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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^2O,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^2O,O')zinc(II)	Chen (2006)	Journal	10.1107/S1600536805040432	SAZCUS
Bis(2-formylphenolato-κ^2O,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^2O,O')manganese(II)	Wang & Fang (2006)	Journal	10.1107/S1600536806021039	IDOVED
Tetraaqua(1,10-phenanthroline-κ^2N,N')copper(II) naphthalene-1,5-disulfonate dihydrate	Liu *et al.* (2006)	Author	10.1107/S1600536806030637	GENYOO
Tetraaqua(1,10-phenanthroline-κ^2N,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^2O,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-1$\kappa^4O^1,O^{1'},O^6,O^{6'}$:2$\kappa^4O^1,N,N',O^{1'}$}(methanol-1κO)-μ-nitrato-1:2κ^2O:O′-dinitrato-1κ^4O,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^2N^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^2N,N')bis(nitrato-κO)zinc(II)	Liu, Zeng & Chen (2007)	Author	10.1107/S1600536807042390	XIKYEW
[N,N′-(o-Phenylene)bis(picolinamido)-κ^4N,N',N'',N''']cobalt(II)	Liu & Zeng (2007*a*)	Author	10.1107/S1600536807044571	XILFII
[N,N′-(o-Phenylene)dipicolinamide-κ^4N]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^2N,N')(3,5-dinitro-2-oxidobenzoato-κ^2O^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

 doi:10.1107/S1600536809054300

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-dinitratoholmium(III)zinc(II)

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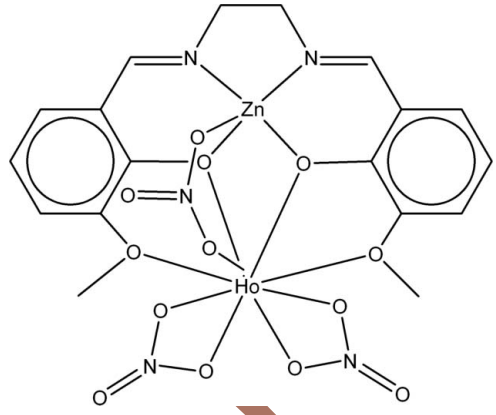
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.008 Å; R factor = 0.034; wR factor = 0.094; data-to-parameter ratio = 13.0.

In the title heteronuclear Zn^{II}–Ho^{III} complex (systematic name: {μ-6,6′-dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato-1$\kappa^4O^1,O^{1'},O^6,O^{6'}$:2$\kappa^4O^1,N,N',O^{1'}$)-μ-nitrato-1:2$\kappa^2O$:$O'$-dinitrato-1$\kappa^4O,O'$-holmium(III)zinc(II)), $[HoZn(C_{18}H_{18}N_2O_4)(NO_3)_3]$, with the hexadentate Schiff base compartmental ligand N,N'-bis(3-methoxysalicylidene)ethylenediamine (H_2L), the Ho 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 Ho^{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 double-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

$[HoZn(C_{18}H_{18}N_2O_4)(NO_3)_3]$
M_r = 742.67
Monoclinic, $P2_1/n$
a = 10.694 (4) Å
b = 16.481 (7) Å
c = 14.921 (6) Å
β = 99.667 (6)°
V = 2592.4 (18) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 4.03 mm^{-1}
T = 293 (2) K
0.16 × 0.16 × 0.10 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.565, T_{max} = 0.689
15217 measured reflections
4499 independent reflections
3377 reflections with $I > 2\sigma(I)$
R_{int} = 0.037

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.093
S = 1.02
4499 reflections
345 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.60 e Å^{-3}
$\Delta\rho_{min}$ = −1.18 e Å^{-3}

Table 1
Selected bond lengths (Å).

Ho1—O1	2.293 (3)	Ho1—O11	2.430 (4)
Ho1—O2	2.298 (3)	Ho1—O12	2.468 (4)
Ho1—O3	2.604 (4)	Zn1—O1	2.005 (4)
Ho1—O4	2.604 (4)	Zn1—O2	2.022 (3)
Ho1—O6	2.323 (4)	Zn1—O5	1.979 (4)
Ho1—O8	2.448 (4)	Zn1—N1	2.047 (4)
Ho1—O9	2.481 (4)	Zn1—N2	2.021 (5)

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	3.377 (7)	174
C10—H10A···O13^{ii}	0.97	2.54	3.483 (8)	165

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

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: AT2567).

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supporting information

Acta Cryst. (2008). E**64**, m804–m805 [doi:10.1107/S1600536808013743]

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

Yi-An Xiao, Yan Sui, Xiu-Guang Yi, Jian-Hong Wu and Li-Ping Zhang

S1. 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 3d-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 3d-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}—Ho^{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 holmium 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 holmium(III) is present in the open and larger portion of the dinucleating compartmental Schiff base ligand.

The Ho^{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 Ho—O bond distances are significantly different, the longest being the Ho—*O* (methoxy) separations and the shortest being the Ho—O (phenolate).

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 0.6067 (4) Å below the mean N_2O_2 plane with an average deviation from the plane of 0.0380 (3) Å, which construct the bottom of square-pyramid. The Zn—O5 (bridging nitrate) separation is 1.979 (4) Å and the angles of this Zn—O vector with the Zn—N or Zn—O bonds lie between 102.5 (4)° and 112.6 (4)°, 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} = 3.377 (7) Å and C10(H10A)···O13^{ii} = 3.483 (8) Å; symmetry codes: (i) -1/2 + *x*, 1/2 - *y*, 1/2 + *z*; (ii) 1 - *x*, -*y*, 2 - *z*]. These link the molecules into a two-dimensional double layer structure (Fig 2).

S2. 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 holmium(III) nitrate hexahydrate (0.459 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 $C_{18}H_{18}HoN_5O_{13}Zn$: C 29.11 H 2.44, Ho 22.21, N 9.43, Zn 8.80%; found: C 29.20, H 2.45, Ho 22.30, N 9.50, Zn 8.90%. IR (KBr, cm^{-1}): 1640 (C=N), 1386,1490 (nitrate).

S3. Refinement

The H atoms were positioned geometrically and treated as riding on their parent atoms, with C—H distances of 0.93 (aromatic), 0.97 (methylene) and 0.96 Å (methyl), 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 N3, O5 and O6 are enforced to be the same.

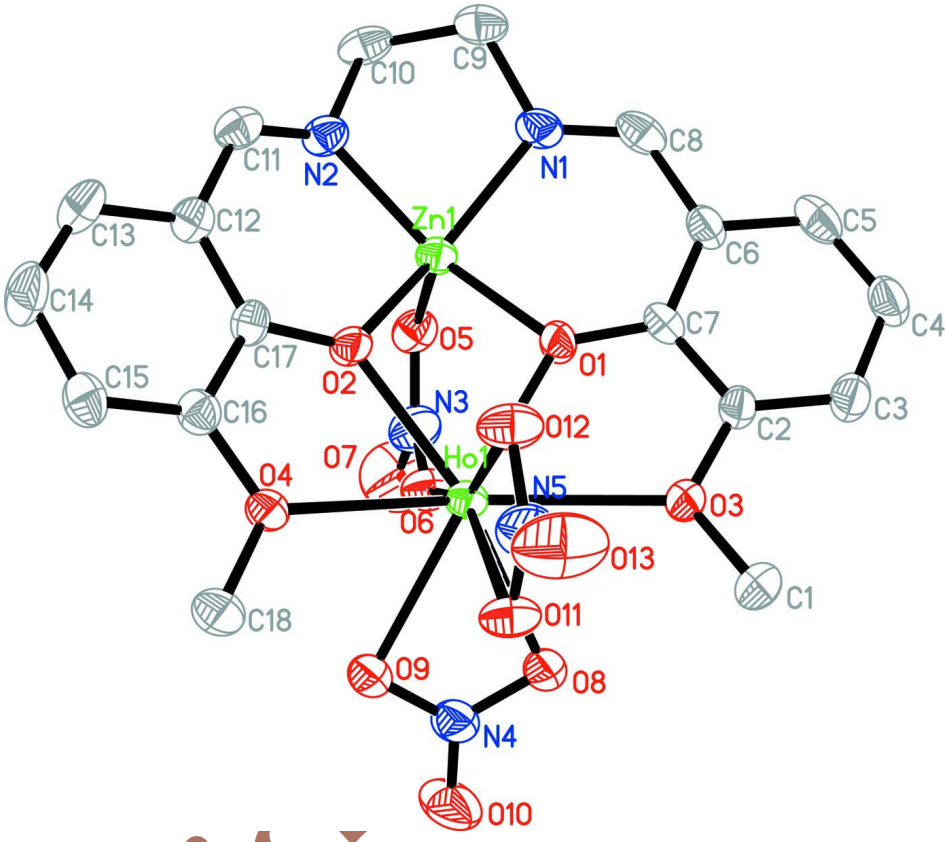

Figure 1

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

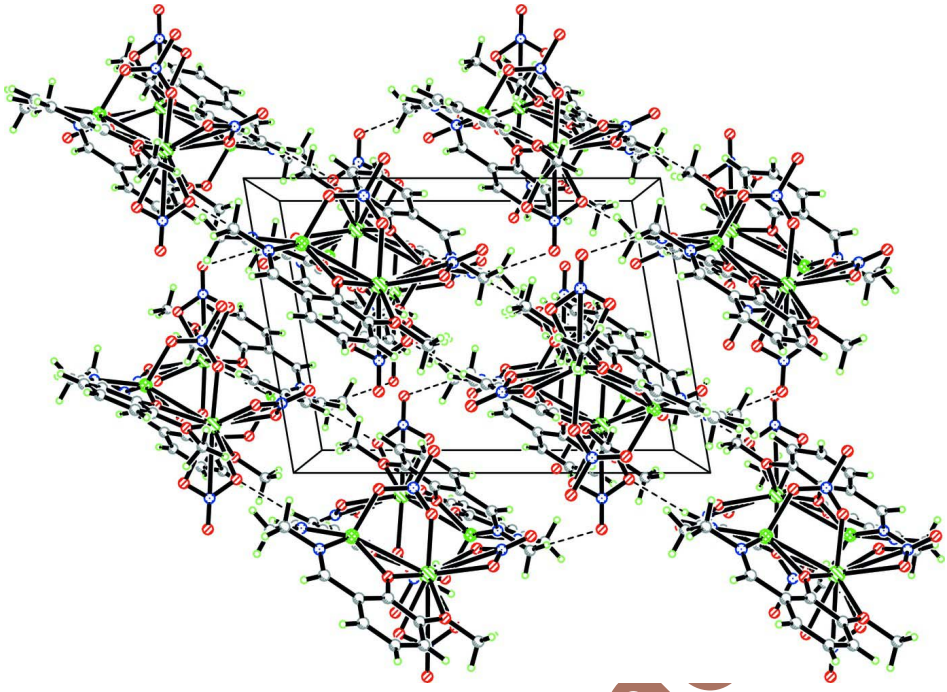

Figure 2

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

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

Crystal data

[HoZn($C_{18}H_{18}N_2O_4$)(NO_3)$_3$]
M_r = 742.67
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 10.694 (4) Å
b = 16.481 (7) Å
c = 14.921 (6) Å
β = 99.667 (6)°
V = 2592.4 (18) Å^3
Z = 4
F(000) = 1448
D_x = 1.903 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5632 reflections
θ = 2.2–25.3°
μ = 4.03 mm^{-1}
T = 293 K
Block, yellow
0.16 × 0.16 × 0.10 mm

Data collection

Bruker APEXII area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.565, T_{max} = 0.689
15217 measured reflections
4499 independent reflections
3377 reflections with $I > 2\sigma(I)$
R_{int} = 0.037
θ_{max} = 25.0°, θ_{min} = 2.2°
h = −12→12
k = −19→19
l = −17→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.093$
$S = 1.02$
4499 reflections
345 parameters
2 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
$w = 1/[\sigma^2(F_o^2) + (0.0558P)^2 + 0.1192P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.61$ e Å^{-3}
$\Delta\rho_{min} = -1.18$ e Å^{-3}

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ho1	0.36187 (2)	0.109293 (15)	0.723858 (16)	0.04439 (11)
Zn1	0.21999 (6)	0.03550 (4)	0.88927 (4)	0.04303 (17)
O1	0.2906 (4)	0.1419 (2)	0.8559 (2)	0.0493 (9)
O12	0.5712 (4)	0.1290 (3)	0.8198 (3)	0.0640 (12)
O2	0.3521 (4)	−0.0016 (2)	0.8158 (2)	0.0497 (9)
O4	0.4894 (3)	−0.0201 (2)	0.6956 (2)	0.0495 (9)
C17	0.4119 (5)	−0.0722 (3)	0.8204 (3)	0.0413 (12)
O8	0.2843 (4)	0.1975 (2)	0.5945 (2)	0.0582 (10)
N4	0.2806 (5)	0.1437 (3)	0.5329 (4)	0.0624 (14)
O6	0.1491 (4)	0.0740 (3)	0.6881 (3)	0.0613 (11)
C3	0.2935 (6)	0.3590 (4)	0.8767 (4)	0.0567 (15)
H3	0.3175	0.4036	0.8452	0.068*
N5	0.6224 (5)	0.1590 (4)	0.7564 (4)	0.0659 (15)
O5	0.0581 (3)	0.0283 (2)	0.8031 (3)	0.0543 (10)
C16	0.4896 (5)	−0.0846 (3)	0.7542 (4)	0.0460 (13)
O9	0.3274 (4)	0.0751 (3)	0.5596 (3)	0.0624 (11)
C2	0.3092 (5)	0.2813 (3)	0.8465 (3)	0.0448 (13)
C12	0.4039 (5)	−0.1325 (3)	0.8854 (4)	0.0457 (13)
N3	0.0556 (5)	0.0490 (3)	0.7206 (4)	0.0695 (14)
O11	0.5537 (4)	0.1634 (3)	0.6792 (3)	0.0612 (11)
O10	0.2350 (6)	0.1567 (3)	0.4552 (3)	0.107 (2)
N1	0.1978 (4)	0.0839 (3)	1.0120 (3)	0.0506 (12)
N2	0.2494 (4)	−0.0675 (3)	0.9634 (3)	0.0488 (11)
C11	0.3278 (5)	−0.1246 (4)	0.9578 (4)	0.0513 (15)
H11	0.3374	−0.1641	1.0030	0.062*

C7	0.2716 (5)	0.2135 (3)	0.8916 (3)	0.0428 (12)
C8	0.1985 (5)	0.1588 (4)	1.0310 (4)	0.0573 (16)
H8	0.1823	0.1728	1.0884	0.069*
C10	0.1754 (6)	−0.0615 (4)	1.0385 (4)	0.0590 (16)
H10A	0.2017	−0.1037	1.0830	0.071*
H10B	0.0859	−0.0688	1.0151	0.071*
C6	0.2222 (5)	0.2248 (3)	0.9720 (4)	0.0500 (14)
C18	0.5665 (6)	−0.0292 (4)	0.6251 (4)	0.0638 (17)
H18A	0.6543	−0.0328	0.6524	0.096*
H18B	0.5544	0.0168	0.5852	0.096*
H18C	0.5421	−0.0777	0.5910	0.096*
C5	0.2056 (6)	0.3045 (4)	1.0014 (4)	0.0631 (17)
H5	0.1699	0.3130	1.0533	0.076*
O13	0.7311 (5)	0.1830 (4)	0.7710 (4)	0.112 (2)
C4	0.2412 (7)	0.3697 (4)	0.9550 (4)	0.0643 (18)
H4	0.2302	0.4219	0.9762	0.077*
C15	0.5530 (6)	−0.1572 (4)	0.7500 (4)	0.0569 (15)
H15	0.6023	−0.1659	0.7052	0.068*
C9	0.1972 (6)	0.0203 (4)	1.0823 (4)	0.0612 (17)
H9A	0.1307	0.0317	1.1174	0.073*
H9B	0.2777	0.0205	1.1234	0.073*
C14	0.5419 (6)	−0.2169 (4)	0.8140 (5)	0.0701 (19)
H14	0.5833	−0.2662	0.8113	0.084*
C13	0.4716 (6)	−0.2043 (4)	0.8802 (4)	0.0623 (17)
H13	0.4683	−0.2446	0.9235	0.075*
O7	−0.0708 (6)	0.0407 (5)	0.6557 (5)	0.142 (3)
O3	0.3629 (4)	0.2616 (2)	0.7706 (2)	0.0502 (9)
C1	0.4246 (7)	0.3260 (4)	0.7307 (4)	0.0661 (17)
H1A	0.3638	0.3673	0.7090	0.099*
H1B	0.4611	0.3051	0.6808	0.099*
H1C	0.4903	0.3486	0.7755	0.099*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ho1	0.05102 (19)	0.04515 (17)	0.04112 (16)	0.00162 (12)	0.01960 (11)	0.00255 (11)
Zn1	0.0470 (4)	0.0447 (4)	0.0411 (3)	−0.0003 (3)	0.0182 (3)	0.0028 (3)
O1	0.067 (3)	0.036 (2)	0.052 (2)	−0.0004 (19)	0.034 (2)	−0.0054 (18)
O12	0.050 (2)	0.091 (3)	0.053 (2)	−0.010 (2)	0.0144 (19)	0.013 (2)
O2	0.064 (3)	0.042 (2)	0.051 (2)	0.0077 (19)	0.0327 (19)	0.0102 (17)
O4	0.060 (2)	0.048 (2)	0.047 (2)	0.0107 (19)	0.0264 (18)	0.0023 (18)
C17	0.035 (3)	0.037 (3)	0.051 (3)	0.003 (2)	0.006 (2)	0.000 (3)
O8	0.081 (3)	0.049 (2)	0.045 (2)	0.013 (2)	0.014 (2)	0.0020 (19)
N4	0.076 (4)	0.063 (3)	0.053 (3)	0.018 (3)	0.024 (3)	0.004 (3)
O6	0.058 (3)	0.074 (3)	0.052 (2)	−0.010 (2)	0.0101 (18)	0.007 (2)
C3	0.068 (4)	0.039 (3)	0.060 (4)	0.001 (3)	0.003 (3)	0.001 (3)
N5	0.056 (4)	0.079 (4)	0.068 (4)	−0.008 (3)	0.024 (3)	0.003 (3)
O5	0.047 (2)	0.055 (2)	0.064 (2)	−0.0028 (19)	0.0182 (19)	0.0082 (19)

C16	0.044 (3)	0.047 (3)	0.048 (3)	0.004 (3)	0.010 (2)	−0.002 (3)
O9	0.088 (3)	0.055 (3)	0.047 (2)	0.015 (2)	0.021 (2)	0.000 (2)
C2	0.053 (3)	0.035 (3)	0.045 (3)	0.003 (3)	0.004 (2)	−0.001 (2)
C12	0.041 (3)	0.044 (3)	0.053 (3)	−0.002 (3)	0.009 (3)	0.002 (3)
N3	0.065 (3)	0.072 (4)	0.072 (3)	−0.007 (3)	0.015 (3)	0.010 (3)
O11	0.060 (3)	0.079 (3)	0.048 (2)	−0.007 (2)	0.021 (2)	0.014 (2)
O10	0.154 (5)	0.118 (5)	0.043 (3)	0.058 (4)	0.003 (3)	0.004 (3)
N1	0.052 (3)	0.062 (3)	0.044 (3)	−0.005 (2)	0.024 (2)	−0.001 (2)
N2	0.047 (3)	0.052 (3)	0.049 (3)	0.001 (2)	0.015 (2)	0.010 (2)
C11	0.049 (4)	0.053 (4)	0.050 (3)	−0.007 (3)	0.003 (3)	0.011 (3)
C7	0.043 (3)	0.049 (3)	0.037 (3)	−0.001 (3)	0.008 (2)	−0.012 (3)
C8	0.055 (4)	0.078 (5)	0.044 (3)	0.000 (3)	0.025 (3)	−0.013 (3)
C10	0.056 (4)	0.070 (4)	0.055 (3)	−0.006 (3)	0.021 (3)	0.024 (3)
C6	0.058 (4)	0.048 (3)	0.045 (3)	0.001 (3)	0.012 (3)	−0.013 (3)
C18	0.071 (4)	0.068 (4)	0.063 (4)	0.011 (3)	0.040 (3)	0.003 (3)
C5	0.069 (4)	0.072 (5)	0.051 (3)	0.010 (4)	0.016 (3)	−0.022 (3)
O13	0.064 (3)	0.173 (6)	0.100 (4)	−0.036 (4)	0.021 (3)	0.026 (4)
C4	0.085 (5)	0.051 (4)	0.056 (4)	0.013 (4)	0.009 (3)	−0.016 (3)
C15	0.053 (4)	0.055 (4)	0.065 (4)	0.014 (3)	0.018 (3)	−0.007 (3)
C9	0.065 (4)	0.077 (5)	0.046 (3)	0.000 (3)	0.023 (3)	0.007 (3)
C14	0.067 (4)	0.046 (4)	0.102 (5)	0.021 (3)	0.025 (4)	0.006 (4)
C13	0.062 (4)	0.045 (4)	0.080 (4)	0.009 (3)	0.013 (3)	0.020 (3)
O7	0.099 (5)	0.175 (7)	0.138 (6)	−0.011 (5)	−0.026 (4)	−0.001 (5)
O3	0.067 (3)	0.038 (2)	0.049 (2)	−0.0051 (19)	0.0216 (18)	0.0003 (18)
C1	0.092 (5)	0.048 (4)	0.063 (4)	−0.013 (4)	0.026 (3)	0.005 (3)

Geometric parameters (Å, º)

Ho1—O1	2.293 (3)	C2—C7	1.398 (7)
Ho1—O2	2.298 (3)	C12—C13	1.396 (8)
Ho1—O3	2.604 (4)	C12—C11	1.463 (8)
Ho1—O4	2.604 (4)	N3—O7	1.531 (8)
Ho1—O6	2.323 (4)	N1—C8	1.267 (8)
Ho1—O8	2.448 (4)	N1—C9	1.484 (7)
Ho1—O9	2.481 (4)	N2—C11	1.273 (7)
Ho1—O11	2.430 (4)	N2—C10	1.480 (6)
Ho1—O12	2.468 (4)	C11—H11	0.9300
Zn1—O1	2.005 (4)	C7—C6	1.401 (7)
Zn1—O2	2.022 (3)	C8—C6	1.449 (8)
Zn1—O5	1.979 (4)	C8—H8	0.9300
Zn1—N1	2.047 (4)	C10—C9	1.498 (9)
Zn1—N2	2.021 (5)	C10—H10A	0.9700
O1—C7	1.324 (6)	C10—H10B	0.9700
O12—N5	1.269 (6)	C6—C5	1.406 (8)
O2—C17	1.325 (6)	C18—H18A	0.9600
O4—C16	1.376 (6)	C18—H18B	0.9600
O4—C18	1.449 (6)	C18—H18C	0.9600
C17—C12	1.402 (7)	C5—C4	1.367 (9)

C17—C16	1.408 (7)	C5—H5	0.9300
O8—N4	1.273 (6)	C4—H4	0.9300
N4—O10	1.199 (6)	C15—C14	1.390 (9)
N4—O9	1.272 (6)	C15—H15	0.9300
O6—N3	1.251 (6)	C9—H9A	0.9700
C3—C2	1.379 (8)	C9—H9B	0.9700
C3—C4	1.389 (9)	C14—C13	1.355 (9)
C3—H3	0.9300	C14—H14	0.9300
N5—O13	1.213 (7)	C13—H13	0.9300
N5—O11	1.260 (6)	O3—C1	1.431 (6)
O5—N3	1.274 (6)	C1—H1A	0.9600
C16—C15	1.382 (8)	C1—H1B	0.9600
C2—O3	1.390 (6)	C1—H1C	0.9600

O1—Ho1—O2	67.54 (12)	C15—C16—C17	120.6 (5)
O1—Ho1—O6	78.56 (14)	N4—O9—Ho1	95.4 (3)
O2—Ho1—O6	78.26 (14)	C3—C2—O3	124.9 (5)
O1—Ho1—O11	124.55 (14)	C3—C2—C7	121.6 (5)
O2—Ho1—O11	125.51 (14)	O3—C2—C7	113.4 (4)
O6—Ho1—O11	150.31 (13)	C13—C12—C17	118.0 (5)
O1—Ho1—O8	114.92 (13)	C13—C12—C11	118.3 (5)
O2—Ho1—O8	154.15 (14)	C17—C12—C11	123.7 (5)
O6—Ho1—O8	77.22 (14)	O6—N3—O5	125.0 (5)
O11—Ho1—O8	75.84 (14)	O6—N3—O7	117.5 (5)
O1—Ho1—O12	82.58 (14)	O5—N3—O7	117.4 (5)
O2—Ho1—O12	83.46 (14)	N5—O11—Ho1	96.7 (3)
O6—Ho1—O12	157.61 (13)	C8—N1—C9	122.1 (5)
O11—Ho1—O12	52.07 (13)	C8—N1—Zn1	125.6 (4)
O8—Ho1—O12	122.24 (14)	C9—N1—Zn1	111.8 (4)
O1—Ho1—O9	152.44 (15)	C11—N2—C10	122.7 (5)
O2—Ho1—O9	113.29 (14)	C11—N2—Zn1	129.0 (4)
O6—Ho1—O9	74.88 (14)	C10—N2—Zn1	107.7 (4)
O11—Ho1—O9	78.74 (14)	N2—C11—C12	124.6 (5)
O8—Ho1—O9	51.77 (13)	N2—C11—H11	117.7
O12—Ho1—O9	124.92 (14)	C12—C11—H11	117.7
O1—Ho1—O4	126.16 (12)	O1—C7—C2	116.2 (4)
O2—Ho1—O4	61.54 (11)	O1—C7—C6	124.6 (5)
O6—Ho1—O4	106.10 (14)	C2—C7—C6	119.1 (5)
O11—Ho1—O4	76.52 (13)	N1—C8—C6	126.2 (5)
O8—Ho1—O4	118.41 (12)	N1—C8—H8	116.9
O12—Ho1—O4	75.69 (14)	C6—C8—H8	116.9
O9—Ho1—O4	69.45 (12)	N2—C10—C9	109.0 (5)
O1—Ho1—O3	62.03 (12)	N2—C10—H10A	109.9
O2—Ho1—O3	127.20 (12)	C9—C10—H10A	109.9
O6—Ho1—O3	105.25 (14)	N2—C10—H10B	109.9
O11—Ho1—O3	75.75 (13)	C9—C10—H10B	109.9
O8—Ho1—O3	67.95 (12)	H10A—C10—H10B	108.3
O12—Ho1—O3	75.82 (14)	C7—C6—C5	118.5 (6)

O9—Ho1—O3	118.46 (12)	C7—C6—C8	123.4 (5)
O4—Ho1—O3	148.63 (12)	C5—C6—C8	117.8 (5)
O5—Zn1—O1	102.49 (16)	O4—C18—H18A	109.5
O5—Zn1—N2	110.09 (18)	O4—C18—H18B	109.5
O1—Zn1—N2	147.12 (18)	H18A—C18—H18B	109.5
O5—Zn1—O2	104.16 (16)	O4—C18—H18C	109.5
O1—Zn1—O2	78.64 (14)	H18A—C18—H18C	109.5
N2—Zn1—O2	89.09 (16)	H18B—C18—H18C	109.5
O5—Zn1—N1	112.60 (18)	C4—C5—C6	121.1 (6)
O1—Zn1—N1	89.23 (17)	C4—C5—H5	119.5
N2—Zn1—N1	82.44 (19)	C6—C5—H5	119.5
O2—Zn1—N1	143.00 (18)	C5—C4—C3	120.8 (6)
C7—O1—Zn1	126.1 (3)	C5—C4—H4	119.6
C7—O1—Ho1	130.6 (3)	C3—C4—H4	119.6
Zn1—O1—Ho1	101.65 (15)	C16—C15—C14	118.9 (6)
N5—O12—Ho1	94.7 (3)	C16—C15—H15	120.5
C17—O2—Zn1	127.8 (3)	C14—C15—H15	120.5
C17—O2—Ho1	131.3 (3)	N1—C9—C10	110.3 (5)
Zn1—O2—Ho1	100.93 (15)	N1—C9—H9A	109.6
C16—O4—C18	116.2 (4)	C10—C9—H9A	109.6
C16—O4—Ho1	118.3 (3)	N1—C9—H9B	109.6
C18—O4—Ho1	125.5 (3)	C10—C9—H9B	109.6
O2—C17—C12	125.0 (5)	H9A—C9—H9B	108.1
O2—C17—C16	115.3 (5)	C13—C14—C15	121.0 (6)
C12—C17—C16	119.7 (5)	C13—C14—H14	119.5
N4—O8—Ho1	96.9 (3)	C15—C14—H14	119.5
O10—N4—O9	122.4 (5)	C14—C13—C12	121.8 (6)
O10—N4—O8	122.1 (5)	C14—C13—H13	119.1
O9—N4—O8	115.4 (5)	C12—C13—H13	119.1
N3—O6—Ho1	144.0 (4)	C2—O3—C1	116.6 (4)
C2—C3—C4	118.8 (6)	C2—O3—Ho1	117.3 (3)
C2—C3—H3	120.6	C1—O3—Ho1	125.8 (3)
C4—C3—H3	120.6	O3—C1—H1A	109.5
O13—N5—O11	122.6 (5)	O3—C1—H1B	109.5
O13—N5—O12	120.9 (6)	H1A—C1—H1B	109.5
O11—N5—O12	116.5 (5)	O3—C1—H1C	109.5
N3—O5—Zn1	119.1 (3)	H1A—C1—H1C	109.5
O4—C16—C15	126.0 (5)	H1B—C1—H1C	109.5
O4—C16—C17	113.3 (5)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1*B*···O11	0.96	2.54	3.167 (8)	123
C5—H5···O11^{i}	0.93	2.45	3.377 (7)	174

C10—H10*A*···O13^{ii}	0.97	2.54	3.483 (8)	165
C18—H18*B*···O9	0.96	2.58	3.100 (8)	114

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