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Retraction of articles

This article reports the retraction of articles published in *Acta Crystallographica Section E* between 2005 and 2009.

After further thorough investigation (see Harrison *et al.*, 2010), articles are retracted as a result of problems with the data sets or incorrect atom assignments. Full details of all the articles are given in Table 1.

Table 1
Details of articles to be retracted, in order of publication.

Title	Reference	DOI	Refcode
Poly[diaquadi-μ_3-malonato-μ-pyrazine-dinickel(II)]	Liu *et al.* (2005)	10.1107/S1600536805026358	GATWAA
catena-Poly[[[diaqua(6-carboxypyridine-2-carboxylato)samarium(II)]-μ-pyridine-2,6-dicarboxylato] tetrahydrate]	Liu *et al.* (2006)	10.1107/S1600536806038141	FONCUH03
Poly[[[μ_4-4,4′-carbonylbis(benzene-3,4-dicarboxylato)]tetrakis(1,10-phenanthroline)-dipalladium(II)] dihydrate]	Li, Wang, Zhang & Yu (2007*e*)	10.1107/S1600536807039050	AFELAZ
Poly[diaqua-μ_3-malonato-μ-pyrazine-diiron(II)]	Li, Liu *et al.* (2007)	10.1107/S1600536807038743	AFELON
Poly[diaqua-di-μ_3-malonato-μ-pyrazine-dimanganese(II)]	Li, Wang, Zhang & Yu (2007*f*)	10.1107/S1600536807039773	VIJZAQ
Poly[[aqua(2,2-bipyridine)(μ_3-pyridine-3,4-dicarboxylato)cobalt(II)] monohydrate]	Li, Wang, Zhang & Yu (2007*g*)	10.1107/S1600536807040275	VIKCIC
catena-Poly[[[diaqua(6-carboxypyridine-2-carboxylato)holmium(III)]-μ-pyridine-2,6-dicarboxylato] tetrahydrate]	Li, Wang, Zhang & Yu (2007*a*)	10.1107/S1600536807041657	DILGEL
catena-Poly[[(2,2′-bipyridine-κ^2N,N')iron(II)]-μ-5-carboxy-4-carboxylatoimidazol-1-ido-$\kappa^4N^3,O^4{:}N^1,O^5$]	Li, Wang, Zhang & Yu (2007*h*)	10.1107/S1600536807042122	XIKWAQ
Poly[[aqua(2,2′-bipyridine)(μ_3-pyridine-3,4-dicarboxylato)nickel(II)] monohydrate]	Li, Wang, Zhang & Yu (2007*b*)	10.1107/S1600536807046466	LEVZAO01
2-(Benzyliminomethyl)-6-methoxyphenol	Li, Wang, Zhang & Yu (2007*i*)	10.1107/S1600536807042134	SILDEX
Poly[aqua(2,2′-bipyridine)(μ_3-pyridine-2,4-dicarboxylato)palladium(II)]	Li, Wang, Zhang & Yu (2007*c*)	10.1107/S1600536807047575	SILXAN
μ-Oxido-bis{chlorido[tris(2-pyridylmethyl)amine]iron(III)} bis(hexafluoridophosphate)	Liu, Dou, Li & Zhang (2007)	10.1107/S1600536807049665	TINRIS
μ-Oxido-bis({4,4′-dibromo-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-manganese(III))	Liu, Dou, Niu & Zhang (2007*a*)	10.1107/S1600536807051008	GIMZAE
Bis[N-(8-quinolyl)pyridine-2-carboxamidato]iron(III) perchlorate monohydrate	Li, Wang, Zhang & Yu (2007*d*)	10.1107/S1600536807048556	WIMZIC
μ-Oxido-bis({4,4′-dibromo-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-chromium(III))	Liu, Dou, Niu & Zhang (2007*b*)	10.1107/S1600536807057996	HIQFIX
μ-Oxido-bis{chlorido[tris(2-pyridylmethyl)amine]chromium(III)} bis(hexafluorido-phosphate)	Li, Wang *et al.* (2008)	10.1107/S1600536807061296	MIRNAD
μ-Oxido-bis({4,4′-dibromo-2,2′-ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-iron(III))	Meng *et al.* (2008*a*)	10.1107/S1600536807063143	MIRWUG
catena-Poly[[bis(1H-benzimidazole-κN^3)palladium(II)]-μ-benzene-1,4-dicarboxylato-$\kappa^2O^1{:}O^4$]	Meng *et al.* (2008*b*)	10.1107/S1600536807065051	XISCAE
Oxalatobis(propane-1,3-diamine)manganese(II) chloride monohydrate	Meng *et al.* (2008*e*)	10.1107/S1600536807065361	SISWIB
μ-Oxido-bis{chlorido[tris(2-pyridylmethyl)amine]manganese(III)} bis(hexafluorido-phosphate)	Meng *et al.* (2008*c*)	10.1107/S1600536807066512	RISRIV
Bis[N-(8-quinolyl)pyridine-2-carboxamidato-κ^3N,N',N'']manganese(III) perchlorate monohydrate	Meng *et al.* (2008*d*)	10.1107/S1600536808000287	GISLEA
Diaquabis(pyridine-2-carboxylato-κ^2N,O)cobalt(II)	Huang (2008)	10.1107/S1600536808010507	WIZPOL
Tetra-μ-2,5-difluorobenzoato-bis[(2,2′-bipyridine)(2,5-difluorobenzoato)gadolinium(III)]	Li, Zhang *et al.* (2008)	10.1107/S1600536808023507	BOFQIX
catena-Poly[[(2,2′-bipyridine-κ^2N,N')nickel(II)]-μ-oxalato-$\kappa^4O^1,O^2{:}O^{1'},O^{2'}$]	Li, Yan *et al.* (2008)	10.1107/S1600536808028389	NOHYUF
catena-Poly[[aqua(2,2′-bipyridyl)cobalt(II)]-μ-5-nitroisophthlalato]	Liu *et al.* (2008)	10.1107/S1600536808038178	AFIREN
Diaquabis(pyridine-2-carboxylato-κ^2N,O)iron(II)	Xia & Sun (2009)	10.1107/S1600536809005765	RONFEG
catena-Poly[[[diaquathulium(III)]-μ-6-carboxynicotinato-μ-pyridine-2,5-dicarboxylato] dihydrate]	Li *et al.* (2009)	10.1107/S1600536809008836	NOQNIR
1-Phenyl-3-(2,4,6-trimethoxyphenyl)prop-2-en-1-one	Liu *et al.* (2009)	10.1107/S1600536809040227	PUGLOT

  doi:10.1107/S1600536811037603

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catena-Poly[[[diaquathulium(III)]-μ-6-carboxynicotinato-μ-pyridine-2,5-dicarboxylato] dihydrate]

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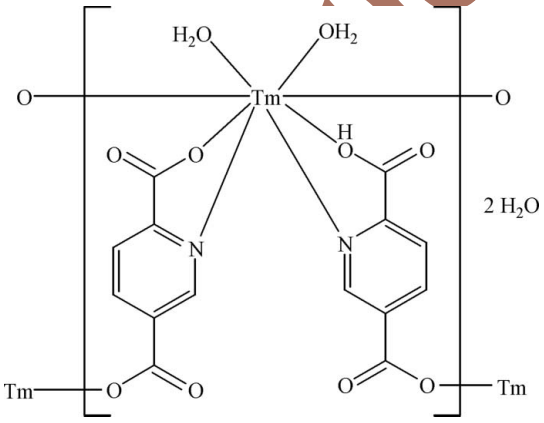
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.013 Å; R factor = 0.043; wR factor = 0.111; data-to-parameter ratio = 11.7.

The title compound, $\{[Tm(C_7H_3NO_4)(C_7H_4NO_4)(H_2O)_2]\cdot 2H_2O\}_n$, is isotypic with the analogous Tb^{III} compound [Li *et al.* (2009). *Acta Cryst.* E**65**, m410]. All interatomic distances and angles and the hydrogen-bond geometries are very similar for the two structures. The refined Flack parameter of 0.49 (2) suggests inversion twinning.

Related literature

For the isotypic Tb^{III} compound, see Li *et al.* (2009). For other related structures, see: Huang *et al.* (2007).



Experimental

Crystal data

$[Tm(C_7H_3NO_4)(C_7H_4NO_4)(H_2O)_2]\cdot 2H_2O$
M_r = 572.21
Tetragonal, $I\overline{4}$
a = 15.1286 (12) Å
c = 14.849 (2) Å
V = 3398.6 (6) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 5.30 mm^{-1}
T = 298 K
0.12 × 0.11 × 0.09 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.569, T_{max} = 0.647
7093 measured reflections
3085 independent reflections
2977 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.111
S = 1.07
3085 reflections
263 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 6.96 e Å^{-3}
$\Delta\rho_{min}$ = −1.18 e Å^{-3}
Absolute structure: Flack (1983), with 1444 Friedel pairs
Flack parameter: 0.49 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O12^{i}	0.85	1.97	2.788 (11)	162
O9—H91···O4^{ii}	0.85	1.83	2.679 (10)	180
O9—H92···O4^{iii}	0.85	1.99	2.842 (10)	180
O10—H101···O7^{iv}	0.85	1.83	2.675 (11)	179
O10—H102···O9^{i}	0.85	2.14	2.996 (10)	179
O11—H111···O5	0.85	2.02	2.872 (11)	179
O11—H112···O2^{iv}	0.85	1.91	2.763 (11)	180
O12—H121···O6^{v}	0.85	2.15	3.004 (12)	179
O12—H122···O6^{vi}	0.85	2.08	2.933 (12)	179

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT-Plus* (Bruker, 2001); 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: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BI2347).

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supporting information

Acta Cryst. (2009). E**65**, m411 [doi:10.1107/S1600536809008836]

catena-Poly[[[diaquathulium(III)]-μ-6-carboxynicotinato-μ-pyridine-2,5-dicarboxylato] dihydrate]

Sheng Li, Yue Chen, Hong-Mei He and Yuan-Fang Ma

S1. Comment

The asymmetric unit of the title compound is shown in Fig. 1. Atom Tm1 displays octa-coordination through two water molecules, four carboxylate O atoms and two pyridyl N atoms from two 2,5-pydc and two 2,5-Hpydc ligands (2,5-pydc = 2,5-pyridinedicarboxylate). The 2,5-pydc and 2,5-Hpydc ligands bridge between Tm^{III} atoms to generate helical coordination polymers along [001] (Fig. 2). An extensive network of O—H···O hydrogen bonds is formed between the coordination polymers and the lattice water molecules (Table 1 and Fig. 3).

S2. Experimental

A mixture of thulium oxide (0.5 mmol), 2,5-pyridinedicarboxylic acid (0.5 mmol), in H_2O (8 ml) and ethanol (8 ml) was sealed in a 25 ml Teflon-lined stainless steel autoclave and kept at 413 K for three days. Colourless crystals were obtained after cooling to room temperature with a yield of 27%. Elemental analysis calculated: C 28.90, H 2.75, N 4.82%; Found: C 28.75, H 2.72, N 4.79%.

S3. Refinement

H atoms bound to C atoms were placed in calculated positions with C—H = 0.93 Å and refined as riding with U_{iso}(H) = 1.2U_{eq}(C). H atoms of the water molecules were placed so as to form a reasonable H-bond network and refined as riding with U_{iso}(H) = 1.5U_{eq}(O). The Flack parameter was refined as a full least-squares parameter, and the refined value of 0.49 (2) suggests inversion twinning. Two relatively large peaks remain in the residual electron density (5.5–7.0 eÅ^{-3}) on the special positions (0,0,0) and (0.5,0,0.25), which may indicate further lattice water molecules. The refinement as a dihydrate is consistent with the isomorphous Tb^{III} compound (Li *et al.*, 2009).

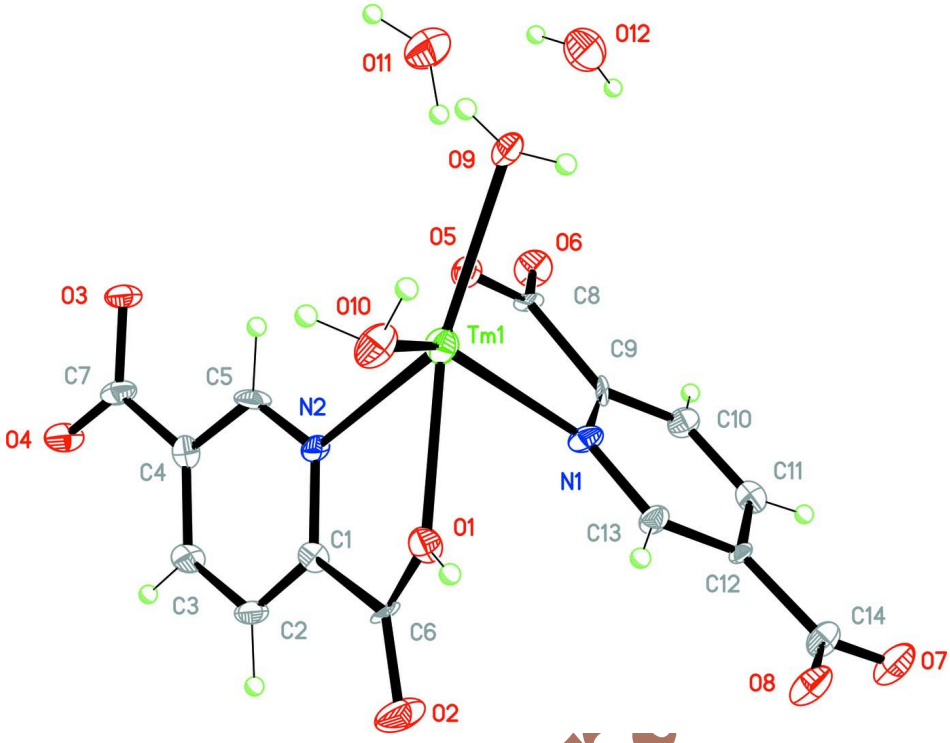

Figure 1

Aysymmetric unit of the title compound, showing 50% probability displacement ellipsoids for non-H atoms.

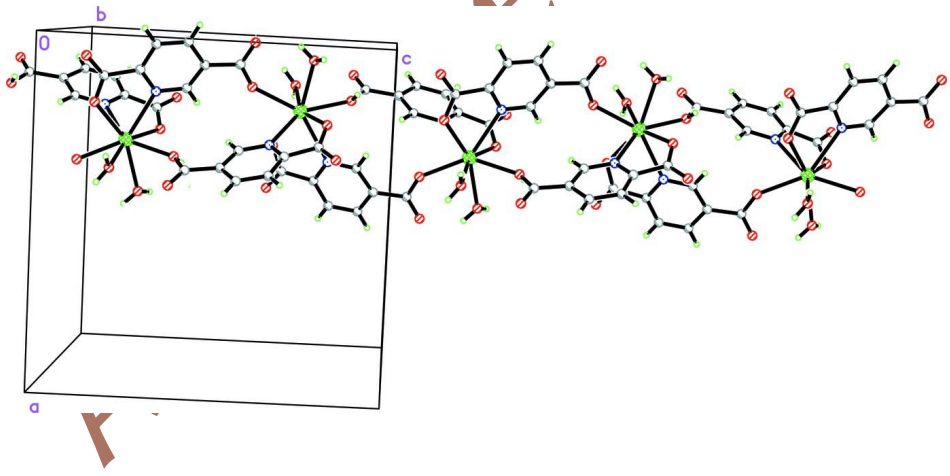

Figure 2

One-dimensional coordination polymer running along [001].

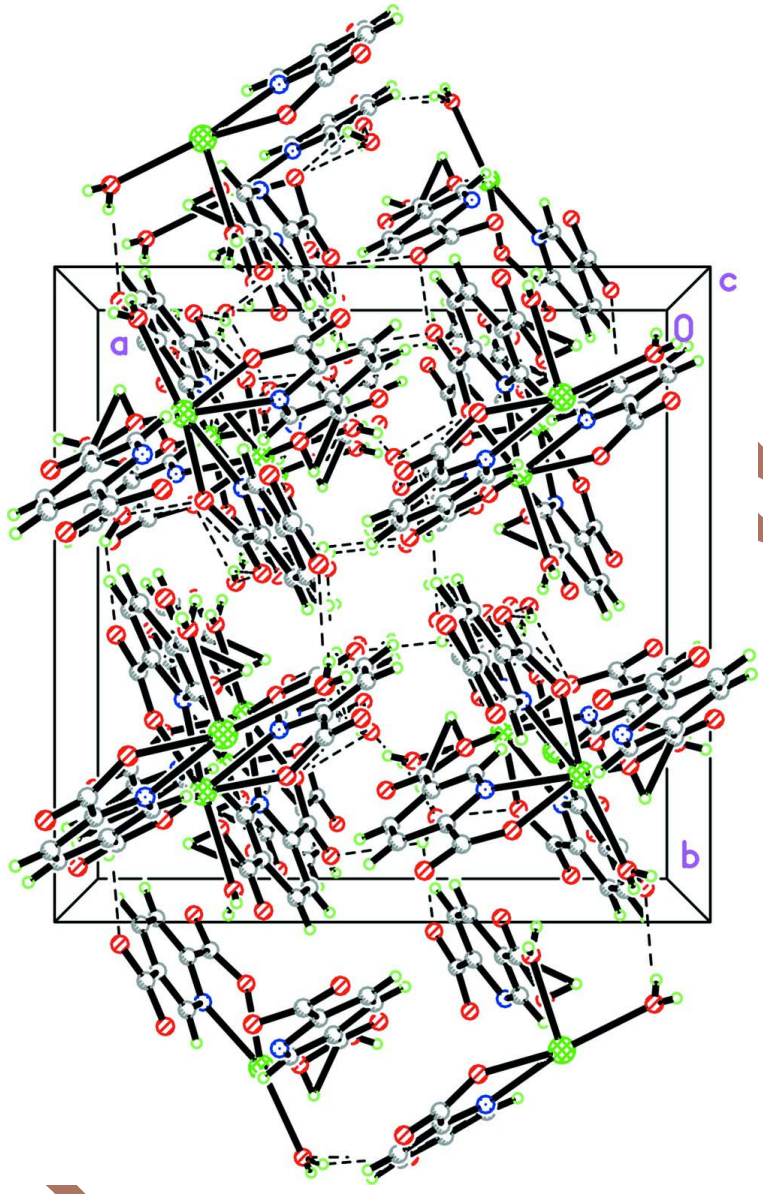

Figure 3

Projection along [001], showing the tetragonal arrangement of coordination polymers. O—H···O hydrogen bonds are shown as dashed lines.

(I)

Crystal data

$[Tm(C_7H_3NO_4)(C_7H_4NO_4)(H_2O)_2]\cdot 2H_2O$
$M_r = 572.21$
Tetragonal, $I\bar{4}$
Hall symbol: I -4
$a = 15.1286\ (12)$ Å
$c = 14.849\ (2)$ Å
$V = 3398.6\ (6)$ Å^3
$Z = 8$
$F(000) = 2224$
$D_x = 2.237$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3085 reflections
$\theta = 1.9$–$25.5°$
$\mu = 5.30$ mm^{-1}
$T = 298$ K
Block, colorless
0.12 × 0.11 × 0.09 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.569, T_{max} = 0.647
7093 measured reflections
3085 independent reflections
2977 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 25.5°, θ_{min} = 1.9°
h = −18→16
k = −18→15
l = −17→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.111
S = 1.07
3085 reflections
263 parameters
0 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
$w = 1/[\sigma^2(F_o^2) + (0.0703P)^2 + 51.4546P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 6.96 e Å^{-3}
$\Delta\rho_{min}$ = −1.18 e Å^{-3}
Absolute structure: Flack (1983), 1444 Friedel pairs
Absolute structure parameter: 0.49 (2)

Special details

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

Refinement. 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 > 2sigma(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	0.30232 (3)	0.22523 (3)	0.22714 (3)	0.01768 (14)
C1	0.1831 (5)	0.4107 (6)	0.1942 (6)	0.0111 (18)
C2	0.1327 (6)	0.4765 (6)	0.1551 (6)	0.0164 (19)
H2A	0.1115	0.5229	0.1900	0.020*
C3	0.1140 (6)	0.4732 (6)	0.0642 (6)	0.0156 (18)
H3A	0.0816	0.5185	0.0376	0.019*
C4	0.1428 (6)	0.4034 (6)	0.0126 (6)	0.0132 (17)
C5	0.1880 (6)	0.3365 (6)	0.0577 (7)	0.0170 (19)
H5A	0.2041	0.2864	0.0253	0.020*
C6	0.2156 (6)	0.4129 (6)	0.2916 (5)	0.0115 (19)
C7	0.1298 (6)	0.3968 (6)	−0.0877 (7)	0.017 (2)
C8	0.1188 (6)	0.1237 (6)	0.1724 (6)	0.0133 (18)
C9	0.0969 (5)	0.1481 (5)	0.2698 (7)	0.0091 (15)
C10	0.0232 (6)	0.1189 (6)	0.3171 (7)	0.0160 (18)
H10A	−0.0196	0.0856	0.2876	0.019*

C11	0.0128 (6)	0.1380 (6)	0.4051 (7)	0.0160 (19)
H11A	−0.0358	0.1162	0.4364	0.019*
C12	0.0768 (6)	0.1922 (6)	0.4506 (6)	0.0103 (16)
C13	0.1453 (6)	0.2202 (6)	0.3982 (6)	0.0136 (18)
H13A	0.1868	0.2571	0.4251	0.016*
C14	0.0689 (6)	0.2110 (7)	0.5496 (6)	0.016 (2)
N1	0.1582 (5)	0.1994 (5)	0.3117 (6)	0.0152 (16)
N2	0.2099 (5)	0.3404 (5)	0.1464 (5)	0.0117 (15)
O1	0.2739 (4)	0.3555 (4)	0.3098 (5)	0.0170 (14)
H1	0.3059	0.3647	0.3559	0.025*
O2	0.1850 (6)	0.4687 (6)	0.3432 (5)	0.0315 (18)
O3	0.1614 (5)	0.3285 (4)	−0.1275 (5)	0.0191 (14)
O4	0.0916 (5)	0.4563 (5)	−0.1268 (5)	0.0221 (15)
O5	0.1938 (4)	0.1458 (4)	0.1461 (5)	0.0177 (14)
O6	0.0627 (5)	0.0860 (5)	0.1274 (5)	0.0221 (15)
O7	0.0051 (5)	0.1854 (6)	0.5920 (5)	0.0281 (17)
O8	0.1335 (4)	0.2552 (5)	0.5835 (5)	0.0215 (15)
O9	0.3709 (5)	0.0809 (4)	0.2010 (4)	0.0189 (14)
H91	0.3827	0.0691	0.2556	0.028*
H92	0.4227	0.0840	0.1790	0.028*
O10	0.4516 (4)	0.2745 (5)	0.2619 (5)	0.0217 (15)
H101	0.4653	0.2877	0.2080	0.033*
H102	0.4887	0.2336	0.2727	0.033*
O11	0.2679 (7)	0.0199 (6)	0.0226 (6)	0.042 (2)
H111	0.2463	0.0571	0.0594	0.063*
H112	0.2823	0.0234	−0.0326	0.063*
O12	0.1257 (6)	−0.0911 (6)	0.0638 (6)	0.041 (2)
H121	0.0724	−0.0900	0.0821	0.061*
H122	0.1146	−0.0831	0.0083	0.061*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Tm1	0.0186 (2)	0.0188 (2)	0.0156 (2)	−0.00011 (16)	−0.00025 (17)	0.00017 (17)
C1	0.006 (4)	0.014 (4)	0.013 (5)	0.002 (3)	−0.006 (3)	0.001 (3)
C2	0.018 (4)	0.014 (4)	0.017 (5)	0.000 (4)	0.004 (4)	−0.006 (4)
C3	0.012 (4)	0.016 (4)	0.019 (4)	0.008 (3)	−0.002 (4)	0.002 (4)
C4	0.011 (4)	0.016 (4)	0.013 (4)	−0.004 (3)	−0.005 (3)	0.001 (3)
C5	0.022 (5)	0.012 (4)	0.017 (5)	0.010 (4)	−0.001 (4)	−0.004 (4)
C6	0.016 (4)	0.015 (4)	0.003 (5)	−0.001 (3)	0.002 (3)	−0.006 (3)
C7	0.017 (5)	0.019 (5)	0.017 (5)	−0.001 (4)	0.001 (4)	−0.009 (4)
C8	0.024 (5)	0.013 (4)	0.003 (4)	0.006 (4)	−0.004 (4)	−0.005 (3)
C9	0.013 (4)	0.010 (4)	0.004 (4)	−0.002 (3)	−0.005 (4)	0.005 (3)
C10	0.016 (4)	0.019 (4)	0.013 (4)	0.000 (3)	−0.002 (4)	−0.002 (4)
C11	0.013 (4)	0.015 (4)	0.021 (5)	0.000 (3)	−0.001 (4)	0.002 (4)
C12	0.012 (4)	0.012 (4)	0.007 (4)	0.005 (3)	0.004 (3)	0.000 (3)
C13	0.016 (4)	0.015 (4)	0.009 (4)	−0.002 (3)	0.000 (3)	−0.003 (3)
C14	0.014 (4)	0.024 (5)	0.011 (5)	0.001 (4)	−0.003 (4)	−0.001 (4)

N1	0.017 (4)	0.017 (4)	0.011 (4)	−0.002 (3)	0.000 (3)	−0.007 (3)
N2	0.015 (4)	0.014 (4)	0.006 (4)	0.003 (3)	−0.002 (3)	0.000 (3)
O1	0.022 (3)	0.015 (3)	0.015 (3)	−0.003 (3)	−0.005 (3)	0.000 (3)
O2	0.047 (5)	0.036 (4)	0.012 (3)	0.021 (4)	−0.004 (3)	−0.005 (3)
O3	0.026 (4)	0.017 (3)	0.014 (3)	0.009 (3)	−0.001 (3)	−0.004 (3)
O4	0.031 (4)	0.022 (4)	0.013 (3)	0.014 (3)	−0.007 (3)	0.000 (3)
O5	0.018 (3)	0.017 (3)	0.018 (4)	−0.003 (3)	0.006 (3)	0.000 (3)
O6	0.019 (3)	0.025 (4)	0.022 (4)	−0.008 (3)	−0.003 (3)	−0.006 (3)
O7	0.030 (4)	0.038 (4)	0.016 (4)	−0.012 (3)	0.007 (3)	−0.007 (3)
O8	0.016 (3)	0.034 (4)	0.015 (3)	−0.008 (3)	0.003 (3)	−0.007 (3)
O9	0.021 (3)	0.022 (3)	0.014 (3)	0.003 (3)	0.007 (3)	0.002 (3)
O10	0.016 (3)	0.032 (4)	0.017 (4)	0.001 (3)	0.001 (3)	−0.001 (3)
O11	0.061 (6)	0.036 (5)	0.029 (4)	0.002 (4)	0.015 (4)	−0.007 (4)
O12	0.044 (5)	0.041 (5)	0.036 (5)	0.019 (4)	0.002 (4)	0.012 (4)

Geometric parameters (Å, º)

Tm1—O1	2.361 (7)	C8—C9	1.529 (13)
Tm1—O8^{i}	2.363 (7)	C9—N1	1.360 (12)
Tm1—O5	2.364 (7)	C9—C10	1.390 (13)
Tm1—O3^{ii}	2.371 (7)	C10—C11	1.347 (15)
Tm1—O10	2.434 (7)	C10—H10A	0.930
Tm1—O9	2.448 (7)	C11—C12	1.438 (13)
Tm1—N2	2.536 (8)	C11—H11A	0.930
Tm1—N1	2.546 (8)	C12—C13	1.363 (13)
C1—N2	1.341 (12)	C12—C14	1.502 (13)
C1—C2	1.381 (13)	C13—N1	1.338 (13)
C1—C6	1.528 (12)	C13—H13A	0.930
C2—C3	1.380 (14)	C14—O7	1.215 (13)
C2—H2A	0.930	C14—O8	1.287 (12)
C3—C4	1.376 (13)	O1—H1	0.850
C3—H3A	0.930	O3—Tm1^{i}	2.371 (7)
C4—C5	1.392 (13)	O8—Tm1^{ii}	2.363 (7)
C4—C7	1.506 (14)	O9—H91	0.850
C5—N2	1.359 (13)	O9—H92	0.850
C5—H5A	0.930	O10—H101	0.850
C6—O2	1.230 (12)	O10—H102	0.850
C6—O1	1.268 (11)	O11—H111	0.850
C7—O4	1.217 (13)	O11—H112	0.850
C7—O3	1.284 (12)	O12—H121	0.850
C8—O6	1.221 (12)	O12—H122	0.850
C8—O5	1.246 (12)		
O1—Tm1—O8^{i}	116.1 (3)	O1—C6—C1	114.3 (8)
O1—Tm1—O5	124.3 (2)	O4—C7—O3	123.6 (9)
O8^{i}—Tm1—O5	83.6 (2)	O4—C7—C4	119.1 (9)
O1—Tm1—O3^{ii}	81.6 (2)	O3—C7—C4	117.4 (9)
O8^{i}—Tm1—O3^{ii}	140.4 (2)	O6—C8—O5	126.0 (9)

O5—Tm1—O3^{ii}	116.7 (2)	O6—C8—C9	118.6 (9)
O1—Tm1—O10	78.6 (2)	O5—C8—C9	115.4 (8)
O8^{i}—Tm1—O10	76.8 (2)	N1—C9—C10	119.8 (9)
O5—Tm1—O10	155.2 (2)	N1—C9—C8	115.0 (8)
O3^{ii}—Tm1—O10	72.4 (2)	C10—C9—C8	125.1 (8)
O1—Tm1—O9	154.7 (2)	C11—C10—C9	121.0 (9)
O8^{i}—Tm1—O9	78.1 (2)	C11—C10—H10A	119.5
O5—Tm1—O9	76.1 (2)	C9—C10—H10A	119.5
O3^{ii}—Tm1—O9	75.0 (2)	C10—C11—C12	120.0 (9)
O10—Tm1—O9	85.1 (2)	C10—C11—H11A	120.0
O1—Tm1—N2	64.7 (2)	C12—C11—H11A	120.0
O8^{i}—Tm1—N2	73.3 (3)	C13—C12—C11	114.9 (8)
O5—Tm1—N2	74.1 (3)	C13—C12—C14	124.1 (8)
O3^{ii}—Tm1—N2	142.5 (2)	C11—C12—C14	120.9 (8)
O10—Tm1—N2	113.6 (3)	N1—C13—C12	125.9 (9)
O9—Tm1—N2	140.5 (2)	N1—C13—H13A	117.0
O1—Tm1—N1	73.5 (3)	C12—C13—H13A	117.0
O8^{i}—Tm1—N1	144.7 (3)	O7—C14—O8	124.5 (9)
O5—Tm1—N1	65.1 (3)	O7—C14—C12	120.7 (9)
O3^{ii}—Tm1—N1	72.3 (3)	O8—C14—C12	114.8 (8)
O10—Tm1—N1	137.5 (3)	C13—N1—C9	118.3 (8)
O9—Tm1—N1	107.7 (2)	C13—N1—Tm1	124.2 (6)
N2—Tm1—N1	82.3 (3)	C9—N1—Tm1	116.5 (7)
N2—C1—C2	121.0 (8)	C1—N2—C5	118.3 (8)
N2—C1—C6	114.9 (7)	C1—N2—Tm1	117.5 (6)
C2—C1—C6	124.0 (8)	C5—N2—Tm1	124.2 (6)
C3—C2—C1	119.9 (8)	C6—O1—Tm1	126.0 (6)
C3—C2—H2A	120.0	C6—O1—H1	117.1
C1—C2—H2A	120.0	Tm1—O1—H1	116.9
C4—C3—C2	120.4 (8)	C7—O3—Tm1^{i}	141.4 (6)
C4—C3—H3A	119.8	C8—O5—Tm1	127.5 (6)
C2—C3—H3A	119.8	C14—O8—Tm1^{ii}	136.9 (6)
C3—C4—C5	116.5 (8)	Tm1—O9—H91	97.2
C3—C4—C7	124.0 (9)	Tm1—O9—H92	113.8
C5—C4—C7	119.5 (8)	H91—O9—H92	100.6
N2—C5—C4	123.6 (8)	Tm1—O10—H101	95.7
N2—C5—H5A	118.2	Tm1—O10—H102	115.4
C4—C5—H5A	118.2	H101—O10—H102	100.8
O2—C6—O1	126.8 (8)	H111—O11—H112	132.5
O2—C6—C1	119.0 (8)	H121—O12—H122	96.9

N2—C1—C2—C3	−4.1 (14)	O3^{ii}—Tm1—N1—C9	−127.0 (7)
C6—C1—C2—C3	173.5 (8)	O10—Tm1—N1—C9	−162.2 (6)
C1—C2—C3—C4	2.0 (14)	O9—Tm1—N1—C9	−59.8 (7)
C2—C3—C4—C5	2.3 (13)	N2—Tm1—N1—C9	80.9 (6)
C2—C3—C4—C7	−176.5 (9)	C2—C1—N2—C5	1.6 (13)
C3—C4—C5—N2	−5.0 (14)	C6—C1—N2—C5	−176.2 (8)
C7—C4—C5—N2	173.9 (9)	C2—C1—N2—Tm1	179.9 (7)

N2—C1—C6—O2	−170.7 (9)	C6—C1—N2—Tm1	2.1 (10)
C2—C1—C6—O2	11.5 (14)	C4—C5—N2—C1	3.1 (14)
N2—C1—C6—O1	10.3 (11)	C4—C5—N2—Tm1	−175.1 (7)
C2—C1—C6—O1	−167.5 (8)	O1—Tm1—N2—C1	−7.8 (6)
C3—C4—C7—O4	0.1 (14)	O8^{i}—Tm1—N2—C1	−138.3 (7)
C5—C4—C7—O4	−178.7 (9)	O5—Tm1—N2—C1	133.7 (7)
C3—C4—C7—O3	178.9 (9)	O3^{ii}—Tm1—N2—C1	20.3 (9)
C5—C4—C7—O3	0.2 (13)	O10—Tm1—N2—C1	−71.3 (7)
O6—C8—C9—N1	−172.2 (8)	O9—Tm1—N2—C1	176.1 (6)
O5—C8—C9—N1	7.3 (11)	N1—Tm1—N2—C1	67.5 (7)
O6—C8—C9—C10	10.7 (13)	O1—Tm1—N2—C5	170.3 (8)
O5—C8—C9—C10	−169.9 (9)	O8^{i}—Tm1—N2—C5	39.8 (8)
N1—C9—C10—C11	−2.3 (13)	O5—Tm1—N2—C5	−48.2 (8)
C8—C9—C10—C11	174.7 (8)	O3^{ii}—Tm1—N2—C5	−161.6 (7)
C9—C10—C11—C12	2.3 (14)	O10—Tm1—N2—C5	106.8 (8)
C10—C11—C12—C13	−0.2 (13)	O9—Tm1—N2—C5	−5.7 (10)
C10—C11—C12—C14	−177.1 (9)	N1—Tm1—N2—C5	−114.3 (8)
C11—C12—C13—N1	−2.1 (14)	O2—C6—O1—Tm1	161.1 (8)
C14—C12—C13—N1	174.7 (9)	C1—C6—O1—Tm1	−20.0 (11)
C13—C12—C14—O7	178.6 (9)	O8^{i}—Tm1—O1—C6	69.8 (7)
C11—C12—C14—O7	−4.8 (14)	O5—Tm1—O1—C6	−30.8 (8)
C13—C12—C14—O8	−1.2 (13)	O3^{ii}—Tm1—O1—C6	−147.5 (7)
C11—C12—C14—O8	175.4 (8)	O10—Tm1—O1—C6	138.9 (7)
C12—C13—N1—C9	2.2 (14)	O9—Tm1—O1—C6	−170.2 (6)
C12—C13—N1—Tm1	−166.1 (7)	N2—Tm1—O1—C6	15.6 (7)
C10—C9—N1—C13	0.1 (13)	N1—Tm1—O1—C6	−73.6 (7)
C8—C9—N1—C13	−177.2 (8)	O4—C7—O3—Tm1^{i}	14.3 (17)
C10—C9—N1—Tm1	169.3 (6)	C4—C7—O3—Tm1^{i}	−164.4 (7)
C8—C9—N1—Tm1	−8.0 (9)	O6—C8—O5—Tm1	176.6 (7)
O1—Tm1—N1—C13	−44.8 (7)	C9—C8—O5—Tm1	−2.8 (11)
O8^{i}—Tm1—N1—C13	−156.8 (7)	O1—Tm1—O5—C8	−46.8 (8)
O5—Tm1—N1—C13	173.4 (8)	O8^{i}—Tm1—O5—C8	−164.2 (8)
O3^{ii}—Tm1—N1—C13	41.5 (7)	O3^{ii}—Tm1—O5—C8	51.6 (8)
O10—Tm1—N1—C13	6.3 (9)	O10—Tm1—O5—C8	158.1 (7)
O9—Tm1—N1—C13	108.7 (7)	O9—Tm1—O5—C8	116.5 (8)
N2—Tm1—N1—C13	−110.6 (8)	N2—Tm1—O5—C8	−89.7 (7)
O1—Tm1—N1—C9	146.7 (7)	N1—Tm1—O5—C8	−0.9 (7)
O8^{i}—Tm1—N1—C9	34.7 (9)	O7—C14—O8—Tm1^{ii}	23.9 (16)
O5—Tm1—N1—C9	4.9 (6)	C12—C14—O8—Tm1^{ii}	−156.4 (6)

Symmetry codes: (i) −*x*+1/2, −*y*+1/2, *z*−1/2; (ii) −*x*+1/2, −*y*+1/2, *z*+1/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O12^{iii}	0.85	1.97	2.788 (11)	162
O9—H91···O4^{ii}	0.85	1.83	2.679 (10)	180
O9—H92···O4^{iv}	0.85	1.99	2.842 (10)	180

O10—H101···O7^{i}	0.85	1.83	2.675 (11)	179
O10—H102···O9^{iii}	0.85	2.14	2.996 (10)	179
O11—H111···O5	0.85	2.02	2.872 (11)	179
O11—H112···O2^{i}	0.85	1.91	2.763 (11)	180
O12—H121···O6^{v}	0.85	2.15	3.004 (12)	179
O12—H122···O6^{vi}	0.85	2.08	2.933 (12)	179

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