Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Poly[tetraaquabis(μ_4-cyclohexane-1,4-dicarboxylato-$\kappa^6O:O,O':O'':O'',O'''$)-hemi($\mu_2$-cyclohexane-1,4-dicarboxylato-$\kappa^2O:O'$)hemi(μ_2-cyclohexane-1,4-dicarboxylato-$\kappa^4O,O':O'',O'''$)-dipraseodymium(III)]

Miao Yu, Shu-Xia Liu,* Lin-Hua Xie, Rui-Ge Cao and Yuan-Hang Ren

Key Laboratory of Polyoxometalates Science of the Ministry of Education, College of Chemistry, Northeast Normal University, Changchun 130024, People's Republic of China
Correspondence e-mail: liusx@nenu.edu.cn

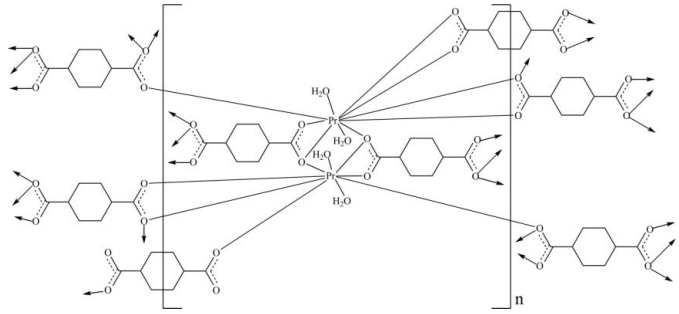
Received 4 June 2007; accepted 11 June 2007

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.006 Å; R factor = 0.024; wR factor = 0.051; data-to-parameter ratio = 13.5.

The title compound, $[Pr_2(C_8H_{10}O_4)_3(H_2O)_4]_n$ is a three-dimensional metal–organic framework built of chains of edge-sharing Pr^{III} polyhedra by the *e*,*e*-*trans*-cyclohexane-1,4-dicarboxylate (chdc) dianions. There are two types of Pr atoms (one in a ten-coordinate and the other in a nine-coordinate geometry) and four types of chdc ligands. One Pr atom is coordinated by eight carboxylate O atoms from five chdc and two water molecules, whereas the other is coordinated by seven carboxylate O atoms from five chdc and two water molecules. Two of the four chdc ligands are located on inversion centers. The ligation of alternate Pr atoms by the carboxylate groups of chdc ligands leads to an infinite chain; the chains are further connected with six neighboring chains through the chdc ligands, resulting in a three-dimensional network.

Related literature

For related literature on metal complexes of cyclohexane-1,4-dicarboxylic acid, see: Kurmoo *et al.* (2003, 2006); Qi *et al.* (2003); Rao *et al.* (2007); Yu *et al.* (2007); Rao *et al.* (2007).



Experimental

Crystal data

$[Pr_2(C_8H_{10}O_4)_3(H_2O)_4]$
M_r = 864.36
Triclinic, $P\overline{1}$
a = 11.439 (2) Å
b = 11.964 (2) Å
c = 12.343 (3) Å
α = 94.794 (18)°
β = 115.82 (3)°
γ = 101.128 (12)°
V = 1464.9 (7) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 3.36 mm^{-1}
T = 298 (2) K
0.27 × 0.26 × 0.24 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.419, T_{max} = 0.443
11551 measured reflections
5116 independent reflections
4548 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.051
S = 1.08
5116 reflections
379 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.51 e Å^{-3}
$\Delta\rho_{min}$ = −0.90 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H2W···O12^{i}	0.85	2.04	2.882 (4)	170
O1W—H1W···O10^{ii}	0.85	1.90	2.720 (4)	163
O2W—H3W···O4W^{i}	0.85	1.94	2.786 (4)	171
O3W—H5W···O9	0.85	1.97	2.722 (4)	147
O3W—H6W···O11^{iii}	0.85	1.95	2.777 (4)	166
O4W—H7W···O12	0.85	1.73	2.551 (4)	161
O4W—H8W···O2W	0.85	2.04	2.874 (4)	165

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

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 1998); software used to prepare material for publication: *SHELXTL* (Bruker, 2001).

This work was supported by the National Science Foundation of China (grant No. 20571014) and the Scientific Research Foundation for Returned Overseas Chinese Scholars, the Ministry of Education.

 doi:10.1107/S1600536807028437

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2275).

References

Brandenburg, K. (1998). *DIAMOND*. Version 2.1. Crystal Impact GbR, Bonn, Germany.

Bruker (2001). *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.

Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.

Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.

Kurmoo, M., Kumagai, H., Akita-Tanaka, M., Inoue, K. & Takagi, S. (2006). *Inorg. Chem.* **45**, 1627–1637.

Kurmoo, M., Kumagai, H., Hughes, S. M. & Kepert, C. J. (2003). *Inorg. Chem.* **42**, 6709–6722.

Qi, Y. J., Wang, Y. H., Hu, C. W., Cao, M. H., Mao, L. & Wang, E. B. (2003). *Inorg. Chem.* **42**, 8519–8523.

Rao, K. P., Thirumurugan, A. & Rao, C. N. R. (2007). *Chem. Eur. J.* **13**, 3193–3201.

Rigaku (1998). *PROCESS-AUTO*. Rigaku Corporation, Tokyo, Japan.

Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

Yu, M., Xie, L. H., Liu, S. X., Wang, C. L., Cheng, H. Y., Ren, Y. H. & Su, Z. M. (2007). *Inorg. Chim. Acta*, **360**, 3108–3112.

supplementary materials

Acta Cryst. (2007). E**63**, m1889-m1890 [**doi:10.1107/S1600536807028437**]

Poly[tetraaquabis(μ_4-cyclohexane-1,4-dicarboxylato-$\kappa^6O:O,O':O'':O'',O'''$)hemi($\mu_2$-cyclohexane-1,4-dicarboxylato-$\kappa^2O:O'$)hemi(μ_2-cyclohexane-1,4-dicarboxylato-$\kappa^4O,O':O'',O'''$)dipraseodymium(III)]

M. Yu, S.-X. Liu, L.-H. Xie, R.-G. Cao and Y.-H. Ren

Comment

Cyclohexane-1,4-dicarboxylic acid ($chdcH_2$) is a flexible ligand for constructing functional metal-organic frameworks (Kurmoo *et al.*, 2003, Kurmoo *et al.*, 2006, Qi *et al.*, 2003, Rao *et al.*, 2007). In our previous work, we have also isolated a photoluminescent zinc cyclohexane-1,4-dicarboxylate (Yu *et al.*, 2007). When investigating the reaction of $chdcH_2$ and Pr^{3+} ions, a compound formulated as $[Pr_2(C_8H_{10}O_4)_3(H_2O)_4]_n$ (I) was obtained.

The compound is a three-dimensional framework built from infinite chains of edge-sharing Pr polyhedra that are interconnected by the $-C_6H_{12}-$ cyclohexane rings of chdc ligands. There are two Pr atoms, three chdc and four coordinated water molecules in the asymmetric unit (Figure 1). There are four types of chdc ligands and two types of Pr atoms. The four chdc dianions are in an *e*,*e*-*trans* conformation. Their coordination modes, shown in Figure 2, are denoted as α, β, γ and δ. The Pr1 is coordinated by eight carboxyl O atoms from five chdc (two α, two β, one γ) and two water molecules in a distorted dicapped square-antiprismatic enviroment whereas the Pr2 is coordinated by seven carboxyl O atoms from five chdc (two α, two β, one δ) and two water molecules in a distorted tricapped trigonal-prismatic enviroment. The Pr—O bond lengths range from 2.451 (3) to 2.828 (3) Å. There are hydrogen bonding interactions involving the water molecules and some carboxyl O atoms. The ligation of alternating Pr1 and Pr2 atoms by the carboxyl groups of chdc ligands leads to an infinite chain (Figure 3). Each chain connects with six neighboring chains through chdc ligands to result in a three-dimensional framework (Figure 4).

Experimental

A mixture of $PrCl_3{\cdot}6H_2O$ (0.5 mmol, 0.178 g), $chdcH_2$ (0.8 mmol, 0.137 g), and water (10 ml) adjusted by dilute NaOH solution to around pH 4 was sealed in Teflon-lined autoclave and heated at 180 °C for 4 days, followed by slow cooling to room temperature. Compound (I) was collected as green block crystals with yield about 75% based on Pr.

Refinement

H atoms on water molecules were located in a difference Fourier map, and fixed with O—H = 0.85 Å and U_{iso}(H) = 1.2 U_{eq}(O). The others on C atoms are placed in calculated positions and refined in the riding model approximation with C—H = 0.97 or 0.98 Å and U_{iso}(H) = 1.2 U_{eq}(C). The highest peak and deepest hole in the final electron-density difference map were 0.506 Å and −0.897 Å, respectively.

Figures

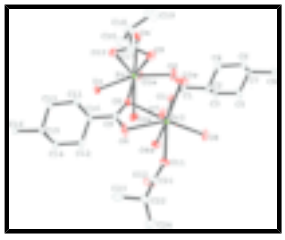


Fig. 1. **Figure 1**. *ORTEP* view of the asymmetric unit of (I) with displacement ellipsoids drawn at 50% probability level.

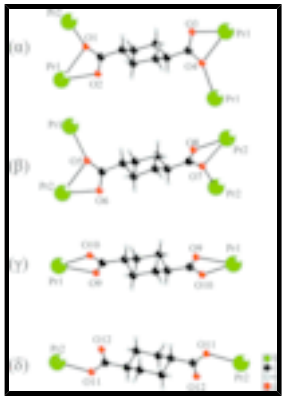


Fig. 2. **Figure 2**. The coordination fashions of the four types of chdc dianions).

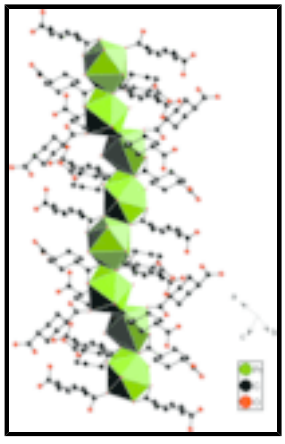


Fig. 3. **Figure 3**. Perspective view of the infinite chain with Pr atoms represented as poly-hedra.

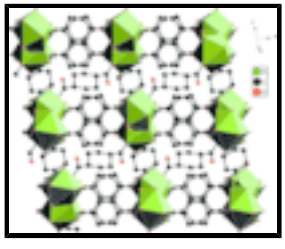


Fig. 4. **Figure 4**. Perspective view of the three-dimensional metal-organic framework along the direction of the infinite chains.

Poly[tetraaquabis(μ$_4$-cyclohexane-1,4-dicarboxylato- κ^6*O*:*O*,*O*':*O*'':*O*'',*O*''')hemi(μ$_2$-cyclohexane- 1,4-di-carboxylato-κ^2*O*:*O*')hemi(μ$_2$-cyclohexane-1,4-dicarboxylato- κ^4*O*,*O*':*O*'',*O*''')dipraseodymium(III)]

Crystal data

$[Pr_2(C_8H_{10}O_4)_3(H_2O)_4]$ $Z = 2$

M_r = 864.36	F_{000} = 856
Triclinic, $P\bar{1}$	D_x = 1.960 Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 11.439 (2) Å	Cell parameters from 776 reflections
b = 11.964 (2) Å	θ = 3.0–25.0º
c = 12.343 (3) Å	μ = 3.36 mm^{-1}
α = 94.794 (18)º	T = 298 (2) K
β = 115.82 (3)º	Block, white
γ = 101.128 (12)º	0.27 × 0.26 × 0.24 mm
V = 1464.9 (7) Å^3	

Data collection

Rigaku R-AXIS RAPID IP diffractometer	5116 independent reflections
Radiation source: fine-focus sealed tube	4548 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.029
Detector resolution: 0 pixels mm^{-1}	θ_{max} = 25.0º
T = 298(2) K	θ_{min} = 3.0º
ω scans	h = −13→12
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	k = −14→14
T_{min} = 0.419, T_{max} = 0.443	l = −14→14
11551 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.024	H-atom parameters constrained
$wR(F^2)$ = 0.051	$w = 1/[\sigma^2(F_o^2) + (0.0084P)^2 + 2.1565P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.08	$(\Delta/\sigma)_{max}$ = 0.001
5116 reflections	$\Delta\rho_{max}$ = 0.51 e Å^{-3}
379 parameters	$\Delta\rho_{min}$ = −0.90 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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	0.488253 (18)	0.430131 (16)	0.319055 (17)	0.01375 (6)
Pr2	0.462496 (17)	0.167914 (16)	0.025852 (16)	0.01346 (6)
C1	0.7123 (3)	0.4174 (3)	0.2526 (3)	0.0201 (8)
C2	0.8420 (3)	0.4200 (3)	0.2469 (3)	0.0226 (8)
H2	0.8221	0.3692	0.1712	0.027*
C3	0.9097 (4)	0.5418 (4)	0.2471 (4)	0.0360 (11)
H3A	0.9243	0.5936	0.3190	0.043*
H3B	0.8515	0.5679	0.1752	0.043*
C4	0.9352 (4)	0.3750 (3)	0.3572 (4)	0.0244 (8)
H4A	0.9435	0.4176	0.4317	0.029*
H4B	0.8945	0.2939	0.3502	0.029*
C5	1.0442 (4)	0.5469 (4)	0.2471 (4)	0.0404 (12)
H5A	1.0292	0.4975	0.1733	0.048*
H5B	1.0847	0.6257	0.2464	0.048*
C6	1.0758 (4)	0.3865 (3)	0.3678 (4)	0.0226 (8)
H6A	1.1335	0.3688	0.4458	0.027*
H6B	1.0700	0.3301	0.3033	0.027*
C7	1.1394 (3)	0.5078 (3)	0.3584 (3)	0.0191 (8)
H7	1.1609	0.5625	0.4321	0.023*
C8	1.2686 (3)	0.5033 (3)	0.3541 (3)	0.0169 (7)
C9	0.2286 (4)	0.2082 (3)	0.0562 (3)	0.0201 (8)
C10	0.0992 (3)	0.2270 (3)	0.0508 (4)	0.0222 (8)
H10	0.1172	0.3063	0.0929	0.027*
C11	0.0512 (3)	0.1417 (3)	0.1181 (3)	0.0206 (8)
H11A	0.0498	0.0640	0.0873	0.025*
H11B	0.1145	0.1614	0.2048	0.025*
C12	−0.0075 (4)	0.2124 (4)	−0.0817 (4)	0.0287 (9)
H12A	−0.0206	0.1365	−0.1262	0.034*
H12B	0.0233	0.2705	−0.1203	0.034*
C13	−0.0887 (3)	0.1431 (3)	0.1022 (3)	0.0226 (8)
H13A	−0.0829	0.2152	0.1489	0.027*
H13B	−0.1196	0.0798	0.1354	0.027*
C14	−0.1411 (4)	0.2248 (4)	−0.0888 (4)	0.0282 (9)
H14A	−0.1291	0.3010	−0.0455	0.034*
H14B	−0.2066	0.2169	−0.1738	0.034*
C15	−0.1914 (3)	0.1317 (3)	−0.0317 (3)	0.0170 (7)
H15	−0.2029	0.0556	−0.0767	0.020*
C16	−0.3234 (3)	0.1365 (3)	−0.0334 (3)	0.0175 (8)
C17	0.4813 (4)	0.2186 (3)	0.4184 (3)	0.0242 (9)
C18	0.4814 (5)	0.1149 (3)	0.4800 (4)	0.0323 (10)

H18	0.4469	0.1289	0.5387	0.039*
C19	0.6205 (5)	0.0967 (4)	0.5510 (4)	0.0467 (12)
H19A	0.6786	0.1656	0.6125	0.056*
H19B	0.6582	0.0841	0.4957	0.056*
C20	0.3862 (5)	0.0083 (4)	0.3863 (4)	0.0440 (12)
H20A	0.4165	−0.0071	0.3257	0.053*
H20B	0.2973	0.0213	0.3445	0.053*
C21	0.2456 (4)	0.1272 (3)	−0.2847 (3)	0.0220 (8)
C22	0.1333 (4)	0.0380 (3)	−0.3917 (3)	0.0273 (9)
H22	0.1574	−0.0363	−0.3880	0.033*
C23	0.0041 (5)	0.0232 (5)	−0.3810 (4)	0.0489 (13)
H23A	−0.0200	0.0966	−0.3819	0.059*
H23B	0.0181	0.0004	−0.3035	0.059*
C24	0.1101 (5)	0.0684 (5)	−0.5141 (4)	0.0491 (13)
H24A	0.1917	0.0748	−0.5222	0.059*
H24B	0.0887	0.1430	−0.5187	0.059*
O1	0.6014 (2)	0.3505 (2)	0.1740 (2)	0.0260 (6)
O2	0.7147 (3)	0.4855 (2)	0.3370 (3)	0.0353 (7)
O3	0.2670 (2)	0.4772 (2)	0.2521 (2)	0.0271 (6)
O4	0.6233 (2)	0.4813 (2)	0.5478 (2)	0.0222 (6)
O5	0.3421 (2)	0.2627 (2)	0.1422 (2)	0.0251 (6)
O6	0.2228 (3)	0.1361 (2)	−0.0272 (3)	0.0350 (7)
O7	0.3943 (2)	−0.0465 (2)	0.0225 (2)	0.0223 (6)
O8	0.6411 (3)	0.2292 (2)	−0.0383 (2)	0.0250 (6)
O9	0.5688 (3)	0.2502 (2)	0.3825 (3)	0.0291 (6)
O10	0.3942 (3)	0.2739 (2)	0.4051 (2)	0.0242 (6)
O11	0.3319 (3)	0.0925 (2)	−0.1981 (2)	0.0242 (6)
O12	0.2456 (3)	0.2317 (2)	−0.2863 (2)	0.0333 (7)
O1W	0.5733 (3)	0.6472 (2)	0.3677 (2)	0.0289 (6)
H1W	0.5998	0.6778	0.4418	0.035*
H2W	0.6316	0.6758	0.3456	0.035*
O2W	0.4036 (3)	0.5128 (2)	0.1098 (2)	0.0301 (6)
H3W	0.4583	0.5631	0.0980	0.036*
H4W	0.3428	0.5457	0.1062	0.036*
O3W	0.6203 (3)	0.1250 (2)	0.2213 (2)	0.0406 (8)
H5W	0.6340	0.1582	0.2909	0.049*
H6W	0.6368	0.0589	0.2269	0.049*
O4W	0.4041 (3)	0.3423 (2)	−0.0683 (2)	0.0238 (6)
H7W	0.3485	0.3204	−0.1440	0.029*
H8W	0.3895	0.3857	−0.0200	0.029*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pr1	0.01010 (10)	0.01528 (10)	0.01643 (11)	0.00264 (8)	0.00685 (8)	0.00308 (8)
Pr2	0.00806 (10)	0.01611 (11)	0.01489 (11)	0.00227 (8)	0.00499 (8)	−0.00001 (8)
C1	0.0129 (18)	0.0218 (19)	0.021 (2)	0.0011 (16)	0.0051 (16)	0.0039 (16)
C2	0.0127 (18)	0.033 (2)	0.021 (2)	0.0034 (17)	0.0091 (16)	−0.0012 (16)

C3	0.018 (2)	0.045 (3)	0.058 (3)	0.018 (2)	0.022 (2)	0.032 (2)
C4	0.0162 (19)	0.023 (2)	0.033 (2)	0.0020 (17)	0.0118 (18)	0.0056 (17)
C5	0.022 (2)	0.063 (3)	0.055 (3)	0.023 (2)	0.024 (2)	0.043 (3)
C6	0.0137 (18)	0.025 (2)	0.029 (2)	0.0056 (16)	0.0093 (17)	0.0049 (17)
C7	0.0117 (18)	0.0210 (19)	0.027 (2)	0.0048 (15)	0.0107 (16)	0.0029 (15)
C8	0.0105 (18)	0.0137 (17)	0.026 (2)	0.0021 (15)	0.0082 (17)	0.0032 (15)
C9	0.0144 (19)	0.0145 (18)	0.031 (2)	0.0001 (16)	0.0117 (18)	0.0055 (16)
C10	0.0111 (18)	0.0197 (19)	0.035 (2)	0.0019 (16)	0.0123 (17)	−0.0006 (16)
C11	0.0141 (18)	0.028 (2)	0.0193 (19)	0.0080 (16)	0.0070 (16)	0.0009 (16)
C12	0.019 (2)	0.041 (2)	0.038 (2)	0.0105 (19)	0.0202 (19)	0.022 (2)
C13	0.0158 (19)	0.031 (2)	0.022 (2)	0.0060 (17)	0.0100 (17)	0.0039 (16)
C14	0.0145 (19)	0.038 (2)	0.038 (2)	0.0088 (18)	0.0143 (19)	0.0211 (19)
C15	0.0125 (17)	0.0184 (18)	0.022 (2)	0.0033 (15)	0.0102 (16)	0.0030 (15)
C16	0.0129 (18)	0.023 (2)	0.0152 (18)	0.0029 (16)	0.0069 (15)	0.0004 (15)
C17	0.035 (2)	0.0175 (19)	0.019 (2)	0.0034 (18)	0.0133 (18)	0.0015 (15)
C18	0.048 (3)	0.022 (2)	0.037 (3)	0.015 (2)	0.025 (2)	0.0127 (18)
C19	0.048 (3)	0.026 (2)	0.041 (3)	−0.007 (2)	0.004 (2)	0.013 (2)
C20	0.043 (3)	0.032 (2)	0.040 (3)	0.001 (2)	0.005 (2)	0.019 (2)
C21	0.019 (2)	0.024 (2)	0.019 (2)	0.0024 (17)	0.0078 (17)	0.0016 (16)
C22	0.023 (2)	0.022 (2)	0.023 (2)	0.0067 (18)	−0.0003 (17)	−0.0024 (16)
C23	0.035 (3)	0.072 (4)	0.018 (2)	−0.015 (3)	0.008 (2)	−0.005 (2)
C24	0.032 (3)	0.071 (4)	0.025 (2)	−0.019 (2)	0.012 (2)	−0.007 (2)
O1	0.0141 (13)	0.0260 (14)	0.0273 (15)	−0.0042 (12)	0.0051 (12)	−0.0017 (12)
O2	0.0206 (15)	0.0397 (17)	0.0434 (18)	0.0003 (13)	0.0197 (14)	−0.0140 (14)
O3	0.0164 (13)	0.0446 (17)	0.0224 (15)	0.0104 (13)	0.0106 (12)	0.0020 (12)
O4	0.0118 (13)	0.0282 (14)	0.0225 (14)	0.0060 (11)	0.0043 (12)	0.0032 (11)
O5	0.0131 (13)	0.0353 (16)	0.0244 (15)	0.0034 (12)	0.0084 (12)	0.0017 (12)
O6	0.0128 (14)	0.0319 (16)	0.0513 (19)	−0.0004 (12)	0.0134 (14)	−0.0151 (14)
O7	0.0172 (13)	0.0217 (14)	0.0327 (16)	0.0043 (12)	0.0158 (12)	0.0064 (11)
O8	0.0199 (14)	0.0232 (14)	0.0402 (17)	0.0076 (12)	0.0201 (13)	0.0068 (12)
O9	0.0427 (17)	0.0249 (14)	0.0368 (17)	0.0188 (14)	0.0280 (15)	0.0143 (12)
O10	0.0315 (15)	0.0195 (13)	0.0281 (15)	0.0088 (13)	0.0181 (13)	0.0066 (11)
O11	0.0216 (14)	0.0284 (14)	0.0173 (14)	0.0105 (12)	0.0030 (12)	0.0017 (11)
O12	0.0361 (17)	0.0226 (15)	0.0232 (15)	0.0028 (13)	−0.0003 (13)	0.0040 (12)
O1W	0.0431 (17)	0.0210 (14)	0.0289 (16)	0.0029 (13)	0.0248 (14)	0.0016 (12)
O2W	0.0356 (16)	0.0315 (15)	0.0332 (16)	0.0112 (14)	0.0223 (14)	0.0142 (13)
O3W	0.061 (2)	0.0359 (17)	0.0158 (15)	0.0285 (16)	0.0040 (15)	0.0004 (12)
O4W	0.0281 (15)	0.0207 (13)	0.0180 (14)	0.0050 (12)	0.0079 (12)	−0.0009 (11)

Geometric parameters (Å, °)

Pr1—O2	2.451 (3)	C11—H11A	0.9700
Pr1—O3	2.493 (2)	C11—H11B	0.9700
Pr1—O4	2.506 (3)	C12—C14	1.529 (5)
Pr1—O1W	2.511 (3)	C12—H12A	0.9700
Pr1—O10	2.516 (3)	C12—H12B	0.9700
Pr1—O5	2.524 (3)	C13—C15	1.530 (5)
Pr1—O9	2.552 (3)	C13—H13A	0.9700
Pr1—O2W	2.684 (3)	C13—H13B	0.9700

Pr1—O4^{i}	2.740 (2)	C14—C15	1.519 (5)
Pr1—O1	2.828 (3)	C14—H14A	0.9700
Pr2—O6	2.466 (3)	C14—H14B	0.9700
Pr2—O1	2.471 (3)	C15—C16	1.513 (4)
Pr2—O3W	2.472 (3)	C15—H15	0.9800
Pr2—O11	2.481 (3)	C16—O8^{v}	1.250 (4)
Pr2—O8	2.503 (2)	C16—O7^{vi}	1.271 (4)
Pr2—O7	2.525 (3)	C17—O10	1.261 (4)
Pr2—O4W	2.533 (2)	C17—O9	1.269 (5)
Pr2—O7^{ii}	2.602 (2)	C17—C18	1.507 (5)
Pr2—O5	2.702 (2)	C18—C20	1.507 (6)
C1—O2	1.255 (4)	C18—C19	1.516 (6)
C1—O1	1.263 (4)	C18—H18	0.9800
C1—C2	1.510 (5)	C19—C20^{vii}	1.535 (6)
C2—C3	1.511 (6)	C19—H19A	0.9700
C2—C4	1.537 (5)	C19—H19B	0.9700
C2—H2	0.9800	C20—C19^{vii}	1.535 (6)
C3—C5	1.527 (5)	C20—H20A	0.9700
C3—H3A	0.9700	C20—H20B	0.9700
C3—H3B	0.9700	C21—O12	1.252 (4)
C4—C6	1.534 (5)	C21—O11	1.266 (4)
C4—H4A	0.9700	C21—C22	1.513 (5)
C4—H4B	0.9700	C22—C24	1.505 (6)
C5—C7	1.514 (5)	C22—C23	1.519 (6)
C5—H5A	0.9700	C22—H22	0.9800
C5—H5B	0.9700	C23—C24^{viii}	1.523 (6)
C6—C7	1.530 (5)	C23—H23A	0.9700
C6—H6A	0.9700	C23—H23B	0.9700
C6—H6B	0.9700	C24—C23^{viii}	1.523 (6)
C7—C8	1.513 (4)	C24—H24A	0.9700
C7—H7	0.9800	C24—H24B	0.9700
C8—O3^{iii}	1.262 (4)	O1W—H1W	0.8500
C8—O4^{iv}	1.264 (4)	O1W—H2W	0.8500
C9—O6	1.257 (4)	O2W—H3W	0.8499
C9—O5	1.263 (4)	O2W—H4W	0.8501
C9—C10	1.513 (5)	O3W—H5W	0.8499
C10—C12	1.525 (5)	O3W—H6W	0.8500
C10—C11	1.535 (5)	O4W—H7W	0.8500
C10—H10	0.9800	O4W—H8W	0.8500
C11—C13	1.528 (5)		
O2—Pr1—O3	146.79 (10)	C6—C7—H7	108.8
O2—Pr1—O4	80.40 (9)	O3^{iii}—C8—O4^{iv}	119.7 (3)
O3—Pr1—O4	110.50 (8)	O3^{iii}—C8—C7	119.7 (3)
O2—Pr1—O1W	70.10 (9)	O4^{iv}—C8—C7	120.5 (3)
O3—Pr1—O1W	82.36 (9)	O6—C9—O5	119.1 (3)
O4—Pr1—O1W	74.75 (9)	O6—C9—C10	119.0 (3)

O2—Pr1—O10	128.45 (10)	O5—C9—C10	121.9 (3)
O3—Pr1—O10	84.50 (9)	C9—C10—C12	110.8 (3)
O4—Pr1—O10	72.71 (9)	C9—C10—C11	109.0 (3)
O1W—Pr1—O10	137.74 (8)	C12—C10—C11	111.2 (3)
O2—Pr1—O5	110.28 (8)	C9—C10—H10	108.6
O3—Pr1—O5	80.23 (9)	C12—C10—H10	108.6
O4—Pr1—O5	143.25 (8)	C11—C10—H10	108.6
O1W—Pr1—O5	141.92 (9)	C13—C11—C10	112.6 (3)
O10—Pr1—O5	73.60 (8)	C13—C11—H11A	109.1
O2—Pr1—O9	79.70 (10)	C10—C11—H11A	109.1
O3—Pr1—O9	132.96 (9)	C13—C11—H11B	109.1
O4—Pr1—O9	74.98 (9)	C10—C11—H11B	109.1
O1W—Pr1—O9	140.08 (10)	H11A—C11—H11B	107.8
O10—Pr1—O9	51.45 (8)	C10—C12—C14	111.4 (3)
O5—Pr1—O9	72.78 (9)	C10—C12—H12A	109.3
O2—Pr1—O2W	87.07 (10)	C14—C12—H12A	109.3
O3—Pr1—O2W	65.97 (9)	C10—C12—H12B	109.3
O4—Pr1—O2W	145.39 (8)	C14—C12—H12B	109.3
O1W—Pr1—O2W	70.65 (9)	H12A—C12—H12B	108.0
O10—Pr1—O2W	137.12 (9)	C11—C13—C15	112.9 (3)
O5—Pr1—O2W	71.35 (9)	C11—C13—H13A	109.0
O9—Pr1—O2W	134.29 (8)	C15—C13—H13A	109.0
O2—Pr1—O4^{i}	131.45 (8)	C11—C13—H13B	109.0
O3—Pr1—O4^{i}	49.08 (8)	C15—C13—H13B	109.0
O4—Pr1—O4^{i}	61.45 (9)	H13A—C13—H13B	107.8
O1W—Pr1—O4^{i}	71.63 (8)	C15—C14—C12	109.3 (3)
O10—Pr1—O4^{i}	69.45 (8)	C15—C14—H14A	109.8
O5—Pr1—O4^{i}	118.26 (8)	C12—C14—H14A	109.8
O9—Pr1—O4^{i}	114.39 (8)	C15—C14—H14B	109.8
O2W—Pr1—O4^{i}	107.14 (8)	C12—C14—H14B	109.8
O2—Pr1—O1	47.90 (8)	H14A—C14—H14B	108.3
O3—Pr1—O1	128.93 (8)	C16—C15—C14	113.7 (3)
O4—Pr1—O1	120.33 (8)	C16—C15—C13	107.2 (3)
O1W—Pr1—O1	105.56 (8)	C14—C15—C13	110.2 (3)
O10—Pr1—O1	113.86 (8)	C16—C15—H15	108.5
O5—Pr1—O1	62.49 (8)	C14—C15—H15	108.5
O9—Pr1—O1	69.17 (8)	C13—C15—H15	108.5
O2W—Pr1—O1	69.60 (8)	O8^{v}—C16—O7^{vi}	120.1 (3)
O4^{i}—Pr1—O1	176.43 (7)	O8^{v}—C16—C15	120.7 (3)
O6—Pr2—O1	112.17 (9)	O7^{vi}—C16—C15	119.1 (3)
O6—Pr2—O3W	119.77 (11)	O10—C17—O9	120.9 (3)
O1—Pr2—O3W	70.03 (10)	O10—C17—C18	118.7 (3)
O6—Pr2—O11	72.91 (9)	O9—C17—C18	120.4 (4)
O1—Pr2—O11	140.80 (9)	C20—C18—C17	109.7 (3)
O3W—Pr2—O11	143.49 (8)	C20—C18—C19	111.4 (4)
O6—Pr2—O8	146.90 (10)	C17—C18—C19	113.1 (4)
O1—Pr2—O8	78.18 (9)	C20—C18—H18	107.5

O3W—Pr2—O8	93.32 (10)	C17—C18—H18	107.5
O11—Pr2—O8	79.83 (9)	C19—C18—H18	107.5
O6—Pr2—O7	77.83 (9)	C18—C19—C20^{vii}	110.5 (4)
O1—Pr2—O7	139.66 (9)	C18—C19—H19A	109.6
O3W—Pr2—O7	71.37 (9)	C20^{vii}—C19—H19A	109.6
O11—Pr2—O7	79.35 (9)	C18—C19—H19B	109.6
O8—Pr2—O7	115.48 (8)	C20^{vii}—C19—H19B	109.6
O6—Pr2—O4W	77.50 (9)	H19A—C19—H19B	108.1
O1—Pr2—O4W	69.00 (9)	C18—C20—C19^{vii}	110.2 (4)
O3W—Pr2—O4W	139.02 (9)	C18—C20—H20A	109.6
O11—Pr2—O4W	74.81 (8)	C19^{vii}—C20—H20A	109.6
O8—Pr2—O4W	77.52 (8)	C18—C20—H20B	109.6
O7—Pr2—O4W	148.44 (8)	C19^{vii}—C20—H20B	109.6
O6—Pr2—O7^{ii}	135.00 (8)	H20A—C20—H20B	108.1
O1—Pr2—O7^{ii}	112.57 (8)	O12—C21—O11	123.8 (3)
O3W—Pr2—O7^{ii}	72.41 (9)	O12—C21—C22	117.4 (3)
O11—Pr2—O7^{ii}	75.79 (8)	O11—C21—C22	118.7 (3)
O8—Pr2—O7^{ii}	50.64 (8)	C24—C22—C21	113.1 (4)
O7—Pr2—O7^{ii}	65.17 (9)	C24—C22—C23	109.5 (3)
O4W—Pr2—O7^{ii}	123.70 (8)	C21—C22—C23	109.8 (3)
O6—Pr2—O5	49.44 (8)	C24—C22—H22	108.1
O1—Pr2—O5	65.04 (8)	C21—C22—H22	108.1
O3W—Pr2—O5	89.86 (9)	C23—C22—H22	108.1
O11—Pr2—O5	118.55 (8)	C22—C23—C24^{viii}	111.1 (4)
O8—Pr2—O5	139.43 (8)	C22—C23—H23A	109.4
O7—Pr2—O5	103.84 (8)	C24^{viii}—C23—H23A	109.4
O4W—Pr2—O5	73.90 (8)	C22—C23—H23B	109.4
O7^{ii}—Pr2—O5	161.22 (8)	C24^{viii}—C23—H23B	109.4
O2—C1—O1	119.1 (3)	H23A—C23—H23B	108.0
O2—C1—C2	118.7 (3)	C22—C24—C23^{viii}	111.3 (4)
O1—C1—C2	122.2 (3)	C22—C24—H24A	109.4
C1—C2—C3	110.6 (3)	C23^{viii}—C24—H24A	109.4
C1—C2—C4	109.2 (3)	C22—C24—H24B	109.4
C3—C2—C4	110.2 (3)	C23^{viii}—C24—H24B	109.4
C1—C2—H2	108.9	H24A—C24—H24B	108.0
C3—C2—H2	108.9	C1—O1—Pr2	152.8 (2)
C4—C2—H2	108.9	C1—O1—Pr1	87.1 (2)
C2—C3—C5	111.3 (3)	Pr2—O1—Pr1	114.27 (9)
C2—C3—H3A	109.4	C1—O2—Pr1	105.5 (2)
C5—C3—H3A	109.4	C8^{v}—O3—Pr1	100.9 (2)
C2—C3—H3B	109.4	C8^{iv}—O4—Pr1	152.0 (2)
C5—C3—H3B	109.4	C8^{iv}—O4—Pr1^{i}	89.1 (2)
H3A—C3—H3B	108.0	Pr1—O4—Pr1^{i}	118.55 (9)
C6—C4—C2	113.3 (3)	C9—O5—Pr1	150.7 (2)

C6—C4—H4A	108.9	C9—O5—Pr2	89.8 (2)
C2—C4—H4A	108.9	Pr1—O5—Pr2	116.90 (9)
C6—C4—H4B	108.9	C9—O6—Pr2	101.3 (2)
C2—C4—H4B	108.9	C16^{vi}—O7—Pr2	153.8 (2)
H4A—C4—H4B	107.7	C16^{vi}—O7—Pr2^{ii}	91.35 (19)
C7—C5—C3	111.4 (3)	Pr2—O7—Pr2^{ii}	114.83 (9)
C7—C5—H5A	109.3	C16^{iii}—O8—Pr2	96.6 (2)
C3—C5—H5A	109.3	C17—O9—Pr1	92.8 (2)
C7—C5—H5B	109.3	C17—O10—Pr1	94.7 (2)
C3—C5—H5B	109.3	C21—O11—Pr2	132.8 (2)
H5A—C5—H5B	108.0	Pr1—O1W—H1W	114.7
C7—C6—C4	112.8 (3)	Pr1—O1W—H2W	116.7
C7—C6—H6A	109.0	H1W—O1W—H2W	109.1
C4—C6—H6A	109.0	Pr1—O2W—H3W	120.1
C7—C6—H6B	109.0	Pr1—O2W—H4W	107.1
C4—C6—H6B	109.0	H3W—O2W—H4W	104.8
H6A—C6—H6B	107.8	Pr2—O3W—H5W	123.1
C8—C7—C5	111.8 (3)	Pr2—O3W—H6W	122.1
C8—C7—C6	107.4 (3)	H5W—O3W—H6W	109.1
C5—C7—C6	111.2 (3)	Pr2—O4W—H7W	109.8
C8—C7—H7	108.8	Pr2—O4W—H8W	108.2
C5—C7—H7	108.8	H7W—O4W—H8W	121.8
O2—C1—C2—C3	−53.6 (5)	O1—Pr1—O4—C8^{iv}	5.7 (5)
O1—C1—C2—C3	125.1 (4)	O2—Pr1—O4—Pr1^{i}	148.93 (12)
O2—C1—C2—C4	67.8 (4)	O3—Pr1—O4—Pr1^{i}	1.51 (13)
O1—C1—C2—C4	−113.5 (4)	O1W—Pr1—O4—Pr1^{i}	77.09 (11)
C1—C2—C3—C5	177.5 (3)	O10—Pr1—O4—Pr1^{i}	−75.57 (11)
C4—C2—C3—C5	56.6 (5)	O5—Pr1—O4—Pr1^{i}	−99.92 (14)
C1—C2—C4—C6	−173.7 (3)	O9—Pr1—O4—Pr1^{i}	−129.26 (12)
C3—C2—C4—C6	−52.0 (4)	O2W—Pr1—O4—Pr1^{i}	78.59 (16)
C2—C3—C5—C7	−59.6 (5)	O4^{i}—Pr1—O4—Pr1^{i}	0.0
C2—C4—C6—C7	49.4 (4)	O1—Pr1—O4—Pr1^{i}	176.45 (8)
C3—C5—C7—C8	175.4 (4)	O6—C9—O5—Pr1	162.5 (3)
C3—C5—C7—C6	55.4 (5)	C10—C9—O5—Pr1	−17.6 (7)
C4—C6—C7—C8	−173.0 (3)	O6—C9—O5—Pr2	5.9 (3)
C4—C6—C7—C5	−50.4 (4)	C10—C9—O5—Pr2	−174.2 (3)
C5—C7—C8—O3^{iii}	−32.6 (5)	O2—Pr1—O5—C9	−148.2 (5)
C6—C7—C8—O3^{iii}	89.6 (4)	O3—Pr1—O5—C9	−0.9 (5)
C5—C7—C8—O4^{iv}	151.6 (4)	O4—Pr1—O5—C9	110.4 (5)
C6—C7—C8—O4^{iv}	−86.2 (4)	O1W—Pr1—O5—C9	−64.9 (5)
O6—C9—C10—C12	−33.1 (5)	O10—Pr1—O5—C9	86.2 (5)
O5—C9—C10—C12	147.0 (4)	O9—Pr1—O5—C9	140.1 (5)
O6—C9—C10—C11	89.6 (4)	O2W—Pr1—O5—C9	−68.7 (5)
O5—C9—C10—C11	−90.3 (4)	O4^{i}—Pr1—O5—C9	31.2 (5)
C9—C10—C11—C13	−172.1 (3)	O1—Pr1—O5—C9	−144.8 (5)

C12—C10—C11—C13	−49.7 (4)	O2—Pr1—O5—Pr2	5.38 (14)
C9—C10—C12—C14	177.0 (3)	O3—Pr1—O5—Pr2	152.67 (12)
C11—C10—C12—C14	55.5 (4)	O4—Pr1—O5—Pr2	−96.01 (14)
C10—C11—C13—C15	49.9 (4)	O1W—Pr1—O5—Pr2	88.67 (15)
C10—C12—C14—C15	−60.7 (4)	O10—Pr1—O5—Pr2	−120.24 (12)
C12—C14—C15—C16	179.7 (3)	O9—Pr1—O5—Pr2	−66.31 (11)
C12—C14—C15—C13	59.3 (4)	O2W—Pr1—O5—Pr2	84.88 (11)
C11—C13—C15—C16	−179.0 (3)	O4^{i}—Pr1—O5—Pr2	−175.23 (8)
C11—C13—C15—C14	−54.8 (4)	O1—Pr1—O5—Pr2	8.71 (9)
C14—C15—C16—O8^{v}	−24.5 (5)	O6—Pr2—O5—C9	−3.5 (2)
C13—C15—C16—O8^{v}	97.6 (4)	O1—Pr2—O5—C9	157.6 (2)
C14—C15—C16—O7^{vi}	159.5 (3)	O3W—Pr2—O5—C9	−134.4 (2)
C13—C15—C16—O7^{vi}	−78.4 (4)	O11—Pr2—O5—C9	21.6 (2)
O10—C17—C18—C20	86.4 (5)	O8—Pr2—O5—C9	130.6 (2)
O9—C17—C18—C20	−94.6 (5)	O7—Pr2—O5—C9	−63.7 (2)
O10—C17—C18—C19	−148.6 (4)	O4W—Pr2—O5—C9	83.7 (2)
O9—C17—C18—C19	30.3 (5)	O7^{ii}—Pr2—O5—C9	−115.4 (3)
C20—C18—C19—C20^{vii}	−57.2 (6)	O6—Pr2—O5—Pr1	−170.85 (18)
C17—C18—C19—C20^{vii}	178.8 (4)	O1—Pr2—O5—Pr1	−9.76 (10)
C17—C18—C20—C19^{vii}	−177.0 (4)	O3W—Pr2—O5—Pr1	58.18 (12)
C19—C18—C20—C19^{vii}	57.1 (6)	O11—Pr2—O5—Pr1	−145.81 (10)
O12—C21—C22—C24	47.3 (5)	O8—Pr2—O5—Pr1	−36.76 (18)
O11—C21—C22—C24	−134.1 (4)	O7—Pr2—O5—Pr1	128.93 (11)
O12—C21—C22—C23	−75.4 (5)	O4W—Pr2—O5—Pr1	−83.68 (12)
O11—C21—C22—C23	103.3 (4)	O7^{ii}—Pr2—O5—Pr1	77.2 (3)
C24—C22—C23—C24^{viii}	56.7 (6)	O5—C9—O6—Pr2	−6.6 (4)
C21—C22—C23—C24^{viii}	−178.6 (4)	C10—C9—O6—Pr2	173.5 (3)
C21—C22—C24—C23^{viii}	−179.6 (4)	O1—Pr2—O6—C9	−15.0 (3)
C23—C22—C24—C23^{viii}	−56.8 (6)	O3W—Pr2—O6—C9	64.0 (3)
O2—C1—O1—Pr2	−149.7 (4)	O11—Pr2—O6—C9	−153.6 (3)
C2—C1—O1—Pr2	31.5 (8)	O8—Pr2—O6—C9	−117.7 (2)
O2—C1—O1—Pr1	−6.6 (3)	O7—Pr2—O6—C9	124.0 (3)
C2—C1—O1—Pr1	174.7 (3)	O4W—Pr2—O6—C9	−75.8 (2)
O6—Pr2—O1—C1	162.9 (5)	O7^{ii}—Pr2—O6—C9	158.6 (2)
O3W—Pr2—O1—C1	47.9 (5)	O5—Pr2—O6—C9	3.5 (2)
O11—Pr2—O1—C1	−107.3 (5)	O6—Pr2—O7—C16^{vi}	−27.6 (5)
O8—Pr2—O1—C1	−50.1 (5)	O1—Pr2—O7—C16^{vi}	82.4 (5)
O7—Pr2—O1—C1	65.5 (6)	O3W—Pr2—O7—C16^{vi}	99.9 (5)
O4W—Pr2—O1—C1	−131.1 (6)	O11—Pr2—O7—C16^{vi}	−102.2 (5)
O7^{ii}—Pr2—O1—C1	−12.2 (6)	O8—Pr2—O7—C16^{vi}	−175.4 (5)
O5—Pr2—O1—C1	147.4 (6)	O4W—Pr2—O7—C16^{vi}	−66.8 (6)
O6—Pr2—O1—Pr1	23.94 (14)	O7^{ii}—Pr2—O7—C16^{vi}	178.7 (6)
O3W—Pr2—O1—Pr1	−91.06 (12)	O5—Pr2—O7—C16^{vi}	14.8 (5)
O11—Pr2—O1—Pr1	113.79 (13)	O6—Pr2—O7—Pr2^{ii}	153.76 (12)

O8—Pr2—O1—Pr1	170.96 (12)	O1—Pr2—O7—Pr2^{ii}	−96.23 (14)
O7—Pr2—O1—Pr1	−73.42 (15)	O3W—Pr2—O7—Pr2^{ii}	−78.73 (12)
O4W—Pr2—O1—Pr1	89.94 (11)	O11—Pr2—O7—Pr2^{ii}	79.15 (11)
O7^{ii}—Pr2—O1—Pr1	−151.11 (9)	O8—Pr2—O7—Pr2^{ii}	5.93 (14)
O5—Pr2—O1—Pr1	8.51 (8)	O4W—Pr2—O7—Pr2^{ii}	114.50 (14)
O2—Pr1—O1—C1	4.0 (2)	O7^{ii}—Pr2—O7—Pr2^{ii}	0.0
O3—Pr1—O1—C1	140.0 (2)	O5—Pr2—O7—Pr2^{ii}	−163.82 (10)
O1W—Pr1—O1—C1	47.3 (2)	O6—Pr2—O8—C16^{iii}	−121.1 (2)
O10—Pr1—O1—C1	−117.1 (2)	O1—Pr2—O8—C16^{iii}	126.3 (2)
O5—Pr1—O1—C1	−171.8 (2)	O3W—Pr2—O8—C16^{iii}	57.5 (2)
O9—Pr1—O1—C1	−91.0 (2)	O11—Pr2—O8—C16^{iii}	−86.4 (2)
O2W—Pr1—O1—C1	109.2 (2)	O7—Pr2—O8—C16^{iii}	−13.4 (2)
O2—Pr1—O1—Pr2	166.46 (18)	O4W—Pr2—O8—C16^{iii}	−162.9 (2)
O3—Pr1—O1—Pr2	−57.52 (15)	O7^{ii}—Pr2—O8—C16^{iii}	−6.47 (19)
O1W—Pr1—O1—Pr2	−150.25 (11)	O5—Pr2—O8—C16^{iii}	151.15 (19)
O10—Pr1—O1—Pr2	45.34 (13)	O10—C17—O9—Pr1	4.0 (4)
O5—Pr1—O1—Pr2	−9.33 (9)	C18—C17—O9—Pr1	−175.0 (3)
O9—Pr1—O1—Pr2	71.52 (12)	O2—Pr1—O9—C17	160.2 (2)
O2W—Pr1—O1—Pr2	−88.32 (12)	O3—Pr1—O9—C17	−26.8 (3)
O1—C1—O2—Pr1	7.9 (4)	O4—Pr1—O9—C17	77.5 (2)
C2—C1—O2—Pr1	−173.3 (3)	O1W—Pr1—O9—C17	119.3 (2)
O3—Pr1—O2—C1	−103.7 (3)	O10—Pr1—O9—C17	−2.2 (2)
O4—Pr1—O2—C1	143.3 (3)	O5—Pr1—O9—C17	−84.7 (2)
O1W—Pr1—O2—C1	−139.5 (3)	O2W—Pr1—O9—C17	−124.3 (2)
O10—Pr1—O2—C1	84.6 (3)	O4^{i}—Pr1—O9—C17	29.2 (2)
O5—Pr1—O2—C1	−0.2 (3)	O1—Pr1—O9—C17	−151.1 (2)
O9—Pr1—O2—C1	67.0 (2)	O9—C17—O10—Pr1	−4.0 (4)
O2W—Pr1—O2—C1	−69.0 (3)	C18—C17—O10—Pr1	174.9 (3)
O4^{i}—Pr1—O2—C1	−179.4 (2)	O2—Pr1—O10—C17	−20.2 (2)
O1—Pr1—O2—C1	−4.1 (2)	O3—Pr1—O10—C17	164.4 (2)
O2—Pr1—O3—C8^{v}	−112.3 (2)	O4—Pr1—O10—C17	−82.1 (2)
O4—Pr1—O3—C8^{v}	−8.1 (2)	O1W—Pr1—O10—C17	−123.3 (2)
O1W—Pr1—O3—C8^{v}	−78.6 (2)	O5—Pr1—O10—C17	83.0 (2)
O10—Pr1—O3—C8^{v}	61.1 (2)	O9—Pr1—O10—C17	2.2 (2)
O5—Pr1—O3—C8^{v}	135.4 (2)	O2W—Pr1—O10—C17	119.2 (2)
O9—Pr1—O3—C8^{v}	80.2 (2)	O4^{i}—Pr1—O10—C17	−147.4 (2)
O2W—Pr1—O3—C8^{v}	−150.8 (2)	O1—Pr1—O10—C17	34.0 (2)
O4^{i}—Pr1—O3—C8^{v}	−6.3 (2)	O12—C21—O11—Pr2	31.6 (6)
O1—Pr1—O3—C8^{v}	177.54 (19)	C22—C21—O11—Pr2	−146.9 (3)
O2—Pr1—O4—C8^{iv}	−21.8 (5)	O6—Pr2—O11—C21	56.6 (3)
O3—Pr1—O4—C8^{iv}	−169.2 (5)	O1—Pr2—O11—C21	−47.7 (4)
O1W—Pr1—O4—C8^{iv}	−93.6 (5)	O3W—Pr2—O11—C21	173.9 (3)
O10—Pr1—O4—C8^{iv}	113.7 (5)	O8—Pr2—O11—C21	−104.4 (3)

O5—Pr1—O4—C8^{iv}	89.4 (5)	O7—Pr2—O11—C21	137.0 (3)
O9—Pr1—O4—C8^{iv}	60.0 (5)	O4W—Pr2—O11—C21	−24.7 (3)
O2W—Pr1—O4—C8^{iv}	−92.1 (5)	O7^{ii}—Pr2—O11—C21	−156.1 (3)
O4^{i}—Pr1—O4—C8^{iv}	−170.7 (6)	O5—Pr2—O11—C21	37.0 (3)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H2W···O12^{ix}	0.85	2.04	2.882 (4)	170
O1W—H1W···O10^{i}	0.85	1.90	2.720 (4)	163
O2W—H3W···O4W^{ix}	0.85	1.94	2.786 (4)	171
O3W—H5W···O9	0.85	1.97	2.722 (4)	147
O3W—H6W···O11^{ii}	0.85	1.95	2.777 (4)	166
O4W—H7W···O12	0.85	1.73	2.551 (4)	161
O4W—H8W···O2W	0.85	2.04	2.874 (4)	165

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

Fig. 1

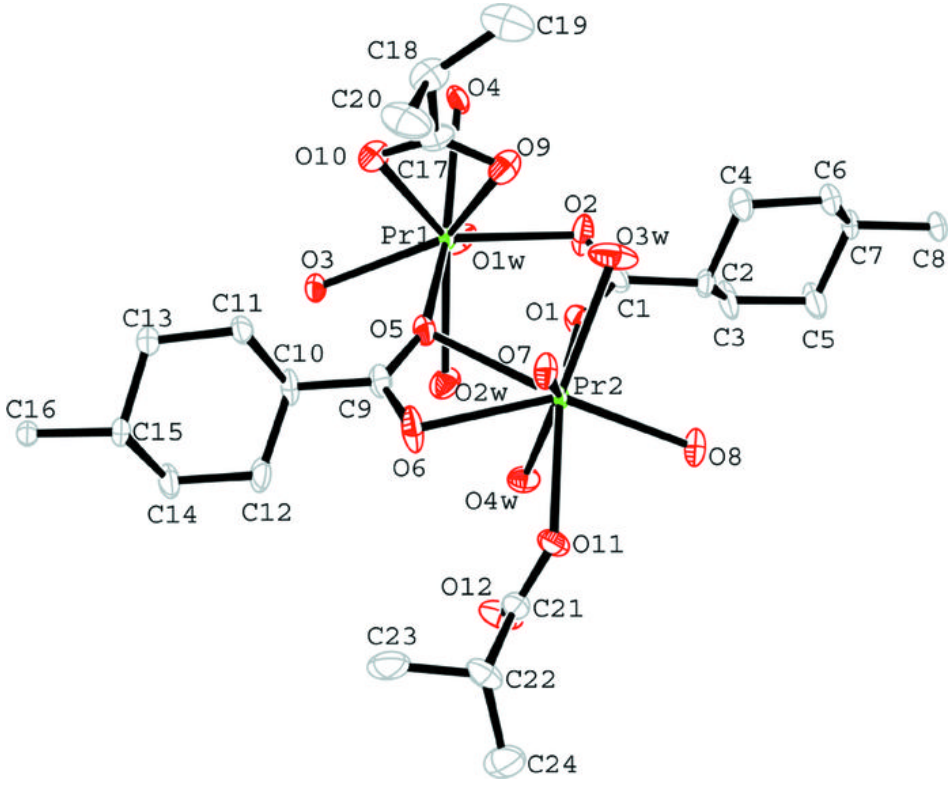

C19
C18
O4
C20
O10
C17
O9
C4
C6
O2
Pr1
O3w
O3
O1w
C2
C7
C8
C13
C11
O1
C1
O5
C3
C5
C10
O7
Pr2
C16
C9
O2w
C15
O6
O8
O4w
C14
C12
O11
O12
C21
C23
C22
C24

Fig. 2

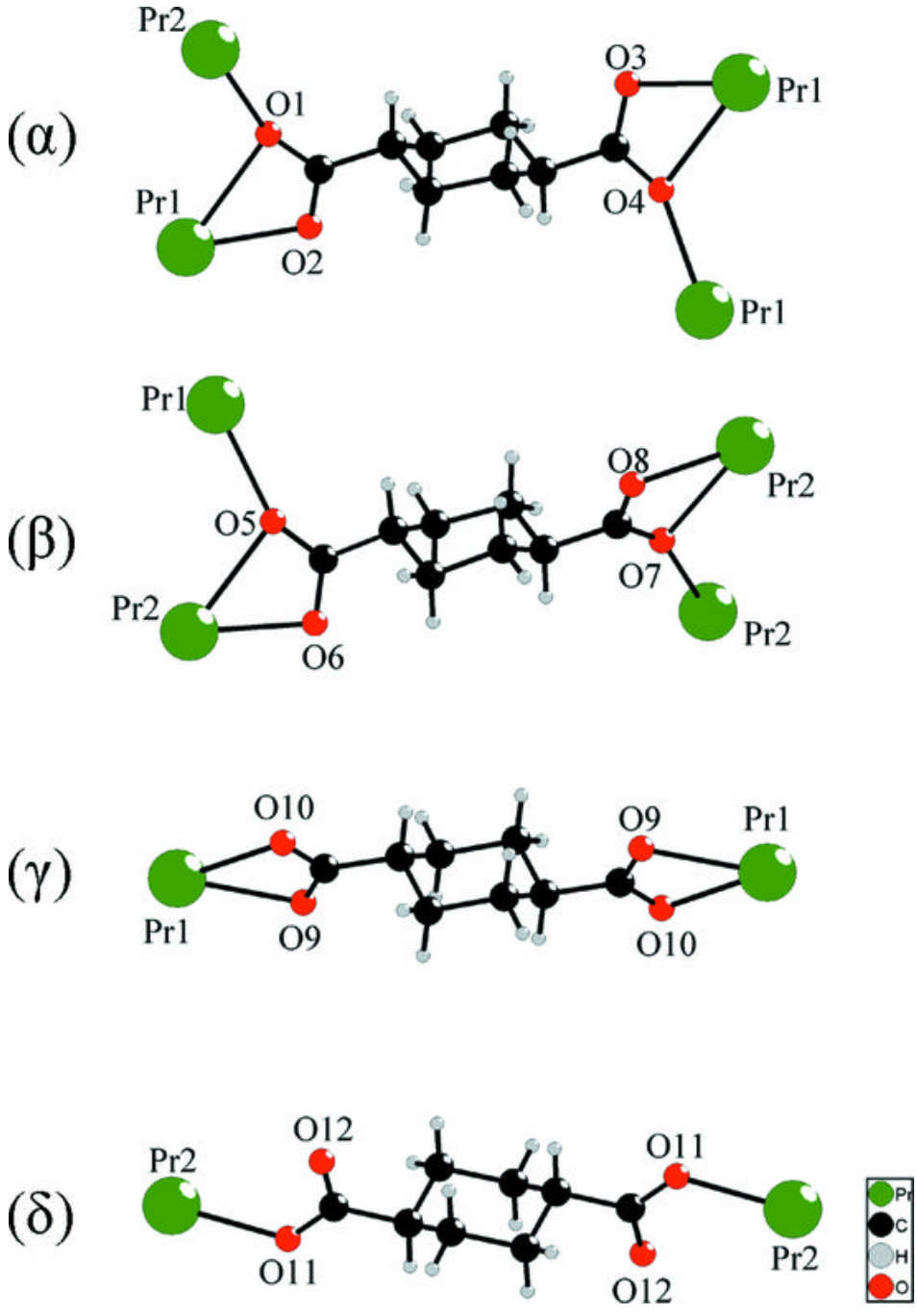

(α)
Pr2
O1
Pr1
O2
O3
Pr1
O4
Pr1
(β)
Pr1
O5
Pr2
O6
O8
Pr2
O7
Pr2
(γ)
O10
Pr1
O9
O9
Pr1
O10
(δ)
Pr2
O12
O11
O11
O12
Pr2
Pr
C
H
O

Fig. 3

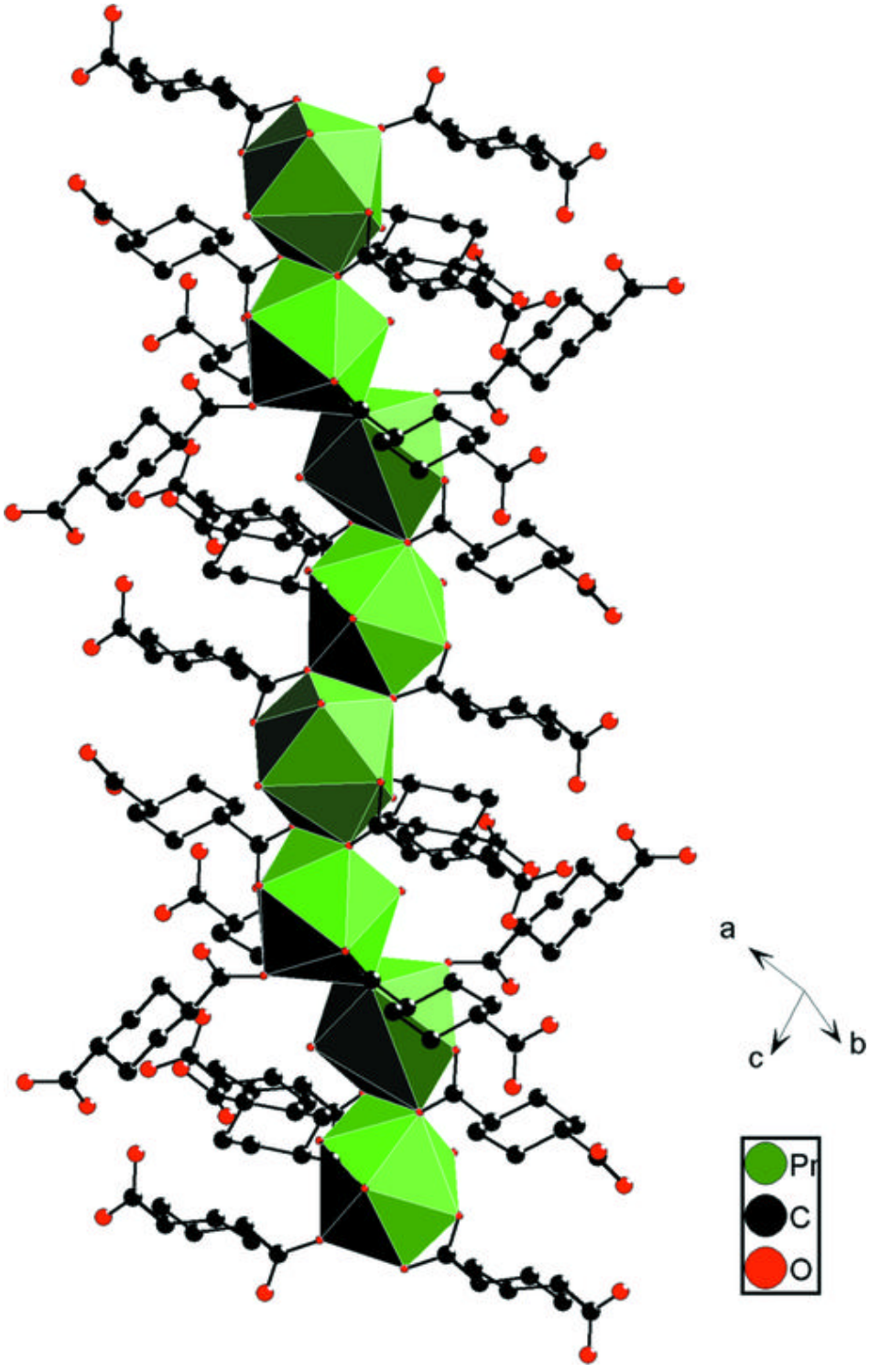


Fig. 4