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# Poly[[diaqua-$\mu_3$-citrato-praseodymium(III)] monohydrate]

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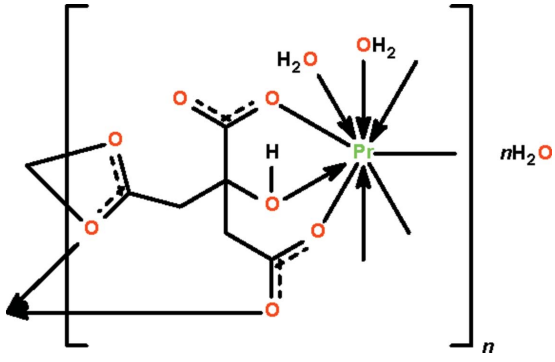
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.026; $wR$ factor = 0.050; data-to-parameter ratio = 13.5.

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 $\mu_3$-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
$\beta$ = 91.0672 (18)°
$V$ = 1039.22 (11) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 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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# supporting information

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## Poly[[diaqua-$\mu_3$-citrato-praseodymium(III)] monohydrate]

**Li-Jun Han, Yuan-Fu Deng and Seik Weng Ng**

### S1. 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-antiprismatic 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 $\mu_3$– 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).

### S2. 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 $Pr_6O_{11}$.

### S3. 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.

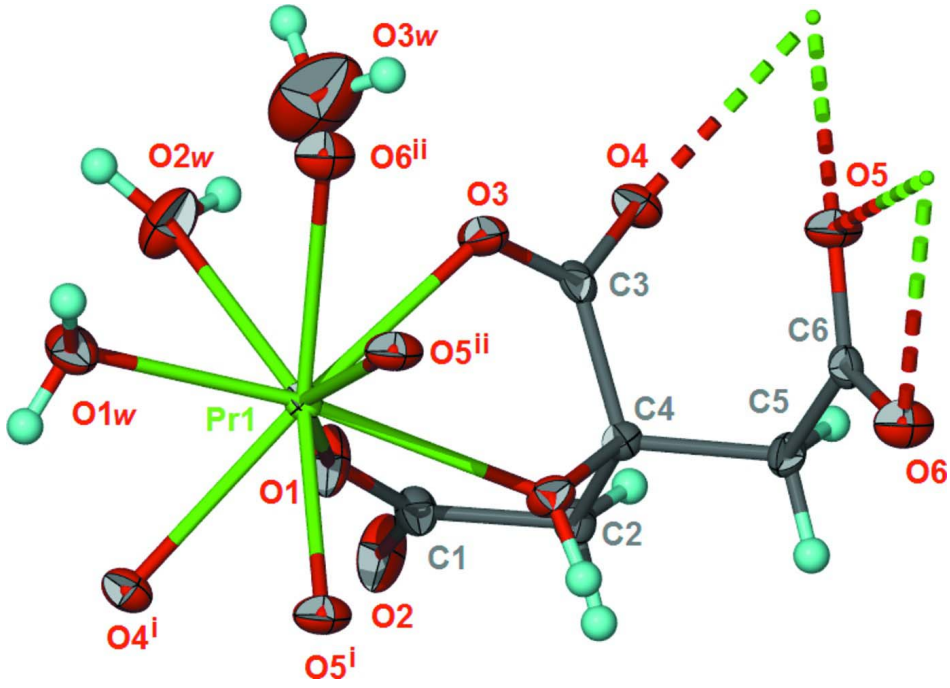


**Figure 1**

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.

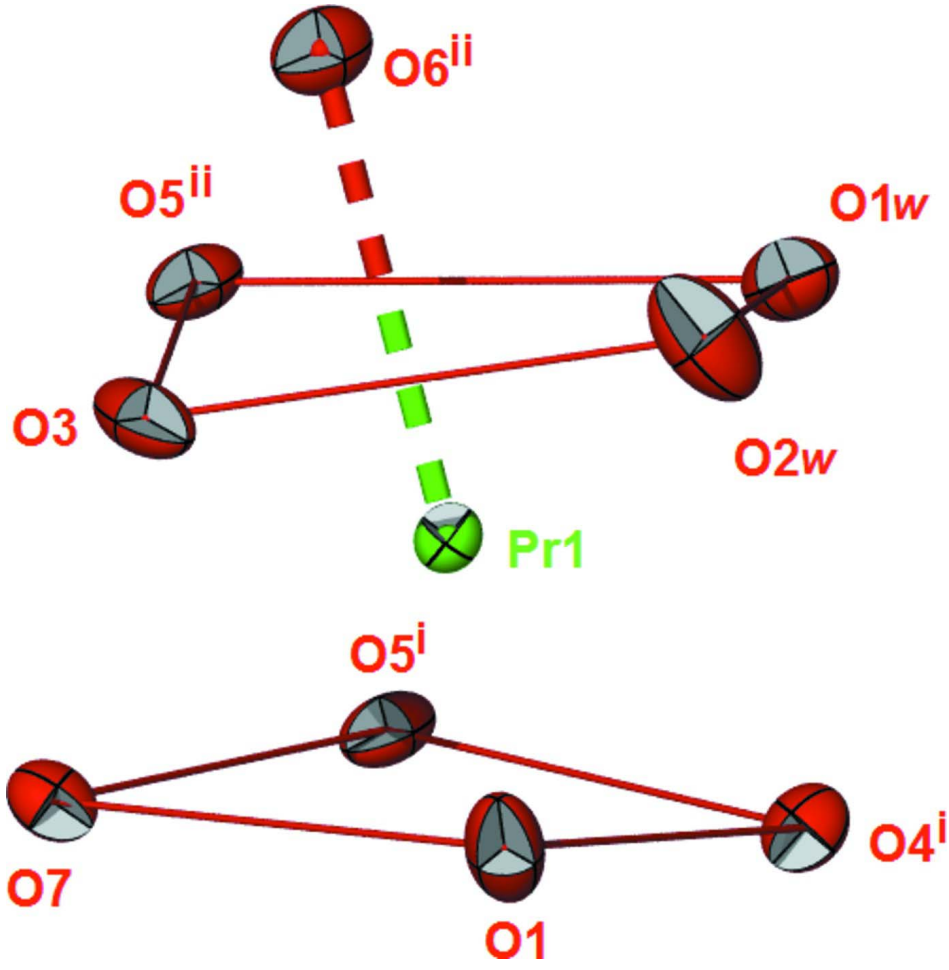


**Figure 2**

Nine-coordinate geometry of $Pr^{III}$.

**Poly[[diaqua-$\mu_3$-citrato-praseodymium(III)] monohydrate]**

*Crystal data*

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

*Data collection*

Rigaku R-AXIS RAPID diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 10.000 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.331$, $T_{max} = 0.649$
9596 measured reflections

2366 independent reflections
2182 reflections with $I > 2\sigma(I)$
$R_{int} = 0.038$
$\theta_{max} = 27.4°$, $\theta_{min} = 3.2°$
$h = -8 \rightarrow 8$
$k = -12 \rightarrow 10$
$l = -22 \rightarrow 22$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.026$
$wR(F^2) = 0.050$
$S = 1.18$
2366 reflections
175 parameters
10 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.P)^2 + 1.4664P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.76$ e Å$^{-3}$
$\Delta\rho_{min} = -0.81$ e Å$^{-3}$

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

| | *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 (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| 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, º)*

| | | | |
|---|---|---|---|
| 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, º)*

| *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: (i) $x-1, y, z$; (iv) $-x+1/2, y+1/2, -z+3/2$; (v) $x-1/2, -y+1/2, z-1/2$; (vi) $-x, -y, -z+1$; (vii) $x, y-1, z$.