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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	HESPEP
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

References

Chen, Q. (2006). *Acta Cryst.* E**62**, m56–m57.
Chen, J.-R., Sui, Y., Luo, Q.-Y. & Jiang, R.-Q. (2007). *Acta Cryst.* E**63**, m2091–m2092.
Chen, J.-R., Sui, Y., Wen, J.-W. & Yin, L.-Y. (2008). *Acta Cryst.* E**64**, m562–m563.
Han, Z.-Q. (2008). *Acta Cryst.* E**64**, m592.
Harrison, W. T. A., Simpson, J. & Weil, M. (2010). *Acta Cryst.* E**66**, e1–e2.
Hu, R.-H., Sui, Y., Chen, L. & He, C.-M. (2008). *Acta Cryst.* E**64**, m8–m9.
Hu, R.-H., Sui, Y., Fang, X.-N. & Chen, H.-M. (2007). *Acta Cryst.* E**63**, m2039–m2040.
Huang, C.-F. & Chen, H.-L. (2007). *Acta Cryst.* E**63**, m2356–m2357.
Huang, Q., Sui, Y.-H. & Zhang, G.-X. (2009). *Acta Cryst.* E**65**, m1161–m1162.
Li, Y.-G. & Chen, H.-J. (2006). *Acta Cryst.* E**62**, m1038–m1039.
Li, N.-G., Tao, R.-M. & Fu, B.-F (2007). *Acta Cryst.* E**63**, o4228.
Li, Z., Zhang, X. & Pu, X. (2008). *Acta Cryst.* E**64**, m215.
Liu, J.-T. & Fan, S.-D. (2006). *Acta Cryst.* E**62**, m2507–m2508.
Liu, J.-T., Fan, S.-D. & Li, D.-Q. (2006). *Acta Cryst.* E**62**, m2165–m2166.
Liu, D., Lin, J., Xu, Y., Huang, C. & Li, X. (2007). *Acta Cryst.* E**63**, m3094.
Liu, Y.-Q. & Wen, H.-R. (2007). *Acta Cryst.* E**63**, m2928.
Liu, Y.-Q. & Zeng, X.-R. (2007*a*). *Acta Cryst.* E**63**, m2547.
Liu, Y.-Q. & Zeng, X.-R. (2007*b*). *Acta Cryst.* E**63**, m2684.
Liu, Y.-Q., Zeng, X.-R. & Chen, W.-T. (2007). *Acta Cryst.* E**63**, m2462.
Liu, Y.-Q., Zeng, X.-R., Luo, Q.-Y. & Xu, Y.-P. (2007*a*). *Acta Cryst.* E**63**, m2396.
Liu, Y.-Q., Zeng, X.-R., Luo, Q.-Y. & Xu, Y.-P. (2007*b*). *Acta Cryst.* E**63**, m2854.
Qadeer, G., Rama, N. H. & Chen, W.-T. (2007*a*). *Acta Cryst.* E**63**, o2892.
Qadeer, G., Rama, N. H. & Chen, W.-T. (2007*b*). *Acta Cryst.* E**63**, o2932.
Qiu, X.-Y. (2006). *Acta Cryst.* E**62**, m1190–m1191.
Sui, Y., Fang, X.-N., Hu, P. & Lin, J. (2007). *Acta Cryst.* E**63**, m2135–m2136.
Sui, Y., Fang, X.-N. & Yuan, M.-W. (2007). *Acta Cryst.* E**63**, m2275–m2276.
Sui, Y., Li, X.-F., Huang, G.-S. & Wang, G.-J. (2007). *Acta Cryst.* E**63**, m2093–m2094.
Sui, Y., Sui, Y.-H., Luo, Q.-Y. & Wang, Y.-D. (2007). *Acta Cryst.* E**63**, m2277–m2278.
Sui, Y., Xiao, Y.-A., Fang, X.-N., Zeng, X.-R. & Li, M.-H. (2006). *Acta Cryst.* E**62**, m3205–m3207.
Sui, Y., Zhang, J.-H., Hu, R.-H. & Jiang, R.-Q. (2007). *Acta Cryst.* E**63**, m2256–m2257.
Sui, Y., Zhang, J.-H., Hu, R.-H. & Yin, L.-Y. (2007). *Acta Cryst.* E**63**, m2089–m2090.
Sun, Y.-X. & Gao, G.-Z. (2005). *Acta Cryst.* E**61**, m354–m355.
Wang, Q. & Fang, Z.-N. (2006). *Acta Cryst.* E**62**, m1492–m1493.
Wang, S., Yang, T., Li, Z. & Yu, X. (2009). *Acta Cryst.* E**65**, o2198.
Xiao, Y.-A., Fu, X.-K., Sui, Y., Wu, Q. & Xiong, S.-H. (2008). *Acta Cryst.* E**64**, m806–m807.
Xiao, Y.-A., Sui, Y., Yi, X.-G., Wu, J.-H. & Zhang, L.-P. (2008). *Acta Cryst.* E**64**, m804–m805.
Xiong, Z.-Y. & Liu, L.-J. (2005). *Acta Cryst.* E**61**, m863–m864.
Yang, X.-M. (2007). *Acta Cryst.* E**63**, o4453.
Yang, Y.-M., Lu, P.-C., Zhu, T.-T. & Liu, C.-H. (2007). *Acta Cryst.* E**63**, m1613.
Zhang, P. (2004). *Acta Cryst.* E**60**, m1808–m1810.

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{6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-methanol-μ-nitrato-dinitrato-samarium(III)nickel(II)

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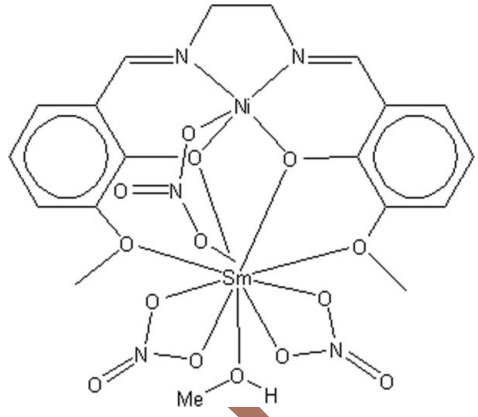
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.008 Å; R factor = 0.037; wR factor = 0.124; data-to-parameter ratio = 17.4.

In the title heteronuclear Ni^{II}–Sm^{III} complex (systematic name: {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-1$\kappa O$)-$\mu$-nitrato-1:2$\kappa^2O$:$O'$-dinitrato-1$\kappa^4O,O'$-nickel(II)-samarium(III)), $[NiSm(C_{18}H_{18}N_2O_4)(NO_3)_3(CH_4O)]$, with the hexadentate Schiff base compartmental ligand N,N'-bis(3-methoxysalicylidene)ethylenediamine, the Ni and Sm atoms are triply bridged by two phenolate O atoms provided by the Schiff base ligand and one nitrate ion. The five-coordinate Ni 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 Sm^{III} center has a tenfold coordination environment of O atoms, involving the phenolate O atoms, two methoxy O atoms, one methanol O atom, and two O atoms from two nitrates and one from the bridging nitrate. Strong intermolecular O—H···O and some weak 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

$[NiSm(C_{18}H_{18}N_2O_4)(NO_3)_3(CH_4O)]$
M_r = 753.48
Monoclinic, $P2_1/n$
a = 9.604 (2) Å
b = 13.805 (3) Å
c = 20.049 (4) Å
β = 91.617 (3)°
V = 2657.3 (10) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.97 mm^{-1}
T = 293 (2) K
0.25 × 0.24 × 0.24 mm

Data collection

Bruker APEX II area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.524, T_{max} = 0.540
(expected range = 0.474–0.490)
19575 measured reflections
6376 independent reflections
5577 reflections with $I > 2\sigma(I)$
R_{int} = 0.018

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.124
S = 1.01
6376 reflections
367 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 2.54 e Å^{-3}
$\Delta\rho_{min}$ = −1.03 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O14—H14A···O9^{i}	0.89 (2)	1.82 (2)	2.691 (4)	166 (6)
C5—H5···O5^{ii}	0.93	2.57	3.432 (6)	155
C7—H7···O11^{ii}	0.93	2.47	3.379 (5)	164

Symmetry codes: (i) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$; (ii) $x+\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *APEX2*; software used to prepare material for publication: *APEX2* and *publCIF* (Westrip, 2007).

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2007317), and the Natural Science Foundation of JiangXi Province (grant No. 0620029).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2269).

References

Baggio, R., Garland, M. T., Moreno, Y., Pena, O., Perec, M. & Spodine, E. (2000). *J. Chem. Soc. Dalton Trans.* pp. 2061–2066.
Bruker (2004). *APEX2* (Version 1.22) and *SADABS* (Version 2004/1). Bruker AXS Inc., Madison, Wisconsin, USA.
Caravan, P., Ellison, J. J., McMurry, T. J. & Lauffer, R. B. (1999). *Chem. Rev.* **99**, 2293–2352.
Edder, C., Piguet, C., Bernardinelli, G., Mareda, J., Bochet, C. G., Bunzli, J.-C. G. & Hopfgartner, G. (2000). *Inorg. Chem.* **39**, 5059–5073.
Knoer, R., Lin, H.-H., Wei, H.-H. & Mohanta, S. (2005). *Inorg. Chem.* **44**, 3524–3536.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sui, Y., Fang, X.-N., Xiao, Y.-A., Luo, Q.-Y. & Li, M.-H. (2006). *Acta Cryst.* E**62**, m2230–m2232.
Sui, Y., He, D.-Y., Fang, X.-N., Chen, L. & Peng, J.-L. (2007). *Acta Cryst.* E**63**, m2013–m2014.
Westrip, S. P. (2007). *publCIF*. In preparation.

supplementary materials

Acta Cryst. (2007). E**63**, m2256-m2257 [**doi:10.1107/S1600536807037130**]

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

Y. Sui, J.-H. Zhang, R.-H. Hu and R.-Q. Jiang

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 Ni^{II}—Sm^{III} complex with salen-type Schiff base *N*,*N*'-bis(3-ethoxysalicylidene) ethylenediamine (H_2L).

Complex (I) crystallizes in the space group $P2_1/n$, with nickel 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 nickel(II), while saramium(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 methanol 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—O(phenolate) and Sm—O8(bridging nitrate).

The Ni^{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 Ni atom is 0.5860 (2)Å below the mean N_2O_2 plane with an average deviation from the plane of 0.0961 (3) Å, which construct the bottom of square-pyramid. The Ni—O9 (bridging nitrate) separation is 2.003 (3)Å and the angles of this Ni—O vector with the Ni—N or Ni—O bonds lie between 103.3 (5)° and 115.6 (6)°, which suggesting that the Ni^{II} is in a slightly distorted square-pyramidal conformation.

Adjacent molecules are held together by strong interactions (O14—H14A···$O9^{i}$=2.691 (4); symmetry codes:(i)3/2 − *x*, 1/2 + *y*, 1/2 − *z*) and weak interactions (C7—H7···$O11^{ii}$=3.379 (5) and C5—H5···$O5^{ii}$=3.432 (6); symmetry codes: (ii)1/2 + *x*, 1/2 − *y*, 1/2 + *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 nickel(II) acetate tetrahydrate (0.217 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 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 methanol solution. Analysis calculated for $C_{19}H_{22}N_5NiO_{14}Sm$: C 30.29, H 2.94, N 9.29, Ni 7.79, Sm 19.96%; found: C 30.01, H 2.98, N 9.40, Ni 7.78, Sm 19.68%. 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) 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 methyl group of methanol was constrainted as idealized non-rotating CH_3 group. The hydroxyl H atom, H14A, was located in a difference Fourier map and refined with the O14—H14A restrained to 0.9 Å.

Figures

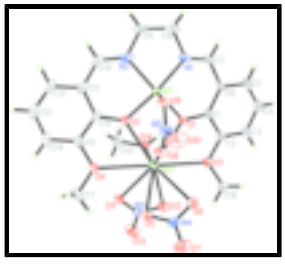

Fig.1. The molecular structure of (I), showing 30% probability displacement ellipsoids.

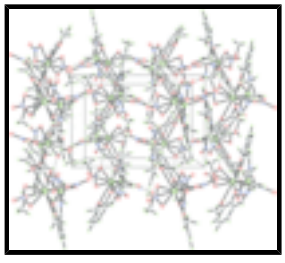

Fig.2. The packing diagram of (I), viewed along the *c* axis; hydrogen bonds are shown as dashed lines.

Table 1. Selected geometric parameters (Å).

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

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

Crystal data

$[NiSm(C_{18}H_{18}N_2O_4)(NO_3)_3(CH_4O)]$	$F_{000} = 1492$
$M_r = 753.48$	$D_x = 1.883$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 6618 reflections
a = 9.604 (2) Å	θ = 1.8–28.3°
b = 13.805 (3) Å	μ = 2.97 mm^{-1}
c = 20.049 (4) Å	*T* = 293 (2) K
β = 91.617 (3)°	Block, red
V = 2657.3 (10) Å^3	0.25 × 0.24 × 0.24 mm
Z = 4	

Data collection

Bruker APEX II area-detector diffractometer	6376 independent reflections
Radiation source: fine-focus sealed tube	5577 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.018$
$T = 293(2)$ K	$\theta_{max} = 28.3°$
φ and ω scans	$\theta_{min} = 1.8°$
Absorption correction: multi-scan (SADABS; Bruker, 2004)	$h = -12 \rightarrow 12$
$T_{min} = 0.524$, $T_{max} = 0.540$	$k = -18 \rightarrow 18$
19575 measured reflections	$l = -26 \rightarrow 26$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.037$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.124$	$w = 1/[\sigma^2(F_o^2) + (0.0827P)^2 + 6.7464P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{max} = 0.001$
6376 reflections	$\Delta\rho_{max} = 2.54$ e Å^{-3}
367 parameters	$\Delta\rho_{min} = -1.03$ e Å^{-3}
1 restraint	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}
Sm1	0.72165 (2)	0.221608 (16)	0.113907 (10)	0.02869 (9)
Ni1	0.68895 (5)	0.12834 (4)	0.27322 (2)	0.02415 (12)
O1	0.8237 (3)	0.2178 (2)	0.22809 (14)	0.0299 (6)

O5	0.7362 (4)	0.1365 (3)	0.00081 (16)	0.0440 (8)
O2	0.5578 (3)	0.1751 (2)	0.19989 (15)	0.0333 (6)
O3	0.9687 (3)	0.3197 (3)	0.14804 (15)	0.0358 (7)
C1	0.9349 (4)	0.2603 (3)	0.2555 (2)	0.0284 (8)
O6	0.9352 (3)	0.1682 (3)	0.04734 (18)	0.0438 (8)
O4	0.4592 (3)	0.1456 (3)	0.08019 (17)	0.0416 (8)
N2	0.5224 (5)	0.1311 (3)	0.3371 (2)	0.0417 (9)
C6	0.9773 (5)	0.2532 (4)	0.3236 (2)	0.0357 (9)
C11	0.3436 (5)	0.1270 (3)	0.2512 (3)	0.0394 (10)
N4	0.8677 (5)	0.1335 (4)	−0.0018 (2)	0.0469 (10)
C3	1.1335 (5)	0.3664 (4)	0.2381 (3)	0.0453 (12)
H3	1.1857	0.4040	0.2096	0.054*
C5	1.0959 (6)	0.3041 (4)	0.3469 (3)	0.0482 (13)
H5	1.1225	0.3002	0.3918	0.058*
C2	1.0163 (4)	0.3176 (3)	0.2138 (2)	0.0327 (9)
C7	0.9013 (6)	0.1986 (4)	0.3737 (2)	0.0398 (11)
H7	0.9339	0.2020	0.4178	0.048*
C10	0.3940 (5)	0.1308 (4)	0.3192 (3)	0.0437 (11)
H10	0.3285	0.1332	0.3525	0.052*
C12	0.2020 (5)	0.1021 (4)	0.2395 (3)	0.0502 (14)
H12	0.1456	0.0919	0.2758	0.060*
C17	0.4074 (6)	0.1210 (5)	0.0148 (3)	0.0565 (15)
H17A	0.3856	0.0531	0.0131	0.085*
H17B	0.4769	0.1353	−0.0173	0.085*
H17C	0.3249	0.1580	0.0045	0.085*
C4	1.1722 (6)	0.3587 (4)	0.3050 (3)	0.0523 (14)
H4	1.2510	0.3910	0.3213	0.063*
C18	1.0641 (6)	0.3586 (5)	0.1011 (3)	0.0491 (13)
H18A	1.0714	0.4274	0.1071	0.074*
H18B	1.0306	0.3449	0.0566	0.074*
H18C	1.1540	0.3294	0.1083	0.074*
O7	0.9247 (6)	0.0977 (6)	−0.0484 (3)	0.103 (2)
O14	0.6425 (4)	0.3820 (2)	0.16112 (17)	0.0381 (7)
O11	0.5703 (4)	0.3179 (3)	0.02337 (17)	0.0428 (8)
O9	0.7472 (3)	−0.0033 (2)	0.24259 (15)	0.0364 (7)
O8	0.7648 (4)	0.0492 (3)	0.13872 (16)	0.0432 (8)
O12	0.7876 (4)	0.3554 (3)	0.02657 (18)	0.0457 (8)
N1	0.7946 (5)	0.1470 (3)	0.36130 (18)	0.0399 (9)
N3	0.6690 (5)	0.3680 (3)	0.00024 (19)	0.0399 (9)
N5	0.7780 (4)	−0.0145 (3)	0.1815 (2)	0.0425 (9)
C16	0.4261 (4)	0.1447 (3)	0.1950 (2)	0.0322 (9)
C15	0.3665 (4)	0.1312 (3)	0.1316 (3)	0.0364 (10)
C14	0.2282 (5)	0.1055 (4)	0.1216 (3)	0.0472 (13)
H14	0.1909	0.0970	0.0787	0.057*
C13	0.1461 (5)	0.0928 (4)	0.1768 (4)	0.0566 (16)
H13	0.0522	0.0777	0.1709	0.068*
C9	0.5660 (7)	0.1387 (5)	0.4080 (2)	0.0524 (14)
H9A	0.5053	0.0998	0.4350	0.063*
H9B	0.5597	0.2055	0.4226	0.063*

C8	0.7147 (7)	0.1033 (4)	0.4163 (2)	0.0510 (13)
H8A	0.7540	0.1232	0.4592	0.061*
H8B	0.7179	0.0332	0.4137	0.061*
C19	0.5000 (6)	0.4105 (5)	0.1618 (4)	0.0596 (16)
H19A	0.4732	0.4378	0.1193	0.071*
H19B	0.4876	0.4578	0.1962	0.071*
H19C	0.4431	0.3549	0.1704	0.071*
O13	0.6481 (6)	0.4245 (4)	−0.0455 (2)	0.0724 (14)
O10	0.8398 (7)	−0.1098 (4)	0.1618 (3)	0.0878 (17)
H14A	0.692 (5)	0.418 (4)	0.190 (2)	0.051 (17)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sm1	0.03071 (13)	0.03499 (14)	0.02022 (12)	−0.00078 (8)	−0.00193 (8)	0.00131 (7)
Ni1	0.0302 (2)	0.0283 (3)	0.0140 (2)	0.00120 (19)	0.00213 (18)	0.00104 (17)
O1	0.0287 (14)	0.0416 (17)	0.0191 (13)	−0.0049 (11)	−0.0057 (11)	0.0014 (11)
O5	0.0440 (18)	0.063 (2)	0.0245 (15)	−0.0011 (16)	−0.0026 (13)	−0.0083 (15)
O2	0.0250 (13)	0.0447 (18)	0.0303 (15)	−0.0056 (13)	0.0021 (11)	0.0071 (13)
O3	0.0308 (14)	0.0480 (19)	0.0282 (15)	−0.0093 (14)	−0.0035 (12)	0.0056 (13)
C1	0.0271 (18)	0.034 (2)	0.0237 (18)	0.0030 (16)	−0.0047 (15)	−0.0061 (16)
O6	0.0338 (16)	0.056 (2)	0.0421 (19)	0.0026 (15)	−0.0003 (14)	−0.0086 (16)
O4	0.0329 (15)	0.058 (2)	0.0328 (16)	−0.0091 (15)	−0.0084 (13)	0.0064 (15)
N2	0.053 (2)	0.046 (2)	0.0271 (18)	0.0022 (19)	0.0142 (17)	0.0003 (16)
C6	0.035 (2)	0.048 (2)	0.024 (2)	0.004 (2)	−0.0086 (17)	−0.0068 (19)
C11	0.033 (2)	0.033 (2)	0.053 (3)	0.0020 (18)	0.015 (2)	0.002 (2)
N4	0.050 (2)	0.055 (3)	0.036 (2)	−0.001 (2)	0.0101 (19)	−0.0092 (19)
C3	0.037 (2)	0.046 (3)	0.053 (3)	−0.008 (2)	−0.007 (2)	−0.008 (2)
C5	0.046 (3)	0.061 (3)	0.037 (3)	0.002 (3)	−0.018 (2)	−0.016 (2)
C2	0.032 (2)	0.037 (2)	0.029 (2)	0.0011 (17)	−0.0048 (16)	−0.0045 (17)
C7	0.051 (3)	0.050 (3)	0.0179 (18)	0.011 (2)	−0.0103 (18)	−0.0029 (18)
C10	0.044 (3)	0.039 (3)	0.050 (3)	−0.001 (2)	0.025 (2)	0.003 (2)
C12	0.032 (2)	0.040 (3)	0.080 (4)	0.000 (2)	0.025 (3)	0.004 (3)
C17	0.054 (3)	0.073 (4)	0.042 (3)	−0.013 (3)	−0.017 (2)	0.000 (3)
C4	0.043 (3)	0.060 (3)	0.052 (3)	−0.010 (2)	−0.016 (2)	−0.018 (3)
C18	0.044 (3)	0.063 (3)	0.040 (3)	−0.016 (2)	0.003 (2)	0.008 (2)
O7	0.083 (4)	0.157 (6)	0.069 (3)	−0.001 (4)	0.033 (3)	−0.061 (4)
O14	0.0402 (17)	0.0355 (17)	0.0384 (17)	0.0038 (14)	−0.0019 (14)	−0.0097 (14)
O11	0.0460 (18)	0.049 (2)	0.0326 (16)	−0.0007 (16)	−0.0131 (14)	0.0041 (15)
O9	0.0513 (19)	0.0316 (15)	0.0264 (14)	0.0037 (13)	0.0031 (13)	0.0027 (12)
O8	0.067 (2)	0.0351 (17)	0.0281 (15)	0.0040 (16)	0.0016 (15)	0.0017 (13)
O12	0.0441 (18)	0.052 (2)	0.0405 (18)	−0.0019 (16)	−0.0026 (15)	0.0127 (16)
N1	0.059 (3)	0.043 (2)	0.0177 (16)	0.0049 (19)	−0.0009 (16)	0.0040 (15)
N3	0.055 (2)	0.039 (2)	0.0259 (17)	0.0008 (18)	−0.0054 (17)	0.0031 (15)
N5	0.046 (2)	0.039 (2)	0.043 (2)	−0.0066 (18)	0.0049 (18)	−0.0002 (18)
C16	0.0237 (18)	0.030 (2)	0.043 (2)	0.0001 (15)	0.0066 (17)	0.0062 (18)
C15	0.0259 (19)	0.035 (2)	0.048 (3)	−0.0022 (16)	−0.0030 (18)	0.0068 (19)
C14	0.027 (2)	0.043 (3)	0.071 (4)	−0.0040 (18)	−0.008 (2)	0.004 (2)

C13	0.025 (2)	0.045 (3)	0.100 (5)	−0.004 (2)	0.006 (3)	0.005 (3)
C9	0.076 (4)	0.057 (3)	0.025 (2)	−0.007 (3)	0.020 (2)	−0.004 (2)
C8	0.081 (4)	0.051 (3)	0.021 (2)	−0.003 (3)	0.006 (2)	0.008 (2)
C19	0.045 (3)	0.066 (4)	0.068 (4)	0.018 (3)	0.000 (3)	−0.015 (3)
O13	0.094 (3)	0.070 (3)	0.052 (2)	−0.006 (3)	−0.020 (2)	0.035 (2)
O10	0.125 (5)	0.061 (3)	0.079 (4)	0.012 (3)	0.029 (3)	0.001 (3)

Geometric parameters (Å, °)

Sm1—O1	2.465 (3)	C5—C4	1.358 (9)
Sm1—O2	2.452 (3)	C5—H5	0.9300
Sm1—O3	2.801 (3)	C7—N1	1.267 (7)
Sm1—O4	2.795 (3)	C7—H7	0.9300
Sm1—O5	2.561 (3)	C10—H10	0.9300
Sm1—O6	2.586 (3)	C12—C13	1.359 (9)
Sm1—O8	2.465 (3)	C12—H12	0.9300
Sm1—O11	2.651 (3)	C17—H17A	0.9600
Sm1—O12	2.635 (4)	C17—H17B	0.9600
Sm1—O14	2.533 (3)	C17—H17C	0.9600
Ni1—N1	2.028 (4)	C4—H4	0.9300
Ni1—N2	2.078 (4)	C18—H18A	0.9600
Ni1—O1	2.021 (3)	C18—H18B	0.9600
Ni1—O2	2.015 (3)	C18—H18C	0.9600
Ni1—O9	2.003 (3)	O14—C19	1.424 (6)
O1—C1	1.324 (5)	O14—H14A	0.89 (2)
O5—N4	1.266 (6)	O11—N3	1.271 (6)
O2—C16	1.333 (5)	O9—N5	1.277 (5)
O3—C2	1.383 (5)	O8—N5	1.233 (5)
O3—C18	1.435 (6)	O12—N3	1.254 (5)
C1—C2	1.405 (6)	N1—C8	1.488 (6)
C1—C6	1.417 (6)	N3—O13	1.216 (5)
O6—N4	1.259 (6)	N5—O10	1.501 (7)
O4—C15	1.395 (6)	C16—C15	1.392 (7)
O4—C17	1.431 (6)	C15—C14	1.384 (6)
N2—C10	1.275 (7)	C14—C13	1.388 (9)
N2—C9	1.474 (6)	C14—H14	0.9300
C6—C5	1.407 (7)	C13—H13	0.9300
C6—C7	1.468 (7)	C9—C8	1.514 (9)
C11—C16	1.416 (6)	C9—H9A	0.9700
C11—C12	1.416 (7)	C9—H9B	0.9700
C11—C10	1.436 (8)	C8—H8A	0.9700
N4—O7	1.202 (6)	C8—H8B	0.9700
C3—C4	1.387 (8)	C19—H19A	0.9600
C3—C2	1.387 (6)	C19—H19B	0.9600
C3—H3	0.9300	C19—H19C	0.9600
O2—Sm1—O8	73.31 (11)	O7—N4—O5	121.5 (5)
O2—Sm1—O1	65.66 (10)	O6—N4—O5	116.6 (4)
O8—Sm1—O1	74.45 (11)	C4—C3—C2	119.7 (5)
O2—Sm1—O14	76.16 (11)	C4—C3—H3	120.1

O8—Sm1—O14	145.02 (11)	C2—C3—H3	120.1
O1—Sm1—O14	77.71 (10)	C4—C5—C6	121.2 (5)
O2—Sm1—O5	123.67 (11)	C4—C5—H5	119.4
O8—Sm1—O5	73.88 (12)	C6—C5—H5	119.4
O1—Sm1—O5	141.46 (11)	O3—C2—C3	124.6 (4)
O14—Sm1—O5	139.15 (12)	O3—C2—C1	113.8 (4)
O2—Sm1—O6	145.31 (12)	C3—C2—C1	121.6 (4)
O8—Sm1—O6	72.39 (12)	N1—C7—C6	124.7 (4)
O1—Sm1—O6	99.96 (11)	N1—C7—H7	117.6
O14—Sm1—O6	133.86 (12)	C6—C7—H7	117.6
O5—Sm1—O6	49.33 (11)	N2—C10—C11	124.4 (4)
O2—Sm1—O12	145.26 (11)	N2—C10—H10	117.8
O8—Sm1—O12	140.28 (12)	C11—C10—H10	117.8
O1—Sm1—O12	122.36 (11)	C13—C12—C11	121.9 (5)
O14—Sm1—O12	73.49 (12)	C13—C12—H12	119.1
O5—Sm1—O12	73.34 (12)	C11—C12—H12	119.1
O6—Sm1—O12	69.39 (12)	O4—C17—H17A	109.5
O2—Sm1—O11	105.22 (11)	O4—C17—H17B	109.5
O8—Sm1—O11	135.12 (12)	H17A—C17—H17B	109.5
O1—Sm1—O11	147.40 (11)	O4—C17—H17C	109.5
O14—Sm1—O11	69.69 (11)	H17A—C17—H17C	109.5
O5—Sm1—O11	70.53 (12)	H17B—C17—H17C	109.5
O6—Sm1—O11	102.54 (12)	C5—C4—C3	120.4 (5)
O12—Sm1—O11	47.97 (11)	C5—C4—H4	119.8
O2—Sm1—O4	58.64 (10)	C3—C4—H4	119.8
O8—Sm1—O4	80.30 (12)	O3—C18—H18A	109.5
O1—Sm1—O4	123.28 (10)	O3—C18—H18B	109.5
O14—Sm1—O4	98.07 (11)	H18A—C18—H18B	109.5
O5—Sm1—O4	71.65 (11)	O3—C18—H18C	109.5
O6—Sm1—O4	119.41 (11)	H18A—C18—H18C	109.5
O12—Sm1—O4	109.54 (11)	H18B—C18—H18C	109.5
O11—Sm1—O4	63.23 (11)	C19—O14—Sm1	122.9 (3)
O2—Sm1—O3	120.73 (10)	C19—O14—H14A	110 (4)
O8—Sm1—O3	106.34 (12)	Sm1—O14—H14A	125 (4)
O1—Sm1—O3	58.09 (9)	N3—O11—Sm1	97.1 (3)
O14—Sm1—O3	75.35 (11)	N5—O9—Ni1	118.6 (3)
O5—Sm1—O3	111.78 (11)	N5—O8—Sm1	147.5 (3)
O6—Sm1—O3	65.48 (11)	N3—O12—Sm1	98.3 (3)
O12—Sm1—O3	66.76 (10)	C7—N1—C8	120.9 (4)
O11—Sm1—O3	111.66 (10)	C7—N1—Ni1	128.6 (3)
O4—Sm1—O3	173.05 (11)	C8—N1—Ni1	109.8 (3)
O9—Ni1—O2	103.96 (13)	O13—N3—O12	122.3 (5)
O9—Ni1—O1	103.26 (13)	O13—N3—O11	121.0 (5)
O2—Ni1—O1	82.67 (12)	O12—N3—O11	116.7 (4)
O9—Ni1—N1	104.17 (15)	O8—N5—O9	124.0 (4)
O2—Ni1—N1	151.86 (16)	O8—N5—O10	118.4 (4)
O1—Ni1—N1	90.09 (15)	O9—N5—O10	117.5 (4)
O9—Ni1—N2	115.62 (15)	O2—C16—C15	118.3 (4)
O2—Ni1—N2	88.16 (15)	O2—C16—C11	123.1 (4)

O1—Ni1—N2	141.12 (15)	C15—C16—C11	118.5 (4)
N1—Ni1—N2	80.53 (18)	C14—C15—C16	122.4 (5)
C1—O1—Ni1	127.2 (3)	C14—C15—O4	124.0 (5)
C1—O1—Sm1	132.1 (3)	C16—C15—O4	113.6 (4)
Ni1—O1—Sm1	100.72 (12)	C15—C14—C13	118.7 (5)
N4—O5—Sm1	97.5 (3)	C15—C14—H14	120.6
C16—O2—Ni1	121.7 (3)	C13—C14—H14	120.6
C16—O2—Sm1	131.1 (3)	C12—C13—C14	120.5 (5)
Ni1—O2—Sm1	101.33 (11)	C12—C13—H13	119.7
C2—O3—C18	115.6 (4)	C14—C13—H13	119.7
C2—O3—Sm1	118.5 (3)	N2—C9—C8	108.9 (4)
C18—O3—Sm1	124.9 (3)	N2—C9—H9A	109.9
O1—C1—C2	117.3 (4)	C8—C9—H9A	109.9
O1—C1—C6	125.1 (4)	N2—C9—H9B	109.9
C2—C1—C6	117.5 (4)	C8—C9—H9B	109.9
N4—O6—Sm1	96.5 (3)	H9A—C9—H9B	108.3
C15—O4—C17	115.5 (4)	N1—C8—C9	107.0 (4)
C15—O4—Sm1	117.7 (3)	N1—C8—H8A	110.3
C17—O4—Sm1	126.8 (3)	C9—C8—H8A	110.3
C10—N2—C9	121.2 (4)	N1—C8—H8B	110.3
C10—N2—Ni1	125.6 (3)	C9—C8—H8B	110.3
C9—N2—Ni1	113.1 (3)	H8A—C8—H8B	108.6
C5—C6—C1	119.6 (5)	O14—C19—H19A	109.5
C5—C6—C7	116.3 (4)	O14—C19—H19B	109.5
C1—C6—C7	124.1 (4)	H19A—C19—H19B	109.5
C16—C11—C12	117.9 (5)	O14—C19—H19C	109.5
C16—C11—C10	124.6 (4)	H19A—C19—H19C	109.5
C12—C11—C10	117.5 (5)	H19B—C19—H19C	109.5
O7—N4—O6	121.9 (5)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O14—H14A···O9^{i}	0.89 (2)	1.82 (2)	2.691 (4)	166 (6)
C5—H5···O5^{ii}	0.93	2.57	3.432 (6)	155
C7—H7···O11^{ii}	0.93	2.47	3.379 (5)	164
C17—H17B···O5	0.96	2.51	3.186 (7)	128
C18—H18B···O12	0.96	2.40	3.011 (7)	121

Symmetry codes: (i) −*x*+3/2, *y*+1/2, −*z*+1/2; (ii) *x*+1/2, −*y*+1/2, *z*+1/2.

Fig. 1

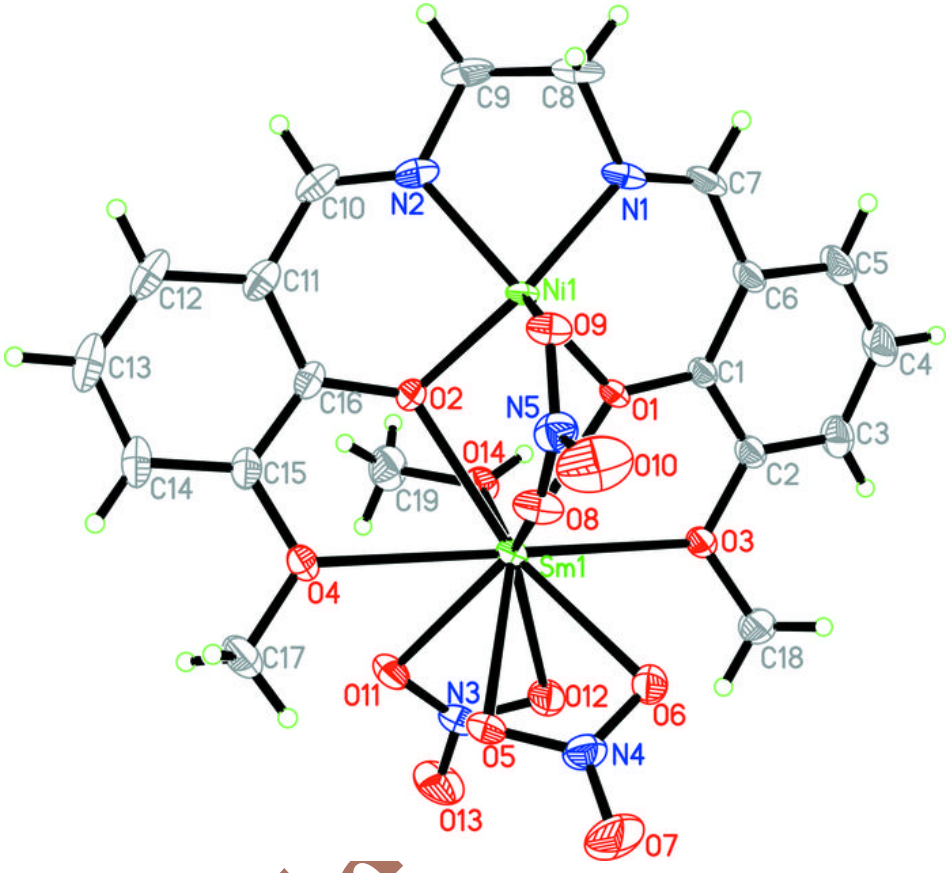

Fig. 2