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Poly[[μ_2-aqua-tetraaquahexakis(μ_4-naphthalene-2,6-dicarboxylato)tetraholmium(III)] 1.75-hydrate]

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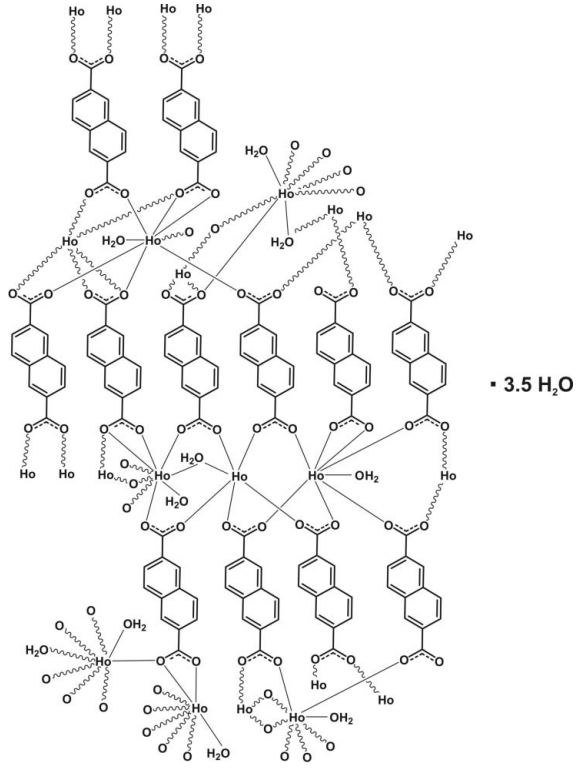
Key indicators: single-crystal X-ray study; T = 180 K; mean σ(C–C) = 0.016 Å; H-atom completeness 73%; disorder in solvent or counterion; R factor = 0.062; wR factor = 0.172; data-to-parameter ratio = 11.2.

In the title compound, $\{[Ho_4(C_{12}H_6O_4)_6(H_2O)_5]\cdot 1.75H_2O\}_n$, which is isostructural with its Tb^{3+}- and Eu^{3+}-containing analogues, there are four crystallographically independent Ho^{3+} centres, each exhibiting a highly distorted HoO_8 bicapped trigonal-prismatic coordination environment. Adjacent polyhedra are interconnected *via* the carboxylate groups and one μ_2-bridging water molecule, forming one-dimensional chains propagating along [100]. The naphthalene-2,6-dicarboxylate ligands further interconnect these chains into a three-dimensional framework, which has zigzag channels housing the water molecules. Two naphthalene-2,6-dicarboxylate bridging ligands have their centroids located on crystallographic centres of inversion. One water O atom has a fixed site occupancy factor of 0.75.

Related literature

For isostructural materials, see: Min & Lee (2002); Zheng, Sun *et al.* (2004). For related structures, see: Zheng, Wang *et al.* (2004); Paz & Klinowski (2003); Almeida Paz & Klinowski (2008); Wang *et al.* (2002). For general background, see: Shi *et al.* (2008); Cunha-Silva *et al.* (2007). For bond-length data, see: Allen (2002).



Experimental

Crystal data

$[Ho_4(C_{12}H_6O_4)_6(H_2O_5)_5]\cdot 1.75H_2O$
M_r = 2066.34
Monoclinic, $P2_1/n$
a = 17.0505 (4) Å
b = 15.1728 (4) Å
c = 24.9142 (6) Å
β = 106.126 (1)°
V = 6191.8 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 5.16 mm^{-1}
T = 180 (2) K
0.12 × 0.12 × 0.01 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
T_{min} = 0.576, T_{max} = 0.950
27842 measured reflections
10664 independent reflections
7421 reflections with $I > 2\sigma(I)$
R_{int} = 0.060

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.062
$wR(F^2)$ = 0.172
S = 1.04
10664 reflections
951 parameters
4 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 9.72 e Å^{-3}
$\Delta\rho_{min}$ = −2.00 e Å^{-3}

  doi:10.1107/S1600536808000378

Table 1
Selected bond lengths (Å).

Ho1—O1	2.313 (8)	Ho3—O8	2.410 (8)
Ho1—O3^{i}	2.335 (7)	Ho3—O12	2.337 (8)
Ho1—O5	2.277 (8)	Ho3—O14	2.356 (8)
Ho1—O10^{ii}	2.314 (8)	Ho3—O17	2.299 (7)
Ho1—O15^{iii}	2.309 (8)	Ho3—O20^{ii}	2.299 (8)
Ho1—O23^{iv}	2.847 (9)	Ho3—O21	2.300 (8)
Ho1—O24^{iv}	2.311 (8)	Ho3—O4*W*	2.469 (8)
Ho1—O2*W*	2.370 (8)	Ho3—O5*W*	2.640 (6)
Ho2—O2	2.299 (8)	Ho4—O4^{v}	2.360 (8)
Ho2—O6	2.316 (8)	Ho4—O9^{vi}	2.382 (7)
Ho2—O7	2.338 (8)	Ho4—O16^{vii}	2.342 (8)
Ho2—O11	2.264 (8)	Ho4—O18	2.337 (7)
Ho2—O13	2.347 (8)	Ho4—O22	2.276 (7)
Ho2—O19^{ii}	2.338 (8)	Ho4—O23^{viii}	2.296 (8)
Ho2—O20^{ii}	2.876 (8)	Ho4—O5*W*	2.671 (6)
Ho2—O3*W*	2.423 (9)	Ho4—O6*W*	2.453 (10)

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

Data collection: *COLLECT* (Nonius 1998); cell refinement: *HKL SCALEPACK* (Otwinowski & Minor 1997); data reduction: *HKL DENZO* (Otwinowski & Minor 1997) and *SCALEPACK*; program(s) used to solve structure: *SIR92* (Altomare *et al.* 1994); program(s) used to refine structure: *SHELXTL* (Bruker, 2001); molecular graphics: *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2668).

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supporting information

Acta Cryst. (2008). E**64**, m336–m337 [doi:10.1107/S1600536808000378]

Poly[[μ_2-aqua-tetraaquahexakis(μ_4-naphthalene-2,6-dicarboxylato)tetraholmium(III)] 1.75-hydrate]

Filipe A. Almeida Paz and Jacek Klinowski

S1. Comment

Multi-dimensional (*i.e.*, one-dimensional, two-dimensional or three-dimensional) networks, known as coordination polymers or metal-organic frameworks (MOFs), in which metallic centres are bridged *via* organic ligands, are of considerable interest. Even though structural diversity can be achieved by selecting different metallic centres (which implies a variation in the number and type of the coordination geometry), fascinating structural architectures are often produced by using uncommon bridging ligands. To reconcile the robustness and crystallinity of the synthesized networks, crystal engineers usually employ *exo*-carboxylate derivatives as the bridging ligands, usually associated with aromatic rings. It is therefore surprising that only a handful of papers reporting lanthanide centres coordinated to residues of naphthalene-2,6-dicarboxylic acid (H_2NDC) have been published (Paz & Klinowski, 2008; Zheng, Sun *et al.*, 2004; Zheng, Wang *et al.*, 2004; Paz & Klinowski, 2003; Wang *et al.*, 2002; Min & Lee, 2002), as confirmed by a search in the Cambridge Structural Database (CSD, Version 5.28 with three updates - August 2007; Allen, 2002).

Following our interest in the hydrothermal synthesis of MOFs, (*e.g.* Shi *et al.*, 2008; Cunha-Silva *et al.*, 2007), we report here the low temperature crystal structure of the title compound, (I), a three-dimensional MOF containing the naphthalene-2,6-dicarboxylate dianion (NDC^{2-}) bound to Ho^{3+}: $[Ho_4(NDC)_6(H_2O)_5]\cdot 1.75H_2O$. Despite being analogous the frameworks reported by Min & Lee (2002) (with Tb^{3+}) and Zheng, Sun *et al.* (2004) (with Eu^{3+}), this new crystal structure provides further insights into the self-assembly process. Thus crystals of a two-dimensional network, $[Ho_2(NDC)_3(H_2O)_6]$, could also be isolated from the same synthetic batch (Paz & Klinowski, 2008). We infer that the ionic radius of the lanthanide employed determines whether a three-dimensional (for the lighter series of lanthanides - up to Dy^{3+}) or a two-dimensional network (for lanthanides after and including Er^{3+}) is obtained. Ho^{3+} always produces a mixture of the two materials, even though it is possible to vary the amount of each framework in the product by adjusting the composition of the synthesis mixture.

Compound (I) contains four crystallographically independent Ho^{3+} centres (Ho1 to Ho4) which are coordinated to a total of six NDC^{2-} ligands (two of these have their centroids located at crystallographic inversion centres) and five water molecules. The coordination sphere of each metallic centre is composed by one unidentate water molecule, with the fifth water (O5W) bridging two neighbouring metallic centres (Ho3 and Ho4 - see Figure 1). Despite the large number of crystallographically independent moieties, the NDC^{2-} moieties coordinate to the Ho^{3+} centres through only two distinct coordination fashions: a *syn,syn*-chelate coupled to a *syn,syn*-μ_2-bridge (for the C56 and C68 carboxylate groups), and simple *syn,syn*-μ_2-bridges (for all remaining carboxylate moieties). The $\{HoO_8\}$ coordination geometries for the Ho^{3+} centres remain strikingly similar, resembling highly distorted bicapped trigonal prisms (Figures 2a to 2 d), with the capping positions being either water molecules or the O-atoms involved in the *syn,syn*-μ_2-bridges coupled to *syn,syn*-chelate mentioned above (O20 and O23 - Figure 2). Disregarding the Ho—O distances related to the O20, O23 and O5W

atoms which occupy the capping positions of the coordination polyhedra, the remaining Ho—O distances are typical and well within the ranges registered for related materials (as revealed by a search in the CSD - 77 entries, range of 2.20–2.82 Å with a median of 2.34 Å): for Ho1 to Ho4, respectively, 2.277 (8)–2.370 (8) Å, 2.264 (8)–2.423 (9) Å, 2.299 (7)–2.469 (8) Å and 2.276 (7)–2.453 (10) Å (Table 1). We emphasize that even though the Ho—O distances associated with these capping positions are unusually long, they are still within the feasible range found in related materials. Moreover, we also note that the longest values of Ho—O for Ho1 to Ho4 found in the ranges given above are those with the coordinated water molecules. In fact, by restricting the search in the CSD to the geometrical parameters for coordinated water molecules to Ho^{3+} centres, the expected range is from 2.28 to 2.55 Å, which is in good agreement with the experimental data for the title compound.

The connection between neighbouring {HoO_8} polyhedra *via* the carboxylate groups and water molecules leads to the formation of a one-dimensional chain of metallic centres running along the [100] crystallographic direction (Figure 2 e). The Ho···Ho distances range from 4.0258 (1) to 5.2585 (1) Å. These chains are interconnected along the [001] direction *via* the NDC^{2-} bridges forming a three-dimensional MOF (Figure 3). There is structural evidence that such connectivity creates small one-dimensional zigzag channels parallel to the *a*-axis, distributed in a typical brick-wall fashion in the *bc* plane containing the water molecules of crystallization O1W and O7W. Although the water H atoms could not be located in the present study, presumably O—H···O hydrogen bonds from the water molecules (both coordinated and uncoordinated) interconnect adjacent chains (not shown).

S2. Experimental

To a solution of $HoCl_3.6H_2O$ (1.062 g, 2.799 mmol) in distilled water (6.04 g), naphthalene-2,6-dicarboxylic acid (0.102 g, 0.472 mmol) and triethylamine (0.089 g, 0.880 mmol) were added and the mixture was stirred thoroughly for 5 minutes at ambient temperature. The suspension, with a molar composition of 5.93 Ho^{3+}: 1.00 H_2NDC: 1.86 TEA: 120 H_2O, was transferred to a Parr teflon-lined stainless steel vessel (*ca* 21 cm^3) and placed for 8 h at 418 K in a preheated oven. Before opening, the reaction vessel was allowed to cool slowly to ambient temperature at a rate of 10 K per hour over a period of 14 h. Colourless plates of (I) were manually selected from the product which also contains $[Ho_2(NDC)_3(H_2O)_6]$ (Paz & Klinowski, 2008).

S3. Refinement

The water molecules O1W, O5W and O7W were refined isotropically. Following structural evidence from unrestrained refinement cycles, the O7W water molecule was given a fixed occupancy of 75% in the final structural model.

It is important to stress that a considerable smeared-out electron density was found surrounding the water molecules O1W and O5W. Attempts to model this disorder (during the last stages of the overall structural refinement) over two (or more) partially occupied sites (for each water molecule) did not produce satisfactory models, with large shifts associated with these chemical moieties being observed. In order to achieve full convergence the positions of O1W and O5W were restrained to be equally distant from, respectively, Ho1 and Ho2, and Ho3 and Ho4 (one free variable for each pair of distances). The difficulties while modelling these two water molecules are attributed to the quality of the crystal used for data collection, which was a very small and thin colourless plate diffracting rather weakly at high angles [*e.g.*, almost no reflections were observed for resolutions higher than 0.80 Å]. The highest difference peak is 0.78Å from O5W.

H atoms associated with all water molecules could not be located from difference Fourier maps, and attempts to place these atoms in calculated positions in order to maximize hydrogen bonding interactions did not lead to chemically reasonable structural models and they were omitted from the refinement. The H atoms bound to carbon were placed at idealized positions (C—H = 0.95 Å) and refined as riding with $U_{iso} = 1.2U_{eq}$(C).

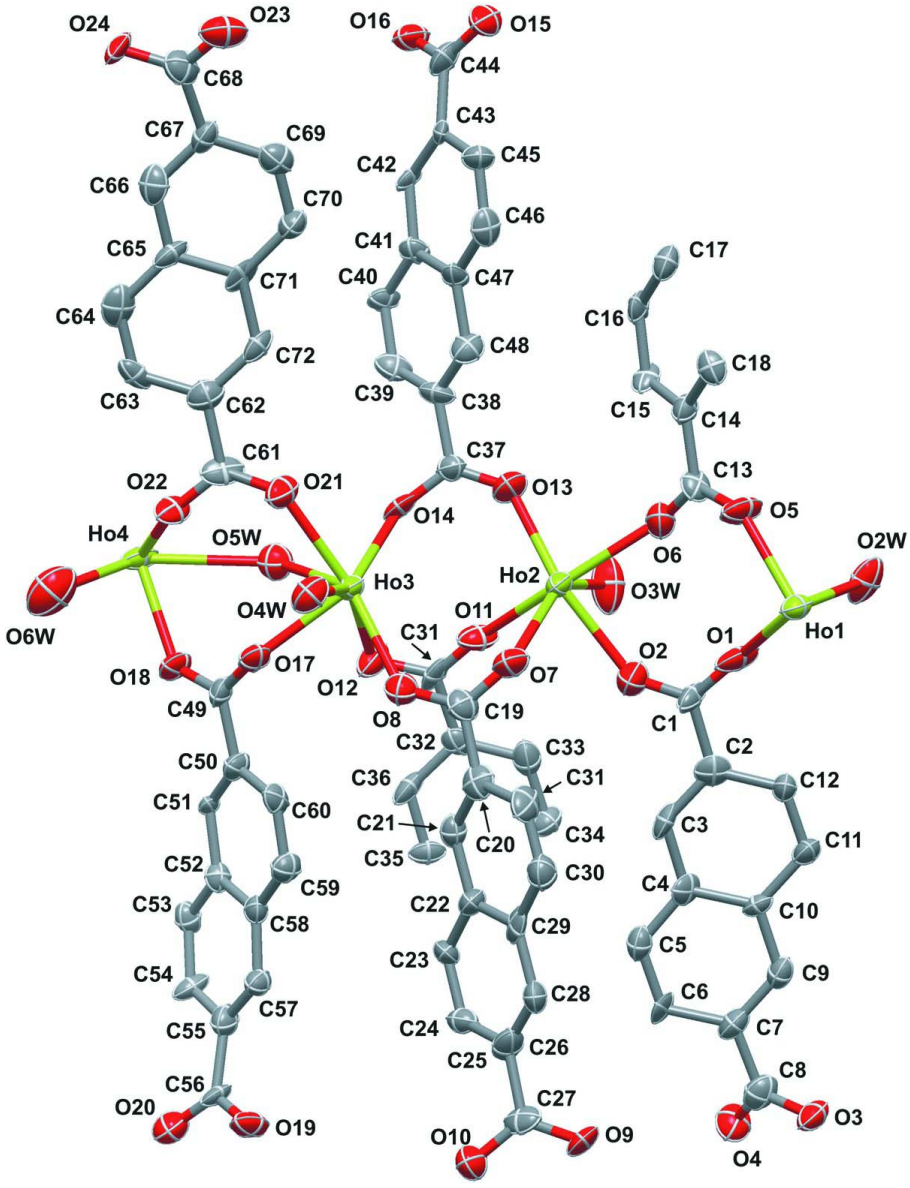

Figure 1

Simplified representation of the asymmetric unit of (I) with displacement ellipsoids drawn at the 80% probability level. Water molecules O1W and O7W, and hydrogen atoms have been omitted for clarity.

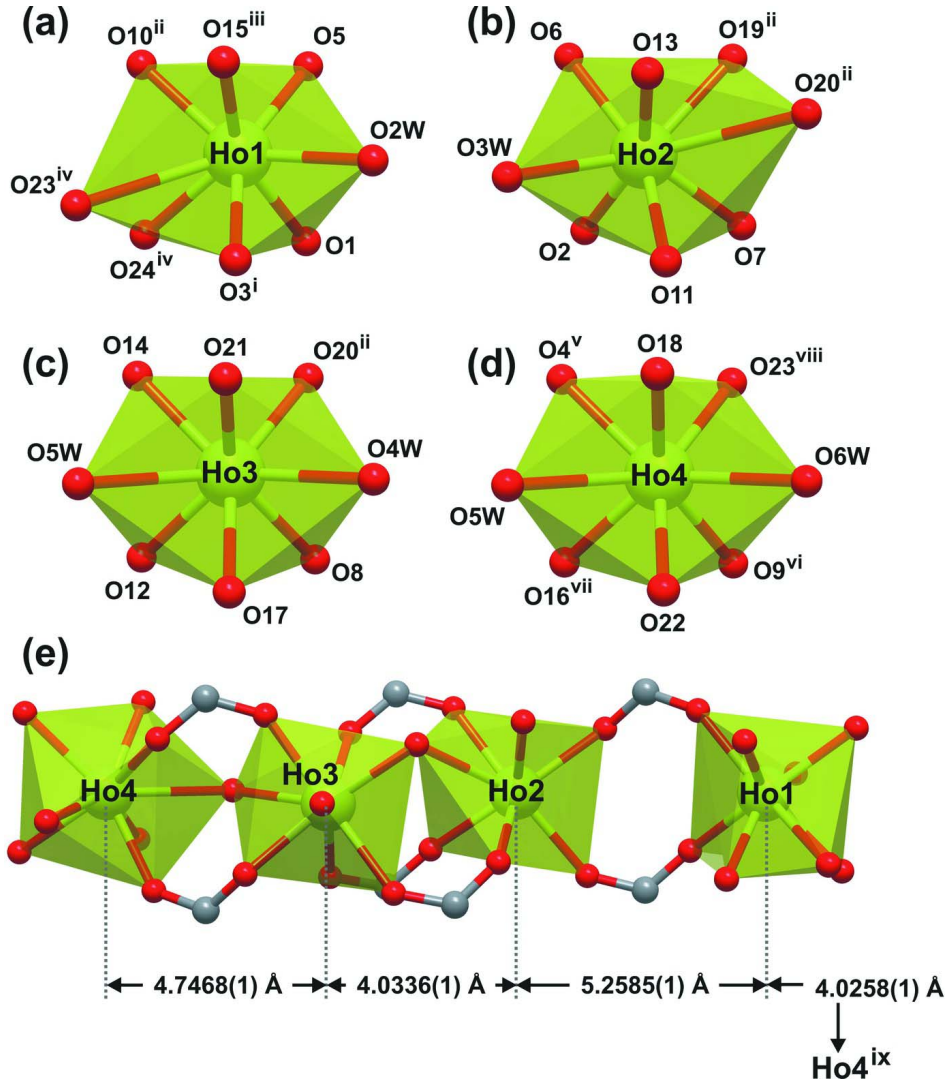

Figure 2

Polyhedral representation of the {HoO_8} coordination environments, which resemble highly distorted bicapped trigonal prisms, for: ***(a)*** Ho1, ***(b)*** Ho2, ***(c)*** Ho3 and ***(d)*** Ho4. ***(e)*** Interconnection of the individual {HoO_8} polyhedra along the [100] crystallographic direction leading to the formation of one-dimensional chains. For selected bond lengths (in Å) see the dedicated Table in the main paper. Symmetry codes used to generate equivalent atoms: (i) *-x + 1*, *-y + 1*, *-z + 2*; (ii) *x-1/2*, *-y + 1/2*, *z-1/2*; (iii) *-x + 1*, *-y + 1*, *-z + 1*; (iv) *x-1/2*, *-y + 1/2*, *z+1/2*; (v) *-x + 2*, *-y + 1*, *-z + 2*; (vi) *x+1/2*, *-y + 1/2*, *z-1/2*; (vii) *-x + 2*, *-y + 1*, *-z + 1*; (viii) *x+1/2*, *-y + 1/2*, *z+1/2*; (ix) *x-1*, *y*, *z*.

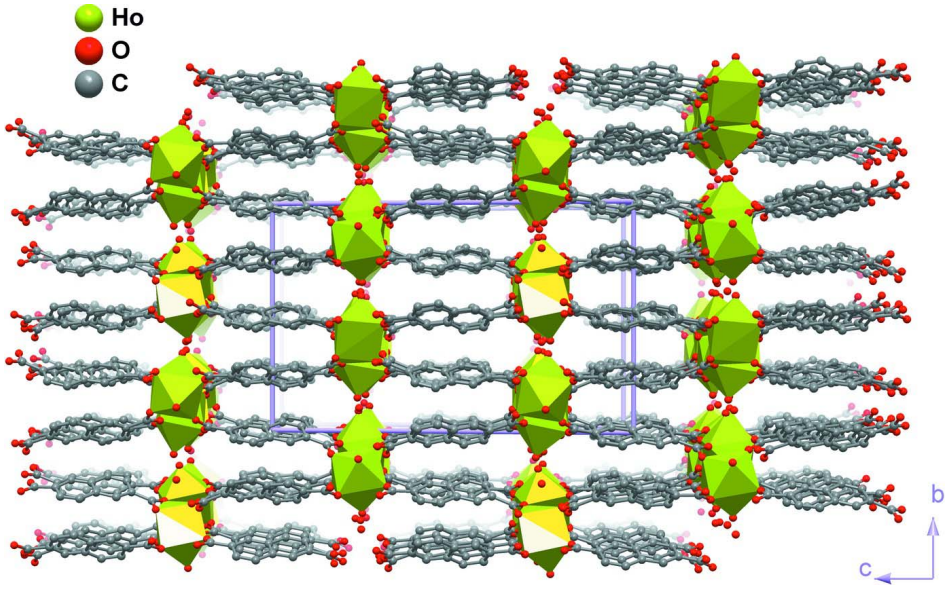

Figure 3

Crystal packing of the title compound viewed in perspective along the [100] direction of the unit cell. Hydrogen atoms have been omitted for clarity.

poly[[μ_2-aqua-tetraaquahexakis(μ_4-naphthalene-2,6-dicarboxylato) tetraholmium(III)] 1.75-hydrate]

Crystal data

$[Ho_4(C_{12}H_6O_4)_6(H_2O_5)_5]\cdot 1.75H_2O$
$M_r = 2066.34$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 17.0505$ (4) Å
$b = 15.1728$ (4) Å
$c = 24.9142$ (6) Å
$\beta = 106.126$ (1)°
$V = 6191.8$ (3) Å^3
$Z = 4$
$F(000) = 3982$
$D_x = 2.217$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 70959 reflections
$\theta = 1.0$–$25.0°$
$\mu = 5.16$ mm^{-1}
$T = 180$ K
Plate, colourless
0.12 × 0.12 × 0.01 mm

Data collection

Nonius Kappa CCD diffractometer
Radiation source: fine-focus sealed tube
Thin slice ω and φ scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
$T_{min} = 0.576$, $T_{max} = 0.950$
27842 measured reflections
10664 independent reflections
7421 reflections with $I > 2\sigma(I)$
$R_{int} = 0.060$
$\theta_{max} = 25.0°$, $\theta_{min} = 3.6°$
$h = -20\rightarrow20$
$k = -18\rightarrow18$
$l = -29\rightarrow29$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.062$
$wR(F^2) = 0.172$
$S = 1.04$
10664 reflections
951 parameters
4 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0951P)^2 + 49.5291P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 9.73$ e Å^{-3}
$\Delta\rho_{min} = -2.01$ e Å^{-3}

Special details

Experimental. See dedicated section in the main paper

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Ho1	0.43036 (3)	0.43328 (3)	0.74931 (2)	0.01641 (16)	
Ho2	0.73944 (3)	0.44550 (4)	0.75148 (2)	0.01864 (16)	
Ho3	0.94596 (3)	0.31502 (3)	0.75250 (2)	0.01782 (16)	
Ho4	1.22082 (3)	0.30713 (4)	0.74454 (2)	0.02020 (16)	
O1W	0.5958 (6)	0.2081 (11)	0.7441 (7)	0.108 (5)*	
O2W	0.4125 (5)	0.5883 (5)	0.7439 (4)	0.028 (2)	
O3W	0.7616 (5)	0.6017 (6)	0.7697 (4)	0.039 (2)	
O4W	0.9089 (5)	0.1577 (5)	0.7388 (3)	0.0251 (18)	
O5W	1.0839 (4)	0.3895 (5)	0.7479 (3)	0.0263 (19)*	
O6W	1.2552 (6)	0.1500 (7)	0.7565 (4)	0.046 (3)	
O7W	0.0661 (11)	0.6098 (13)	0.7506 (7)	0.080 (5)*	0.75
O1	0.5535 (5)	0.4870 (6)	0.8042 (3)	0.0273 (19)	
O2	0.6872 (5)	0.4687 (6)	0.8260 (4)	0.030 (2)	
O3	0.6279 (5)	0.5218 (5)	1.1807 (3)	0.0226 (18)	
O4	0.7584 (5)	0.5611 (5)	1.2030 (3)	0.0265 (19)	
O5	0.4886 (5)	0.4701 (6)	0.6805 (3)	0.0274 (19)	
O6	0.6189 (5)	0.5100 (5)	0.7000 (3)	0.0251 (18)	
O7	0.7555 (5)	0.3124 (5)	0.8006 (3)	0.0257 (19)	
O8	0.8854 (5)	0.2691 (5)	0.8246 (3)	0.0224 (17)	
O9	0.7805 (5)	0.2343 (6)	1.1724 (3)	0.0272 (19)	
O10	0.9123 (5)	0.1926 (5)	1.1948 (3)	0.0271 (19)	
O11	0.8714 (5)	0.4522 (5)	0.8033 (3)	0.0221 (18)	
O12	0.9998 (5)	0.4138 (6)	0.8254 (3)	0.0263 (19)	
O13	0.7983 (5)	0.4924 (6)	0.6817 (3)	0.0286 (19)	
O14	0.9277 (5)	0.4469 (5)	0.7005 (3)	0.0255 (19)	
O15	0.7017 (5)	0.5512 (6)	0.3068 (3)	0.029 (2)	
O16	0.8295 (5)	0.5917 (6)	0.3278 (3)	0.0275 (19)	
O17	1.0540 (4)	0.2363 (5)	0.8072 (3)	0.0193 (17)	
O18	1.1862 (5)	0.2690 (6)	0.8260 (3)	0.0255 (19)	

O19	1.1803 (5)	0.1574 (6)	1.1822 (3)	0.0244 (18)
O20	1.3118 (5)	0.1900 (5)	1.2001 (3)	0.0279 (19)
O21	0.9784 (4)	0.2705 (6)	0.6730 (3)	0.0237 (18)
O22	1.1109 (4)	0.2322 (5)	0.6914 (3)	0.0205 (17)
O23	0.8546 (5)	0.2013 (5)	0.2970 (3)	0.029 (2)
O24	0.9861 (5)	0.1763 (6)	0.3129 (3)	0.027 (2)
C1	0.6227 (6)	0.4803 (8)	0.8388 (5)	0.018 (2)
C2	0.6267 (7)	0.4936 (7)	0.8990 (5)	0.017 (2)
C3	0.6942 (6)	0.4698 (7)	0.9413 (5)	0.017 (2)
H3	0.7390	0.4426	0.9321	0.020*
C4	0.6985 (6)	0.4851 (8)	0.9988 (5)	0.018 (2)
C5	0.7657 (7)	0.4613 (7)	1.0441 (5)	0.018 (2)
H5	0.8115	0.4337	1.0367	0.021*
C6	0.7666 (7)	0.4770 (8)	1.0988 (5)	0.021 (3)
H6	0.8137	0.4634	1.1284	0.025*
C7	0.6966 (7)	0.5137 (7)	1.1106 (5)	0.019 (2)
C8	0.6950 (7)	0.5322 (8)	1.1689 (5)	0.023 (3)
C9	0.6303 (7)	0.5372 (7)	1.0675 (5)	0.017 (2)
H9	0.5837	0.5621	1.0756	0.021*
C10	0.6301 (6)	0.5250 (7)	1.0112 (4)	0.013 (2)
C11	0.5608 (7)	0.5494 (7)	0.9665 (5)	0.019 (2)
H11	0.5152	0.5765	0.9746	0.023*
C12	0.5597 (6)	0.5342 (7)	0.9130 (5)	0.016 (2)
H12	0.5131	0.5510	0.8839	0.019*
C13	0.5503 (6)	0.4905 (7)	0.6661 (5)	0.017 (2)
C14	0.5434 (6)	0.5002 (7)	0.6056 (5)	0.016 (2)
C15	0.6068 (6)	0.5430 (7)	0.5885 (4)	0.017 (2)
H15	0.6541	0.5631	0.6158	0.020*
C16	0.5998 (6)	0.5554 (7)	0.5329 (5)	0.017 (2)
H16	0.6416	0.5861	0.5222	0.020*
C17	0.5312 (6)	0.5233 (7)	0.4910 (5)	0.017 (2)
C18	0.4772 (6)	0.4677 (7)	0.5661 (5)	0.015 (2)
H18	0.4357	0.4382	0.5778	0.018*
C19	0.8176 (7)	0.2826 (8)	0.8349 (5)	0.021 (3)
C20	0.8111 (7)	0.2621 (7)	0.8932 (5)	0.019 (2)
C21	0.8757 (6)	0.2863 (7)	0.9394 (5)	0.016 (2)
H21	0.9242	0.3103	0.9337	0.019*
C22	0.8690 (7)	0.2752 (8)	0.9943 (5)	0.021 (3)
C23	0.9341 (7)	0.2967 (8)	1.0427 (5)	0.020 (2)
H23	0.9828	0.3228	1.0387	0.024*
C24	0.9259 (7)	0.2794 (7)	1.0947 (4)	0.018 (2)
H24	0.9704	0.2916	1.1264	0.021*
C25	0.8527 (7)	0.2439 (8)	1.1029 (5)	0.024 (3)
C26	0.8468 (7)	0.2230 (7)	1.1597 (5)	0.021 (3)
C27	0.7881 (6)	0.2240 (7)	1.0570 (5)	0.019 (2)
H27	0.7388	0.2011	1.0621	0.023*
C28	0.7956 (7)	0.2380 (7)	1.0023 (5)	0.018 (2)
C29	0.7310 (7)	0.2155 (8)	0.9532 (5)	0.021 (3)

H29	0.6820	0.1906	0.9577	0.026*
C30	0.7375 (6)	0.2283 (8)	0.9012 (5)	0.023 (3)
H30	0.6929	0.2148	0.8698	0.027*
C31	0.9407 (7)	0.4500 (7)	0.8369 (5)	0.019 (2)
C32	0.9522 (7)	0.4816 (7)	0.8958 (5)	0.018 (2)
C33	0.8895 (7)	0.5255 (7)	0.9109 (5)	0.023 (3)
H33	0.8419	0.5425	0.8827	0.028*
C34	0.8955 (7)	0.5444 (7)	0.9651 (5)	0.018 (2)
H34	0.8516	0.5726	0.9747	0.021*
C35	1.0323 (7)	0.4782 (7)	0.9923 (4)	0.017 (2)
C36	1.0245 (7)	0.4606 (8)	0.9367 (5)	0.021 (3)
H36	1.0684	0.4341	0.9261	0.025*
C37	0.8618 (7)	0.4769 (7)	0.6682 (4)	0.017 (2)
C38	0.8630 (7)	0.4925 (7)	0.6092 (4)	0.019 (2)
C39	0.9333 (7)	0.5273 (7)	0.5949 (5)	0.021 (3)
H39	0.9816	0.5403	0.6236	0.026*
C40	0.9309 (6)	0.5418 (7)	0.5409 (4)	0.016 (2)
H40	0.9775	0.5658	0.5325	0.019*
C41	0.8605 (6)	0.5219 (7)	0.4964 (4)	0.015 (2)
C42	0.8534 (6)	0.5405 (7)	0.4398 (4)	0.013 (2)
H42	0.8984	0.5668	0.4303	0.015*
C43	0.7835 (6)	0.5220 (7)	0.3975 (4)	0.015 (2)
C44	0.7714 (7)	0.5548 (8)	0.3403 (5)	0.021 (3)
C45	0.7181 (7)	0.4779 (7)	0.4120 (4)	0.017 (2)
H45	0.6710	0.4612	0.3832	0.021*
C46	0.7218 (6)	0.4594 (7)	0.4660 (5)	0.018 (2)
H46	0.6772	0.4307	0.4745	0.021*
C47	0.7923 (6)	0.4830 (7)	0.5103 (4)	0.015 (2)
C48	0.7949 (7)	0.4712 (7)	0.5676 (5)	0.018 (2)
H48	0.7485	0.4481	0.5768	0.021*
C49	1.1229 (6)	0.2538 (7)	0.8407 (5)	0.017 (2)
C50	1.1273 (6)	0.2519 (7)	0.9011 (5)	0.017 (2)
C51	1.1979 (6)	0.2820 (7)	0.9410 (4)	0.013 (2)
H51	1.2405	0.3098	0.9294	0.016*
C52	1.2048 (6)	0.2704 (7)	0.9985 (4)	0.014 (2)
C53	1.2777 (6)	0.2962 (7)	1.0406 (5)	0.017 (2)
H53	1.3196	0.3276	1.0303	0.020*
C54	1.2864 (7)	0.2755 (7)	1.0951 (4)	0.018 (2)
H54	1.3353	0.2908	1.1226	0.022*
C55	1.2227 (6)	0.2308 (8)	1.1113 (5)	0.020 (2)
C56	1.2393 (7)	0.1930 (7)	1.1688 (4)	0.017 (2)
C57	1.1509 (6)	0.2115 (7)	1.0724 (4)	0.016 (2)
H57	1.1080	0.1843	1.0838	0.019*
C58	1.1396 (6)	0.2314 (7)	1.0155 (4)	0.015 (2)
C59	1.0675 (6)	0.2059 (7)	0.9728 (5)	0.018 (2)
H59	1.0224	0.1819	0.9832	0.021*
C60	1.0627 (6)	0.2154 (7)	0.9185 (5)	0.017 (2)
H60	1.0147	0.1970	0.8912	0.020*

C61	1.0416 (7)	0.2537 (7)	0.6579 (4)	0.020 (3)
C62	1.0362 (7)	0.2519 (7)	0.5969 (5)	0.021 (3)
C63	1.1013 (6)	0.2124 (7)	0.5797 (5)	0.016 (2)
H63	1.1487	0.1917	0.6067	0.019*
C64	1.0947 (7)	0.2049 (7)	0.5240 (5)	0.023 (3)
H64	1.1384	0.1796	0.5125	0.027*
C65	1.0234 (6)	0.2345 (7)	0.4826 (4)	0.017 (2)
C66	1.0120 (7)	0.2199 (7)	0.4252 (5)	0.021 (3)
H66	1.0551	0.1945	0.4131	0.025*
C67	0.9396 (7)	0.2414 (7)	0.3858 (5)	0.018 (2)
C68	0.9257 (7)	0.2056 (8)	0.3278 (5)	0.023 (3)
C69	0.8791 (7)	0.2877 (7)	0.4044 (5)	0.021 (2)
H69	0.8306	0.3070	0.3778	0.025*
C70	0.8896 (7)	0.3041 (7)	0.4580 (5)	0.019 (2)
H70	0.8482	0.3351	0.4690	0.023*
C71	0.9601 (6)	0.2772 (7)	0.4996 (4)	0.015 (2)
C72	0.9682 (6)	0.2855 (7)	0.5576 (5)	0.016 (2)
H72	0.9266	0.3143	0.5698	0.019*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ho1	0.0159 (3)	0.0228 (3)	0.0110 (3)	−0.0031 (2)	0.00474 (19)	−0.0011 (2)
Ho2	0.0156 (3)	0.0290 (3)	0.0126 (3)	0.0039 (2)	0.0060 (2)	−0.0003 (2)
Ho3	0.0158 (3)	0.0273 (3)	0.0115 (3)	0.0032 (2)	0.0057 (2)	−0.0002 (2)
Ho4	0.0173 (3)	0.0331 (3)	0.0116 (3)	−0.0074 (2)	0.0063 (2)	−0.0006 (2)
O2W	0.029 (5)	0.023 (4)	0.043 (5)	−0.006 (4)	0.026 (4)	−0.002 (4)
O3W	0.026 (5)	0.026 (5)	0.065 (7)	0.000 (4)	0.012 (4)	−0.011 (5)
O4W	0.026 (5)	0.026 (4)	0.026 (5)	−0.004 (4)	0.012 (4)	−0.003 (4)
O6W	0.050 (6)	0.044 (6)	0.052 (7)	−0.012 (5)	0.030 (5)	−0.006 (5)
O1	0.027 (5)	0.044 (5)	0.015 (4)	−0.011 (4)	0.013 (4)	−0.003 (4)
O2	0.024 (5)	0.045 (5)	0.024 (5)	0.008 (4)	0.009 (4)	−0.001 (4)
O3	0.022 (4)	0.031 (5)	0.018 (4)	0.000 (3)	0.011 (3)	−0.004 (3)
O4	0.021 (4)	0.031 (5)	0.026 (5)	−0.003 (4)	0.003 (4)	−0.006 (4)
O5	0.023 (4)	0.046 (5)	0.016 (4)	−0.008 (4)	0.011 (3)	0.003 (4)
O6	0.021 (4)	0.030 (5)	0.027 (5)	0.007 (4)	0.009 (4)	0.004 (4)
O7	0.027 (5)	0.035 (5)	0.018 (4)	0.002 (4)	0.010 (4)	0.005 (4)
O8	0.021 (4)	0.027 (4)	0.019 (4)	0.001 (3)	0.005 (3)	−0.002 (3)
O9	0.028 (5)	0.041 (5)	0.020 (4)	0.009 (4)	0.018 (4)	0.004 (4)
O10	0.020 (4)	0.037 (5)	0.024 (5)	0.006 (4)	0.005 (4)	0.006 (4)
O11	0.022 (4)	0.031 (5)	0.012 (4)	−0.009 (4)	0.002 (3)	−0.003 (3)
O12	0.019 (4)	0.040 (5)	0.022 (4)	−0.002 (4)	0.009 (3)	−0.010 (4)
O13	0.027 (5)	0.039 (5)	0.024 (5)	0.006 (4)	0.014 (4)	0.007 (4)
O14	0.027 (5)	0.039 (5)	0.016 (4)	0.006 (4)	0.016 (4)	0.002 (4)
O15	0.013 (4)	0.053 (6)	0.018 (4)	0.002 (4)	0.000 (3)	−0.002 (4)
O16	0.022 (4)	0.047 (5)	0.015 (4)	0.001 (4)	0.007 (3)	0.004 (4)
O17	0.024 (4)	0.020 (4)	0.017 (4)	0.002 (3)	0.012 (3)	0.004 (3)
O18	0.018 (4)	0.044 (5)	0.018 (4)	0.002 (4)	0.011 (3)	0.006 (4)

O19	0.021 (4)	0.036 (5)	0.018 (4)	−0.002 (4)	0.007 (3)	0.011 (4)
O20	0.030 (5)	0.034 (5)	0.022 (5)	0.003 (4)	0.011 (4)	−0.002 (4)
O21	0.015 (4)	0.038 (5)	0.019 (4)	−0.002 (4)	0.005 (3)	−0.005 (4)
O22	0.013 (4)	0.033 (5)	0.014 (4)	−0.007 (3)	0.001 (3)	−0.005 (3)
O23	0.031 (5)	0.036 (5)	0.019 (4)	−0.010 (4)	0.006 (4)	0.001 (4)
O24	0.021 (4)	0.046 (5)	0.018 (4)	0.009 (4)	0.010 (3)	−0.009 (4)
C1	0.010 (5)	0.033 (7)	0.014 (6)	−0.003 (5)	0.005 (4)	−0.007 (5)
C2	0.019 (6)	0.015 (5)	0.019 (6)	−0.007 (5)	0.008 (5)	0.003 (5)
C3	0.016 (6)	0.016 (6)	0.024 (6)	0.000 (4)	0.013 (5)	−0.006 (5)
C4	0.010 (5)	0.027 (6)	0.019 (6)	−0.004 (5)	0.007 (4)	0.002 (5)
C5	0.015 (6)	0.017 (6)	0.024 (7)	0.001 (4)	0.009 (5)	0.000 (5)
C6	0.014 (6)	0.033 (7)	0.021 (6)	0.004 (5)	0.014 (5)	0.004 (5)
C7	0.021 (6)	0.022 (6)	0.019 (6)	−0.001 (5)	0.012 (5)	−0.002 (5)
C8	0.024 (7)	0.023 (6)	0.027 (7)	−0.003 (5)	0.014 (5)	0.002 (5)
C9	0.018 (6)	0.016 (6)	0.021 (6)	0.001 (4)	0.011 (5)	0.000 (5)
C10	0.018 (6)	0.013 (5)	0.010 (5)	−0.002 (4)	0.008 (4)	0.000 (4)
C11	0.021 (6)	0.023 (6)	0.017 (6)	0.005 (5)	0.011 (5)	0.003 (5)
C12	0.015 (6)	0.019 (6)	0.015 (6)	0.005 (4)	0.006 (4)	0.002 (4)
C13	0.010 (5)	0.021 (6)	0.017 (6)	−0.003 (5)	−0.001 (4)	−0.005 (5)
C14	0.012 (5)	0.020 (6)	0.018 (6)	0.000 (4)	0.006 (4)	−0.003 (5)
C15	0.013 (5)	0.023 (6)	0.013 (6)	−0.002 (5)	0.003 (4)	−0.012 (5)
C16	0.009 (5)	0.022 (6)	0.022 (6)	0.002 (4)	0.008 (4)	0.001 (5)
C17	0.014 (5)	0.017 (6)	0.022 (6)	−0.001 (4)	0.008 (5)	−0.006 (5)
C18	0.013 (5)	0.009 (5)	0.021 (6)	−0.002 (4)	0.002 (4)	−0.002 (4)
C19	0.016 (6)	0.026 (6)	0.019 (6)	−0.002 (5)	0.002 (5)	−0.001 (5)
C20	0.023 (6)	0.011 (5)	0.022 (6)	0.000 (5)	0.006 (5)	−0.004 (5)
C21	0.014 (5)	0.013 (5)	0.021 (6)	0.001 (4)	0.006 (4)	0.001 (4)
C22	0.019 (6)	0.032 (7)	0.015 (6)	0.008 (5)	0.009 (5)	0.003 (5)
C23	0.017 (6)	0.029 (6)	0.013 (6)	0.010 (5)	0.004 (4)	0.006 (5)
C24	0.025 (6)	0.016 (6)	0.012 (6)	0.003 (5)	0.004 (4)	0.002 (4)
C25	0.028 (7)	0.023 (6)	0.028 (7)	0.007 (5)	0.019 (5)	0.011 (5)
C26	0.036 (7)	0.014 (6)	0.015 (6)	0.003 (5)	0.010 (5)	−0.004 (5)
C27	0.014 (6)	0.025 (6)	0.019 (6)	0.008 (5)	0.005 (4)	0.002 (5)
C28	0.021 (6)	0.011 (5)	0.027 (7)	0.008 (4)	0.015 (5)	0.001 (5)
C29	0.017 (6)	0.024 (6)	0.025 (7)	0.003 (5)	0.007 (5)	0.002 (5)
C30	0.010 (5)	0.034 (7)	0.022 (6)	−0.001 (5)	0.001 (4)	−0.005 (5)
C31	0.022 (6)	0.020 (6)	0.023 (6)	0.000 (5)	0.019 (5)	0.001 (5)
C32	0.017 (6)	0.019 (6)	0.019 (6)	−0.001 (5)	0.006 (5)	0.006 (5)
C33	0.018 (6)	0.022 (6)	0.031 (7)	0.005 (5)	0.011 (5)	0.009 (5)
C34	0.018 (6)	0.020 (6)	0.016 (6)	−0.002 (5)	0.006 (5)	−0.004 (5)
C35	0.021 (6)	0.018 (6)	0.013 (6)	−0.006 (5)	0.006 (5)	0.002 (4)
C36	0.019 (6)	0.028 (6)	0.021 (6)	−0.003 (5)	0.014 (5)	−0.008 (5)
C37	0.021 (6)	0.017 (6)	0.014 (6)	0.002 (5)	0.007 (5)	0.001 (4)
C38	0.024 (6)	0.020 (6)	0.011 (6)	0.001 (5)	0.001 (5)	0.004 (4)
C39	0.019 (6)	0.025 (6)	0.016 (6)	−0.003 (5)	−0.001 (5)	0.000 (5)
C40	0.015 (6)	0.023 (6)	0.012 (6)	−0.003 (5)	0.006 (4)	0.004 (4)
C41	0.017 (6)	0.014 (5)	0.015 (6)	0.000 (4)	0.005 (4)	0.005 (4)
C42	0.011 (5)	0.019 (5)	0.011 (6)	−0.002 (4)	0.008 (4)	−0.002 (4)

C43	0.012 (5)	0.022 (6)	0.010 (5)	0.011 (4)	0.004 (4)	−0.001 (4)
C44	0.019 (6)	0.026 (6)	0.024 (7)	−0.001 (5)	0.014 (5)	−0.002 (5)
C45	0.020 (6)	0.020 (6)	0.012 (6)	0.001 (5)	0.005 (4)	0.002 (4)
C46	0.011 (5)	0.016 (6)	0.027 (7)	−0.005 (4)	0.007 (5)	0.001 (5)
C47	0.014 (5)	0.018 (6)	0.015 (6)	0.003 (4)	0.006 (4)	0.008 (4)
C48	0.017 (6)	0.018 (6)	0.017 (6)	−0.005 (5)	0.004 (5)	−0.005 (5)
C49	0.014 (6)	0.021 (6)	0.019 (6)	0.002 (5)	0.009 (5)	−0.002 (5)
C50	0.014 (5)	0.024 (6)	0.016 (6)	0.000 (5)	0.008 (4)	0.002 (5)
C51	0.013 (5)	0.020 (6)	0.010 (5)	0.006 (4)	0.007 (4)	0.005 (4)
C52	0.012 (5)	0.013 (5)	0.017 (6)	−0.001 (4)	0.003 (4)	−0.002 (4)
C53	0.013 (5)	0.016 (6)	0.022 (6)	0.000 (4)	0.005 (4)	0.003 (5)
C54	0.021 (6)	0.024 (6)	0.012 (6)	−0.007 (5)	0.010 (4)	−0.006 (5)
C55	0.015 (6)	0.026 (6)	0.020 (6)	0.002 (5)	0.006 (5)	−0.001 (5)
C56	0.017 (6)	0.026 (6)	0.011 (5)	−0.003 (5)	0.010 (4)	−0.002 (4)
C57	0.013 (5)	0.023 (6)	0.013 (6)	0.000 (5)	0.005 (4)	0.000 (5)
C58	0.015 (5)	0.016 (5)	0.017 (6)	0.005 (4)	0.006 (4)	0.002 (4)
C59	0.015 (6)	0.021 (6)	0.018 (6)	−0.002 (5)	0.006 (4)	0.001 (5)
C60	0.008 (5)	0.023 (6)	0.019 (6)	0.000 (4)	0.003 (4)	0.005 (5)
C61	0.019 (6)	0.025 (6)	0.014 (6)	−0.015 (5)	0.001 (5)	−0.006 (5)
C62	0.023 (6)	0.021 (6)	0.020 (6)	−0.005 (5)	0.008 (5)	−0.001 (5)
C63	0.012 (5)	0.014 (5)	0.019 (6)	−0.002 (4)	0.001 (4)	0.009 (4)
C64	0.020 (6)	0.018 (6)	0.035 (7)	−0.004 (5)	0.015 (5)	0.003 (5)
C65	0.017 (6)	0.024 (6)	0.014 (6)	−0.007 (5)	0.010 (4)	−0.007 (5)
C66	0.022 (6)	0.013 (6)	0.030 (7)	0.000 (5)	0.009 (5)	−0.002 (5)
C67	0.019 (6)	0.018 (6)	0.020 (6)	0.001 (5)	0.012 (5)	−0.001 (5)
C68	0.016 (6)	0.028 (6)	0.023 (6)	−0.003 (5)	0.003 (5)	0.001 (5)
C69	0.018 (6)	0.022 (6)	0.021 (6)	−0.002 (5)	0.004 (5)	0.004 (5)
C70	0.019 (6)	0.023 (6)	0.017 (6)	0.003 (5)	0.008 (5)	−0.003 (5)
C71	0.013 (5)	0.018 (6)	0.019 (6)	−0.009 (4)	0.013 (4)	−0.005 (5)
C72	0.014 (5)	0.019 (6)	0.019 (6)	−0.005 (4)	0.011 (4)	−0.006 (5)

Geometric parameters (Å, º)

Ho1—O1	2.313 (8)	C17—C18^{iii}	1.395 (16)
Ho1—O3^{i}	2.335 (7)	C17—C17^{iii}	1.45 (2)
Ho1—O5	2.277 (8)	C18—C17^{iii}	1.395 (16)
Ho1—O10^{ii}	2.314 (8)	C18—H18	0.9500
Ho1—O15^{iii}	2.309 (8)	C19—C20	1.519 (16)
Ho1—O23^{iv}	2.847 (9)	C20—C21	1.402 (15)
Ho1—O24^{iv}	2.311 (8)	C20—C30	1.420 (16)
Ho1—O2W	2.370 (8)	C21—C22	1.415 (15)
Ho2—O2	2.299 (8)	C21—H21	0.9500
Ho2—O6	2.316 (8)	C22—C23	1.431 (16)
Ho2—O7	2.338 (8)	C22—C28	1.437 (16)
Ho2—O11	2.264 (8)	C23—C24	1.365 (15)
Ho2—O13	2.347 (8)	C23—H23	0.9500
Ho2—O19^{ii}	2.338 (8)	C24—C25	1.425 (16)
Ho2—O20^{ii}	2.876 (8)	C24—H24	0.9500

Ho2—O3W	2.423 (9)	C25—C27	1.383 (16)
Ho3—O8	2.410 (8)	C25—C26	1.482 (16)
Ho3—O12	2.337 (8)	C27—C28	1.420 (16)
Ho3—O14	2.356 (8)	C27—H27	0.9500
Ho3—O17	2.299 (7)	C28—C29	1.441 (16)
Ho3—O20^{ii}	2.299 (8)	C29—C30	1.346 (16)
Ho3—O21	2.300 (8)	C29—H29	0.9500
Ho3—O4W	2.469 (8)	C30—H30	0.9500
Ho3—O5W	2.640 (6)	C31—C32	1.503 (16)
Ho4—O4^{v}	2.360 (8)	C32—C33	1.397 (16)
Ho4—O9^{vi}	2.382 (7)	C32—C36	1.400 (16)
Ho4—O16^{vii}	2.342 (8)	C33—C34	1.357 (16)
Ho4—O18	2.337 (7)	C33—H33	0.9500
Ho4—O22	2.276 (7)	C34—C35^{v}	1.426 (15)
Ho4—O23^{viii}	2.296 (8)	C34—H34	0.9500
Ho4—O5W	2.671 (6)	C35—C36	1.380 (16)
Ho4—O6W	2.453 (10)	C35—C35^{v}	1.43 (2)
O1—C1	1.258 (13)	C35—C34^{v}	1.426 (15)
O2—C1	1.239 (13)	C36—H36	0.9500
O3—C8	1.269 (14)	C37—C38	1.494 (15)
O3—Ho1^{i}	2.335 (7)	C38—C48	1.364 (15)
O4—C8	1.254 (14)	C38—C39	1.443 (16)
O4—Ho4^{v}	2.360 (8)	C39—C40	1.352 (16)
O5—C13	1.240 (13)	C39—H39	0.9500
O6—C13	1.272 (13)	C40—C41	1.421 (15)
O7—C19	1.246 (14)	C40—H40	0.9500
O8—C19	1.269 (14)	C41—C42	1.410 (15)
O9—C26	1.268 (14)	C41—C47	1.429 (15)
O9—Ho4^{iv}	2.382 (7)	C42—C43	1.383 (15)
O10—C26	1.297 (14)	C42—H42	0.9500
O10—Ho1^{viii}	2.314 (8)	C43—C45	1.429 (15)
O11—C31	1.245 (14)	C43—C44	1.470 (16)
O12—C31	1.249 (13)	C44—Ho4^{vii}	3.005 (12)
O13—C37	1.241 (13)	C45—C46	1.359 (16)
O14—C37	1.271 (13)	C45—H45	0.9500
O15—C44	1.249 (14)	C46—C47	1.433 (15)
O15—Ho1^{iii}	2.309 (7)	C46—H46	0.9500
O16—C44	1.250 (13)	C47—C48	1.428 (15)
O16—Ho4^{vii}	2.342 (8)	C48—H48	0.9500
O17—C49	1.266 (13)	C49—C50	1.486 (15)
O18—C49	1.255 (13)	C50—C60	1.404 (14)
O19—C56	1.266 (13)	C50—C51	1.408 (15)
O19—Ho2^{viii}	2.338 (8)	C51—C52	1.417 (14)
O20—C56	1.266 (14)	C51—H51	0.9500
O20—Ho3^{viii}	2.299 (8)	C52—C58	1.424 (15)
O20—Ho2^{viii}	2.876 (8)	C52—C53	1.439 (15)
O21—C61	1.263 (13)	C53—C54	1.361 (15)
O22—C61	1.285 (13)	C53—H53	0.9500

O23—C68	1.243 (14)	C54—C55	1.431 (15)
O23—Ho4^{ii}	2.296 (8)	C54—H54	0.9500
O23—Ho1^{vi}	2.847 (9)	C55—C57	1.366 (15)
O24—C68	1.267 (14)	C55—C56	1.495 (15)
O24—Ho1^{vi}	2.311 (8)	C56—Ho2^{viii}	2.942 (11)
C1—C2	1.496 (15)	C57—C58	1.409 (15)
C2—C3	1.375 (16)	C57—H57	0.9500
C2—C12	1.422 (15)	C58—C59	1.438 (15)
C3—C4	1.433 (16)	C59—C60	1.340 (15)
C3—H3	0.9500	C59—H59	0.9500
C4—C5	1.414 (16)	C60—H60	0.9500
C4—C10	1.422 (15)	C61—C62	1.496 (16)
C5—C6	1.379 (16)	C62—C72	1.390 (16)
C5—H5	0.9500	C62—C63	1.428 (15)
C6—C7	1.419 (15)	C63—C64	1.366 (16)
C6—H6	0.9500	C63—H63	0.9500
C7—C9	1.373 (16)	C64—C65	1.431 (16)
C7—C8	1.485 (16)	C64—H64	0.9500
C9—C10	1.415 (15)	C65—C66	1.406 (16)
C9—H9	0.9500	C65—C71	1.421 (14)
C10—C11	1.428 (15)	C66—C67	1.386 (16)
C11—C12	1.349 (15)	C66—H66	0.9500
C11—H11	0.9500	C67—C69	1.428 (15)
C12—H12	0.9500	C67—C68	1.500 (16)
C13—C14	1.487 (15)	C68—Ho1^{vi}	2.890 (12)
C14—C18	1.367 (15)	C69—C70	1.322 (16)
C14—C15	1.423 (15)	C69—H69	0.9500
C15—C16	1.371 (16)	C70—C71	1.412 (15)
C15—H15	0.9500	C70—H70	0.9500
C16—C17	1.421 (15)	C71—C72	1.419 (15)
C16—H16	0.9500	C72—H72	0.9500

O5—Ho1—O15^{iii}	94.3 (3)	C9—C10—C11	120.8 (10)
O5—Ho1—O24^{iv}	120.7 (3)	C4—C10—C11	119.5 (10)
O15^{iii}—Ho1—O24^{iv}	129.4 (3)	C12—C11—C10	120.5 (10)
O5—Ho1—O1	81.0 (3)	C12—C11—H11	119.8
O15^{iii}—Ho1—O1	153.5 (3)	C10—C11—H11	119.8
O24^{iv}—Ho1—O1	73.5 (3)	C11—C12—C2	121.6 (10)
O5—Ho1—O10^{ii}	77.0 (3)	C11—C12—H12	119.2
O15^{iii}—Ho1—O10^{ii}	77.3 (3)	C2—C12—H12	119.2
O24^{iv}—Ho1—O10^{ii}	76.7 (3)	O5—C13—O6	124.3 (10)
O1—Ho1—O10^{ii}	126.1 (3)	O5—C13—C14	118.9 (9)
O5—Ho1—O3^{i}	148.8 (3)	O6—C13—C14	116.6 (9)
O15^{iii}—Ho1—O3^{i}	82.9 (3)	C18—C14—C15	119.5 (10)
O24^{iv}—Ho1—O3^{i}	83.0 (3)	C18—C14—C13	120.7 (10)
O1—Ho1—O3^{i}	87.7 (3)	C15—C14—C13	119.7 (9)
O10^{ii}—Ho1—O3^{i}	131.6 (3)	C16—C15—C14	120.3 (10)
O5—Ho1—O2W	77.9 (3)	C16—C15—H15	119.8

O15^{iii}—Ho1—O2W	77.1 (3)	C14—C15—H15	119.8
O24^{iv}—Ho1—O2W	140.8 (3)	C15—C16—C17	121.2 (10)
O1—Ho1—O2W	76.4 (3)	C15—C16—H16	119.4
O10^{ii}—Ho1—O2W	142.3 (3)	C17—C16—H16	119.4
O3^{i}—Ho1—O2W	71.2 (3)	C18^{iii}—C17—C16	123.1 (10)
O5—Ho1—O23^{iv}	146.5 (3)	C18^{iii}—C17—C17^{iii}	119.2 (12)
O15^{iii}—Ho1—O23^{iv}	81.2 (3)	C16—C17—C17^{iii}	117.7 (13)
O24^{iv}—Ho1—O23^{iv}	49.1 (2)	C14—C18—C17^{iii}	121.9 (10)
O1—Ho1—O23^{iv}	116.7 (3)	C14—C18—H18	119.0
O10^{ii}—Ho1—O23^{iv}	69.6 (3)	C17^{iii}—C18—H18	119.0
O3^{i}—Ho1—O23^{iv}	64.0 (3)	O7—C19—O8	124.6 (11)
O2W—Ho1—O23^{iv}	132.0 (2)	O7—C19—C20	117.2 (10)
O5—Ho1—C68^{iv}	142.0 (3)	O8—C19—C20	118.2 (10)
O15^{iii}—Ho1—C68^{iv}	106.2 (3)	C21—C20—C30	120.2 (10)
O24^{iv}—Ho1—C68^{iv}	25.2 (3)	C21—C20—C19	118.8 (10)
O1—Ho1—C68^{iv}	92.7 (3)	C30—C20—C19	120.6 (10)
O10^{ii}—Ho1—C68^{iv}	76.8 (3)	C20—C21—C22	120.5 (10)
O3^{i}—Ho1—C68^{iv}	67.1 (3)	C20—C21—H21	119.8
O2W—Ho1—C68^{iv}	137.3 (3)	C22—C21—H21	119.8
O23^{iv}—Ho1—C68^{iv}	25.0 (3)	C21—C22—C23	122.5 (10)
O11—Ho2—O2	94.6 (3)	C21—C22—C28	119.2 (10)
O11—Ho2—O6	152.3 (3)	C23—C22—C28	118.3 (10)
O2—Ho2—O6	84.2 (3)	C24—C23—C22	119.7 (11)
O11—Ho2—O19^{ii}	127.4 (3)	C24—C23—H23	120.1
O2—Ho2—O19^{ii}	120.9 (3)	C22—C23—H23	120.1
O6—Ho2—O19^{ii}	74.8 (3)	C23—C24—C25	122.2 (11)
O11—Ho2—O7	77.7 (3)	C23—C24—H24	118.9
O2—Ho2—O7	74.0 (3)	C25—C24—H24	118.9
O6—Ho2—O7	127.7 (3)	C27—C25—C24	119.5 (10)
O19^{ii}—Ho2—O7	76.9 (3)	C27—C25—C26	119.5 (10)
O11—Ho2—O13	81.2 (3)	C24—C25—C26	120.9 (11)
O2—Ho2—O13	153.4 (3)	O9—C26—O10	122.8 (10)
O6—Ho2—O13	87.6 (3)	O9—C26—C25	120.8 (10)
O19^{ii}—Ho2—O13	80.9 (3)	O10—C26—C25	116.4 (10)
O7—Ho2—O13	129.6 (3)	C25—C27—C28	119.8 (10)
O11—Ho2—O3W	76.8 (3)	C25—C27—H27	120.1
O2—Ho2—O3W	76.9 (3)	C28—C27—H27	120.1
O6—Ho2—O3W	76.0 (3)	C27—C28—C22	120.4 (10)
O19^{ii}—Ho2—O3W	143.6 (3)	C27—C28—C29	121.8 (10)
O7—Ho2—O3W	139.2 (3)	C22—C28—C29	117.8 (10)
O13—Ho2—O3W	76.5 (3)	C30—C29—C28	122.3 (11)
O11—Ho2—O20^{ii}	78.7 (3)	C30—C29—H29	118.9
O2—Ho2—O20^{ii}	141.2 (3)	C28—C29—H29	118.9
O6—Ho2—O20^{ii}	118.7 (3)	C29—C30—C20	120.0 (10)
O19^{ii}—Ho2—O20^{ii}	49.0 (2)	C29—C30—H30	120.0
O7—Ho2—O20^{ii}	67.2 (3)	C20—C30—H30	120.0
O13—Ho2—O20^{ii}	64.0 (3)	O11—C31—O12	122.1 (11)
O3W—Ho2—O20^{ii}	136.0 (3)	O11—C31—C32	119.4 (9)

O11—Ho2—C56^{ii}	103.8 (3)	O12—C31—C32	118.0 (10)
O2—Ho2—C56^{ii}	138.5 (3)	O11—C31—Ho3	75.5 (6)
O6—Ho2—C56^{ii}	94.9 (3)	O12—C31—Ho3	49.1 (6)
O19^{ii}—Ho2—C56^{ii}	24.5 (3)	C32—C31—Ho3	153.4 (7)
O7—Ho2—C56^{ii}	74.1 (3)	C33—C32—C36	119.8 (11)
O13—Ho2—C56^{ii}	67.4 (3)	C33—C32—C31	120.8 (10)
O3W—Ho2—C56^{ii}	143.1 (3)	C36—C32—C31	119.2 (10)
O20^{ii}—Ho2—C56^{ii}	25.1 (3)	C34—C33—C32	121.1 (11)
O20^{ii}—Ho3—O17	145.8 (3)	C34—C33—H33	119.5
O20^{ii}—Ho3—O21	86.6 (3)	C32—C33—H33	119.5
O17—Ho3—O21	90.7 (3)	C33—C34—C35^{v}	120.1 (10)
O20^{ii}—Ho3—O12	125.3 (3)	C33—C34—H34	119.9
O17—Ho3—O12	78.2 (3)	C35^{v}—C34—H34	119.9
O21—Ho3—O12	136.1 (3)	C36—C35—C35^{v}	119.6 (13)
O20^{ii}—Ho3—O14	75.9 (3)	C36—C35—C34^{v}	121.6 (10)
O17—Ho3—O14	136.8 (3)	C35^{v}—C35—C34^{v}	118.8 (12)
O21—Ho3—O14	78.6 (3)	C35—C36—C32	120.4 (10)
O12—Ho3—O14	81.1 (3)	C35—C36—H36	119.8
O20^{ii}—Ho3—O8	81.3 (3)	C32—C36—H36	119.8
O17—Ho3—O8	81.2 (3)	O13—C37—O14	125.4 (10)
O21—Ho3—O8	144.2 (3)	O13—C37—C38	119.2 (10)
O12—Ho3—O8	76.3 (3)	O14—C37—C38	115.4 (9)
O14—Ho3—O8	129.5 (3)	C48—C38—C39	119.3 (10)
O20^{ii}—Ho3—O4W	73.3 (3)	C48—C38—C37	118.0 (10)
O17—Ho3—O4W	73.2 (3)	C39—C38—C37	122.7 (10)
O21—Ho3—O4W	73.2 (3)	C40—C39—C38	120.5 (10)
O12—Ho3—O4W	139.3 (3)	C40—C39—H39	119.7
O14—Ho3—O4W	139.1 (3)	C38—C39—H39	119.7
O8—Ho3—O4W	71.1 (3)	C39—C40—C41	121.8 (10)
O20^{ii}—Ho3—O5W	138.4 (3)	C39—C40—H40	119.1
O17—Ho3—O5W	70.8 (2)	C41—C40—H40	119.1
O21—Ho3—O5W	70.1 (3)	C42—C41—C40	123.8 (10)
O12—Ho3—O5W	66.2 (3)	C42—C41—C47	118.4 (10)
O14—Ho3—O5W	66.2 (3)	C40—C41—C47	117.8 (10)
O8—Ho3—O5W	136.6 (2)	C43—C42—C41	122.5 (9)
O4W—Ho3—O5W	127.3 (2)	C43—C42—H42	118.8
O20^{ii}—Ho3—C31	101.9 (3)	C41—C42—H42	118.8
O17—Ho3—C31	96.7 (3)	C42—C43—C45	118.1 (10)
O21—Ho3—C31	151.5 (3)	C42—C43—C44	121.9 (10)
O12—Ho3—C31	23.8 (3)	C45—C43—C44	119.6 (9)
O14—Ho3—C31	77.1 (3)	O15—C44—O16	121.7 (11)
O8—Ho3—C31	64.3 (3)	O15—C44—C43	119.0 (10)
O4W—Ho3—C31	135.3 (3)	O16—C44—C43	119.0 (10)
O5W—Ho3—C31	86.4 (3)	O15—C44—Ho4^{vii}	77.3 (7)
O22—Ho4—O23^{viii}	146.1 (3)	O16—C44—Ho4^{vii}	47.1 (6)
O22—Ho4—O18	90.9 (3)	C43—C44—Ho4^{vii}	153.7 (8)
O23^{viii}—Ho4—O18	86.7 (3)	C46—C45—C43	121.4 (10)
O22—Ho4—O16^{vii}	79.3 (3)	C46—C45—H45	119.3

O23^{viii}—Ho4—O16^{vii}	124.6 (3)	C43—C45—H45	119.3
O18—Ho4—O16^{vii}	134.8 (3)	C45—C46—C47	120.6 (10)
O22—Ho4—O4^{v}	135.9 (3)	C45—C46—H46	119.7
O23^{viii}—Ho4—O4^{v}	76.1 (3)	C47—C46—H46	119.7
O18—Ho4—O4^{v}	76.4 (3)	C48—C47—C41	119.5 (10)
O16^{vii}—Ho4—O4^{v}	80.7 (3)	C48—C47—C46	121.6 (10)
O22—Ho4—O9^{vi}	83.4 (3)	C41—C47—C46	118.8 (10)
O23^{viii}—Ho4—O9^{vi}	81.4 (3)	C38—C48—C47	120.9 (10)
O18—Ho4—O9^{vi}	148.5 (3)	C38—C48—H48	119.5
O16^{vii}—Ho4—O9^{vi}	74.6 (3)	C47—C48—H48	119.5
O4^{v}—Ho4—O9^{vi}	127.6 (3)	O18—C49—O17	124.2 (10)
O22—Ho4—O6W	73.5 (3)	O18—C49—C50	119.6 (10)
O23^{viii}—Ho4—O6W	73.2 (3)	O17—C49—C50	116.1 (9)
O18—Ho4—O6W	76.3 (3)	C60—C50—C51	120.0 (10)
O16^{vii}—Ho4—O6W	139.0 (3)	C60—C50—C49	119.8 (10)
O4^{v}—Ho4—O6W	139.6 (3)	C51—C50—C49	120.1 (9)
O9^{vi}—Ho4—O6W	72.4 (3)	C50—C51—C52	119.3 (9)
O22—Ho4—O5W	70.5 (3)	C50—C51—H51	120.4
O23^{viii}—Ho4—O5W	138.4 (3)	C52—C51—H51	120.4
O18—Ho4—O5W	69.8 (3)	C51—C52—C58	120.0 (9)
O16^{vii}—Ho4—O5W	65.3 (3)	C51—C52—C53	121.0 (9)
O4^{v}—Ho4—O5W	65.4 (3)	C58—C52—C53	119.0 (10)
O9^{vi}—Ho4—O5W	135.1 (3)	C54—C53—C52	119.7 (10)
O6W—Ho4—O5W	129.2 (3)	C54—C53—H53	120.1
O22—Ho4—C44^{vii}	97.5 (3)	C52—C53—H53	120.1
O23^{viii}—Ho4—C44^{vii}	102.0 (3)	C53—C54—C55	120.7 (10)
O18—Ho4—C44^{vii}	148.7 (3)	C53—C54—H54	119.6
O16^{vii}—Ho4—C44^{vii}	23.0 (3)	C55—C54—H54	119.6
O4^{v}—Ho4—C44^{vii}	76.7 (3)	C57—C55—C54	120.1 (10)
O9^{vi}—Ho4—C44^{vii}	62.7 (3)	C57—C55—C56	119.4 (10)
O6W—Ho4—C44^{vii}	135.0 (3)	C54—C55—C56	119.8 (10)
O5W—Ho4—C44^{vii}	84.6 (3)	O19—C56—O20	122.3 (10)
Ho3—O5W—Ho4	126.7 (3)	O19—C56—C55	117.6 (10)
C1—O1—Ho1	154.4 (8)	O20—C56—C55	119.7 (9)
C1—O2—Ho2	143.2 (8)	O19—C56—Ho2^{viii}	50.0 (5)
C8—O3—Ho1^{i}	137.4 (8)	O20—C56—Ho2^{viii}	74.5 (6)
C8—O4—Ho4^{v}	129.9 (8)	C55—C56—Ho2^{viii}	155.2 (8)
C13—O5—Ho1	149.4 (7)	C55—C57—C58	120.9 (10)
C13—O6—Ho2	141.3 (7)	C55—C57—H57	119.5
C19—O7—Ho2	128.7 (8)	C58—C57—H57	119.5
C19—O8—Ho3	135.0 (7)	C57—C58—C52	119.2 (10)
C26—O9—Ho4^{iv}	138.6 (7)	C57—C58—C59	122.5 (10)
C26—O10—Ho1^{viii}	129.6 (7)	C52—C58—C59	118.0 (10)
C31—O11—Ho2	171.8 (7)	C60—C59—C58	121.2 (10)
C31—O12—Ho3	107.0 (7)	C60—C59—H59	119.4
C37—O13—Ho2	136.7 (7)	C58—C59—H59	119.4
C37—O14—Ho3	127.7 (7)	C59—C60—C50	121.4 (10)
C44—O15—Ho1^{iii}	170.7 (8)	C59—C60—H60	119.3

C44—O16—Ho4^{vii}	109.8 (7)	C50—C60—H60	119.3
C49—O17—Ho3	136.5 (7)	O21—C61—O22	124.3 (10)
C49—O18—Ho4	138.1 (7)	O21—C61—C62	119.3 (10)
C56—O19—Ho2^{viii}	105.6 (7)	O22—C61—C62	116.2 (10)
C56—O20—Ho3^{viii}	176.9 (7)	C72—C62—C63	120.5 (10)
C56—O20—Ho2^{viii}	80.4 (6)	C72—C62—C61	120.8 (10)
Ho3^{viii}—O20—Ho2^{viii}	101.8 (3)	C63—C62—C61	118.6 (10)
C61—O21—Ho3	138.2 (7)	C64—C63—C62	119.3 (10)
C61—O22—Ho4	135.3 (7)	C64—C63—H63	120.4
C68—O23—Ho4^{ii}	176.8 (8)	C62—C63—H63	120.4
C68—O23—Ho1^{vi}	79.4 (7)	C63—C64—C65	121.3 (10)
Ho4^{ii}—O23—Ho1^{vi}	102.5 (3)	C63—C64—H64	119.3
C68—O24—Ho1^{vi}	103.9 (7)	C65—C64—H64	119.3
O2—C1—O1	124.4 (10)	C66—C65—C71	118.3 (10)
O2—C1—C2	118.8 (10)	C66—C65—C64	122.2 (10)
O1—C1—C2	116.7 (9)	C71—C65—C64	119.4 (10)
C3—C2—C12	119.0 (10)	C67—C66—C65	121.9 (10)
C3—C2—C1	121.8 (10)	C67—C66—H66	119.1
C12—C2—C1	119.2 (10)	C65—C66—H66	119.1
C2—C3—C4	121.5 (10)	C66—C67—C69	117.9 (10)
C2—C3—H3	119.2	C66—C67—C68	117.9 (10)
C4—C3—H3	119.2	C69—C67—C68	123.8 (10)
C5—C4—C10	117.8 (10)	O23—C68—O24	122.3 (11)
C5—C4—C3	124.3 (10)	O23—C68—C67	118.6 (10)
C10—C4—C3	118.0 (10)	O24—C68—C67	119.1 (10)
C6—C5—C4	122.0 (10)	O23—C68—Ho1^{vi}	75.6 (7)
C6—C5—H5	119.0	O24—C68—Ho1^{vi}	50.9 (6)
C4—C5—H5	119.0	C67—C68—Ho1^{vi}	152.8 (8)
C5—C6—C7	119.6 (11)	C70—C69—C67	120.8 (10)
C5—C6—H6	120.2	C70—C69—H69	119.6
C7—C6—H6	120.2	C67—C69—H69	119.6
C9—C7—C6	119.8 (10)	C69—C70—C71	122.5 (10)
C9—C7—C8	118.7 (10)	C69—C70—H70	118.8
C6—C7—C8	121.4 (10)	C71—C70—H70	118.8
O4—C8—O3	123.2 (11)	C70—C71—C72	122.9 (10)
O4—C8—C7	118.9 (10)	C70—C71—C65	118.3 (10)
O3—C8—C7	117.8 (10)	C72—C71—C65	118.6 (10)
C7—C9—C10	121.1 (10)	C62—C72—C71	120.7 (10)
C7—C9—H9	119.5	C62—C72—H72	119.7
C10—C9—H9	119.5	C71—C72—H72	119.7
C9—C10—C4	119.7 (10)		

O20^{ii}—Ho3—O5W—Ho4	−119.2 (4)	C20—C21—C22—C28	0.6 (16)
O17—Ho3—O5W—Ho4	38.6 (3)	C21—C22—C23—C24	−176.0 (10)
O21—Ho3—O5W—Ho4	−59.5 (4)	C28—C22—C23—C24	1.7 (16)
O12—Ho3—O5W—Ho4	123.8 (4)	C22—C23—C24—C25	−2.8 (17)
O14—Ho3—O5W—Ho4	−145.6 (4)	C23—C24—C25—C27	1.5 (17)
O8—Ho3—O5W—Ho4	91.3 (5)	C23—C24—C25—C26	177.8 (10)

O4W—Ho3—O5W—Ho4	−11.0 (5)	Ho4^{iv}—O9—C26—O10	−14.1 (19)
C31—Ho3—O5W—Ho4	136.9 (4)	Ho4^{iv}—O9—C26—C25	165.6 (8)
O22—Ho4—O5W—Ho3	38.8 (4)	Ho1^{viii}—O10—C26—O9	52.1 (15)
O23^{viii}—Ho4—O5W—Ho3	−119.3 (4)	Ho1^{viii}—O10—C26—C25	−127.6 (9)
O18—Ho4—O5W—Ho3	−59.7 (4)	C27—C25—C26—O9	−39.3 (16)
O16^{vii}—Ho4—O5W—Ho3	125.6 (5)	C24—C25—C26—O9	144.3 (11)
O4^{v}—Ho4—O5W—Ho3	−143.5 (5)	C27—C25—C26—O10	140.3 (11)
O9^{vi}—Ho4—O5W—Ho3	96.9 (5)	C24—C25—C26—O10	−36.0 (15)
O6W—Ho4—O5W—Ho3	−8.5 (6)	C24—C25—C27—C28	0.9 (17)
C44^{vii}—Ho4—O5W—Ho3	138.7 (4)	C26—C25—C27—C28	−175.5 (10)
O5—Ho1—O1—C1	−111.2 (17)	C25—C27—C28—C22	−1.9 (16)
O15^{iii}—Ho1—O1—C1	167.1 (15)	C25—C27—C28—C29	177.8 (11)
O24^{iv}—Ho1—O1—C1	14.6 (16)	C21—C22—C28—C27	178.4 (10)
O10^{ii}—Ho1—O1—C1	−44.6 (18)	C23—C22—C28—C27	0.6 (16)
O3^{i}—Ho1—O1—C1	97.9 (17)	C21—C22—C28—C29	−1.3 (16)
O2W—Ho1—O1—C1	169.2 (17)	C23—C22—C28—C29	−179.2 (10)
O23^{iv}—Ho1—O1—C1	38.7 (17)	C27—C28—C29—C30	−179.9 (11)
C68^{iv}—Ho1—O1—C1	31.0 (17)	C22—C28—C29—C30	−0.2 (17)
O11—Ho2—O2—C1	174.7 (14)	C28—C29—C30—C20	2.4 (18)
O6—Ho2—O2—C1	22.5 (14)	C21—C20—C30—C29	−3.2 (17)
O19^{ii}—Ho2—O2—C1	−46.0 (15)	C19—C20—C30—C29	−176.0 (10)
O7—Ho2—O2—C1	−109.5 (14)	Ho3—O12—C31—O11	−20.8 (13)
O13—Ho2—O2—C1	95.3 (15)	Ho3—O12—C31—C32	151.5 (8)
O3W—Ho2—O2—C1	99.4 (14)	O20^{ii}—Ho3—C31—O11	−7.7 (7)
O20^{ii}—Ho2—O2—C1	−107.6 (13)	O17—Ho3—C31—O11	−158.8 (6)
C56^{ii}—Ho2—O2—C1	−68.4 (15)	O21—Ho3—C31—O11	97.2 (8)
O15^{iii}—Ho1—O5—C13	168.4 (16)	O12—Ho3—C31—O11	161.9 (11)
O24^{iv}—Ho1—O5—C13	−50.0 (16)	O14—Ho3—C31—O11	64.7 (6)
O1—Ho1—O5—C13	14.7 (15)	O8—Ho3—C31—O11	−81.9 (6)
O10^{ii}—Ho1—O5—C13	−115.7 (16)	O4W—Ho3—C31—O11	−85.9 (7)
O3^{i}—Ho1—O5—C13	84.9 (17)	O5W—Ho3—C31—O11	131.0 (6)
O2W—Ho1—O5—C13	92.6 (16)	O20^{ii}—Ho3—C31—O12	−169.6 (7)
O23^{iv}—Ho1—O5—C13	−111.1 (15)	O17—Ho3—C31—O12	39.3 (8)
C68^{iv}—Ho1—O5—C13	−68.3 (17)	O21—Ho3—C31—O12	−64.7 (10)
O11—Ho2—O6—C13	166.5 (10)	O14—Ho3—C31—O12	−97.2 (7)
O2—Ho2—O6—C13	−104.7 (12)	O8—Ho3—C31—O12	116.2 (8)
O19^{ii}—Ho2—O6—C13	19.5 (11)	O4W—Ho3—C31—O12	112.2 (7)
O7—Ho2—O6—C13	−40.0 (13)	O5W—Ho3—C31—O12	−30.9 (7)
O13—Ho2—O6—C13	100.7 (12)	O20^{ii}—Ho3—C31—C32	120.3 (16)
O3W—Ho2—O6—C13	177.4 (12)	O17—Ho3—C31—C32	−30.8 (17)
O20^{ii}—Ho2—O6—C13	42.3 (12)	O21—Ho3—C31—C32	−134.8 (15)
C56^{ii}—Ho2—O6—C13	33.7 (12)	O12—Ho3—C31—C32	−70.1 (17)
O11—Ho2—O7—C19	−0.8 (9)	O14—Ho3—C31—C32	−167.3 (17)
O2—Ho2—O7—C19	−99.2 (10)	O8—Ho3—C31—C32	46.1 (16)
O6—Ho2—O7—C19	−168.5 (9)	O4W—Ho3—C31—C32	42.1 (18)
O19^{ii}—Ho2—O7—C19	132.8 (10)	O5W—Ho3—C31—C32	−100.9 (16)
O13—Ho2—O7—C19	66.7 (10)	O11—C31—C32—C33	−9.9 (16)
O3W—Ho2—O7—C19	−53.0 (11)	O12—C31—C32—C33	177.6 (10)

O20^{ii}—Ho2—O7—C19	82.0 (9)	Ho3—C31—C32—C33	−128.7 (14)
C56^{ii}—Ho2—O7—C19	107.6 (10)	O11—C31—C32—C36	165.2 (10)
O20^{ii}—Ho3—O8—C19	−32.2 (10)	O12—C31—C32—C36	−7.3 (16)
O17—Ho3—O8—C19	177.4 (11)	Ho3—C31—C32—C36	46 (2)
O21—Ho3—O8—C19	−103.7 (11)	C36—C32—C33—C34	−3.4 (17)
O12—Ho3—O8—C19	97.5 (10)	C31—C32—C33—C34	171.6 (10)
O14—Ho3—O8—C19	31.5 (11)	C32—C33—C34—C35^{v}	2.0 (17)
O4W—Ho3—O8—C19	−107.4 (11)	C35^{v}—C35—C36—C32	−3.0 (19)
O5W—Ho3—O8—C19	127.9 (10)	C34^{v}—C35—C36—C32	178.6 (10)
C31—Ho3—O8—C19	75.6 (10)	C33—C32—C36—C35	3.9 (17)
O20^{ii}—Ho3—O12—C31	12.5 (9)	C31—C32—C36—C35	−171.2 (10)
O17—Ho3—O12—C31	−140.0 (8)	Ho2—O13—C37—O14	−22.7 (19)
O21—Ho3—O12—C31	141.4 (7)	Ho2—O13—C37—C38	156.1 (8)
O14—Ho3—O12—C31	78.2 (7)	Ho3—O14—C37—O13	57.0 (15)
O8—Ho3—O12—C31	−56.3 (7)	Ho3—O14—C37—C38	−121.8 (9)
O4W—Ho3—O12—C31	−93.9 (8)	O13—C37—C38—C48	−38.8 (15)
O5W—Ho3—O12—C31	146.0 (8)	O14—C37—C38—C48	140.0 (11)
O11—Ho2—O13—C37	38.7 (11)	O13—C37—C38—C39	142.3 (11)
O2—Ho2—O13—C37	121.3 (11)	O14—C37—C38—C39	−38.9 (15)
O6—Ho2—O13—C37	−166.7 (11)	C48—C38—C39—C40	2.3 (17)
O19^{ii}—Ho2—O13—C37	−91.7 (11)	C37—C38—C39—C40	−178.8 (10)
O7—Ho2—O13—C37	−27.2 (13)	C38—C39—C40—C41	−1.2 (17)
O3W—Ho2—O13—C37	117.1 (12)	C39—C40—C41—C42	176.2 (11)
O20^{ii}—Ho2—O13—C37	−43.0 (11)	C39—C40—C41—C47	−2.1 (16)
C56^{ii}—Ho2—O13—C37	−70.4 (11)	C40—C41—C42—C43	−178.7 (10)
O20^{ii}—Ho3—O14—C37	5.3 (8)	C47—C41—C42—C43	−0.4 (16)
O17—Ho3—O14—C37	173.3 (8)	C41—C42—C43—C45	−3.5 (15)
O21—Ho3—O14—C37	94.6 (9)	C41—C42—C43—C44	169.5 (10)
O12—Ho3—O14—C37	−124.6 (9)	Ho4^{vii}—O16—C44—O15	22.1 (14)
O8—Ho3—O14—C37	−60.6 (10)	Ho4^{vii}—O16—C44—C43	−152.1 (8)
O4W—Ho3—O14—C37	47.6 (10)	C42—C43—C44—O15	−166.0 (10)
O5W—Ho3—O14—C37	167.6 (9)	C45—C43—C44—O15	7.0 (16)
C31—Ho3—O14—C37	−100.6 (9)	C42—C43—C44—O16	8.4 (16)
O20^{ii}—Ho3—O17—C49	−166.4 (9)	C45—C43—C44—O16	−178.7 (10)
O21—Ho3—O17—C49	108.6 (10)	C42—C43—C44—Ho4^{vii}	−42 (2)
O12—Ho3—O17—C49	−28.6 (10)	C45—C43—C44—Ho4^{vii}	130.7 (14)
O14—Ho3—O17—C49	34.6 (11)	C42—C43—C45—C46	4.1 (16)
O8—Ho3—O17—C49	−106.3 (10)	C44—C43—C45—C46	−169.1 (10)
O4W—Ho3—O17—C49	−179.2 (10)	C43—C45—C46—C47	−0.7 (16)
O5W—Ho3—O17—C49	40.1 (9)	C42—C41—C47—C48	−174.1 (9)
C31—Ho3—O17—C49	−43.7 (10)	C40—C41—C47—C48	4.3 (15)
O22—Ho4—O18—C49	−31.4 (12)	C42—C41—C47—C46	3.8 (15)
O23^{viii}—Ho4—O18—C49	−177.7 (12)	C40—C41—C47—C46	−177.8 (10)
O16^{vii}—Ho4—O18—C49	44.2 (13)	C45—C46—C47—C48	174.6 (10)
O4^{v}—Ho4—O18—C49	105.9 (12)	C45—C46—C47—C41	−3.3 (16)
O9^{vi}—Ho4—O18—C49	−110.2 (11)	C39—C38—C48—C47	−0.1 (17)
O6W—Ho4—O18—C49	−104.2 (12)	C37—C38—C48—C47	−179.0 (10)
O5W—Ho4—O18—C49	37.4 (11)	C41—C47—C48—C38	−3.3 (16)

C44^{vii}—Ho4—O18—C49	74.5 (13)	C46—C47—C48—C38	178.9 (11)
O20^{ii}—Ho3—O21—C61	179.4 (12)	Ho4—O18—C49—O17	17.4 (18)
O17—Ho3—O21—C61	−34.7 (11)	Ho4—O18—C49—C50	−165.5 (8)
O12—Ho3—O21—C61	38.9 (13)	Ho3—O17—C49—O18	−83.7 (14)
O14—Ho3—O21—C61	103.1 (12)	Ho3—O17—C49—C50	99.1 (11)
O8—Ho3—O21—C61	−110.6 (11)	O18—C49—C50—C60	−165.1 (10)
O4W—Ho3—O21—C61	−107.0 (12)	O17—C49—C50—C60	12.2 (15)
O5W—Ho3—O21—C61	34.5 (11)	O18—C49—C50—C51	11.2 (16)
C31—Ho3—O21—C61	70.7 (14)	O17—C49—C50—C51	−171.4 (10)
O23^{viii}—Ho4—O22—C61	−167.4 (9)	C60—C50—C51—C52	3.5 (16)
O18—Ho4—O22—C61	107.3 (10)	C49—C50—C51—C52	−172.8 (9)
O16^{vii}—Ho4—O22—C61	−28.3 (10)	C50—C51—C52—C58	−2.0 (15)
O4^{v}—Ho4—O22—C61	36.1 (11)	C50—C51—C52—C53	176.9 (10)
O9^{vi}—Ho4—O22—C61	−103.8 (10)	C51—C52—C53—C54	−172.7 (10)
O6W—Ho4—O22—C61	−177.3 (10)	C58—C52—C53—C54	6.2 (16)
O5W—Ho4—O22—C61	39.1 (10)	C52—C53—C54—C55	−2.1 (16)
C44^{vii}—Ho4—O22—C61	−42.5 (10)	C53—C54—C55—C57	−2.5 (17)
Ho2—O2—C1—O1	−4 (2)	C53—C54—C55—C56	168.0 (10)
Ho2—O2—C1—C2	−179.4 (8)	Ho2^{viii}—O19—C56—O20	−19.2 (12)
Ho1—O1—C1—O2	92 (2)	Ho2^{viii}—O19—C56—C55	153.9 (8)
Ho1—O1—C1—C2	−92.3 (18)	Ho2^{viii}—O20—C56—O19	15.1 (10)
O2—C1—C2—C3	−18.2 (17)	Ho2^{viii}—O20—C56—C55	−157.9 (10)
O1—C1—C2—C3	165.8 (11)	C57—C55—C56—O19	−12.4 (16)
O2—C1—C2—C12	160.1 (11)	C54—C55—C56—O19	177.0 (10)
O1—C1—C2—C12	−15.9 (15)	C57—C55—C56—O20	161.0 (10)
C12—C2—C3—C4	−0.2 (16)	C54—C55—C56—O20	−9.6 (16)
C1—C2—C3—C4	178.1 (10)	C57—C55—C56—Ho2^{viii}	41 (2)
C2—C3—C4—C5	179.2 (11)	C54—C55—C56—Ho2^{viii}	−129.7 (15)
C2—C3—C4—C10	0.8 (16)	C54—C55—C57—C58	2.9 (17)
C10—C4—C5—C6	−1.1 (16)	C56—C55—C57—C58	−167.6 (10)
C3—C4—C5—C6	−179.5 (11)	C55—C57—C58—C52	1.3 (16)
C4—C5—C6—C7	3.6 (17)	C55—C57—C58—C59	175.0 (11)
C5—C6—C7—C9	−3.2 (17)	C51—C52—C58—C57	173.1 (9)
C5—C6—C7—C8	−179.6 (10)	C53—C52—C58—C57	−5.8 (15)
Ho4^{v}—O4—C8—O3	−55.0 (16)	C51—C52—C58—C59	−0.9 (15)
Ho4^{v}—O4—C8—C7	121.4 (10)	C53—C52—C58—C59	−179.9 (9)
Ho1^{i}—O3—C8—O4	14.9 (19)	C57—C58—C59—C60	−171.3 (10)
Ho1^{i}—O3—C8—C7	−161.5 (8)	C52—C58—C59—C60	2.6 (16)
C9—C7—C8—O4	−138.4 (12)	C58—C59—C60—C50	−1.2 (17)
C6—C7—C8—O4	38.0 (16)	C51—C50—C60—C59	−1.9 (17)
C9—C7—C8—O3	38.2 (16)	C49—C50—C60—C59	174.4 (10)
C6—C7—C8—O3	−145.4 (11)	Ho3—O21—C61—O22	22.6 (18)
C6—C7—C9—C10	0.4 (17)	Ho3—O21—C61—C62	−161.9 (8)
C8—C7—C9—C10	176.9 (10)	Ho4—O22—C61—O21	−85.9 (14)
C7—C9—C10—C4	2.1 (16)	Ho4—O22—C61—C62	98.5 (11)
C7—C9—C10—C11	179.8 (10)	O21—C61—C62—C72	13.2 (16)
C5—C4—C10—C9	−1.7 (16)	O22—C61—C62—C72	−171.0 (10)
C3—C4—C10—C9	176.8 (9)	O21—C61—C62—C63	−165.0 (10)

C5—C4—C10—C11	−179.5 (10)	O22—C61—C62—C63	10.9 (15)
C3—C4—C10—C11	−0.9 (16)	C72—C62—C63—C64	−2.6 (16)
C9—C10—C11—C12	−177.2 (10)	C61—C62—C63—C64	175.6 (10)
C4—C10—C11—C12	0.5 (16)	C62—C63—C64—C65	−1.0 (16)
C10—C11—C12—C2	0.1 (16)	C63—C64—C65—C66	−173.8 (10)
C3—C2—C12—C11	−0.3 (16)	C63—C64—C65—C71	3.8 (16)
C1—C2—C12—C11	−178.6 (10)	C71—C65—C66—C67	−3.6 (16)
Ho1—O5—C13—O6	−10 (2)	C64—C65—C66—C67	173.9 (10)
Ho1—O5—C13—C14	175.0 (10)	C65—C66—C67—C69	6.3 (16)
Ho2—O6—C13—O5	88.6 (15)	C65—C66—C67—C68	−166.6 (10)
Ho2—O6—C13—C14	−96.4 (13)	Ho1^{vi}—O23—C68—O24	21.2 (11)
O5—C13—C14—C18	−15.3 (16)	Ho1^{vi}—O23—C68—C67	−154.9 (10)
O6—C13—C14—C18	169.3 (10)	Ho1^{vi}—O24—C68—O23	−26.8 (13)
O5—C13—C14—C15	165.3 (10)	C66—C67—C68—O23	159.0 (11)
O6—C13—C14—C15	−10.0 (15)	C69—C67—C68—O23	−13.5 (17)
C18—C14—C15—C16	3.1 (16)	C66—C67—C68—O24	−17.2 (16)
C13—C14—C15—C16	−177.5 (10)	C69—C67—C68—O24	170.3 (11)
C14—C15—C16—C17	−2.4 (16)	C66—C67—C68—Ho1^{vi}	43 (2)
C15—C16—C17—C18^{iii}	−178.1 (10)	C69—C67—C68—Ho1^{vi}	−129.5 (15)
C15—C16—C17—C17^{iii}	−0.1 (18)	C66—C67—C69—C70	−4.5 (16)
C15—C14—C18—C17^{iii}	−1.3 (16)	C68—C67—C69—C70	168.0 (11)
C13—C14—C18—C17^{iii}	179.3 (10)	C67—C69—C70—C71	−0.1 (17)
Ho2—O7—C19—O8	−57.9 (16)	C69—C70—C71—C72	−172.6 (11)
Ho2—O7—C19—C20	121.5 (9)	C69—C70—C71—C65	2.9 (16)
Ho3—O8—C19—O7	15.9 (18)	C66—C65—C71—C70	−1.0 (15)
Ho3—O8—C19—C20	−163.5 (7)	C64—C65—C71—C70	−178.7 (10)
O7—C19—C20—C21	−137.2 (11)	C66—C65—C71—C72	174.7 (10)
O8—C19—C20—C21	42.2 (15)	C64—C65—C71—C72	−3.0 (15)
O7—C19—C20—C30	35.8 (16)	C63—C62—C72—C71	3.3 (16)
O8—C19—C20—C30	−144.8 (11)	C61—C62—C72—C71	−174.8 (9)
C30—C20—C21—C22	1.7 (16)	C70—C71—C72—C62	175.0 (10)
C19—C20—C21—C22	174.6 (10)	C65—C71—C72—C62	−0.5 (15)
C20—C21—C22—C23	178.3 (11)		

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