Acta Crystallographica Section E
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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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{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-1$\kappa O$)-$\mu$-nitrato-1:2$\kappa^2O$:$O'$-dinitrato-1$\kappa^4O,O'$-samarium(III)zinc(II)

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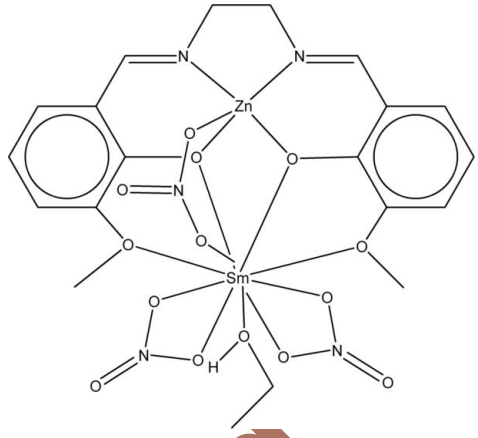
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.006 Å; R factor = 0.027; wR factor = 0.079; data-to-parameter ratio = 12.6.

In the title heteronuclear Zn^{II}–Sm^{III} complex, $[SmZn(C_{18}H_{18}N_2O_4)(NO_3)_3(CH_3CH_2OH)]$, with the hexadentate Schiff base compartmental ligand N,N'-bis(3-methoxysalicylidene)ethylenediamine (H_2L), the Sm^{III} and Zn^{II} ions are triply bridged by two phenolate O atoms from the Schiff base ligand and one nitrate anion. The five-coordinate Zn^{II} ion is in a square-pyramidal geometry formed by the donor centers of two imine N atoms, two phenolate O atoms and one of the bridging nitrate O atoms. The Sm^{III} center is in a ten-fold coordination of O atoms, involving the phenolate O atoms, two methoxy O atoms, one ethanol O atom, and two O atoms from two nitrate anions and one from the bridging nitrate anion. In the crystal, intermolecular O—H···O and C—H···O interactions generate a layer structure extending parallel to (101).

Related literature

For the preparation, magnetic and optical properties of 3*d*-4*f* hetorometallic dinuclear complexes, see: Baggio *et al.* (2000); Caravan *et al.* (1999); Edder *et al.* (2000); Knoer *et al.* (2005).



Experimental

Crystal data

$[SmZn(C_{18}H_{18}N_2O_4)(NO_3)_3(C_2H_6O)]$
M_r = 774.16
Monoclinic, $P2_1/n$
a = 9.975 (3) Å
b = 13.780 (4) Å
c = 19.889 (6) Å
β = 91.745 (4)°
V = 2732.4 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 3.08 mm^{-1}
T = 293 K
0.26 × 0.23 × 0.19 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.501, T_{max} = 0.592
16112 measured reflections
4741 independent reflections
4175 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.079
S = 1.08
4741 reflections
377 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.67 e Å^{-3}
$\Delta\rho_{min}$ = −0.70 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C18—H18B···O9	0.96	2.52	3.237 (6)	132
O14—H14S···O6^{i}	0.855 (19)	1.87 (2)	2.718 (4)	171 (5)
C8—H8···O11^{ii}	0.93	2.55	3.440 (5)	160

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXL97*; software used to prepare material for publication: *SHELXL97* and *publCIF* (Westrip, 2009).

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Province of China (2008GQC0002).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2862).

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supporting information

Acta Cryst. (2009). E**65**, m1161–m1162 [doi:10.1107/S1600536809033558]

{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-1$\kappa O$)-$\mu$-nitrato-1:2$\kappa^2O$:$O'$-dinitrato-1$\kappa^4O,O'$-samarium(III)zinc(II)

Qiang Huang, Yu-Hua Sui and Guo-Xiang 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 3 d-4f hetorometallic dinuclear complexes (Baggio *et al.*, 2000; Caravan *et al.*, 1999; Edder *et al.*, 2000; Knoer *et al.*, 2005). we report here the synthesis and X-ray crystal structure analysis of the title complex, (I), a new Zn^{II}—Sm^{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 samarium triply bridged by two phenolate O atoms provided by a salen-type Schiff base ligand and one nitrate. The inner salen-type cavity is occupied by zinc(II), while samarium(III) is present in the open and larger portion of the dinucleating compartmental Schiff base ligand.

The Sm^{III} center has a decacoordination environment of O atoms, involving the phenolate O atoms, two methoxy O atoms, one ethanol O atom, two O atoms from two nitrates and one from the bridging nitrate. The five kinds of Sm—O bond distances are significantly different, the longest being the Sm—*O*(methoxy) separations and the shortest being the Sm—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.

Adjacent molecules are held together by typical O—H···O hydrogen bonds and weak C—H···O interactions. these link the molecules into a two-dimensional 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 ethanol solution (80 ml) under reflux for 3 h and then for another 3 h after the addition of samarium(III) nitrate hexahydrate(0.444 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 ethanol solution. Analysis calculated for $C_{20}H_{24}N_5O_{14}SmZn$: C 31.03, H 3.12, N 9.05, Sm 19.42, Zn 8.45%; found: C 31.10, H 2.98, N 8.99, Sm 20.01, Zn 8.40%. 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 0.97 (methylene), 0.96 Å (methyl) and 0.93 Å (aromatic), and with U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms and 1.2U_{eq}(C) for other H atoms. The hydroxyl H atom, H14s, was located in a difference Fourier map and the O14—H14s was restrained

to 0.88 Å.

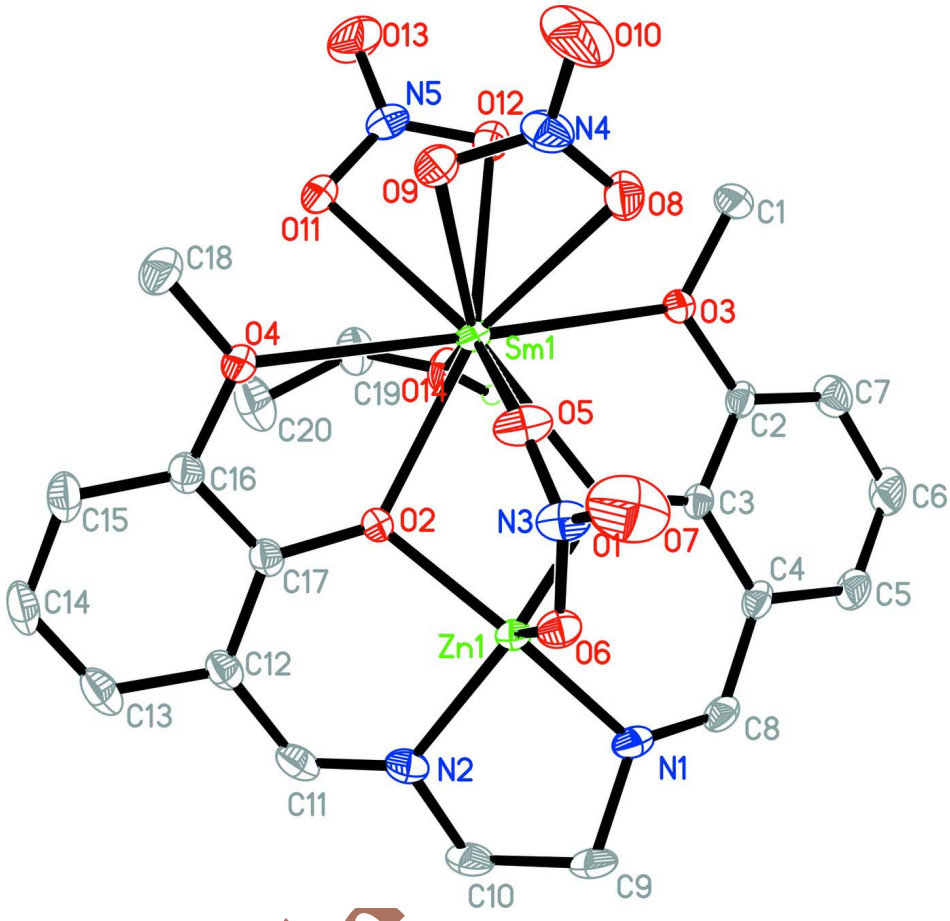

Figure 1

The molecular structure of (I), showing 30% probability displacement ellipsoids.

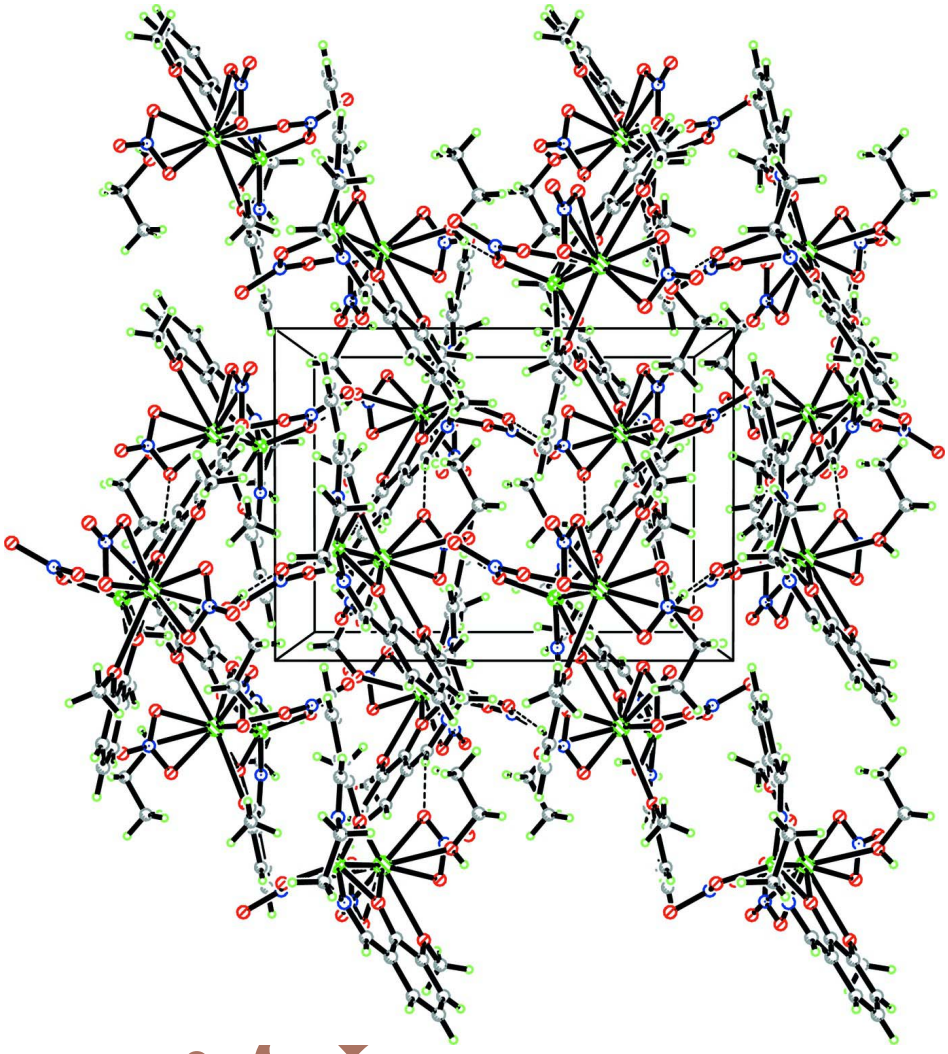

Figure 2

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

{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-1$\kappa O$)- μ-nitrato-1:2κ^2O:O'-dinitrato-1κ^4O,O'- samarium(III)zinc(II)

Crystal data

[SmZn($C_{18}H_{18}N_2O_4$)(NO_3)$_3$(C_2H_6O)]
M_r = 774.16
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 9.975 (3) Å
b = 13.780 (4) Å
c = 19.889 (6) Å
β = 91.745 (4)°
V = 2732.4 (13) Å^3
Z = 4
F(000) = 1532
D_x = 1.882 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5725 reflections
θ = 2.5–28.2°
μ = 3.08 mm^{-1}
T = 293 K
Block, yellow
0.26 × 0.23 × 0.19 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} = 0.501, T_{max} = 0.592
16112 measured reflections
4741 independent reflections
4175 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
θ_{max} = 25.0°, θ_{min} = 1.8°
h = −11→11
k = −15→16
l = −23→23

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.079
S = 1.08
4741 reflections
377 parameters
3 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
$w = 1/[\sigma^2(F_o^2) + (0.045P)^2 + 4.1668P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.67 e Å^{-3}
$\Delta\rho_{min}$ = −0.70 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}
C1	0.5387 (4)	0.1513 (4)	0.1046 (2)	0.0435 (11)
H1A	0.6226	0.1846	0.1108	0.065*
H1B	0.5050	0.1609	0.0594	0.065*
H1C	0.5517	0.0832	0.1126	0.065*
C2	0.4878 (4)	0.1904 (3)	0.21745 (19)	0.0287 (8)
C3	0.4091 (4)	0.2491 (3)	0.25846 (18)	0.0248 (8)
C4	0.4475 (4)	0.2570 (3)	0.32728 (19)	0.0309 (9)
C5	0.5626 (4)	0.2059 (3)	0.3513 (2)	0.0405 (11)
H5	0.5894	0.2119	0.3963	0.049*
C6	0.6343 (5)	0.1489 (4)	0.3106 (2)	0.0468 (12)
H6	0.7083	0.1151	0.3280	0.056*
C7	0.5978 (4)	0.1404 (3)	0.2430 (2)	0.0416 (10)
H7	0.6473	0.1011	0.2150	0.050*
C8	0.3727 (4)	0.3097 (3)	0.37649 (19)	0.0325 (9)
H8	0.4042	0.3070	0.4209	0.039*

C9	0.1883 (5)	0.4013 (3)	0.4187 (2)	0.0419 (11)
H9A	0.1913	0.4716	0.4174	0.050*
H9B	0.2236	0.3797	0.4621	0.050*
C10	0.0444 (5)	0.3652 (4)	0.4069 (2)	0.0432 (11)
H10A	0.0380	0.2976	0.4201	0.052*
H10B	−0.0162	0.4027	0.4340	0.052*
C11	−0.1155 (4)	0.3718 (3)	0.3160 (2)	0.0376 (10)
H11	−0.1793	0.3652	0.3488	0.045*
C12	−0.1630 (4)	0.3768 (3)	0.2471 (2)	0.0337 (9)
C13	−0.3008 (4)	0.3975 (3)	0.2340 (3)	0.0454 (11)
H13	−0.3576	0.4041	0.2700	0.054*
C14	−0.3520 (4)	0.4080 (3)	0.1702 (3)	0.0482 (12)
H14	−0.4427	0.4212	0.1631	0.058*
C15	−0.2698 (4)	0.3991 (3)	0.1159 (2)	0.0419 (11)
H15	−0.3044	0.4081	0.0724	0.050*
C16	−0.1355 (4)	0.3769 (3)	0.1268 (2)	0.0327 (9)
C17	−0.0801 (4)	0.3635 (3)	0.1915 (2)	0.0291 (8)
C18	−0.0918 (5)	0.3868 (4)	0.0095 (2)	0.0523 (13)
H18A	−0.1594	0.3406	−0.0040	0.078*
H18B	−0.0188	0.3835	−0.0207	0.078*
H18C	−0.1295	0.4509	0.0085	0.078*
C19	0.0334 (4)	0.0595 (3)	0.1448 (3)	0.0453 (11)
H19A	0.0360	0.0054	0.1761	0.054*
H19B	0.0421	0.0337	0.0998	0.054*
C20	−0.0964 (5)	0.1103 (4)	0.1492 (3)	0.0640 (15)
H20A	−0.1040	0.1376	0.1934	0.096*
H20B	−0.1683	0.0651	0.1409	0.096*
H20C	−0.1014	0.1612	0.1163	0.096*
H14S	0.189 (4)	0.093 (3)	0.1907 (18)	0.045 (14)*
N1	0.2671 (4)	0.3598 (3)	0.36409 (16)	0.0334 (8)
N2	0.0069 (4)	0.3757 (3)	0.33567 (17)	0.0365 (8)
N3	0.2742 (4)	0.5201 (3)	0.18223 (18)	0.0429 (8)
N4	0.3575 (4)	0.3693 (3)	−0.00107 (19)	0.0461 (10)
N5	0.1636 (4)	0.1430 (3)	−0.00124 (17)	0.0380 (8)
O1	0.3020 (3)	0.29131 (19)	0.22943 (13)	0.0285 (6)
O2	0.0480 (2)	0.3360 (2)	0.19722 (13)	0.0310 (6)
O3	0.4443 (3)	0.1886 (2)	0.15072 (13)	0.0340 (6)
O4	−0.0437 (3)	0.3650 (2)	0.07643 (14)	0.0378 (7)
O5	0.2537 (3)	0.4574 (2)	0.13814 (15)	0.0460 (8)
O6	0.2370 (3)	0.5111 (2)	0.24316 (13)	0.0334 (6)
O7	0.3498 (5)	0.6110 (3)	0.1638 (3)	0.0920 (15)
O8	0.4194 (3)	0.3382 (2)	0.05096 (16)	0.0441 (7)
O9	0.2306 (3)	0.3687 (2)	−0.00015 (14)	0.0422 (7)
O10	0.4160 (5)	0.3958 (4)	−0.0499 (2)	0.0997 (17)
O11	0.0688 (3)	0.1928 (2)	0.02181 (14)	0.0383 (7)
O12	0.2775 (3)	0.1549 (2)	0.02628 (15)	0.0408 (7)
O13	0.1458 (4)	0.0871 (3)	−0.04800 (19)	0.0694 (11)
O14	0.1442 (3)	0.1242 (2)	0.16021 (15)	0.0361 (7)

Sm1	0.209482 (19)	0.287372 (15)	0.113944 (9)	0.02816 (9)
Zn1	0.17006 (4)	0.38157 (3)	0.27338 (2)	0.02711 (12)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.035 (2)	0.060 (3)	0.036 (2)	0.016 (2)	0.0029 (18)	−0.011 (2)
C2	0.0245 (19)	0.034 (2)	0.027 (2)	−0.0018 (16)	−0.0040 (15)	0.0050 (16)
C3	0.0228 (19)	0.028 (2)	0.0233 (19)	−0.0031 (15)	−0.0020 (14)	0.0067 (15)
C4	0.028 (2)	0.038 (2)	0.027 (2)	−0.0031 (17)	−0.0074 (16)	0.0051 (17)
C5	0.035 (2)	0.058 (3)	0.028 (2)	0.001 (2)	−0.0093 (18)	0.0101 (19)
C6	0.036 (2)	0.058 (3)	0.046 (3)	0.012 (2)	−0.012 (2)	0.015 (2)
C7	0.036 (2)	0.045 (3)	0.044 (3)	0.0095 (19)	0.0013 (19)	0.007 (2)
C8	0.036 (2)	0.041 (2)	0.0203 (19)	−0.0063 (18)	−0.0052 (16)	0.0038 (17)
C9	0.056 (3)	0.049 (3)	0.021 (2)	0.003 (2)	0.0044 (18)	−0.0073 (19)
C10	0.052 (3)	0.053 (3)	0.026 (2)	0.004 (2)	0.0140 (19)	−0.0007 (19)
C11	0.035 (2)	0.036 (2)	0.043 (3)	−0.0011 (18)	0.0172 (19)	−0.0053 (19)
C12	0.026 (2)	0.031 (2)	0.045 (2)	−0.0022 (16)	0.0072 (17)	−0.0053 (18)
C13	0.028 (2)	0.041 (3)	0.068 (3)	−0.0012 (19)	0.015 (2)	−0.008 (2)
C14	0.022 (2)	0.049 (3)	0.074 (4)	0.0056 (19)	−0.004 (2)	−0.007 (2)
C15	0.029 (2)	0.038 (3)	0.057 (3)	0.0059 (18)	−0.010 (2)	−0.005 (2)
C16	0.029 (2)	0.027 (2)	0.042 (2)	0.0032 (16)	−0.0028 (17)	−0.0083 (17)
C17	0.025 (2)	0.024 (2)	0.038 (2)	0.0009 (15)	0.0006 (16)	−0.0061 (16)
C18	0.051 (3)	0.066 (3)	0.039 (3)	0.017 (2)	−0.013 (2)	−0.001 (2)
C19	0.038 (3)	0.038 (3)	0.060 (3)	−0.002 (2)	−0.002 (2)	0.006 (2)
C20	0.036 (3)	0.059 (3)	0.097 (5)	−0.002 (2)	0.009 (3)	−0.003 (3)
N1	0.043 (2)	0.0359 (19)	0.0215 (16)	−0.0051 (16)	0.0014 (14)	−0.0033 (14)
N2	0.040 (2)	0.041 (2)	0.0291 (18)	−0.0007 (16)	0.0111 (15)	0.0003 (15)
N3	0.058 (2)	0.038 (2)	0.0329 (14)	0.0040 (17)	0.0048 (15)	−0.0028 (12)
N4	0.053 (3)	0.048 (2)	0.038 (2)	0.0035 (18)	0.0141 (18)	0.0109 (18)
N5	0.047 (2)	0.038 (2)	0.0287 (18)	−0.0019 (17)	−0.0023 (16)	−0.0059 (16)
O1	0.0244 (14)	0.0385 (16)	0.0221 (14)	0.0051 (11)	−0.0042 (10)	−0.0010 (11)
O2	0.0226 (13)	0.0421 (16)	0.0282 (14)	0.0061 (12)	−0.0005 (11)	−0.0067 (12)
O3	0.0251 (14)	0.0489 (17)	0.0279 (15)	0.0091 (12)	−0.0016 (11)	−0.0054 (12)
O4	0.0317 (15)	0.0516 (18)	0.0298 (15)	0.0093 (13)	−0.0054 (12)	−0.0056 (13)
O5	0.071 (2)	0.0360 (17)	0.0308 (15)	−0.0057 (15)	0.0056 (15)	−0.0015 (11)
O6	0.0410 (16)	0.0288 (15)	0.0303 (12)	−0.0026 (12)	0.0015 (11)	−0.0031 (11)
O7	0.114 (4)	0.069 (3)	0.095 (4)	−0.018 (3)	0.033 (3)	−0.002 (2)
O8	0.0332 (16)	0.053 (2)	0.0460 (19)	−0.0035 (14)	−0.0014 (13)	0.0090 (15)
O9	0.0420 (18)	0.054 (2)	0.0309 (16)	0.0052 (14)	−0.0023 (13)	0.0070 (14)
O10	0.085 (3)	0.143 (5)	0.074 (3)	0.015 (3)	0.042 (3)	0.058 (3)
O11	0.0355 (16)	0.0480 (18)	0.0310 (16)	0.0025 (13)	−0.0073 (12)	−0.0040 (13)
O12	0.0341 (17)	0.0488 (19)	0.0393 (17)	0.0041 (13)	−0.0037 (13)	−0.0085 (14)
O13	0.082 (3)	0.069 (3)	0.056 (2)	−0.001 (2)	−0.013 (2)	−0.036 (2)
O14	0.0323 (16)	0.0368 (17)	0.0386 (17)	−0.0058 (12)	−0.0078 (13)	0.0112 (13)
Sm1	0.02985 (13)	0.03342 (14)	0.02110 (13)	0.00080 (8)	−0.00085 (8)	−0.00187 (8)
Zn1	0.0286 (2)	0.0328 (3)	0.0200 (2)	−0.00050 (18)	0.00205 (17)	−0.00135 (17)

Geometric parameters (Å, º)

C1—O3	1.430 (5)	C17—O2	1.334 (5)
C1—H1A	0.9600	C18—O4	1.433 (5)
C1—H1B	0.9600	C18—H18A	0.9600
C1—H1C	0.9600	C18—H18B	0.9600
C2—C7	1.379 (6)	C18—H18C	0.9600
C2—O3	1.384 (5)	C19—O14	1.446 (5)
C2—C3	1.406 (6)	C19—C20	1.477 (7)
C3—O1	1.333 (4)	C19—H19A	0.9700
C3—C4	1.414 (5)	C19—H19B	0.9700
C4—C5	1.418 (6)	C20—H20A	0.9600
C4—C8	1.444 (6)	C20—H20B	0.9600
C5—C6	1.348 (7)	C20—H20C	0.9600
C5—H5	0.9300	N1—Zn1	2.043 (3)
C6—C7	1.387 (6)	N2—Zn1	2.077 (3)
C6—H6	0.9300	N3—O5	1.244 (5)
C7—H7	0.9300	N3—O6	1.284 (4)
C8—N1	1.277 (5)	N3—O7	1.512 (6)
C8—H8	0.9300	N4—O10	1.205 (5)
C9—N1	1.474 (5)	N4—O8	1.264 (5)
C9—C10	1.530 (7)	N4—O9	1.267 (5)
C9—H9A	0.9700	N5—O13	1.217 (5)
C9—H9B	0.9700	N5—O12	1.257 (4)
C10—N2	1.462 (5)	N5—O11	1.265 (5)
C10—H10A	0.9700	O1—Zn1	2.028 (3)
C10—H10B	0.9700	O1—Sm1	2.450 (3)
C11—N2	1.272 (6)	O2—Zn1	2.014 (3)
C11—C12	1.438 (6)	O2—Sm1	2.439 (3)
C11—H11	0.9300	O3—Sm1	2.787 (3)
C12—C17	1.413 (6)	O4—Sm1	2.822 (3)
C12—C13	1.420 (6)	O5—Sm1	2.429 (3)
C13—C14	1.362 (7)	O6—Zn1	2.004 (3)
C13—H13	0.9300	O8—Sm1	2.570 (3)
C14—C15	1.380 (7)	O9—Sm1	2.545 (3)
C14—H14	0.9300	O11—Sm1	2.621 (3)
C15—C16	1.385 (6)	O12—Sm1	2.627 (3)
C15—H15	0.9300	O14—Sm1	2.523 (3)
C16—O4	1.387 (5)	O14—H14S	0.855 (19)
C16—C17	1.398 (6)		
O3—C1—H1A	109.5	O5—N3—O7	118.5 (4)
O3—C1—H1B	109.5	O6—N3—O7	118.0 (3)
H1A—C1—H1B	109.5	O10—N4—O8	121.8 (4)
O3—C1—H1C	109.5	O10—N4—O9	121.5 (4)
H1A—C1—H1C	109.5	O8—N4—O9	116.7 (3)
H1B—C1—H1C	109.5	O13—N5—O12	121.7 (4)
C7—C2—O3	124.6 (4)	O13—N5—O11	121.8 (4)

C7—C2—C3	121.7 (4)	O12—N5—O11	116.6 (3)
O3—C2—C3	113.7 (3)	C3—O1—Zn1	127.1 (2)
O1—C3—C2	117.0 (3)	C3—O1—Sm1	132.1 (2)
O1—C3—C4	125.1 (3)	Zn1—O1—Sm1	100.77 (10)
C2—C3—C4	117.8 (3)	C17—O2—Zn1	122.1 (2)
C3—C4—C5	118.7 (4)	C17—O2—Sm1	132.1 (2)
C3—C4—C8	124.4 (4)	Zn1—O2—Sm1	101.52 (10)
C5—C4—C8	116.8 (4)	C2—O3—C1	115.4 (3)
C6—C5—C4	121.8 (4)	C2—O3—Sm1	118.7 (2)
C6—C5—H5	119.1	C1—O3—Sm1	124.9 (2)
C4—C5—H5	119.1	C16—O4—C18	115.8 (3)
C5—C6—C7	120.1 (4)	C16—O4—Sm1	117.3 (2)
C5—C6—H6	119.9	C18—O4—Sm1	126.7 (3)
C7—C6—H6	119.9	N3—O5—Sm1	146.6 (3)
C2—C7—C6	119.9 (4)	N3—O6—Zn1	118.6 (2)
C2—C7—H7	120.1	N4—O8—Sm1	96.1 (2)
C6—C7—H7	120.1	N4—O9—Sm1	97.2 (2)
N1—C8—C4	125.5 (4)	N5—O11—Sm1	97.6 (2)
N1—C8—H8	117.3	N5—O12—Sm1	97.6 (2)
C4—C8—H8	117.3	C19—O14—Sm1	132.6 (2)
N1—C9—C10	106.2 (3)	C19—O14—H14S	103 (3)
N1—C9—H9A	110.5	Sm1—O14—H14S	125 (3)
C10—C9—H9A	110.5	O5—Sm1—O2	73.74 (10)
N1—C9—H9B	110.5	O5—Sm1—O1	74.45 (10)
C10—C9—H9B	110.5	O2—Sm1—O1	66.10 (9)
H9A—C9—H9B	108.7	O5—Sm1—O14	146.58 (10)
N2—C10—C9	109.1 (3)	O2—Sm1—O14	79.28 (10)
N2—C10—H10A	109.9	O1—Sm1—O14	76.81 (9)
C9—C10—H10A	109.9	O5—Sm1—O9	74.48 (10)
N2—C10—H10B	109.9	O2—Sm1—O9	123.96 (10)
C9—C10—H10B	109.9	O1—Sm1—O9	141.92 (10)
H10A—C10—H10B	108.3	O14—Sm1—O9	138.33 (10)
N2—C11—C12	125.3 (4)	O5—Sm1—O8	71.83 (11)
N2—C11—H11	117.4	O2—Sm1—O8	145.17 (10)
C12—C11—H11	117.4	O1—Sm1—O8	99.31 (9)
C17—C12—C13	118.0 (4)	O14—Sm1—O8	130.09 (10)
C17—C12—C11	123.7 (4)	O9—Sm1—O8	49.82 (10)
C13—C12—C11	118.2 (4)	O5—Sm1—O11	135.09 (10)
C14—C13—C12	121.6 (4)	O2—Sm1—O11	105.13 (9)
C14—C13—H13	119.2	O1—Sm1—O11	147.66 (9)
C12—C13—H13	119.2	O14—Sm1—O11	70.91 (9)
C13—C14—C15	120.4 (4)	O9—Sm1—O11	69.69 (10)
C13—C14—H14	119.8	O8—Sm1—O11	102.80 (10)
C15—C14—H14	119.8	O5—Sm1—O12	138.80 (10)
C14—C15—C16	119.5 (4)	O2—Sm1—O12	146.17 (9)
C14—C15—H15	120.3	O1—Sm1—O12	122.69 (9)
C16—C15—H15	120.3	O14—Sm1—O12	72.40 (10)
C15—C16—O4	124.8 (4)	O9—Sm1—O12	71.60 (10)

C15—C16—C17	121.8 (4)	O8—Sm1—O12	68.60 (10)
O4—C16—C17	113.5 (3)	O11—Sm1—O12	48.25 (9)
O2—C17—C16	117.8 (3)	O5—Sm1—O3	105.83 (10)
O2—C17—C12	123.5 (4)	O2—Sm1—O3	121.53 (8)
C16—C17—C12	118.6 (4)	O1—Sm1—O3	58.34 (8)
O4—C18—H18A	109.5	O14—Sm1—O3	72.15 (9)
O4—C18—H18B	109.5	O9—Sm1—O3	110.93 (9)
H18A—C18—H18B	109.5	O8—Sm1—O3	64.54 (9)
O4—C18—H18C	109.5	O11—Sm1—O3	111.62 (9)
H18A—C18—H18C	109.5	O12—Sm1—O3	66.62 (8)
H18B—C18—H18C	109.5	O5—Sm1—O4	80.93 (10)
O14—C19—C20	111.1 (4)	O2—Sm1—O4	58.08 (8)
O14—C19—H19A	109.4	O1—Sm1—O4	123.23 (8)
C20—C19—H19A	109.4	O14—Sm1—O4	101.26 (9)
O14—C19—H19B	109.4	O9—Sm1—O4	72.24 (9)
C20—C19—H19B	109.4	O8—Sm1—O4	120.25 (9)
H19A—C19—H19B	108.0	O11—Sm1—O4	63.13 (9)
C19—C20—H20A	109.5	O12—Sm1—O4	109.57 (9)
C19—C20—H20B	109.5	O3—Sm1—O4	173.01 (9)
H20A—C20—H20B	109.5	O6—Zn1—O2	104.55 (12)
C19—C20—H20C	109.5	O6—Zn1—O1	100.96 (11)
H20A—C20—H20C	109.5	O2—Zn1—O1	82.54 (10)
H20B—C20—H20C	109.5	O6—Zn1—N1	104.02 (13)
C8—N1—C9	121.5 (3)	O2—Zn1—N1	151.32 (13)
C8—N1—Zn1	128.0 (3)	O1—Zn1—N1	89.69 (12)
C9—N1—Zn1	110.2 (3)	O6—Zn1—N2	119.22 (13)
C11—N2—C10	120.6 (4)	O2—Zn1—N2	88.27 (13)
C11—N2—Zn1	125.5 (3)	O1—Zn1—N2	139.80 (13)
C10—N2—Zn1	113.6 (3)	N1—Zn1—N2	79.99 (14)
O5—N3—O6	123.4 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1*B*···O12	0.96	2.35	2.995 (5)	125
C18—H18*B*···O9	0.96	2.52	3.237 (6)	132
O14—H14*S*···O6^{i}	0.86 (2)	1.87 (2)	2.718 (4)	171 (5)
C8—H8···O11^{ii}	0.93	2.55	3.440 (5)	160

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