (17)	0.0485 (13)
H20	0.996917	1.167448	0.316952	0.058*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pr1	0.01815 (13)	0.01481 (12)	0.02073 (14)	0.00126 (7)	0.00452 (9)	0.00299 (8)
Pr2	0.01974 (13)	0.01567 (12)	0.01921 (14)	0.00040 (7)	0.00422 (9)	0.00159 (8)
O7	0.0247 (15)	0.0284 (14)	0.0302 (17)	0.0052 (12)	0.0009 (13)	-0.0047 (12)
O2	0.0305 (15)	0.0164 (12)	0.0310 (16)	0.0006 (11)	0.0054 (13)	0.0040 (11)
O12	0.0186 (14)	0.0230 (13)	0.0278 (16)	0.0040 (11)	-0.0032 (12)	0.0000 (11)
O5	0.0222 (14)	0.0220 (13)	0.0300 (16)	-0.0022 (11)	0.0078 (12)	0.0052 (12)
O8	0.0312 (15)	0.0179 (12)	0.0184 (15)	-0.0023 (11)	0.0024 (12)	-0.0003 (11)
O15W	0.0267 (16)	0.0304 (15)	0.046 (2)	0.0023 (12)	-0.0064 (15)	-0.0147 (14)
O9	0.0262 (15)	0.0207 (12)	0.0280 (16)	-0.0066 (11)	0.0077 (12)	0.0032 (11)
O4	0.0362 (17)	0.0229 (13)	0.0292 (17)	0.0071 (12)	0.0155 (14)	0.0060 (11)
O10	0.0278 (15)	0.0332 (15)	0.0245 (16)	-0.0063 (12)	0.0020 (12)	0.0058 (12)
O6	0.0262 (15)	0.0261 (14)	0.0288 (16)	0.0055 (11)	0.0032 (13)	0.0105 (12)
O3	0.052 (2)	0.0198 (13)	0.0305 (17)	0.0036 (13)	0.0216 (15)	0.0004 (12)
O14W	0.0332 (16)	0.0228 (13)	0.0256 (16)	0.0057 (12)	0.0024 (13)	0.0019 (11)
O11	0.0314 (16)	0.0359 (15)	0.0299 (17)	0.0070 (13)	-0.0053 (13)	-0.0145 (13)
O1	0.0379 (17)	0.0202 (13)	0.0386 (18)	0.0036 (12)	0.0206 (14)	0.0074 (12)
N1	0.0259 (17)	0.0156 (14)	0.0306 (19)	0.0024 (13)	0.0097 (15)	0.0037 (14)
O16W	0.046 (2)	0.059 (2)	0.046 (2)	0.0062 (18)	-0.0142 (18)	0.0038 (17)
O13W	0.072 (3)	0.054 (2)	0.044 (2)	0.0244 (19)	-0.0162 (19)	0.0018 (17)

C15	0.023 (2)	0.0133 (16)	0.024 (2)	-0.0063 (15)	0.0044 (17)	0.0010 (15)
C22	0.021 (2)	0.0225 (18)	0.023 (2)	0.0021 (16)	0.0008 (16)	0.0015 (16)
C17	0.023 (2)	0.0228 (18)	0.022 (2)	0.0010 (16)	0.0028 (16)	0.0041 (16)
C23	0.020 (2)	0.0191 (17)	0.025 (2)	0.0008 (15)	0.0029 (17)	0.0022 (16)
C6	0.030 (2)	0.0174 (16)	0.024 (2)	0.0029 (16)	0.0075 (18)	0.0038 (16)
C16	0.021 (2)	0.0173 (17)	0.025 (2)	0.0039 (15)	0.0078 (17)	0.0030 (16)
C2	0.020 (2)	0.0177 (17)	0.022 (2)	0.0009 (14)	0.0037 (16)	-0.0003 (15)
C8	0.022 (2)	0.0146 (16)	0.021 (2)	0.0011 (15)	0.0046 (16)	-0.0022 (15)
C5	0.024 (2)	0.0221 (18)	0.023 (2)	0.0001 (16)	0.0077 (17)	0.0028 (16)
C1	0.023 (2)	0.0170 (17)	0.019 (2)	-0.0009 (15)	0.0020 (16)	0.0020 (14)
C14	0.0198 (19)	0.0174 (17)	0.021 (2)	-0.0037 (14)	0.0003 (16)	0.0019 (14)
C7	0.028 (2)	0.0210 (19)	0.023 (2)	-0.0004 (16)	0.0091 (18)	0.0012 (16)
C18	0.027 (2)	0.035 (2)	0.047 (3)	0.0083 (19)	0.004 (2)	-0.007 (2)
C21	0.026 (2)	0.034 (2)	0.044 (3)	0.0017 (19)	-0.001 (2)	-0.009 (2)
C4	0.029 (2)	0.0241 (19)	0.039 (3)	0.0037 (17)	0.014 (2)	0.0032 (18)
C11	0.029 (2)	0.046 (3)	0.033 (3)	-0.0025 (19)	0.015 (2)	0.003 (2)
C3	0.032 (2)	0.0202 (18)	0.029 (2)	0.0065 (16)	0.0095 (18)	0.0060 (16)
C10	0.028 (2)	0.0261 (19)	0.028 (2)	0.0016 (17)	0.0112 (18)	0.0018 (17)
C9	0.0182 (19)	0.0225 (18)	0.024 (2)	-0.0012 (15)	0.0035 (16)	0.0002 (16)
C13	0.039 (3)	0.0239 (19)	0.027 (2)	0.0015 (17)	0.005 (2)	0.0052 (17)
C12	0.043 (3)	0.039 (2)	0.033 (3)	-0.006 (2)	0.018 (2)	0.014 (2)
C19	0.026 (2)	0.053 (3)	0.056 (3)	0.018 (2)	0.000 (2)	-0.010 (3)
C20	0.018 (2)	0.063 (3)	0.063 (4)	0.002 (2)	-0.008 (2)	-0.012 (3)

Geometric parameters (Å, °)

Pr1—Pr1 ⁱ	4.0877 (4)	N1—C2	1.352 (4)
Pr1—O7 ⁱⁱ	2.536 (3)	O16W—H16A	0.8495
Pr1—O2 ⁱⁱⁱ	2.580 (2)	O16W—H16B	0.8500
Pr1—O5 ⁱ	2.473 (2)	O13W—H13A	0.8548
Pr1—O8 ⁱⁱ	2.689 (2)	O13W—H13B	0.8552
Pr1—O8 ^{iv}	2.473 (3)	C15—C14	1.497 (5)
Pr1—O6	2.446 (3)	C22—C17	1.391 (5)
Pr1—O1	2.439 (2)	C22—C23	1.499 (5)
Pr1—N1	2.696 (3)	C22—C21	1.387 (5)
Pr1—O13W	2.571 (4)	C17—C16	1.513 (5)
Pr1—C15 ⁱⁱ	2.984 (4)	C17—C18	1.376 (5)
Pr2—O12 ^{iv}	2.514 (2)	C6—H6	0.9300
Pr2—O15W	2.413 (3)	C6—C5	1.393 (5)
Pr2—O9 ^v	2.691 (3)	C2—C1	1.504 (5)
Pr2—O9	2.469 (2)	C2—C3	1.370 (5)
Pr2—O4	2.526 (2)	C8—C9	1.523 (5)
Pr2—O10 ^v	2.510 (3)	C5—C7	1.507 (5)
Pr2—O3	2.575 (3)	C5—C4	1.375 (5)
Pr2—O14W	2.460 (2)	C14—C9	1.392 (5)
Pr2—O11 ^{iv}	2.529 (3)	C14—C13	1.373 (5)
Pr2—C23 ^{iv}	2.891 (4)	C18—H18	0.9300
Pr2—C16 ^v	2.986 (4)	C18—C19	1.380 (6)

O7—C15	1.256 (5)	C21—H21	0.9300
O2—C1	1.254 (4)	C21—C20	1.374 (6)
O12—C23	1.271 (4)	C4—H4	0.9300
O5—C8	1.253 (4)	C4—C3	1.390 (5)
O8—C15	1.276 (4)	C11—H11	0.9300
O15W—H15A	0.8498	C11—C10	1.375 (5)
O15W—H15B	0.8499	C11—C12	1.386 (5)
O9—C16	1.274 (4)	C3—H3	0.9300
O4—C7	1.281 (4)	C10—H10	0.9300
O10—C16	1.250 (4)	C10—C9	1.391 (5)
O6—C8	1.252 (4)	C13—H13	0.9300
O3—C7	1.229 (4)	C13—C12	1.379 (5)
O14W—H14A	0.8511	C12—H12	0.9300
O14W—H14B	0.8512	C19—H19	0.9300
O11—C23	1.256 (4)	C19—C20	1.368 (6)
O1—C1	1.255 (4)	C20—H20	0.9300
N1—C6	1.332 (4)		
O7 ⁱⁱ —Pr1—Pr1 ⁱ	82.31 (6)	C23 ^{iv} —Pr2—C16 ^v	109.32 (10)
O7 ⁱⁱ —Pr1—O2 ⁱⁱⁱ	81.68 (8)	C15—O7—Pr1 ⁱⁱ	98.1 (2)
O7 ⁱⁱ —Pr1—O8 ⁱⁱ	49.76 (8)	C1—O2—Pr1 ^{iv}	119.2 (2)
O7 ⁱⁱ —Pr1—N1	150.37 (10)	C23—O12—Pr2 ⁱⁱⁱ	93.8 (2)
O7 ⁱⁱ —Pr1—O13W	70.46 (10)	C8—O5—Pr1 ⁱ	138.9 (2)
O7 ⁱⁱ —Pr1—C15 ⁱⁱ	24.63 (10)	Pr1 ⁱⁱⁱ —O8—Pr1 ⁱⁱ	104.62 (8)
O2 ⁱⁱⁱ —Pr1—Pr1 ⁱ	123.65 (6)	C15—O8—Pr1 ⁱⁱⁱ	142.8 (2)
O2 ⁱⁱⁱ —Pr1—O8 ⁱⁱ	98.79 (7)	C15—O8—Pr1 ⁱⁱ	90.4 (2)
O2 ⁱⁱⁱ —Pr1—N1	74.17 (8)	Pr2—O15W—H15A	126.8
O2 ⁱⁱⁱ —Pr1—C15 ⁱⁱ	92.20 (8)	Pr2—O15W—H15B	127.9
O5 ⁱ —Pr1—Pr1 ⁱ	67.00 (6)	H15A—O15W—H15B	104.5
O5 ⁱ —Pr1—O7 ⁱⁱ	69.95 (8)	Pr2—O9—Pr2 ^v	113.13 (9)
O5 ⁱ —Pr1—O2 ⁱⁱⁱ	148.44 (9)	C16—O9—Pr2	156.4 (3)
O5 ⁱ —Pr1—O8 ⁱⁱ	73.52 (7)	C16—O9—Pr2 ^v	90.4 (2)
O5 ⁱ —Pr1—N1	126.85 (8)	C7—O4—Pr2	94.3 (2)
O5 ⁱ —Pr1—O13W	90.61 (11)	C16—O10—Pr2 ^v	99.7 (2)
O5 ⁱ —Pr1—C15 ⁱⁱ	67.57 (8)	C8—O6—Pr1	136.3 (2)
O8 ^{iv} —Pr1—Pr1 ⁱ	39.54 (6)	C7—O3—Pr2	93.4 (2)
O8 ⁱⁱ —Pr1—Pr1 ⁱ	35.83 (6)	Pr2—O14W—H14A	109.5
O8 ^{iv} —Pr1—O7 ⁱⁱ	118.78 (9)	Pr2—O14W—H14B	109.6
O8 ^{iv} —Pr1—O2 ⁱⁱⁱ	138.56 (8)	H14A—O14W—H14B	104.5
O8 ^{iv} —Pr1—O5 ⁱ	70.29 (9)	C23—O11—Pr2 ⁱⁱⁱ	93.5 (2)
O8 ^{iv} —Pr1—O8 ⁱⁱ	75.37 (8)	C1—O1—Pr1	129.2 (2)
O8 ⁱⁱ —Pr1—N1	150.31 (9)	C6—N1—Pr1	125.4 (2)
O8 ^{iv} —Pr1—N1	90.82 (9)	C6—N1—C2	117.5 (3)
O8 ^{iv} —Pr1—O13W	151.68 (10)	C2—N1—Pr1	116.7 (2)
O8 ^{iv} —Pr1—C15 ⁱⁱ	96.50 (10)	H16A—O16W—H16B	104.5
O8 ⁱⁱ —Pr1—C15 ⁱⁱ	25.31 (9)	Pr1—O13W—H13A	109.6
O6—Pr1—Pr1 ⁱ	68.41 (6)	Pr1—O13W—H13B	109.6
O6—Pr1—O7 ⁱⁱ	110.62 (9)	H13A—O13W—H13B	104.4

O6—Pr1—O2 ⁱⁱⁱ	67.76 (9)	O7—C15—Pr1 ⁱⁱ	57.32 (19)
O6—Pr1—O5 ⁱ	134.86 (9)	O7—C15—O8	121.0 (3)
O6—Pr1—O8 ^{iv}	71.19 (9)	O7—C15—C14	118.5 (3)
O6—Pr1—O8 ⁱⁱ	74.76 (8)	O8—C15—Pr1 ⁱⁱ	64.34 (18)
O6—Pr1—N1	75.93 (9)	O8—C15—C14	120.2 (3)
O6—Pr1—O13W	133.39 (12)	C14—C15—Pr1 ⁱⁱ	165.5 (2)
O6—Pr1—C15 ⁱⁱ	94.57 (9)	C17—C22—C23	121.4 (3)
O1—Pr1—Pr1 ⁱ	116.18 (7)	C21—C22—C17	118.9 (3)
O1—Pr1—O7 ⁱⁱ	119.27 (9)	C21—C22—C23	119.6 (3)
O1—Pr1—O2 ⁱⁱⁱ	118.80 (9)	C22—C17—C16	123.4 (3)
O1—Pr1—O5 ⁱ	67.30 (8)	C18—C17—C22	119.5 (4)
O1—Pr1—O8 ⁱⁱ	140.00 (8)	C18—C17—C16	117.1 (3)
O1—Pr1—O8 ^{iv}	84.05 (9)	O12—C23—Pr2 ⁱⁱⁱ	60.15 (18)
O1—Pr1—O6	130.10 (9)	O12—C23—C22	119.2 (3)
O1—Pr1—N1	61.47 (8)	O11—C23—Pr2 ⁱⁱⁱ	60.80 (19)
O1—Pr1—O13W	69.03 (11)	O11—C23—O12	121.0 (3)
O1—Pr1—C15 ⁱⁱ	131.64 (9)	O11—C23—C22	119.8 (4)
N1—Pr1—Pr1 ⁱ	125.47 (7)	C22—C23—Pr2 ⁱⁱⁱ	179.4 (3)
N1—Pr1—C15 ⁱⁱ	165.50 (9)	N1—C6—H6	118.3
O13W—Pr1—Pr1 ⁱ	149.66 (8)	N1—C6—C5	123.4 (3)
O13W—Pr1—O2 ⁱⁱⁱ	66.39 (11)	C5—C6—H6	118.3
O13W—Pr1—O8 ⁱⁱ	120.15 (9)	O9—C16—Pr2 ^v	64.3 (2)
O13W—Pr1—N1	84.09 (11)	O9—C16—C17	120.9 (3)
O13W—Pr1—C15 ⁱⁱ	95.07 (11)	O10—C16—Pr2 ^v	56.0 (2)
C15 ⁱⁱ —Pr1—Pr1 ⁱ	58.24 (8)	O10—C16—O9	120.3 (4)
O12 ^{iv} —Pr2—O9 ^v	78.00 (8)	O10—C16—C17	118.6 (3)
O12 ^{iv} —Pr2—O4	79.32 (8)	C17—C16—Pr2 ^v	172.4 (2)
O12 ^{iv} —Pr2—O3	129.85 (8)	N1—C2—C1	114.8 (3)
O12 ^{iv} —Pr2—O11 ^{iv}	51.70 (9)	N1—C2—C3	122.7 (3)
O12 ^{iv} —Pr2—C23 ^{iv}	26.01 (9)	C3—C2—C1	122.5 (3)
O12 ^{iv} —Pr2—C16 ^v	83.43 (9)	O5—C8—C9	115.7 (3)
O15W—Pr2—O12 ^{iv}	123.55 (9)	O6—C8—O5	126.7 (3)
O15W—Pr2—O9 ^v	138.66 (9)	O6—C8—C9	117.5 (3)
O15W—Pr2—O9	84.33 (10)	C6—C5—C7	119.8 (3)
O15W—Pr2—O4	102.48 (10)	C4—C5—C6	118.1 (3)
O15W—Pr2—O10 ^v	145.79 (9)	C4—C5—C7	122.1 (3)
O15W—Pr2—O3	78.21 (10)	O2—C1—O1	124.8 (3)
O15W—Pr2—O14W	75.74 (9)	O2—C1—C2	118.6 (3)
O15W—Pr2—O11 ^{iv}	73.99 (9)	O1—C1—C2	116.5 (3)
O15W—Pr2—C23 ^{iv}	98.70 (10)	C9—C14—C15	123.4 (3)
O15W—Pr2—C16 ^v	150.18 (9)	C13—C14—C15	117.1 (3)
O9—Pr2—O12 ^{iv}	74.68 (8)	C13—C14—C9	119.3 (3)
O9—Pr2—O9 ^v	66.86 (9)	O4—C7—C5	117.2 (3)
O9—Pr2—O4	152.26 (8)	O3—C7—O4	121.4 (3)
O9—Pr2—O10 ^v	116.47 (9)	O3—C7—C5	121.4 (3)
O9—Pr2—O3	155.19 (8)	C17—C18—H18	119.5
O9—Pr2—O11 ^{iv}	81.57 (9)	C17—C18—C19	121.1 (4)
O9 ^v —Pr2—C23 ^{iv}	102.54 (10)	C19—C18—H18	119.5

O9—Pr2—C23 ^{iv}	76.84 (9)	C22—C21—H21	119.6
O9—Pr2—C16 ^v	92.12 (10)	C20—C21—C22	120.9 (4)
O9 ^v —Pr2—C16 ^v	25.27 (8)	C20—C21—H21	119.6
O4—Pr2—O9 ^v	116.93 (9)	C5—C4—H4	120.4
O4—Pr2—O3	50.80 (8)	C5—C4—C3	119.2 (3)
O4—Pr2—O11 ^{iv}	74.77 (9)	C3—C4—H4	120.4
O4—Pr2—C23 ^{iv}	75.56 (9)	C10—C11—H11	120.0
O4—Pr2—C16 ^v	94.37 (10)	C10—C11—C12	120.0 (4)
O10 ^v —Pr2—O12 ^{iv}	89.35 (8)	C12—C11—H11	120.0
O10 ^v —Pr2—O9 ^v	49.64 (8)	C2—C3—C4	119.0 (3)
O10 ^v —Pr2—O4	72.22 (9)	C2—C3—H3	120.5
O10 ^v —Pr2—O3	72.59 (9)	C4—C3—H3	120.5
O10 ^v —Pr2—O11 ^{iv}	132.78 (8)	C11—C10—H10	119.7
O10 ^v —Pr2—C23 ^{iv}	111.90 (10)	C11—C10—C9	120.5 (4)
O10 ^v —Pr2—C16 ^v	24.37 (8)	C9—C10—H10	119.7
O3—Pr2—O9 ^v	116.93 (9)	C14—C9—C8	121.8 (3)
O3—Pr2—C23 ^{iv}	122.92 (10)	C10—C9—C8	118.6 (3)
O3—Pr2—C16 ^v	94.34 (10)	C10—C9—C14	119.5 (3)
O14W—Pr2—O12 ^{iv}	143.58 (9)	C14—C13—H13	119.2
O14W—Pr2—O9 ^v	69.69 (8)	C14—C13—C12	121.5 (4)
O14W—Pr2—O9	77.46 (8)	C12—C13—H13	119.2
O14W—Pr2—O4	130.24 (8)	C11—C12—H12	120.4
O14W—Pr2—O10 ^v	82.48 (9)	C13—C12—C11	119.3 (3)
O14W—Pr2—O3	81.23 (9)	C13—C12—H12	120.4
O14W—Pr2—O11 ^{iv}	144.54 (9)	C18—C19—H19	120.2
O14W—Pr2—C23 ^{iv}	154.13 (9)	C20—C19—C18	119.6 (4)
O14W—Pr2—C16 ^v	74.59 (9)	C20—C19—H19	120.2
O11 ^{iv} —Pr2—O9 ^v	126.43 (8)	C21—C20—H20	120.0
O11 ^{iv} —Pr2—O3	109.85 (9)	C19—C20—C21	120.0 (4)
O11 ^{iv} —Pr2—C23 ^{iv}	25.69 (10)	C19—C20—H20	120.0
O11 ^{iv} —Pr2—C16 ^v	134.86 (9)		
Pr1 ⁱⁱ —O7—C15—O8	10.0 (3)	N1—C2—C1—O1	-3.9 (5)
Pr1 ⁱⁱ —O7—C15—C14	-163.8 (2)	N1—C2—C3—C4	-2.2 (6)
Pr1 ^{iv} —O2—C1—O1	46.5 (5)	C15—C14—C9—C8	11.8 (6)
Pr1 ^{iv} —O2—C1—C2	-131.6 (3)	C15—C14—C9—C10	-172.9 (4)
Pr1 ⁱ —O5—C8—O6	3.6 (6)	C15—C14—C13—C12	173.7 (4)
Pr1 ⁱ —O5—C8—C9	179.2 (2)	C22—C17—C16—O9	-88.4 (4)
Pr1 ⁱⁱⁱ —O8—C15—Pr1 ⁱⁱ	-115.2 (3)	C22—C17—C16—O10	96.6 (4)
Pr1 ⁱⁱⁱ —O8—C15—O7	-124.5 (4)	C22—C17—C18—C19	-0.3 (6)
Pr1 ⁱⁱ —O8—C15—O7	-9.3 (3)	C22—C21—C20—C19	-0.9 (8)
Pr1 ⁱⁱ —O8—C15—C14	164.4 (3)	C17—C22—C23—O12	-15.5 (5)
Pr1 ⁱⁱⁱ —O8—C15—C14	49.2 (5)	C17—C22—C23—O11	164.4 (4)
Pr1—O6—C8—O5	-21.5 (6)	C17—C22—C21—C20	-0.5 (6)
Pr1—O6—C8—C9	162.9 (2)	C17—C18—C19—C20	-1.1 (7)
Pr1—O1—C1—O2	174.8 (3)	C23—C22—C17—C16	5.7 (6)
Pr1—O1—C1—C2	-7.1 (5)	C23—C22—C17—C18	-177.2 (4)
Pr1—N1—C6—C5	173.0 (3)	C23—C22—C21—C20	177.9 (4)

Pr1—N1—C2—C1	11.0 (4)	C6—N1—C2—C1	-175.6 (3)
Pr1—N1—C2—C3	-171.3 (3)	C6—N1—C2—C3	2.1 (6)
Pr1 ⁱⁱ —C15—C14—C9	161.5 (9)	C6—C5—C7—O4	-165.8 (4)
Pr1 ⁱⁱ —C15—C14—C13	-13.1 (13)	C6—C5—C7—O3	13.7 (6)
Pr2 ⁱⁱⁱ —O12—C23—O11	-0.1 (4)	C6—C5—C4—C3	2.2 (6)
Pr2 ⁱⁱⁱ —O12—C23—C22	179.8 (3)	C16—C17—C18—C19	176.9 (4)
Pr2—O9—C16—Pr2 ^v	-176.4 (6)	C2—N1—C6—C5	0.2 (6)
Pr2 ^v —O9—C16—O10	1.1 (3)	C5—C4—C3—C2	0.0 (6)
Pr2—O9—C16—O10	-175.3 (4)	C1—C2—C3—C4	175.3 (4)
Pr2—O9—C16—C17	9.8 (8)	C14—C13—C12—C11	0.7 (7)
Pr2 ^v —O9—C16—C17	-173.8 (3)	C7—C5—C4—C3	-175.8 (4)
Pr2—O4—C7—O3	-4.0 (4)	C18—C17—C16—O9	94.5 (4)
Pr2—O4—C7—C5	175.5 (3)	C18—C17—C16—O10	-80.5 (5)
Pr2 ^v —O10—C16—O9	-1.2 (4)	C18—C19—C20—C21	1.8 (8)
Pr2 ^v —O10—C16—C17	173.8 (3)	C21—C22—C17—C16	-175.8 (4)
Pr2—O3—C7—O4	3.9 (4)	C21—C22—C17—C18	1.2 (6)
Pr2—O3—C7—C5	-175.5 (3)	C21—C22—C23—O12	166.1 (4)
Pr2 ⁱⁱⁱ —O11—C23—O12	0.1 (4)	C21—C22—C23—O11	-14.0 (6)
Pr2 ⁱⁱⁱ —O11—C23—C22	-179.8 (3)	C4—C5—C7—O4	12.2 (6)
O7—C15—C14—C9	-129.3 (4)	C4—C5—C7—O3	-168.4 (4)
O7—C15—C14—C13	56.1 (5)	C11—C10—C9—C8	173.9 (4)
O5—C8—C9—C14	39.7 (5)	C11—C10—C9—C14	-1.5 (6)
O5—C8—C9—C10	-135.6 (4)	C3—C2—C1—O2	-3.4 (6)
O8—C15—C14—C9	56.9 (5)	C3—C2—C1—O1	178.4 (4)
O8—C15—C14—C13	-117.7 (4)	C10—C11—C12—C13	-0.6 (7)
O6—C8—C9—C14	-144.3 (4)	C9—C14—C13—C12	-1.2 (6)
O6—C8—C9—C10	40.4 (5)	C13—C14—C9—C8	-173.7 (4)
N1—C6—C5—C7	175.6 (4)	C13—C14—C9—C10	1.6 (6)
N1—C6—C5—C4	-2.4 (6)	C12—C11—C10—C9	1.0 (7)
N1—C2—C1—O2	174.4 (3)		

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O13 W —H13A \cdots O11 ^{vi}	0.85	2.57	3.003 (5)	113
O13 W —H13A \cdots O16 W ^{vi}	0.85	2.26	2.881 (5)	130
O13 W —H13B \cdots O2 ⁱⁱⁱ	0.86	2.52	2.820 (4)	102
O14 W —H14A \cdots O12 ^{vii}	0.85	1.95	2.766 (4)	160
O14 W —H14B \cdots O4 ⁱⁱⁱ	0.85	2.04	2.887 (4)	174
O14 W —H14B \cdots O10 ^{vii}	0.85	2.58	2.912 (4)	104
O15 W —H15A \cdots O16 W	0.85	1.75	2.595 (4)	170
O15 W —H15B \cdots O4 ⁱⁱⁱ	0.85	1.92	2.725 (3)	158
O16 W —H16B \cdots O7 ^{viii}	0.85	2.31	2.709 (4)	109
O16 W —H16B \cdots O1 ^{ix}	0.85	2.13	2.938 (5)	158
C11—H11 \cdots O14 W	0.93	2.51	3.375 (5)	156

Symmetry codes: (iii) $x, y+1, z$; (vi) $-x+3/2, y-1, -z+1$; (vii) $-x+3/2, -y+5/2, -z+1/2$; (viii) $x+1/2, -y+2, z$; (ix) $-x+3/2, y+1, -z+1$.