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Poly[diaquapentakis(μ_4-benzene-1,2-dicarboxylato)(μ_3-benzene-1,2-dicarboxylato)tetrathulium(III)]

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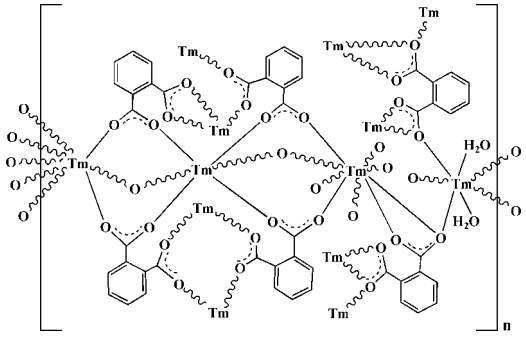
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.012 Å; R factor = 0.042; wR factor = 0.109; data-to-parameter ratio = 13.2.

The title compound, $[Tm_4(C_8H_4O_4)_6(H_2O)_2]_n$, has been synthesized hydrothermally. The asymmetric unit has four unique Tm^{III} ions that are six-, seven-, eight- and nine-coordinate. The cations are interconnected by bridging benzene-1,2-dicarboxylate (BDC) anions to form an infinite two-dimensional framework, in which the BDC ligands adopt three different coordination modes. Adjacent sheets are further packed to form a three-dimensional supramolecular framework through O—H···O hydrogen bonds.

Related literature

For background to the structures and applications of coordination polymers, see: Meares & Wensel, (1984); Scott & Horrocks, (1992); Reineke *et al.* (1999); Eddaoudi *et al.* (2001). For related structures involving multi-dimensional networks formed by multi-functional carboxylate ligands, see: Choi *et al.* (1998); MacGillivray *et al.* (1998); Evans *et al.* (1999); Chen *et al.* (2001); Suresh *et al.* (2001); Kumagai *et al.* (2002); Lu & Babb (2003); Song *et al.* (2003); Zhang *et al.* (2004); Wang *et al.* (2007).



Experimental

Crystal data

$[Tm_4(C_8H_4O_4)_6(H_2O)_2]$
M_r = 1696.42
Triclinic, $P\overline{1}$
a = 12.5716 (4) Å
b = 13.7737 (2) Å
c = 15.8867 (3) Å
α = 75.301 (4)°
β = 69.112 (2)°
γ = 65.617 (2)°
V = 2322.45 (9) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 7.67 mm^{-1}
T = 295 (2) K
0.30 × 0.14 × 0.02 mm

Data collection

Bruker APEX area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.207, T_{max} = 0.862
18519 measured reflections
9421 independent reflections
8260 reflections with $I > 2\sigma(I)$
R_{int} = 0.044

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.108
S = 1.02
9421 reflections
715 parameters
6 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 2.34 e Å^{-3}
$\Delta\rho_{min}$ = −2.67 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O25—H25A···O14^{i}	0.824 (10)	2.06 (2)	2.872 (7)	169 (9)
O25—H25B···O17^{i}	0.821 (10)	2.32 (7)	2.729 (7)	111 (6)
O25—H25B···O19^{i}	0.821 (10)	2.45 (3)	3.232 (7)	161 (7)
O26—H26A···O7^{ii}	0.816 (10)	2.08 (5)	2.822 (7)	151 (9)
O26—H26B···O22^{iii}	0.817 (10)	2.40 (2)	3.208 (7)	168 (9)
O26—H26B···O5^{ii}	0.817 (10)	2.62 (6)	3.072 (7)	116 (5)

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

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT-Plus* (Bruker, 2002); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2461).

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supplementary materials

Acta Cryst. (2008). E**64**, m468-m469 [**doi:10.1107/S1600536808003620**]

Poly[diaquapentakis($_4$-benzene-1,2-dicarboxylato)($_3$-benzene-1,2-dicarboxylato)tetrathulium(III)]

G.-M. Wang, C.-S. Duan, H.-L. Liu and H. Li

Comment

Research into the design, synthesis and characterization of metal coordination polymers is still of great interest because of their intriguing topological architectures and their potential applications as functional materials (Meares & Wensel, 1984; Scott & Horrocks, 1992; Reineke *et al.*, 1999; Eddaoudi *et al.*, 2001). In these studies, multifunctional ligands such as poly-carboxylate compounds are used as bridging groups to construct one-, two- and three-dimensional networks (Choi *et al.*, 1998; MacGillivray *et al.*, 1998; Evans *et al.*, 1999; Chen *et al.*, 2001; Suresh *et al.*, 2001; Kumagai *et al.*, 2002; Lu & Babb, 2003; Song *et al.*, 2003; Zhang *et al.*, 2004). Numerous architectures have been assembled from particular combinations of appropriate metal centers and versatile polydentate ligands. In our pursuit of the synthesis of novel coordination polymers in the presence of benzene-1,2-dicarboxylic and isonicotinic acids (Wang *et al.*, 2007), we obtained the title compound (I), Fig. 1, which exhibits an infinite two dimensional structure.

The asymmetric unit of (I) contains four independent thulium cations, six BDC ligands and two coordinated water molecules. Tm1 is coordinated to eight carboxylate oxygen atoms of six BDC anions; Tm2 binds to six carboxylate oxygen atoms of six individual BDC anions; Tm3 is nine-coordinated binding to nine carboxylate oxygen atoms from six BDC anions; finally, Tm4 is seven-coordinate binding to carboxylate oxygen atoms from five BDC anions and two coordinated water molecules. Compounds with four different types of metal ion coordination environments are rarely found in lanthanide coordination chemistry.

The Tm centers are each interconnected by BDC bridges to form an infinite two-dimensional network in the *ac* plane, as shown in Fig. 2. Interestingly, the sheet is made up from alternating infinite chains, in which the four Tm ions of the asymmetric unit are arranged in reverse order with Tm···Tm distances in the range 4.214 (6)–4.625 (9) Å. The six independent BDC ligands, however, adopt three discrete coordination modes (Fig. 3) linking the Tm cations into an extended network. O—H···O hydrogen bonds join adjacent sheets into a three dimensional supramolecular framework with O···O distances in the range 2.729 (7)–3.232 (7) Å, Table 1.

Experimental

The title compound was prepared under mild hydrothermal conditions. Typically, a mixture of Tm_2O_3 (0.193 g,0.5 mmol), isonicotinic acid (0.10 g,0.80 mmol), H_2BDC (0.251 g,1.50 mmol) and H_2O (10 mL) was sealed in a 25 ml Teflon-lined steel autoclave and heated under autogenous pressure at 443 K for 5 days. The colorless plate-like crystals obtained were recovered by filtration, washed with distilled water and dried in air.

Refinement

All the H atoms bound to C atoms were positioned geometrically, with C—H = 0.93 Å for aromatic H and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C). The hydrogen atoms of water molecule were located in a difference Fourier

map and their positions and isotropic displacement parameters were refined. In the final difference map a number of peaks of height approximately 2.0 e $Å^{-3}$ were found at close to the Tm atoms but no chemical significance can be attached to them.

Figures

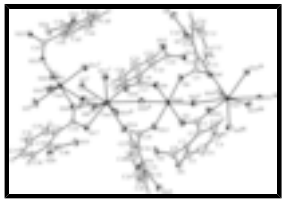

Fig. 1. The molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes: (i) −2 − *x*, 2 − *y*, 2 − *z*; (ii) −1 − *x*, 2 − *y*, 2 − *z*; (iii) −1 + *x*, *y*, 1 + *z*; (iiii) −2 − *x*, 2 − *y*, 3 − *z*].

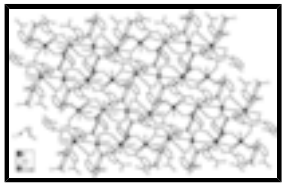

Fig. 2. Crystal packing of (I) showing the two-dimensional layer structure.

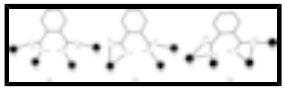

Fig. 3. Coordination modes of the BDC ligand found in (I).

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Crystal data

$[Tm_4(C_8H_4O_4)_6(H_2O)_2]$	$Z = 2$
$M_r = 1696.42$	$F_{000} = 1600$
Triclinic, $P\bar{1}$	$D_x = 2.426$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 12.5716$ (4) Å	Cell parameters from 9365 reflections
$b = 13.7737$ (2) Å	$\theta = 2.8$–$28.3°$
$c = 15.8867$ (3) Å	$\mu = 7.67$ mm^{-1}
$\alpha = 75.301$ (4)°	$T = 295$ (2) K
$\beta = 69.112$ (2)°	Plate, colorless
$\gamma = 65.617$ (2)°	0.30 × 0.14 × 0.02 mm
$V = 2322.45$ (9) $Å^3$	

Data collection

Bruker APEX area-detector diffractometer	9421 independent reflections
Radiation source: fine-focus sealed tube	8260 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.044$
$T = 295(2)$ K	$\theta_{max} = 26.5°$
φ and ω scans	$\theta_{min} = 1.4°$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -15 \rightarrow 15$

T_{min} = 0.207, T_{max} = 0.862
18519 measured reflections

k = −17→17
l = −19→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.108
S = 1.02
9421 reflections
715 parameters
6 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
$w = 1/[\sigma^2(F_o^2) + (0.0519P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 2.34 e Å^{-3}
$\Delta\rho_{min}$ = −2.67 e Å^{-3}
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 $F^2 > 2$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}
Tm1	−0.31816 (2)	0.12071 (2)	0.463579 (18)	0.01666 (9)
Tm2	−0.00120 (2)	0.00357 (2)	0.241350 (18)	0.01670 (9)
Tm3	0.30710 (2)	−0.11202 (2)	0.002946 (18)	0.01663 (9)
Tm4	0.51486 (2)	0.04932 (2)	−0.258514 (18)	0.01669 (9)
O1	−0.1567 (4)	0.1696 (5)	0.4135 (4)	0.0365 (13)
O2	0.0298 (4)	0.0745 (4)	0.3378 (3)	0.0289 (12)
O3	0.2956 (4)	0.0633 (4)	0.3023 (3)	0.0354 (13)
O4	0.2189 (4)	−0.0054 (4)	0.4425 (3)	0.0282 (11)
O5	−0.3224 (4)	0.1930 (4)	0.3206 (3)	0.0265 (11)
O6	−0.1474 (4)	0.1583 (4)	0.2105 (3)	0.0241 (11)
O7	−0.3531 (4)	0.1884 (4)	0.1302 (3)	0.0249 (11)
O8	−0.3630 (4)	0.3019 (4)	0.0065 (3)	0.0276 (11)
O9	−0.0324 (4)	−0.0860 (4)	0.1619 (3)	0.0265 (11)
O10	0.1308 (4)	−0.1341 (4)	0.0439 (4)	0.0355 (13)

O11	−0.3142 (4)	−0.1192 (4)	0.2113 (3)	0.0302 (12)
O12	−0.2293 (4)	−0.0281 (4)	0.0877 (3)	0.0274 (11)
O13	0.1513 (4)	−0.1479 (4)	0.2665 (3)	0.0275 (11)
O14	0.3183 (4)	−0.1874 (4)	0.1483 (3)	0.0275 (11)
O15	0.3801 (4)	−0.2562 (4)	0.4525 (3)	0.0253 (11)
O16	0.3972 (5)	−0.1774 (4)	0.3097 (3)	0.0296 (12)
O17	0.5130 (4)	−0.1881 (4)	−0.0108 (3)	0.0254 (11)
O18	0.5131 (4)	−0.0711 (4)	−0.1315 (3)	0.0279 (11)
O19	0.6707 (4)	−0.0348 (4)	−0.0425 (3)	0.0249 (11)
O20	0.8564 (4)	−0.0430 (4)	−0.1219 (3)	0.0251 (11)
O21	0.5023 (4)	0.1011 (4)	−0.4038 (3)	0.0197 (10)
O22	0.4733 (4)	0.1920 (4)	−0.5335 (3)	0.0253 (11)
O23	0.1458 (4)	0.0407 (4)	−0.3581 (3)	0.0261 (11)
O24	0.3314 (4)	0.0309 (4)	−0.4389 (3)	0.0261 (11)
O25	0.4742 (5)	0.1444 (5)	−0.1427 (3)	0.0359 (13)
O26	0.4781 (5)	−0.0892 (5)	−0.2904 (4)	0.0360 (13)
C1	−0.0433 (6)	0.1453 (6)	0.3882 (4)	0.0216 (14)
C2	0.0057 (6)	0.2099 (6)	0.4160 (4)	0.0208 (14)
C3	−0.0740 (7)	0.3070 (6)	0.4508 (5)	0.0333 (18)
H3	−0.1578	0.3266	0.4630	0.040*
C4	−0.0269 (8)	0.3731 (7)	0.4667 (6)	0.043 (2)
H4	−0.0795	0.4363	0.4915	0.052*
C5	0.0940 (8)	0.3469 (7)	0.4466 (6)	0.042 (2)
H5	0.1237	0.3949	0.4541	0.050*
C6	0.1761 (7)	0.2499 (7)	0.4150 (5)	0.0347 (18)
H6	0.2595	0.2316	0.4032	0.042*
C7	0.1294 (6)	0.1807 (5)	0.4014 (4)	0.0205 (14)
C8	0.2211 (6)	0.0706 (6)	0.3786 (5)	0.0242 (15)
C9	−0.2531 (5)	0.2181 (5)	0.2461 (4)	0.0189 (13)
C10	−0.3008 (6)	0.3307 (6)	0.2024 (4)	0.0198 (14)
C11	−0.2968 (7)	0.4109 (6)	0.2387 (5)	0.0290 (16)
H11	−0.2646	0.3919	0.2874	0.035*
C12	−0.3396 (8)	0.5178 (7)	0.2041 (5)	0.0366 (19)
H12	−0.3377	0.5702	0.2301	0.044*
C13	−0.3853 (7)	0.5465 (6)	0.1304 (6)	0.040 (2)
H13	−0.4120	0.6182	0.1057	0.048*
C14	−0.3913 (7)	0.4700 (6)	0.0937 (5)	0.0306 (17)
H14	−0.4231	0.4901	0.0447	0.037*
C15	−0.3498 (6)	0.3608 (6)	0.1294 (4)	0.0203 (14)
C16	−0.3577 (5)	0.2801 (6)	0.0867 (4)	0.0204 (14)
C17	0.0328 (6)	−0.1417 (5)	0.0971 (5)	0.0193 (14)
C18	−0.0077 (6)	−0.2241 (6)	0.0859 (4)	0.0210 (14)
C19	0.0831 (6)	−0.3190 (6)	0.0542 (5)	0.0285 (16)
H19	0.1648	−0.3266	0.0367	0.034*
C20	0.0510 (8)	−0.4018 (7)	0.0489 (6)	0.040 (2)
H20	0.1114	−0.4645	0.0272	0.049*
C21	−0.0675 (7)	−0.3920 (7)	0.0751 (6)	0.043 (2)
H21	−0.0882	−0.4479	0.0711	0.052*
C22	−0.1584 (6)	−0.2989 (6)	0.1079 (5)	0.0279 (16)

H22	−0.2395	−0.2932	0.1269	0.034*
C23	−0.1287 (6)	−0.2141 (6)	0.1125 (4)	0.0214 (14)
C24	−0.2311 (5)	−0.1127 (6)	0.1400 (4)	0.0194 (14)
C25	0.2553 (6)	−0.2075 (6)	0.2276 (4)	0.0208 (14)
C26	0.3052 (5)	−0.3180 (5)	0.2776 (4)	0.0188 (14)
C27	0.2949 (7)	−0.4028 (6)	0.2527 (5)	0.0305 (17)
H27	0.2622	−0.3910	0.2053	0.037*
C28	0.3340 (8)	−0.5060 (7)	0.2992 (6)	0.043 (2)
H28	0.3290	−0.5631	0.2816	0.052*
C29	0.3802 (8)	−0.5236 (6)	0.3712 (6)	0.039 (2)
H29	0.4050	−0.5921	0.4025	0.047*
C30	0.3891 (7)	−0.4394 (6)	0.3960 (5)	0.0295 (16)
H30	0.4182	−0.4510	0.4453	0.035*
C31	0.3552 (6)	−0.3363 (6)	0.3483 (4)	0.0216 (15)
C32	0.3785 (6)	−0.2512 (6)	0.3731 (4)	0.0206 (14)
C33	0.5698 (5)	−0.1514 (5)	−0.0863 (4)	0.0179 (13)
C34	0.7019 (5)	−0.2149 (5)	−0.1220 (4)	0.0182 (13)
C35	0.7286 (7)	−0.3091 (6)	−0.1544 (5)	0.0303 (17)
H35	0.6656	−0.3291	−0.1526	0.036*
C36	0.8467 (7)	−0.3730 (7)	−0.1891 (6)	0.041 (2)
H36	0.8634	−0.4350	−0.2122	0.049*
C37	0.9415 (7)	−0.3461 (7)	−0.1900 (6)	0.040 (2)
H37	1.0218	−0.3908	−0.2120	0.048*
C38	0.9158 (6)	−0.2520 (6)	−0.1578 (5)	0.0271 (16)
H38	0.9793	−0.2334	−0.1585	0.033*
C39	0.7962 (5)	−0.1850 (5)	−0.1247 (4)	0.0194 (14)
C40	0.7718 (6)	−0.0829 (6)	−0.0942 (4)	0.0202 (14)
C41	0.4315 (6)	0.1676 (5)	−0.4498 (4)	0.0182 (13)
C42	0.3013 (5)	0.2301 (5)	−0.4029 (4)	0.0183 (13)
C43	0.2790 (7)	0.3312 (6)	−0.3869 (5)	0.0297 (17)
H43	0.3426	0.3570	−0.4059	0.036*
C44	0.1616 (7)	0.3961 (7)	−0.3424 (5)	0.0370 (19)
H44	0.1477	0.4632	−0.3294	0.044*
C45	0.0666 (7)	0.3585 (6)	−0.3180 (5)	0.0360 (19)
H45	−0.0123	0.4019	−0.2906	0.043*
C46	0.0882 (6)	0.2577 (6)	−0.3339 (5)	0.0265 (16)
H46	0.0235	0.2336	−0.3170	0.032*
C47	0.2054 (5)	0.1908 (6)	−0.3752 (4)	0.0193 (14)
C48	0.2280 (6)	0.0824 (6)	−0.3906 (4)	0.0198 (14)
H25A	0.528 (6)	0.165 (7)	−0.146 (5)	0.050*
H25B	0.440 (7)	0.127 (7)	−0.0899 (18)	0.050*
H26A	0.422 (5)	−0.096 (7)	−0.246 (3)	0.050*
H26B	0.481 (7)	−0.107 (7)	−0.337 (3)	0.050*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Tm1	0.01355 (14)	0.01940 (17)	0.01543 (15)	−0.00609 (12)	−0.00262 (11)	−0.00136 (11)

Tm2	0.01188 (15)	0.01966 (18)	0.01674 (15)	−0.00620 (13)	0.00029 (11)	−0.00466 (12)
Tm3	0.01472 (15)	0.01797 (17)	0.01583 (15)	−0.00678 (12)	−0.00276 (11)	−0.00056 (12)
Tm4	0.01315 (14)	0.02015 (17)	0.01376 (15)	−0.00586 (12)	−0.00174 (10)	−0.00035 (11)
O1	0.016 (2)	0.043 (4)	0.051 (3)	−0.013 (2)	−0.008 (2)	−0.005 (3)
O2	0.028 (3)	0.034 (3)	0.030 (3)	−0.012 (2)	−0.005 (2)	−0.015 (2)
O3	0.016 (2)	0.036 (3)	0.036 (3)	−0.003 (2)	0.006 (2)	−0.004 (2)
O4	0.026 (3)	0.027 (3)	0.024 (3)	−0.002 (2)	−0.010 (2)	−0.001 (2)
O5	0.019 (2)	0.034 (3)	0.020 (2)	−0.011 (2)	−0.0013 (19)	0.004 (2)
O6	0.018 (2)	0.025 (3)	0.022 (2)	−0.006 (2)	0.0006 (19)	−0.002 (2)
O7	0.030 (3)	0.022 (3)	0.023 (2)	−0.013 (2)	−0.006 (2)	0.001 (2)
O8	0.035 (3)	0.027 (3)	0.020 (2)	−0.009 (2)	−0.009 (2)	−0.004 (2)
O9	0.024 (2)	0.032 (3)	0.025 (3)	−0.010 (2)	−0.004 (2)	−0.010 (2)
O10	0.024 (3)	0.036 (3)	0.044 (3)	−0.017 (2)	0.007 (2)	−0.012 (3)
O11	0.017 (2)	0.042 (3)	0.026 (3)	−0.010 (2)	−0.004 (2)	0.001 (2)
O12	0.027 (3)	0.023 (3)	0.027 (3)	−0.006 (2)	−0.011 (2)	0.005 (2)
O13	0.019 (2)	0.023 (3)	0.026 (3)	0.001 (2)	−0.001 (2)	0.000 (2)
O14	0.027 (3)	0.030 (3)	0.021 (2)	−0.009 (2)	−0.003 (2)	−0.002 (2)
O15	0.028 (3)	0.029 (3)	0.019 (2)	−0.011 (2)	−0.0050 (19)	−0.004 (2)
O16	0.043 (3)	0.033 (3)	0.022 (3)	−0.025 (3)	−0.012 (2)	0.005 (2)
O17	0.020 (2)	0.031 (3)	0.019 (2)	−0.012 (2)	0.0006 (19)	0.003 (2)
O18	0.023 (2)	0.025 (3)	0.028 (3)	0.001 (2)	−0.011 (2)	−0.001 (2)
O19	0.018 (2)	0.029 (3)	0.026 (3)	−0.008 (2)	0.0003 (19)	−0.010 (2)
O20	0.020 (2)	0.034 (3)	0.023 (2)	−0.017 (2)	−0.0003 (19)	0.000 (2)
O21	0.017 (2)	0.025 (3)	0.017 (2)	−0.010 (2)	−0.0047 (18)	0.0013 (19)
O22	0.016 (2)	0.034 (3)	0.019 (2)	−0.007 (2)	−0.0030 (18)	0.002 (2)
O23	0.021 (2)	0.037 (3)	0.020 (2)	−0.019 (2)	0.0019 (19)	−0.001 (2)
O24	0.015 (2)	0.025 (3)	0.033 (3)	−0.007 (2)	0.004 (2)	−0.013 (2)
O25	0.033 (3)	0.058 (4)	0.022 (3)	−0.018 (3)	−0.005 (2)	−0.014 (3)
O26	0.048 (3)	0.046 (4)	0.024 (3)	−0.029 (3)	−0.006 (2)	−0.006 (3)
C1	0.021 (3)	0.026 (4)	0.017 (3)	−0.011 (3)	−0.003 (3)	0.001 (3)
C2	0.019 (3)	0.024 (4)	0.018 (3)	−0.005 (3)	−0.006 (3)	−0.003 (3)
C3	0.030 (4)	0.022 (4)	0.040 (4)	0.003 (3)	−0.012 (3)	−0.009 (3)
C4	0.051 (5)	0.027 (5)	0.051 (5)	0.002 (4)	−0.022 (4)	−0.018 (4)
C5	0.066 (6)	0.033 (5)	0.047 (5)	−0.029 (5)	−0.029 (4)	0.001 (4)
C6	0.043 (4)	0.039 (5)	0.037 (4)	−0.025 (4)	−0.018 (4)	−0.002 (4)
C7	0.021 (3)	0.019 (4)	0.017 (3)	−0.005 (3)	−0.005 (3)	0.000 (3)
C8	0.021 (3)	0.025 (4)	0.029 (4)	−0.011 (3)	−0.006 (3)	−0.004 (3)
C9	0.014 (3)	0.018 (4)	0.025 (3)	−0.003 (3)	−0.009 (3)	−0.003 (3)
C10	0.016 (3)	0.022 (4)	0.018 (3)	−0.006 (3)	−0.001 (2)	−0.004 (3)
C11	0.035 (4)	0.031 (4)	0.027 (4)	−0.015 (3)	−0.009 (3)	−0.006 (3)
C12	0.049 (5)	0.028 (5)	0.037 (4)	−0.018 (4)	−0.008 (4)	−0.010 (4)
C13	0.039 (5)	0.012 (4)	0.053 (5)	−0.003 (4)	−0.006 (4)	−0.002 (4)
C14	0.035 (4)	0.023 (4)	0.031 (4)	−0.010 (3)	−0.010 (3)	0.001 (3)
C15	0.020 (3)	0.018 (4)	0.016 (3)	−0.004 (3)	0.000 (2)	−0.001 (3)
C16	0.014 (3)	0.021 (4)	0.025 (4)	−0.006 (3)	0.000 (3)	−0.009 (3)
C17	0.016 (3)	0.016 (3)	0.028 (4)	−0.008 (3)	−0.007 (3)	−0.001 (3)
C18	0.022 (3)	0.026 (4)	0.018 (3)	−0.010 (3)	−0.005 (3)	−0.006 (3)
C19	0.025 (4)	0.025 (4)	0.031 (4)	−0.007 (3)	0.000 (3)	−0.010 (3)
C20	0.039 (5)	0.028 (5)	0.048 (5)	−0.005 (4)	−0.003 (4)	−0.019 (4)

C21	0.037 (4)	0.031 (5)	0.068 (6)	−0.017 (4)	−0.013 (4)	−0.013 (4)
C22	0.028 (4)	0.024 (4)	0.037 (4)	−0.015 (3)	−0.010 (3)	−0.002 (3)
C23	0.019 (3)	0.022 (4)	0.020 (3)	−0.010 (3)	0.000 (3)	0.000 (3)
C24	0.013 (3)	0.028 (4)	0.015 (3)	−0.006 (3)	−0.003 (2)	−0.003 (3)
C25	0.020 (3)	0.027 (4)	0.020 (3)	−0.011 (3)	−0.008 (3)	−0.004 (3)
C26	0.016 (3)	0.018 (4)	0.018 (3)	−0.004 (3)	0.000 (2)	−0.005 (3)
C27	0.031 (4)	0.026 (4)	0.038 (4)	−0.010 (3)	−0.015 (3)	−0.005 (3)
C28	0.060 (6)	0.023 (5)	0.051 (5)	−0.019 (4)	−0.021 (4)	0.000 (4)
C29	0.049 (5)	0.016 (4)	0.045 (5)	−0.010 (4)	−0.012 (4)	0.003 (4)
C30	0.036 (4)	0.020 (4)	0.027 (4)	−0.005 (3)	−0.012 (3)	0.004 (3)
C31	0.019 (3)	0.020 (4)	0.023 (3)	−0.009 (3)	0.000 (3)	−0.002 (3)
C32	0.015 (3)	0.025 (4)	0.021 (3)	−0.007 (3)	−0.003 (2)	−0.004 (3)
C33	0.013 (3)	0.022 (4)	0.019 (3)	−0.003 (3)	−0.007 (2)	−0.006 (3)
C34	0.015 (3)	0.018 (4)	0.017 (3)	−0.008 (3)	0.000 (2)	0.001 (3)
C35	0.030 (4)	0.023 (4)	0.037 (4)	−0.007 (3)	−0.005 (3)	−0.014 (3)
C36	0.036 (4)	0.031 (5)	0.050 (5)	−0.006 (4)	−0.001 (4)	−0.022 (4)
C37	0.025 (4)	0.025 (5)	0.047 (5)	0.003 (3)	0.003 (3)	−0.005 (4)
C38	0.013 (3)	0.028 (4)	0.032 (4)	−0.007 (3)	0.000 (3)	0.000 (3)
C39	0.017 (3)	0.016 (4)	0.018 (3)	−0.004 (3)	−0.002 (2)	0.001 (3)
C40	0.022 (3)	0.029 (4)	0.015 (3)	−0.015 (3)	−0.008 (3)	0.003 (3)
C41	0.021 (3)	0.021 (4)	0.017 (3)	−0.012 (3)	−0.005 (2)	−0.001 (3)
C42	0.015 (3)	0.022 (4)	0.014 (3)	−0.008 (3)	−0.001 (2)	0.002 (3)
C43	0.031 (4)	0.020 (4)	0.031 (4)	−0.008 (3)	−0.008 (3)	0.005 (3)
C44	0.044 (5)	0.025 (4)	0.036 (4)	−0.010 (4)	−0.005 (4)	−0.007 (4)
C45	0.031 (4)	0.026 (4)	0.034 (4)	−0.001 (3)	0.002 (3)	−0.005 (3)
C46	0.015 (3)	0.025 (4)	0.027 (4)	−0.001 (3)	0.003 (3)	−0.004 (3)
C47	0.015 (3)	0.024 (4)	0.016 (3)	−0.006 (3)	−0.001 (2)	−0.005 (3)
C48	0.023 (3)	0.024 (4)	0.015 (3)	−0.012 (3)	−0.007 (3)	0.000 (3)

Geometric parameters (Å, °)

Tm1—O4^{i}	2.190 (5)	O26—H26B	0.817 (10)
Tm1—O1	2.216 (5)	C1—C2	1.488 (9)
Tm1—O5	2.248 (5)	C2—C7	1.380 (9)
Tm1—O15^{i}	2.278 (5)	C2—C3	1.403 (10)
Tm1—O24^{ii}	2.300 (5)	C3—C4	1.383 (12)
Tm1—O22^{iii}	2.377 (4)	C3—H3	0.9300
Tm1—O21^{iii}	2.536 (4)	C4—C5	1.343 (12)
Tm1—O23^{ii}	2.787 (5)	C4—H4	0.9300
Tm1—C41^{iii}	2.811 (6)	C5—C6	1.391 (12)
Tm1—C48^{ii}	2.924 (7)	C5—H5	0.9300
Tm2—O9	2.194 (5)	C6—C7	1.400 (10)
Tm2—O2	2.225 (5)	C6—H6	0.9300
Tm2—O13	2.238 (5)	C7—C8	1.516 (9)
Tm2—O20^{iv}	2.244 (4)	C9—C10	1.493 (9)
Tm2—O6	2.244 (5)	C10—C11	1.395 (9)
Tm2—O23^{ii}	2.248 (4)	C10—C15	1.396 (9)

Tm3—O12^{ii}	2.188 (5)	C11—C12	1.381 (11)
Tm3—O10	2.203 (4)	C11—H11	0.9300
Tm3—O17	2.306 (4)	C12—C13	1.383 (12)
Tm3—O14	2.308 (5)	C12—H12	0.9300
Tm3—O7^{ii}	2.380 (5)	C13—C14	1.366 (11)
Tm3—O19^{iv}	2.408 (5)	C13—H13	0.9300
Tm3—O8^{ii}	2.442 (5)	C14—C15	1.409 (10)
Tm3—C16^{ii}	2.758 (7)	C14—H14	0.9300
Tm3—O20^{iv}	2.830 (5)	C15—C16	1.493 (9)
Tm3—O18	2.870 (5)	C16—Tm3^{ii}	2.758 (7)
Tm3—C33	2.963 (6)	C17—C18	1.491 (9)
Tm4—O11^{ii}	2.205 (4)	C18—C23	1.381 (9)
Tm4—O3^{iv}	2.210 (5)	C18—C19	1.400 (10)
Tm4—O18	2.264 (5)	C19—C20	1.386 (11)
Tm4—O21	2.278 (4)	C19—H19	0.9300
Tm4—O16^{iv}	2.289 (5)	C20—C21	1.354 (11)
Tm4—O25	2.315 (5)	C20—H20	0.9300
Tm4—O26	2.344 (5)	C21—C22	1.388 (11)
O1—C1	1.254 (8)	C21—H21	0.9300
O2—C1	1.253 (8)	C22—C23	1.389 (9)
O3—C8	1.237 (8)	C22—H22	0.9300
O3—Tm4^{iv}	2.210 (5)	C23—C24	1.492 (9)
O4—C8	1.261 (8)	C25—C26	1.515 (9)
O4—Tm1^{i}	2.190 (5)	C26—C27	1.390 (9)
O5—C9	1.258 (7)	C26—C31	1.396 (9)
O6—C9	1.250 (7)	C27—C28	1.398 (11)
O7—C16	1.267 (8)	C27—H27	0.9300
O7—Tm3^{ii}	2.380 (5)	C28—C29	1.386 (12)
O8—C16	1.252 (8)	C28—H28	0.9300
O8—Tm3^{ii}	2.442 (5)	C29—C30	1.373 (11)
O9—C17	1.265 (8)	C29—H29	0.9300
O10—C17	1.251 (7)	C30—C31	1.399 (10)
O11—C24	1.252 (7)	C30—H30	0.9300
O11—Tm4^{ii}	2.205 (4)	C31—C32	1.487 (9)
O12—C24	1.251 (8)	C33—C34	1.492 (8)
O12—Tm3^{ii}	2.188 (5)	C34—C35	1.386 (9)
O13—C25	1.249 (8)	C34—C39	1.391 (9)
O14—C25	1.258 (7)	C35—C36	1.366 (10)
O15—C32	1.253 (8)	C35—H35	0.9300
O15—Tm1^{i}	2.278 (5)	C36—C37	1.380 (11)
O16—C32	1.270 (8)	C36—H36	0.9300
O16—Tm4^{iv}	2.289 (5)	C37—C38	1.386 (11)
O17—C33	1.258 (7)	C37—H37	0.9300
O18—C33	1.248 (8)	C38—C39	1.387 (9)
O19—C40	1.251 (8)	C38—H38	0.9300

O19—Tm3^{iv}	2.408 (5)	C39—C40	1.480 (9)
O20—C40	1.286 (7)	C41—C42	1.506 (8)
O20—Tm2^{iv}	2.244 (4)	C41—Tm1^{v}	2.811 (6)
O20—Tm3^{iv}	2.830 (5)	C42—C43	1.375 (10)
O21—C41	1.272 (8)	C42—C47	1.406 (8)
O21—Tm1^{v}	2.536 (4)	C43—C44	1.401 (10)
O22—C41	1.256 (7)	C43—H43	0.9300
O22—Tm1^{v}	2.377 (4)	C44—C45	1.387 (11)
O23—C48	1.274 (7)	C44—H44	0.9300
O23—Tm2^{ii}	2.248 (4)	C45—C46	1.373 (10)
O23—Tm1^{ii}	2.787 (5)	C45—H45	0.9300
O24—C48	1.259 (8)	C46—C47	1.396 (9)
O24—Tm1^{ii}	2.300 (5)	C46—H46	0.9300
O25—H25A	0.824 (10)	C47—C48	1.468 (9)
O25—H25B	0.821 (10)	C48—Tm1^{ii}	2.924 (7)
O26—H26A	0.816 (10)		
O4^{i}—Tm1—O1	82.99 (19)	C48—O23—Tm1^{ii}	83.2 (4)
O4^{i}—Tm1—O5	149.43 (17)	Tm2^{ii}—O23—Tm1^{ii}	116.9 (2)
O1—Tm1—O5	78.74 (18)	C48—O24—Tm1^{ii}	106.8 (4)
O4^{i}—Tm1—O15^{i}	91.43 (18)	Tm4—O25—H25A	115 (5)
O1—Tm1—O15^{i}	78.58 (18)	Tm4—O25—H25B	122 (6)
O5—Tm1—O15^{i}	108.50 (18)	H25A—O25—H25B	112 (3)
O4^{i}—Tm1—O24^{ii}	82.45 (19)	Tm4—O26—H26A	102 (5)
O1—Tm1—O24^{ii}	127.61 (18)	Tm4—O26—H26B	134 (6)
O5—Tm1—O24^{ii}	89.52 (18)	H26A—O26—H26B	115 (3)
O15^{i}—Tm1—O24^{ii}	151.59 (15)	O2—C1—O1	124.3 (6)
O4^{i}—Tm1—O22^{iii}	133.10 (16)	O2—C1—C2	118.5 (6)
O1—Tm1—O22^{iii}	139.67 (19)	O1—C1—C2	117.1 (6)
O5—Tm1—O22^{iii}	73.92 (15)	C7—C2—C3	119.3 (7)
O15^{i}—Tm1—O22^{iii}	82.61 (17)	C7—C2—C1	121.1 (6)
O24^{ii}—Tm1—O22^{iii}	81.57 (17)	C3—C2—C1	119.4 (6)
O4^{i}—Tm1—O21^{iii}	80.83 (16)	C4—C3—C2	119.4 (7)
O1—Tm1—O21^{iii}	147.00 (18)	C4—C3—H3	120.3
O5—Tm1—O21^{iii}	126.42 (15)	C2—C3—H3	120.3
O15^{i}—Tm1—O21^{iii}	73.30 (15)	C5—C4—C3	120.7 (8)
O24^{ii}—Tm1—O21^{iii}	78.34 (15)	C5—C4—H4	119.6
O22^{iii}—Tm1—O21^{iii}	52.83 (15)	C3—C4—H4	119.6
O4^{i}—Tm1—O23^{ii}	76.67 (16)	C4—C5—C6	121.7 (7)
O1—Tm1—O23^{ii}	77.80 (17)	C4—C5—H5	119.2
O5—Tm1—O23^{ii}	75.65 (16)	C6—C5—H5	119.2
O15^{i}—Tm1—O23^{ii}	154.64 (15)	C5—C6—C7	118.1 (7)
O24^{ii}—Tm1—O23^{ii}	49.89 (13)	C5—C6—H6	121.0

O22^{iii}—Tm1—O23^{ii}	121.86 (15)	C7—C6—H6	121.0
O21^{iii}—Tm1—O23^{ii}	125.32 (15)	C2—C7—C6	120.7 (7)
O4^{i}—Tm1—C41^{iii}	107.72 (18)	C2—C7—C8	123.4 (6)
O1—Tm1—C41^{iii}	149.9 (2)	C6—C7—C8	115.7 (6)
O5—Tm1—C41^{iii}	100.28 (17)	O3—C8—O4	125.6 (7)
O15^{i}—Tm1—C41^{iii}	73.19 (17)	O3—C8—C7	118.4 (6)
O24^{ii}—Tm1—C41^{iii}	82.27 (17)	O4—C8—C7	115.8 (6)
O22^{iii}—Tm1—C41^{iii}	26.36 (17)	O6—C9—O5	124.8 (6)
O21^{iii}—Tm1—C41^{iii}	26.89 (16)	O6—C9—C10	119.3 (6)
O23^{ii}—Tm1—C41^{iii}	131.59 (16)	O5—C9—C10	115.8 (5)
O4^{i}—Tm1—C48^{ii}	77.03 (18)	C11—C10—C15	118.4 (7)
O1—Tm1—C48^{ii}	103.25 (19)	C11—C10—C9	116.7 (6)
O5—Tm1—C48^{ii}	83.54 (18)	C15—C10—C9	124.9 (6)
O15^{i}—Tm1—C48^{ii}	167.89 (18)	C12—C11—C10	121.6 (7)
O24^{ii}—Tm1—C48^{ii}	24.35 (15)	C12—C11—H11	119.2
O22^{iii}—Tm1—C48^{ii}	102.50 (17)	C10—C11—H11	119.2
O21^{iii}—Tm1—C48^{ii}	100.86 (16)	C11—C12—C13	119.6 (7)
O23^{ii}—Tm1—C48^{ii}	25.63 (15)	C11—C12—H12	120.2
C41^{iii}—Tm1—C48^{ii}	106.56 (18)	C13—C12—H12	120.2
O9—Tm2—O2	171.67 (18)	C14—C13—C12	120.3 (8)
O9—Tm2—O13	86.46 (19)	C14—C13—H13	119.9
O2—Tm2—O13	88.27 (19)	C12—C13—H13	119.9
O9—Tm2—O20^{iv}	91.61 (17)	C13—C14—C15	120.7 (8)
O2—Tm2—O20^{iv}	94.30 (17)	C13—C14—H14	119.7
O13—Tm2—O20^{iv}	84.49 (17)	C15—C14—H14	119.7
O9—Tm2—O6	93.86 (18)	C10—C15—C14	119.5 (7)
O2—Tm2—O6	91.72 (19)	C10—C15—C16	121.8 (6)
O13—Tm2—O6	177.17 (15)	C14—C15—C16	118.6 (6)
O20^{iv}—Tm2—O6	92.69 (17)	O8—C16—O7	120.4 (6)
O9—Tm2—O23^{ii}	86.23 (17)	O8—C16—C15	119.7 (6)
O2—Tm2—O23^{ii}	87.80 (17)	O7—C16—C15	119.8 (6)
O13—Tm2—O23^{ii}	94.83 (17)	O8—C16—Tm3^{ii}	62.3 (4)
O20^{iv}—Tm2—O23^{ii}	177.77 (16)	O7—C16—Tm3^{ii}	59.5 (3)
O6—Tm2—O23^{ii}	87.99 (17)	C15—C16—Tm3^{ii}	165.0 (4)
O12^{ii}—Tm3—O10	85.95 (19)	O10—C17—O9	123.9 (6)
O12^{ii}—Tm3—O17	122.74 (16)	O10—C17—C18	118.2 (6)
O10—Tm3—O17	147.99 (19)	O9—C17—C18	117.8 (5)
O12^{ii}—Tm3—O14	148.40 (18)	C23—C18—C19	119.7 (6)
O10—Tm3—O14	86.65 (19)	C23—C18—C17	122.9 (6)
O17—Tm3—O14	75.42 (16)	C19—C18—C17	117.2 (6)
O12^{ii}—Tm3—O7^{ii}	77.54 (18)	C20—C19—C18	119.8 (7)
O10—Tm3—O7^{ii}	86.24 (18)	C20—C19—H19	120.1

O17—Tm3—O7^{ii}	86.73 (17)	C18—C19—H19	120.1
O14—Tm3—O7^{ii}	132.48 (17)	C21—C20—C19	120.5 (8)
O12^{ii}—Tm3—O19^{iv}	75.28 (18)	C21—C20—H20	119.7
O10—Tm3—O19^{iv}	122.56 (17)	C19—C20—H20	119.7
O17—Tm3—O19^{iv}	81.89 (17)	C20—C21—C22	120.2 (7)
O14—Tm3—O19^{iv}	83.07 (17)	C20—C21—H21	119.9
O7^{ii}—Tm3—O19^{iv}	138.07 (15)	C22—C21—H21	119.9
O12^{ii}—Tm3—O8^{ii}	128.53 (17)	C21—C22—C23	120.4 (7)
O10—Tm3—O8^{ii}	75.95 (18)	C21—C22—H22	119.8
O17—Tm3—O8^{ii}	74.70 (17)	C23—C22—H22	119.8
O14—Tm3—O8^{ii}	78.84 (17)	C18—C23—C22	119.4 (7)
O7^{ii}—Tm3—O8^{ii}	53.88 (16)	C18—C23—C24	122.9 (6)
O19^{iv}—Tm3—O8^{ii}	153.32 (16)	C22—C23—C24	117.5 (6)
O12^{ii}—Tm3—C16^{ii}	102.3 (2)	O12—C24—O11	125.1 (6)
O10—Tm3—C16^{ii}	76.62 (18)	O12—C24—C23	117.1 (5)
O17—Tm3—C16^{ii}	82.96 (18)	O11—C24—C23	117.7 (6)
O14—Tm3—C16^{ii}	105.80 (19)	O13—C25—O14	126.1 (7)
O7^{ii}—Tm3—C16^{ii}	27.30 (18)	O13—C25—C26	116.6 (6)
O19^{iv}—Tm3—C16^{ii}	159.87 (16)	O14—C25—C26	117.0 (6)
O8^{ii}—Tm3—C16^{ii}	26.99 (18)	C27—C26—C31	119.9 (7)
O12^{ii}—Tm3—O20^{iv}	76.45 (17)	C27—C26—C25	116.9 (6)
O10—Tm3—O20^{iv}	74.39 (16)	C31—C26—C25	123.1 (6)
O17—Tm3—O20^{iv}	122.62 (15)	C26—C27—C28	119.7 (7)
O14—Tm3—O20^{iv}	71.97 (16)	C26—C27—H27	120.1
O7^{ii}—Tm3—O20^{iv}	148.42 (15)	C28—C27—H27	120.1
O19^{iv}—Tm3—O20^{iv}	48.69 (13)	C29—C28—C27	120.4 (8)
O8^{ii}—Tm3—O20^{iv}	139.11 (14)	C29—C28—H28	119.8
C16^{ii}—Tm3—O20^{iv}	151.00 (15)	C27—C28—H28	119.8
O12^{ii}—Tm3—O18	74.97 (16)	C30—C29—C28	119.6 (8)
O10—Tm3—O18	152.24 (18)	C30—C29—H29	120.2
O17—Tm3—O18	48.03 (15)	C28—C29—H29	120.2
O14—Tm3—O18	119.99 (15)	C29—C30—C31	121.1 (7)
O7^{ii}—Tm3—O18	70.26 (15)	C29—C30—H30	119.5
O19^{iv}—Tm3—O18	72.22 (14)	C31—C30—H30	119.5
O8^{ii}—Tm3—O18	100.23 (15)	C26—C31—C30	119.2 (7)
C16^{ii}—Tm3—O18	87.78 (16)	C26—C31—C32	122.6 (6)
O20^{iv}—Tm3—O18	118.94 (14)	C30—C31—C32	118.2 (7)
O12^{ii}—Tm3—C33	99.60 (18)	O15—C32—O16	124.0 (6)
O10—Tm3—C33	158.80 (18)	O15—C32—C31	119.9 (6)
O17—Tm3—C33	23.68 (17)	O16—C32—C31	116.1 (6)
O14—Tm3—C33	98.32 (17)	O18—C33—O17	119.9 (6)
O7^{ii}—Tm3—C33	75.17 (16)	O18—C33—C34	122.8 (6)

O19^{iv}—Tm3—C33	78.59 (16)	O17—C33—C34	117.0 (6)
O8^{ii}—Tm3—C33	84.77 (17)	O18—C33—Tm3	73.5 (3)
C16^{ii}—Tm3—C33	82.21 (17)	O17—C33—Tm3	47.4 (3)
O20^{iv}—Tm3—C33	126.77 (15)	C34—C33—Tm3	157.5 (4)
O18—Tm3—C33	24.63 (15)	C35—C34—C39	119.7 (6)
O11^{ii}—Tm4—O3^{iv}	163.2 (2)	C35—C34—C33	115.8 (6)
O11^{ii}—Tm4—O18	89.47 (17)	C39—C34—C33	124.5 (6)
O3^{iv}—Tm4—O18	81.73 (18)	C36—C35—C34	120.6 (7)
O11^{ii}—Tm4—O21	88.24 (16)	C36—C35—H35	119.7
O3^{iv}—Tm4—O21	92.44 (18)	C34—C35—H35	119.7
O18—Tm4—O21	150.61 (17)	C35—C36—C37	120.5 (7)
O11^{ii}—Tm4—O16^{iv}	112.53 (19)	C35—C36—H36	119.8
O3^{iv}—Tm4—O16^{iv}	83.94 (19)	C37—C36—H36	119.8
O18—Tm4—O16^{iv}	129.82 (17)	C36—C37—C38	119.3 (7)
O21—Tm4—O16^{iv}	77.53 (16)	C36—C37—H37	120.3
O11^{ii}—Tm4—O25	75.59 (19)	C38—C37—H37	120.3
O3^{iv}—Tm4—O25	115.2 (2)	C37—C38—C39	120.7 (6)
O18—Tm4—O25	74.5 (2)	C37—C38—H38	119.6
O21—Tm4—O25	132.8 (2)	C39—C38—H38	119.6
O16^{iv}—Tm4—O25	68.97 (18)	C38—C39—C34	119.1 (6)
O11^{ii}—Tm4—O26	83.4 (2)	C38—C39—C40	119.4 (6)
O3^{iv}—Tm4—O26	80.5 (2)	C34—C39—C40	121.4 (6)
O18—Tm4—O26	74.75 (19)	O19—C40—O20	119.6 (6)
O21—Tm4—O26	75.88 (18)	O19—C40—C39	121.3 (5)
O16^{iv}—Tm4—O26	148.45 (17)	O20—C40—C39	119.0 (6)
O25—Tm4—O26	142.58 (19)	O22—C41—O21	120.1 (6)
C1—O1—Tm1	150.0 (5)	O22—C41—C42	118.8 (6)
C1—O2—Tm2	130.1 (4)	O21—C41—C42	120.4 (5)
C8—O3—Tm4^{iv}	130.2 (5)	O22—C41—Tm1^{v}	57.2 (3)
C8—O4—Tm1^{i}	144.7 (4)	O21—C41—Tm1^{v}	64.4 (3)
C9—O5—Tm1	139.6 (4)	C42—C41—Tm1^{v}	159.4 (4)
C9—O6—Tm2	141.4 (4)	C43—C42—C47	120.0 (6)
C16—O7—Tm3^{ii}	93.2 (4)	C43—C42—C41	115.9 (5)
C16—O8—Tm3^{ii}	90.7 (4)	C47—C42—C41	124.1 (6)
C17—O9—Tm2	135.3 (4)	C42—C43—C44	120.9 (7)
C17—O10—Tm3	156.6 (5)	C42—C43—H43	119.5
C24—O11—Tm4^{ii}	137.6 (4)	C44—C43—H43	119.5
C24—O12—Tm3^{ii}	152.0 (4)	C45—C44—C43	118.9 (7)
C25—O13—Tm2	142.0 (4)	C45—C44—H44	120.5
C25—O14—Tm3	143.2 (4)	C43—C44—H44	120.5
C32—O15—Tm1^{i}	129.4 (5)	C46—C45—C44	120.4 (7)
C32—O16—Tm4^{iv}	145.1 (4)	C46—C45—H45	119.8
C33—O17—Tm3	108.9 (4)	C44—C45—H45	119.8

C33—O18—Tm4	149.3 (4)	C45—C46—C47	121.1 (6)
C33—O18—Tm3	81.9 (4)	C45—C46—H46	119.4
Tm4—O18—Tm3	128.13 (19)	C47—C46—H46	119.4
C40—O19—Tm3^{iv}	106.2 (4)	C46—C47—C42	118.5 (6)
C40—O20—Tm2^{iv}	145.9 (4)	C46—C47—C48	120.7 (6)
C40—O20—Tm3^{iv}	85.1 (4)	C42—C47—C48	120.7 (6)
Tm2^{iv}—O20—Tm3^{iv}	120.00 (19)	O24—C48—O23	119.7 (6)
C41—O21—Tm4	141.4 (4)	O24—C48—C47	118.3 (5)
C41—O21—Tm1^{v}	88.7 (3)	O23—C48—C47	122.0 (6)
Tm4—O21—Tm1^{v}	122.08 (18)	O24—C48—Tm1^{ii}	48.9 (3)
C41—O22—Tm1^{v}	96.5 (4)	O23—C48—Tm1^{ii}	71.2 (4)
C48—O23—Tm2^{ii}	151.2 (4)	C47—C48—Tm1^{ii}	165.3 (4)
O4^{i}—Tm1—O1—C1	47.0 (10)	C10—C15—C16—O8	−156.4 (6)
O5—Tm1—O1—C1	−108.4 (10)	C14—C15—C16—O8	22.5 (9)
O15^{i}—Tm1—O1—C1	139.9 (10)	C10—C15—C16—O7	20.2 (9)
O24^{ii}—Tm1—O1—C1	−27.8 (11)	C14—C15—C16—O7	−160.9 (6)
O22^{iii}—Tm1—O1—C1	−156.3 (9)	C10—C15—C16—Tm3^{ii}	−63 (2)
O21^{iii}—Tm1—O1—C1	108.0 (10)	C14—C15—C16—Tm3^{ii}	116.0 (18)
O23^{ii}—Tm1—O1—C1	−30.8 (10)	Tm3—O10—C17—O9	37.6 (17)
C41^{iii}—Tm1—O1—C1	160.5 (9)	Tm3—O10—C17—C18	−140.1 (10)
C48^{ii}—Tm1—O1—C1	−27.9 (10)	Tm2—O9—C17—O10	−21.7 (11)
O9—Tm2—O2—C1	−100.3 (12)	Tm2—O9—C17—C18	155.9 (5)
O13—Tm2—O2—C1	−151.1 (6)	O10—C17—C18—C23	−153.5 (7)
O20^{iv}—Tm2—O2—C1	124.6 (6)	O9—C17—C18—C23	28.7 (10)
O6—Tm2—O2—C1	31.8 (6)	O10—C17—C18—C19	32.2 (10)
O23^{ii}—Tm2—O2—C1	−56.1 (6)	O9—C17—C18—C19	−145.6 (7)
O4^{i}—Tm1—O5—C9	−36.3 (9)	C23—C18—C19—C20	0.6 (11)
O1—Tm1—O5—C9	18.1 (7)	C17—C18—C19—C20	175.1 (7)
O15^{i}—Tm1—O5—C9	91.9 (7)	C18—C19—C20—C21	−0.7 (13)
O24^{ii}—Tm1—O5—C9	−110.5 (7)	C19—C20—C21—C22	−0.2 (14)
O22^{iii}—Tm1—O5—C9	168.2 (7)	C20—C21—C22—C23	1.2 (13)
O21^{iii}—Tm1—O5—C9	174.4 (6)	C19—C18—C23—C22	0.4 (11)
O23^{ii}—Tm1—O5—C9	−62.0 (7)	C17—C18—C23—C22	−173.8 (6)
C41^{iii}—Tm1—O5—C9	167.5 (7)	C19—C18—C23—C24	−175.0 (6)
C48^{ii}—Tm1—O5—C9	−86.8 (7)	C17—C18—C23—C24	10.8 (11)
O9—Tm2—O6—C9	105.1 (7)	C21—C22—C23—C18	−1.3 (11)
O2—Tm2—O6—C9	−68.7 (7)	C21—C22—C23—C24	174.3 (7)
O13—Tm2—O6—C9	−158 (3)	Tm3^{ii}—O12—C24—O11	−59.1 (13)
O20^{iv}—Tm2—O6—C9	−163.1 (7)	Tm3^{ii}—O12—C24—C23	117.8 (9)
O23^{ii}—Tm2—O6—C9	19.0 (7)	Tm4^{ii}—O11—C24—O12	38.9 (11)
O2—Tm2—O9—C17	−103.5 (12)	Tm4^{ii}—O11—C24—C23	−138.0 (6)
O13—Tm2—O9—C17	−52.7 (7)	C18—C23—C24—O12	50.0 (9)

O20^{iv}—Tm2—O9—C17	31.7 (7)	C22—C23—C24—O12	−125.5 (7)
O6—Tm2—O9—C17	124.5 (7)	C18—C23—C24—O11	−132.9 (7)
O23^{ii}—Tm2—O9—C17	−147.8 (7)	C22—C23—C24—O11	51.6 (9)
O12^{ii}—Tm3—O10—C17	−119.9 (13)	Tm2—O13—C25—O14	8.4 (12)
O17—Tm3—O10—C17	84.6 (13)	Tm2—O13—C25—C26	−166.0 (5)
O14—Tm3—O10—C17	29.3 (12)	Tm3—O14—C25—O13	−39.0 (11)
O7^{ii}—Tm3—O10—C17	162.3 (13)	Tm3—O14—C25—C26	135.4 (6)
O19^{iv}—Tm3—O10—C17	−50.3 (13)	O13—C25—C26—C27	98.5 (7)
O8^{ii}—Tm3—O10—C17	108.7 (13)	O14—C25—C26—C27	−76.4 (8)
C16^{ii}—Tm3—O10—C17	136.4 (13)	O13—C25—C26—C31	−78.8 (8)
O20^{iv}—Tm3—O10—C17	−42.9 (12)	O14—C25—C26—C31	106.2 (7)
O18—Tm3—O10—C17	−166.1 (11)	C31—C26—C27—C28	0.4 (10)
C33—Tm3—O10—C17	133.8 (11)	C25—C26—C27—C28	−177.0 (7)
O9—Tm2—O13—C25	70.2 (7)	C26—C27—C28—C29	1.5 (12)
O2—Tm2—O13—C25	−116.2 (7)	C27—C28—C29—C30	−1.0 (13)
O20^{iv}—Tm2—O13—C25	−21.7 (7)	C28—C29—C30—C31	−1.6 (12)
O6—Tm2—O13—C25	−26 (4)	C27—C26—C31—C30	−2.9 (9)
O23^{ii}—Tm2—O13—C25	156.2 (7)	C25—C26—C31—C30	174.4 (6)
O12^{ii}—Tm3—O14—C25	57.0 (9)	C27—C26—C31—C32	174.7 (6)
O10—Tm3—O14—C25	−19.7 (8)	C25—C26—C31—C32	−8.1 (9)
O17—Tm3—O14—C25	−172.9 (8)	C29—C30—C31—C26	3.5 (10)
O7^{ii}—Tm3—O14—C25	−101.5 (8)	C29—C30—C31—C32	−174.1 (7)
O19^{iv}—Tm3—O14—C25	103.7 (8)	Tm1^{i}—O15—C32—O16	35.3 (9)
O8^{ii}—Tm3—O14—C25	−96.0 (8)	Tm1^{i}—O15—C32—C31	−145.6 (5)
C16^{ii}—Tm3—O14—C25	−94.8 (8)	Tm4^{iv}—O16—C32—O15	23.4 (13)
O20^{iv}—Tm3—O14—C25	55.0 (7)	Tm4^{iv}—O16—C32—C31	−155.8 (6)
O18—Tm3—O14—C25	168.5 (7)	C26—C31—C32—O15	154.0 (6)
C33—Tm3—O14—C25	−179.0 (7)	C30—C31—C32—O15	−28.4 (9)
O12^{ii}—Tm3—O17—C33	−13.4 (5)	C26—C31—C32—O16	−26.8 (9)
O10—Tm3—O17—C33	137.0 (4)	C30—C31—C32—O16	150.8 (6)
O14—Tm3—O17—C33	−165.0 (5)	Tm4—O18—C33—O17	−179.0 (6)
O7^{ii}—Tm3—O17—C33	59.5 (4)	Tm3—O18—C33—O17	−10.2 (6)
O19^{iv}—Tm3—O17—C33	−80.1 (4)	Tm4—O18—C33—C34	−5.9 (13)
O8^{ii}—Tm3—O17—C33	112.9 (4)	Tm3—O18—C33—C34	162.9 (6)
C16^{ii}—Tm3—O17—C33	86.6 (4)	Tm4—O18—C33—Tm3	−168.8 (9)
O20^{iv}—Tm3—O17—C33	−108.1 (4)	Tm3—O17—C33—O18	13.3 (7)
O18—Tm3—O17—C33	−6.7 (4)	Tm3—O17—C33—C34	−160.1 (4)
O11^{ii}—Tm4—O18—C33	175.0 (9)	O12^{ii}—Tm3—C33—O18	0.6 (4)
O3^{iv}—Tm4—O18—C33	9.4 (9)	O10—Tm3—C33—O18	104.4 (6)
O21—Tm4—O18—C33	89.6 (10)	O17—Tm3—C33—O18	−168.0 (7)
O16^{iv}—Tm4—O18—C33	−65.6 (10)	O14—Tm3—C33—O18	−153.3 (4)
O25—Tm4—O18—C33	−109.8 (9)	O7^{ii}—Tm3—C33—O18	74.9 (4)
O26—Tm4—O18—C33	91.8 (9)	O19^{iv}—Tm3—C33—O18	−72.1 (4)

O11^{ii}—Tm4—O18—Tm3	9.2 (3)	O8^{ii}—Tm3—C33—O18	128.8 (4)
O3^{iv}—Tm4—O18—Tm3	−156.5 (3)	C16^{ii}—Tm3—C33—O18	101.8 (4)
O21—Tm4—O18—Tm3	−76.3 (4)	O20^{iv}—Tm3—C33—O18	−79.6 (4)
O16^{iv}—Tm4—O18—Tm3	128.6 (3)	O12^{ii}—Tm3—C33—O17	168.6 (4)
O25—Tm4—O18—Tm3	84.4 (3)	O10—Tm3—C33—O17	−87.7 (7)
O26—Tm4—O18—Tm3	−74.1 (3)	O14—Tm3—C33—O17	14.7 (4)
O12^{ii}—Tm3—O18—C33	−179.4 (4)	O7^{ii}—Tm3—C33—O17	−117.2 (4)
O10—Tm3—O18—C33	−131.2 (5)	O19^{iv}—Tm3—C33—O17	95.8 (4)
O17—Tm3—O18—C33	6.5 (4)	O8^{ii}—Tm3—C33—O17	−63.2 (4)
O14—Tm3—O18—C33	30.9 (4)	C16^{ii}—Tm3—C33—O17	−90.2 (4)
O7^{ii}—Tm3—O18—C33	−97.5 (4)	O20^{iv}—Tm3—C33—O17	88.4 (4)
O19^{iv}—Tm3—O18—C33	101.6 (4)	O18—Tm3—C33—O17	168.0 (7)
O8^{ii}—Tm3—O18—C33	−52.0 (4)	O12^{ii}—Tm3—C33—C34	−139.0 (11)
C16^{ii}—Tm3—O18—C33	−76.1 (4)	O10—Tm3—C33—C34	−35.2 (14)
O20^{iv}—Tm3—O18—C33	115.8 (4)	O17—Tm3—C33—C34	52.4 (11)
O12^{ii}—Tm3—O18—Tm4	−6.6 (3)	O14—Tm3—C33—C34	67.1 (11)
O10—Tm3—O18—Tm4	41.5 (5)	O7^{ii}—Tm3—C33—C34	−64.7 (11)
O17—Tm3—O18—Tm4	179.2 (4)	O19^{iv}—Tm3—C33—C34	148.3 (12)
O14—Tm3—O18—Tm4	−156.3 (2)	O8^{ii}—Tm3—C33—C34	−10.8 (11)
O7^{ii}—Tm3—O18—Tm4	75.3 (3)	C16^{ii}—Tm3—C33—C34	−37.8 (11)
O19^{iv}—Tm3—O18—Tm4	−85.7 (3)	O20^{iv}—Tm3—C33—C34	140.8 (11)
O8^{ii}—Tm3—O18—Tm4	120.7 (3)	O18—Tm3—C33—C34	−139.6 (13)
C16^{ii}—Tm3—O18—Tm4	96.7 (3)	O18—C33—C34—C35	−99.9 (8)
O20^{iv}—Tm3—O18—Tm4	−71.4 (3)	O17—C33—C34—C35	73.3 (8)
C33—Tm3—O18—Tm4	172.7 (6)	Tm3—C33—C34—C35	32.4 (15)
O11^{ii}—Tm4—O21—C41	22.2 (6)	O18—C33—C34—C39	79.7 (9)
O3^{iv}—Tm4—O21—C41	−174.6 (6)	O17—C33—C34—C39	−107.0 (7)
O18—Tm4—O21—C41	108.0 (7)	Tm3—C33—C34—C39	−147.9 (9)
O16^{iv}—Tm4—O21—C41	−91.3 (6)	C39—C34—C35—C36	−0.1 (11)
O25—Tm4—O21—C41	−46.2 (7)	C33—C34—C35—C36	179.6 (7)
O26—Tm4—O21—C41	105.8 (6)	C34—C35—C36—C37	1.8 (13)
O11^{ii}—Tm4—O21—Tm1^{v}	160.1 (2)	C35—C36—C37—C38	−1.9 (13)
O3^{iv}—Tm4—O21—Tm1^{v}	−36.7 (2)	C36—C37—C38—C39	0.2 (12)
O18—Tm4—O21—Tm1^{v}	−114.2 (3)	C37—C38—C39—C34	1.6 (11)
O16^{iv}—Tm4—O21—Tm1^{v}	46.5 (2)	C37—C38—C39—C40	−177.5 (7)
O25—Tm4—O21—Tm1^{v}	91.6 (3)	C35—C34—C39—C38	−1.6 (10)
O26—Tm4—O21—Tm1^{v}	−116.3 (3)	C33—C34—C39—C38	178.7 (6)
Tm2—O2—C1—O1	21.3 (10)	C35—C34—C39—C40	177.5 (6)
Tm2—O2—C1—C2	−154.8 (5)	C33—C34—C39—C40	−2.2 (10)
Tm1—O1—C1—O2	41.8 (14)	Tm3^{iv}—O19—C40—O20	−6.7 (7)
Tm1—O1—C1—C2	−142.0 (8)	Tm3^{iv}—O19—C40—C39	173.4 (5)
O2—C1—C2—C7	−11.8 (10)	Tm2^{iv}—O20—C40—O19	−134.8 (7)

O1—C1—C2—C7	171.7 (6)	Tm3^{iv}—O20—C40—O19	5.5 (6)
O2—C1—C2—C3	162.8 (7)	Tm2^{iv}—O20—C40—C39	45.1 (11)
O1—C1—C2—C3	−13.7 (10)	Tm3^{iv}—O20—C40—C39	−174.6 (6)
C7—C2—C3—C4	2.2 (11)	C38—C39—C40—O19	−160.5 (6)
C1—C2—C3—C4	−172.5 (7)	C34—C39—C40—O19	20.4 (10)
C2—C3—C4—C5	2.1 (13)	C38—C39—C40—O20	19.6 (9)
C3—C4—C5—C6	−4.3 (14)	C34—C39—C40—O20	−159.4 (6)
C4—C5—C6—C7	2.1 (13)	Tm1^{v}—O22—C41—O21	−14.6 (6)
C3—C2—C7—C6	−4.3 (10)	Tm1^{v}—O22—C41—C42	156.4 (5)
C1—C2—C7—C6	170.3 (6)	Tm4—O21—C41—O22	158.9 (5)
C3—C2—C7—C8	169.9 (7)	Tm1^{v}—O21—C41—O22	13.6 (6)
C1—C2—C7—C8	−15.5 (10)	Tm4—O21—C41—C42	−11.9 (10)
C5—C6—C7—C2	2.2 (11)	Tm1^{v}—O21—C41—C42	−157.2 (5)
C5—C6—C7—C8	−172.4 (7)	Tm4—O21—C41—Tm1^{v}	145.3 (6)
Tm4^{iv}—O3—C8—O4	−27.1 (10)	O22—C41—C42—C43	−75.5 (8)
Tm4^{iv}—O3—C8—C7	148.1 (5)	O21—C41—C42—C43	95.5 (7)
Tm1^{i}—O4—C8—O3	64.5 (12)	Tm1^{v}—C41—C42—C43	−2.6 (16)
Tm1^{i}—O4—C8—C7	−110.8 (8)	O22—C41—C42—C47	105.0 (8)
C2—C7—C8—O3	113.1 (8)	O21—C41—C42—C47	−84.0 (8)
C6—C7—C8—O3	−72.4 (9)	Tm1^{v}—C41—C42—C47	177.9 (9)
C2—C7—C8—O4	−71.3 (9)	C47—C42—C43—C44	0.6 (11)
C6—C7—C8—O4	103.2 (7)	C41—C42—C43—C44	−178.9 (7)
Tm2—O6—C9—O5	−11.6 (11)	C42—C43—C44—C45	−2.8 (12)
Tm2—O6—C9—C10	164.1 (5)	C43—C44—C45—C46	2.6 (12)
Tm1—O5—C9—O6	48.3 (11)	C44—C45—C46—C47	−0.3 (12)
Tm1—O5—C9—C10	−127.5 (6)	C45—C46—C47—C42	−1.9 (11)
O6—C9—C10—C11	−99.1 (7)	C45—C46—C47—C48	178.9 (7)
O5—C9—C10—C11	76.9 (7)	C43—C42—C47—C46	1.7 (10)
O6—C9—C10—C15	81.8 (8)	C41—C42—C47—C46	−178.8 (6)
O5—C9—C10—C15	−102.2 (8)	C43—C42—C47—C48	−179.1 (6)
C15—C10—C11—C12	−0.2 (10)	C41—C42—C47—C48	0.4 (10)
C9—C10—C11—C12	−179.4 (6)	Tm1^{ii}—O24—C48—O23	7.2 (7)
C10—C11—C12—C13	−1.4 (11)	Tm1^{ii}—O24—C48—C47	−171.4 (5)
C11—C12—C13—C14	1.9 (12)	Tm2^{ii}—O23—C48—O24	130.9 (8)
C12—C13—C14—C15	−0.8 (12)	Tm1^{ii}—O23—C48—O24	−5.7 (6)
C11—C10—C15—C14	1.2 (9)	Tm2^{ii}—O23—C48—C47	−50.5 (13)
C9—C10—C15—C14	−179.7 (6)	Tm1^{ii}—O23—C48—C47	172.8 (6)
C11—C10—C15—C16	−179.9 (6)	Tm2^{ii}—O23—C48—Tm1^{ii}	136.7 (9)
C9—C10—C15—C16	−0.8 (9)	C46—C47—C48—O24	170.4 (6)
C13—C14—C15—C10	−0.8 (10)	C42—C47—C48—O24	−8.8 (9)
C13—C14—C15—C16	−179.7 (6)	C46—C47—C48—O23	−8.2 (10)
Tm3^{ii}—O8—C16—O7	−13.5 (6)	C42—C47—C48—O23	172.7 (6)
Tm3^{ii}—O8—C16—C15	163.1 (5)	C46—C47—C48—Tm1^{ii}	143.9 (15)
Tm3^{ii}—O7—C16—O8	13.9 (6)	C42—C47—C48—Tm1^{ii}	−35 (2)

Tm3^{ii}—O7—C16—C15	−162.7 (5)

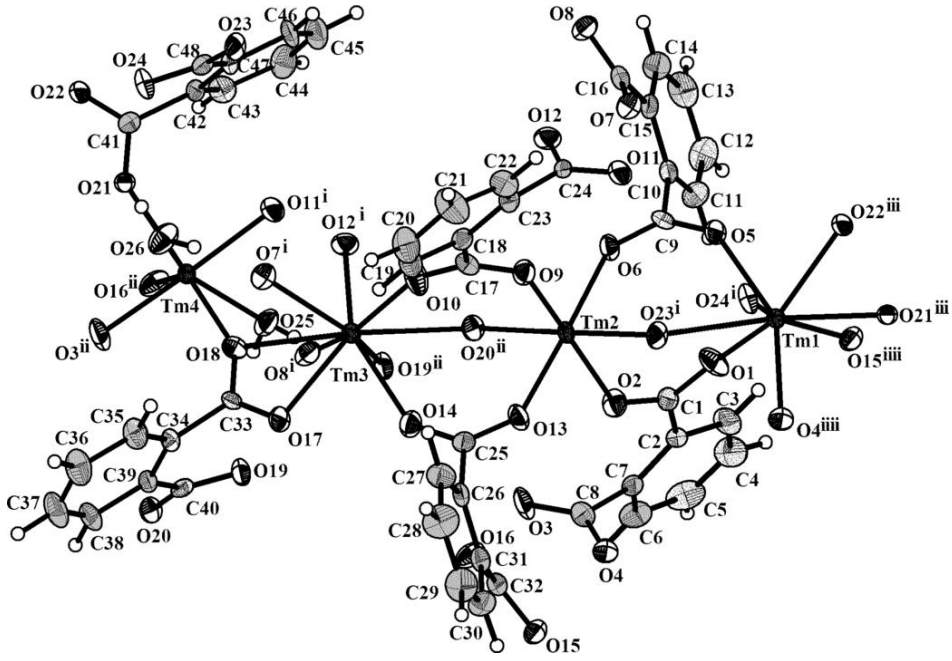
Symmetry codes: (i) −*x*, −*y*, −*z*+1; (ii) −*x*, −*y*, −*z*; (iii) *x*−1, *y*, *z*+1; (iv) −*x*+1, −*y*, −*z*; (v) *x*+1, *y*, *z*−1.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O25—H25A···O14^{iv}	0.824 (10)	2.06 (2)	2.872 (7)	169 (9)
O25—H25B···O17^{iv}	0.821 (10)	2.32 (7)	2.729 (7)	111 (6)
O25—H25B···O19^{iv}	0.821 (10)	2.45 (3)	3.232 (7)	161 (7)
O26—H26A···O7^{ii}	0.816 (10)	2.08 (5)	2.822 (7)	151 (9)
O26—H26B···O22^{vi}	0.817 (10)	2.40 (2)	3.208 (7)	168 (9)
O26—H26B···O5^{ii}	0.817 (10)	2.62 (6)	3.072 (7)	116 (5)

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

Fig. 1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C48
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C42
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O21
O26
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O11i
O12i
O7i
C20
C21
C22
C23
C24
O12
O11
C10
C11
C12
C13
C14
O8
C16
O7
C15
C18
C19
C17
O9
O10
O6
C9
O5
O22iii
O24i
O23i
Tm2
Tm1
O21iii
O15iiii
O25
O18
O8i
Tm3
O19ii
O20ii
O2
O1
C1
C3
O4iiii
C2
C4
C5
C6
C7
C8
O3
O4
C35
C34
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O17
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C37
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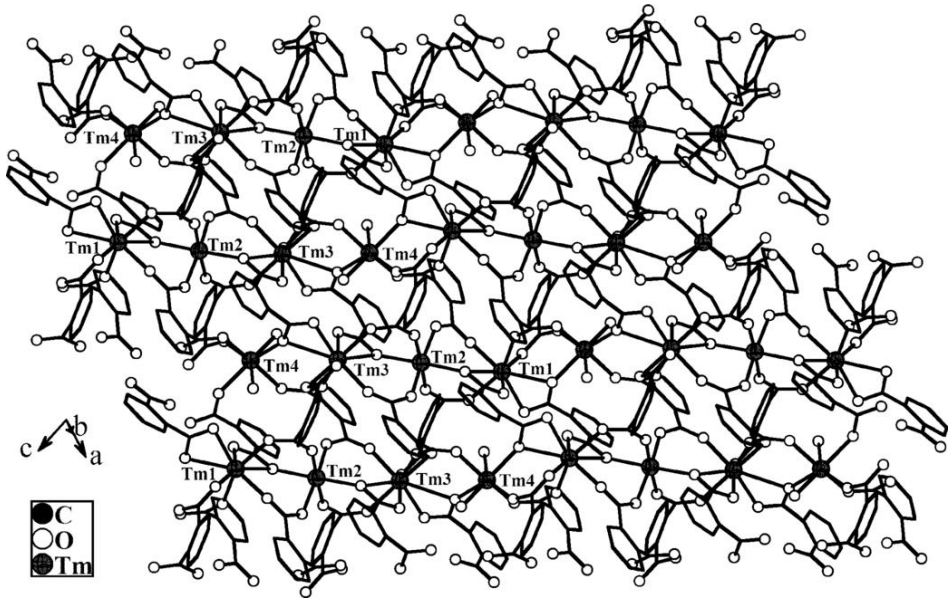
C30
O15

Fig. 2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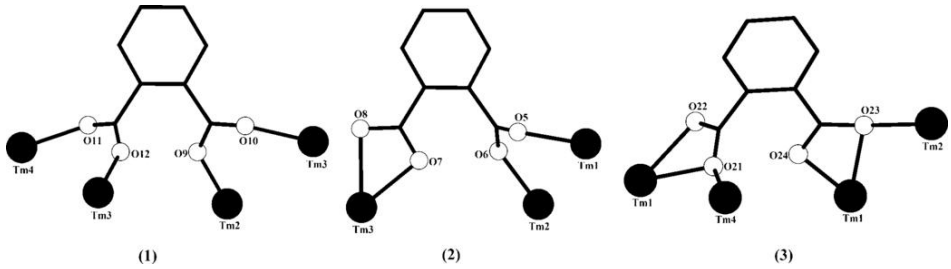
c
b
a
C
O
Tm

Fig. 3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O22
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O21
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Tm2
Tm1
Tm4
Tm1
(3)