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Retraction of articles by H. Zhong *et al.*

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A series of 41 papers by H. Zhong *et al.* are retracted.

As a result of problems with the data sets and incorrect atom assignments, 41 papers by H. Zhong *et al.* are retracted. Full details of all the articles are given in Table 1.

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

Title	Reference	DOI	Refcode
Aquachlorobis(1,10-phenanthroline)cobalt(II) chloride thiourea solvate	Zhong, Zeng, Liu & Luo (2006*a*)	10.1107/S1600536806041122	KERQEE
cis-Dichlorobis(1,10-phenanthroline)cobalt(II)	Zhong, Zeng & Luo (2006)	10.1107/S1600536806047295	MEQFOE
Tris(quinolin-8-olato-κ^2N,O)cobalt(III) glyoxal hemisolvate monohydrate	Zhong, Zeng, Liu & Luo (2006*b*)	10.1107/S1600536806050240	MEQHEW
(8-Quinolinol-κ^2N,O)bis(8-quinolinolato-κ^2N,O)nickel(II) glyoxal hemisolvate monohydrate	Zhong, Zeng, Liu & Luo (2007)	10.1107/S1600536806053232	METVUD
Aquachlorobis(1,10-phenanthroline)cobalt(II) chloride thioacetamide solvate	Zhong, Zeng & Luo (2007)	10.1107/S1600536806053530	METQIM
(8-Quinolinol-κ^2N,O)-bis(8-quinolinolato-κ^2N,O)zinc(II) glyoxal hemisolvate monohydrate	Zhong, Zeng, Luo, Li & Xiao (2007)	10.1107/S1600536807001171	DEXTEG
(Dimethylglyoxime-κ^2N,N')bis(1,10-phenanthroline-κ^2N,N')nickel(II) dinitrate dihydrate	Zhong, Zeng, Yang, Luo & Li (2007*a*)	10.1107/S1600536807004102	YEYGOZ
(Dimethylglyoxime-κ^2N,N')bis(1,10-phenanthroline-κ^2N,N')zinc(II) dinitrate dihydrate	Zhong, Zeng, Yang, Luo & Li (2007*b*)	10.1107/S1600536807004096	YEYGUF
Chloridobis(1,10-phenanthroline-$\kappa N,N'$)copper(I) hexahydrate	Zhong, Zeng, Yang, Luo & Xiao (2007)	10.1107/S160053680700791X	HEGKOU01
Tetrakis(pyridine-κN)bis(thiocyanato-κN)cobalt(II)	Zhong, Zeng, Yang & Luo (2007*a*)	10.1107/S1600536807017461	ITCPCO01
Tetrakis(pyridine-κN)bis(thiocyanato-κN)copper(II)	Zhong, Zeng, Yang & Luo (2007*b*)	10.1107/S160053680701879X	AVUJEG02
Tetrakis(nitrato-κ^2O,O')bis(4-phenylpyridine-κN)cerium(IV)	Zhong, Zeng, Yang & Luo (2007*c*)	10.1107/S1600536807018831	CICDOI
Bis(4,4′-bipyridine-κ^2N,N')tetrakis(nitrato-κ^2O,O')cerium(IV)	Zhong, Zeng, Yang & Luo (2007*d*)	10.1107/S1600536807021502	YIDNEF
(1,10-Phenanthroline)tris(phenoxyacetato)lanthanum(III)	Zhong, Zeng, Yang, Luo & Xu (2007)	10.1107/S1600536807027171	EDUROL
(1,10-Phenanthroline)tris(phenoxyacetato)cerium(III)	Zhong, Yang, Luo & Xu (2007*a*)	10.1107/S1600536807028061	EDUTUT
(1,10-Phenanthroline)tri(3-phenylpropanoato)lanthanum(III)	Zhong, Yang, Luo & Xu (2007*b*)	10.1107/S1600536807028693	RIGQEE
(1,10-Phenanthroline-κ^2N,N')tris(phenoxyacetato)-$\kappa O;\kappa O;\kappa O,O'$-neodymium(III)	Zhong, Yang, Luo & Xu (2007*c*)	10.1107/S1600536807030371	UDUMEM
Bis(2,2′-bipyridyl-κ^2N,N')bis(thiocyanato-κN)nickel(II)	Zhong, Yang, Luo & Xu (2007*d*)	10.1107/S1600536807031613	YEJGOJ01
Bis(2,2′-bipyridyl-κ^2N,N')bis(isothiocyanato-κN)copper(II)	Zhong, Yang, Luo & Xu (2007*e*)	10.1107/S1600536807033181	UFAPOH
Bis(2,2′-bipyridyl-κ^2N,N')bis(thiocyanato-κN)zinc(II)	Zhong, Yang, Luo & Xu (2007*f*)	10.1107/S1600536807035337	TIGFAR
(1,10-Phenanthroline-κ^2N,N')tris(3-phenylpropanoato-κO)neodymium(III)	Zhong, Yang, Luo & Xu (2007*g*)	10.1107/S1600536807035350	TIGFEV
2-Fluoro-3,5-dinitrobenzamide monohydrate	Zhong, Yang, Xie & Luo (2007*j*)	10.1107/S1600536807038676	VIKGAY
2-Fluoro-3,5-dinitrobenzoic acid-ammonia (1/1)	Zhong, Yang, Xie & Luo (2007*k*)	10.1107/S1600536807039724	KILKIA
1-Hydroxy-4,6-dinitropyridine-2-carboxamide monohydrate	Zhong, Yang, Xie & Luo (2007*l*)	10.1107/S1600536807040779	AFETAH
N-(2-Hydroxyphenyl)carbamic acid-ammonia (1/1)	Zhong, Yang, Xie & Luo (2007*m*)	10.1107/S160053680704086X	AFINAF
catena-Poly[[bis(μ-anilinoacetato-$\kappa^2O:O'$)bis(μ-anilinoacetato-$\kappa^3O,O':O$)bis[(1,10-phenanthroline-κ^2N,N')samarium(III)]-μ-anilinoacetato-$\kappa^2O:O'$]	Zhong, Yang, Xie & Luo (2007*a*)	10.1107/S1600536807043528	PILDAQ
2-Hydroxy-5-nitrobenzene-1,3-dicarboxylic acid monohydrate	Zhong, Yang, Xie & Luo (2007*n*)	10.1107/S1600536807045199	XILWIZ
catena-Poly[[tetra-μ-anilinoacetato-bis(1,10-phenanthroline)-dineodymium(III)]-di-μ-anilinoacetato]	Zhong, Yang, Xie & Luo (2007*b*)	10.1107/S1600536807048489	WIMWEV
Hexaaquacopper(II) bis(4-methylbenzenesulfonate)	Zhong, Yang, Xie & Luo (2007*c*)	10.1107/S1600536807049525	TOLSCV01

Table 1 (continued)

Title	Reference	DOI	Refcode
catena-Poly[[tetra-μ-anilinoacetato-bis(1,10-phenanthroline)-dilanthanum(III)]-di-μ-anilinoacetato]	Zhong, Yang, Xie & Luo (2007*d*)	10.1107/S1600536807051240	GIMZEI
Hexaaquachromium(II) bis(4-methylbenzenesulfonate)	Zhong, Yang, Xie & Luo (2007*e*)	10.1107/S1600536807051227	GIMZIM
Hexaaquamanganese(II) bis(4-methylbenzenesulfonate)	Zhong, Yang, Xie & Luo (2007*f*)	10.1107/S1600536807052051	QUKQES01
catena-Poly[[(acetato-κO)(1,10-phenanthroline-κ^2N,N')cobalt(II)]-μ-acetato-$\kappa^2O:O'$]	Zhong, Yang, Xie & Luo (2007*g*)	10.1107/S1600536807053494	NIQLAB
Hexaaquanickel(II) bis(4-aminobenzenesulfonate)	Zhong, Zhong, Xie & Luo (2007*a*)	10.1107/S1600536807054372	HIPZOW
catena-Poly[[(acetato-κO)(1,10-phenanthroline-κ^2N,N')copper(II)]-μ-acetato-$\kappa^2O:O'$]	Zhong, Yang, Xie & Luo (2007*h*)	10.1107/S160053680705622X	XIRGOV
Hexaaquazinc(II) bis(4-aminobenzenesulfonate)	Zhong, Zhong, Xie & Luo (2007*b*)	10.1107/S1600536807056498	XIRJEO
catena-Poly[[(acetato-κO)(1,10-phenanthroline-κ^2N,N')nickel(II)]-μ-acetato-$\kappa^2O:O'$]	Zhong, Yang, Xie & Luo (2007*i*)	10.1107/S1600536807058540	HIQJOH
Hexaaquacobalt(II) bis(4-aminobenzenesulfonate)	Zhong, Xie & Luo (2007)	10.1107/S1600536807058527	HIQJUN
catena-Poly[[tetra-μ-anilinoacetato-bis(1,10-phenanthroline)-dieuropium(III)]-di-μ-anilinoacetato]	Zhong, Yang, Duan & Hong (2007)	10.1107/S1600536807060643	YIQMAN
(Dimethylglyoxime-κ^2N,N')bis(1,10-phenanthroline-κ^2N,N')copper(II) dinitrate dihydrate	Zhong, Yang, Luo & Li (2007)	10.1107/S1600536807061193	YIQNUI
catena-Poly[[(1,10-phenanthroline-κ^2N,N')praseodymium(III)]-di-μ-phenoxyacetato-$\kappa^4O:O'$-[(1,10-phenanthroline-κ^2N,N')-praseodymium(III)]-di-μ-phenoxyacetato-$\kappa^4O:O'$-di-μ-phenoxyacetato-$\kappa^3O,O':O;\kappa^3O:O,O'$]	Zhong, Yang, Luo & Xu (2008)	10.1107/S1600536807068614	GISJIC

References

Zhong, H., Xie, H.-L. & Luo, C.-J. (2007). *Acta Cryst.* E**63**, m3054.
Zhong, H., Yang, X.-M., Duan, S.-H. & Hong, Y.-P. (2007). *Acta Cryst.* E**63**, m3142–m3143.
Zhong, H., Yang, X.-M., Luo, C.-J. & Li, M.-L. (2007). *Acta Cryst.* E**63**, m3160–m3161.
Zhong, H., Yang, X.-M., Luo, Q.-Y. & Xu, Y.-P. (2007*a*). *Acta Cryst.* E**63**, m1885–m1886.
Zhong, H., Yang, X.-M., Luo, Q.-Y. & Xu, Y.-P. (2007*b*). *Acta Cryst.* E**63**, m1909.
Zhong, H., Yang, X.-M., Luo, Q.-Y. & Xu, Y.-P. (2007*c*). *Acta Cryst.* E**63**, m2019.
Zhong, H., Yang, X.-M., Luo, Q.-Y. & Xu, Y.-P. (2007*d*). *Acta Cryst.* E**63**, m2062.
Zhong, H., Yang, X.-M., Luo, Q.-Y. & Xu, Y.-P. (2007*e*). *Acta Cryst.* E**63**, m2141.
Zhong, H., Yang, X.-M., Luo, Q.-Y. & Xu, Y.-P. (2007*f*). *Acta Cryst.* E**63**, m2208.
Zhong, H., Yang, X.-M., Luo, Q.-Y. & Xu, Y.-P. (2007*g*). *Acta Cryst.* E**63**, m2209–m2210.
Zhong, H., Yang, X.-M., Luo, Q.-Y. & Xu, Y.-P. (2008). *Acta Cryst.* E**64**, m317–m318.
Zhong, H., Yang, X.-M., Xie, H.-L. & Luo, C.-J. (2007*a*). *Acta Cryst.* E**63**, m2508–m2509.
Zhong, H., Yang, X.-M., Xie, H.-L. & Luo, C.-J. (2007*b*). *Acta Cryst.* E**63**, m2680–m2681.
Zhong, H., Yang, X.-M., Xie, H.-L. & Luo, C.-J. (2007*c*). *Acta Cryst.* E**63**, m2724–m2725.
Zhong, H., Yang, X.-M., Xie, H.-L. & Luo, C.-J. (2007*d*). *Acta Cryst.* E**63**, m2772–m2773.
Zhong, H., Yang, X.-M., Xie, H.-L. & Luo, C.-J. (2007*e*). *Acta Cryst.* E**63**, m2774.
Zhong, H., Yang, X.-M., Xie, H.-L. & Luo, C.-J. (2007*f*). *Acta Cryst.* E**63**, m2825.
Zhong, H., Yang, X.-M., Xie, H.-L. & Luo, C.-J. (2007*g*). *Acta Cryst.* E**63**, m2895–m2896.
Zhong, H., Yang, X.-M., Xie, H.-L. & Luo, C.-J. (2007*h*). *Acta Cryst.* E**63**, m2979.
Zhong, H., Yang, X.-M., Xie, H.-L. & Luo, C.-J. (2007*i*). *Acta Cryst.* E**63**, m3053.
Zhong, H., Yang, X.-M., Xie, H.-L. & Luo, C.-J. (2007*j*). *Acta Cryst.* E**63**, o3780.
Zhong, H., Yang, X.-M., Xie, H.-L. & Luo, C.-J. (2007*k*). *Acta Cryst.* E**63**, o3831.
Zhong, H., Yang, X.-M., Xie, H.-L. & Luo, C.-J. (2007*l*). *Acta Cryst.* E**63**, o3881.
Zhong, H., Yang, X.-M., Xie, H.-L. & Luo, C.-J. (2007*m*). *Acta Cryst.* E**63**, o3882.
Zhong, H., Yang, X.-M., Xie, H.-L. & Luo, C.-J. (2007*n*). *Acta Cryst.* E**63**, o4191.
Zhong, H., Zeng, X.-R., Liu, Y.-Q. & Luo, Q.-Y. (2006*a*). *Acta Cryst.* E**62**, m2925–m2927.
Zhong, H., Zeng, X.-R., Liu, Y.-Q. & Luo, Q.-Y. (2006*b*). *Acta Cryst.* E**62**, m3557–m3559.
Zhong, H., Zeng, X.-R., Liu, Y.-Q. & Luo, Q.-Y. (2007). *Acta Cryst.* E**63**, m187–m189.
Zhong, H., Zeng, X.-R. & Luo, Q.-Y. (2006). *Acta Cryst.* E**62**, m3330–m3332.
Zhong, H., Zeng, X.-R. & Luo, Q.-Y. (2007). *Acta Cryst.* E**63**, m221–m223.
Zhong, H., Zeng, X.-R., Luo, Q.-Y., Li, M.-L. & Xiao, S.-Z. (2007). *Acta Cryst.* E**63**, m492–m494.
Zhong, H., Zeng, X.-R., Yang, X.-M. & Luo, Q.-Y. (2007*a*). *Acta Cryst.* E**63**, m1379.
Zhong, H., Zeng, X.-R., Yang, X.-M. & Luo, Q.-Y. (2007*b*). *Acta Cryst.* E**63**, m1445.
Zhong, H., Zeng, X.-R., Yang, X.-M. & Luo, Q.-Y. (2007*c*). *Acta Cryst.* E**63**, m1455.
Zhong, H., Zeng, X.-R., Yang, X.-M. & Luo, Q.-Y. (2007*d*). *Acta Cryst.* E**63**, m1592–m1593.
Zhong, H., Zeng, X.-R., Yang, X.-M., Luo, Q.-Y. & Li, M.-L. (2007*a*). *Acta Cryst.* E**63**, m639–m641.
Zhong, H., Zeng, X.-R., Yang, X.-M., Luo, Q.-Y. & Li, M.-L. (2007*b*). *Acta Cryst.* E**63**, m642–m644.
Zhong, H., Zeng, X.-R., Yang, X.-M., Luo, Q.-Y. & Xiao, S.-Z. (2007). *Acta Cryst.* E**63**, m826–m828.
Zhong, H., Zeng, X.-R., Yang, X.-M., Luo, Q.-Y. & Xu, Y.-P. (2007). *Acta Cryst.* E**63**, m1868–m1869.
Zhong, H., Zhong, Q. Y., Xie, H.-L. & Luo, C.-J. (2007*a*). *Acta Cryst.* E**63**, m2913–m2914.
Zhong, H., Zhong, Q.-Y., Xie, H.-L. & Luo, C.-J. (2007*b*). *Acta Cryst.* E**63**, m2990.

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catena-Poly[[bis(μ-anilinoacetato-κ^2O:O')bis(μ-anilinoacetato-κ^3O,O':O)-bis[(1,10-phenanthroline-κ^2N,N')-samarium(III)]-μ-anilinoacetato-κ^2O:O']

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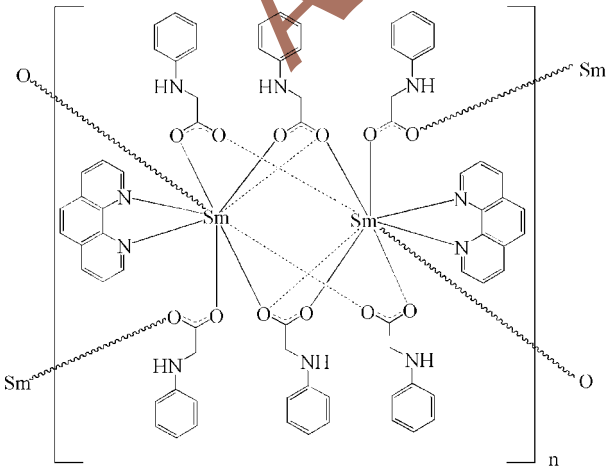
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.013 Å; R factor = 0.050; wR factor = 0.152; data-to-parameter ratio = 18.7.

In the crystal structure of the title compound, $[Sm_2(C_8H_8NO_2)_6(C_{12}H_8N_2)_2]_n$, the Sm^{III} atoms are bridged by two terdentate, two bidentate and four mondentate carboxylate groups with an inversion centre between the two Sm^{III} ions. Each Sm atom is nine-coordinated by two N atoms of 1,10-phenanthroline and seven O atoms of four anilinoacetate ligands. In the crystal structure, the chains are linked by hydrogen bonds into a polymeric ribbon structure.

Related literature

For related literature, see: Allen *et al.* (1987); Daiguebonne *et al.* (2000); Farrugia *et al.* (2000); Kay *et al.* (1972); Ma *et al.* (1999); Mao *et al.* (1998); Starynowicz (1991, 1993); Tsukube & Shinoda (2002); Zhang *et al.* (2005); Zeng *et al.* (2000).



Experimental

Crystal data

$[Sm_2(C_8H_8NO_2)_6(C_{12}H_8N_2)_2]$
M_r = 1562.04
Monoclinic, $P2_1/n$
a = 19.998 (3) Å
b = 8.498 (2) Å
c = 20.783 (2) Å
β = 106.998 (5)°
V = 3377.7 (10) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.79 mm^{-1}
T = 273 (2) K
0.33 × 0.12 × 0.08 mm

Data collection

Bruker APEX II area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.590, T_{max} = 0.871
27195 measured reflections
7519 independent reflections
4974 reflections with $I > 2\sigma(I)$
R_{int} = 0.043

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.152
S = 0.98
7519 reflections
403 parameters
3 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.54 e Å^{-3}
$\Delta\rho_{min}$ = −0.81 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Sm1—O1	2.559 (3)	Sm1—O5	2.414 (3)
Sm1—O2	2.822 (4)	Sm1—O6^{ii}	2.537 (4)
Sm1—O2^{i}	2.421 (4)	Sm1—N1	2.728 (4)
Sm1—O3	2.480 (3)	Sm1—N2	2.710 (4)
Sm1—O4^{i}	2.533 (3)		
O1—Sm1—O2	48.11 (10)	O3—Sm1—N1	127.29 (13)
O1—Sm1—O3	73.35 (12)	O5—Sm1—N1	77.22 (13)
O1—Sm1—O5	139.14 (12)	O1—Sm1—N2	74.31 (12)
O2—Sm1—O3	65.25 (11)	O2—Sm1—N2	118.35 (11)
O2—Sm1—O5	139.49 (11)	O3—Sm1—N2	80.65 (13)
O3—Sm1—O5	145.83 (12)	O5—Sm1—N2	96.87 (12)
O1—Sm1—N1	63.68 (12)	N1—Sm1—N2	60.01 (14)
O2—Sm1—N1	102.42 (13)		

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

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

D—H···A	D—H	H···A	D···A	D—H···A
N5—H5···O6	0.86	2.32	2.658 (5)	103
N3—H3A···O4	0.86	2.27	2.628 (5)	105
C22—H22B···O5^{iii}	0.97	2.40	3.345 (7)	163
C12—H12···N5^{ii}	0.93	2.60	3.441 (8)	151
C12—H12···O6^{ii}	0.93	2.47	3.059 (8)	121
C10—H10···O1^{iv}	0.93	2.35	3.218 (7)	156
C1—H1···O4^{i}	0.93	2.41	3.108 (8)	132

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1996); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2392).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Bruker (2005). *APEX2*. Bruker AXS Inc., Madison, Wisconsin, USA.
Daiguebonne, C., Guillou, O. & Boubekeur, K. (2000). *Inorg. Chim. Acta*, **304**, 161–169.
Farrugia, L. J., Peacock, R. D. & Stewart, B. (2000). *Acta Cryst.* C**56**, e435–e436.
Kay, J., Moore, J. W. & Glick, M. D. (1972). *Inorg. Chem.* **11**, 2818–2827.
Ma, L., Evans, O. R., Foxman, B. M. & Lin, W. B. (1999). *Inorg. Chem.* **38**, 5837–5840.
Mao, J. G., Zhang, H. J., Ni, J. Z., Wang, S. B. & Mak, T. C. W. (1998). *J. Chem. Crystallogr.* **17**, 3999–4009.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Siemens (1996). *SAINT* and *SHELXTL*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Starynowicz, P. (1991). *Acta Cryst.* C**47**, 294–297.
Starynowicz, P. (1993). *Acta Cryst.* C**49**, 1895–1897.
Tsukube, H. & Shinoda, S. (2002). *Chem. Rev.* **102**, 2389–2404.
Zeng, X.-R., Xu, Y., Xiong, R.-G., Zhang, L.-J. & You, X.-Z. (2000). *Acta Cryst.* C**56**, e325–e326.
Zhang, Z.-H., Shen, Z.-L., Okamura, T.-A., Zhu, H.-F., Sun, W.-Y. & Ueyama, N. (2005). *Cryst. Growth Des.* **5**, 1191–1197.

supplementary materials

Acta Cryst. (2007). E**63**, m2508-m2509 [**doi:10.1107/S1600536807043528**]

catena-Poly[[bis(μ-anilinoacetato-κ^2O:O')bis(μ-anilinoacetato-κ^3O,O':O)bis[(1,10-phenanthroline-κ^2N,N')samarium(III)]-μ-anilinoacetato-κ^2O:O']

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Comment

In recent years, there has been great interest in the synthesis of metal organic frameworks (MOFs) with organic ligands and rare earth metals because of their novel structures, fascinating properties and important roles in special materials having optical, electronic, magnetic and biological importance potential applications (Daiguebonne *et al.*, 2000; Farrugia *et al.*, 2000; Tsukube & Shinoda, 2002; Zhang *et al.*, 2005). These compounds are usually prepared by the reaction of rare-earth metal ions with bi- or multidentate ligands (Starynowicz, 1991, 1993; Kay *et al.*, 1972; Ma *et al.*, 1999; Zeng *et al.*, 2000; Mao *et al.*, 1998). We report herein the crystal structure of the title compound, (I).

In the molecule of (I) (Fig. 1), the ligand bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The title compound, $[Sm_2(C_8H_8NO_2)_6(C_{12}H_8N_2)_2]_n$, which are the metal organic framework synthesized by the anilinoacetate ligand and the rare earth metal Sm, are bridged by two terdentate, two bidentate and four mondentate carboxyl groups with an inversion centre between the two Sm^{III} ions. Each Sm atom is nine-coordinated by two N atoms of 1,10-phenanthroline (phen) ligand and seven O atoms of four anilinoacetate ligands (Table 1). The Sm—O bond lengths are in the range 2.414 (3) to 2.822 (4) Å. The Sm—N bond lengths are in the range 2.710 (4) to 2.728 (4) Å. In the crystal structure, N—H···O, C—H···N and C—H···O hydrogen bonds (Fig. 2 and Table 2) seem to be effective in the stabilization of the structure, resulting in the formation of a supramolecular network structure.

Experimental

Crystals of the title compound (I) were synthesized using hydrothermal method in a 23 ml Teflon-lined Parr bomb, which was then sealed. Samarium (III) nitrate hexahydrate (218.5 mg, 0.5 mmol), phen (198 mg, 1 mmol), anilinoacetic acid (146.2 mg, 1 mmol), ammonia (0.5 mol/l, 2 ml) and distilled water (6 g) were placed into the bomb and sealed. The bomb was then heated under autogenous pressure up to 423 K over the course of 7 d and allowed to cool at room temperature for 24 h. Upon opening the bomb, a clear colourless solution was decanted from small colorless crystals. These crystals were washed with distilled water followed by ethanol, and allowed to air-dry at room temperature.

Refinement

The H atoms were positioned geometrically, with N— H = 0.86 Å (for NH) and C—H = 0.93 − 0.97 Å (for CH), and constrained to ride on their parent atoms, with U_{iso}(H) = xU_{eq}(C, N), where x = 1.2 for aromatic H atoms and x = 1.5 for all other H atoms.

Figures

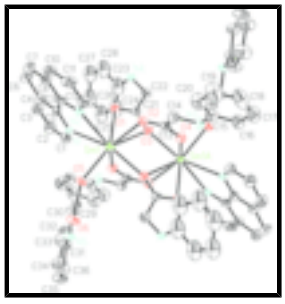

Fig. 1. The structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level [symmetry code (A): $2-x, -y, 2-z$]. All H atoms have been omitted for clarity.

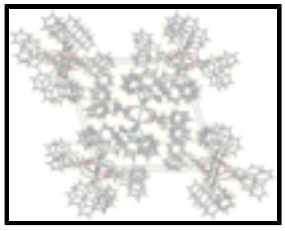

Fig. 2. A packing diagram of (I). Hydrogen bonds are shown as dashed lines.

catena-Poly[[bis(μ-anilinoacetato-κ^2*O*:*O*')bis(μ-\ anilinoacetato-κ^3*O*,*O*':*O*)bis[(1,10-phenanthroline-\ κ^2*N*,*N*')samarium(III)]- bis-(μ-anilinoacetato-κ^2*O*:*O*')]

Crystal data

$[Sm_2(C_8H_8NO_2)_6(C_{12}H_8N_2)_2]$	F_{000} = 1572
M_r = 1562.04	D_x = 1.536 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 8997 reflections
a = 19.998 (3) Å	θ = 2.7–26.7º
b = 8.498 (2) Å	μ = 1.79 mm^{-1}
c = 20.783 (2) Å	T = 273 (2) K
β = 106.998 (5)º	Plane, colourless
V = 3377.7 (10) Å^3	0.33 × 0.12 × 0.08 mm
Z = 2	

Data collection

Bruker APEX II area-detector diffractometer	7519 independent reflections
Radiation source: fine-focus sealed tube	4974 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.043
T = 273(2) K	θ_{max} = 27.4º
φ and ω scans	θ_{min} = 2.1º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −25→25
T_{min} = 0.590, T_{max} = 0.871	k = −10→11
27195 measured reflections	l = −26→26

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.050$

$wR(F^2) = 0.152$

$S = 0.98$

7519 reflections

403 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-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.1002P)^2 + 0.285P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.002$

$\Delta\rho_{max} = 1.54$ e Å^{-3}

$\Delta\rho_{min} = -0.81$ e Å^{-3}

Extinction correction: none

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	0.931196 (13)	0.19068 (3)	0.964300 (12)	0.03994 (12)
O1	0.84626 (17)	−0.0361 (4)	0.91902 (17)	0.0413 (8)
O2	0.94708 (19)	−0.1388 (5)	0.97740 (18)	0.0480 (9)
O3	0.97071 (19)	0.0614 (4)	0.87480 (17)	0.0447 (8)
O4	1.06691 (19)	−0.0829 (4)	0.92152 (17)	0.0473 (9)
O5	0.94009 (19)	0.4211 (4)	1.03423 (17)	0.0447 (8)
O6	1.0073 (2)	0.6128 (5)	1.09082 (17)	0.0531 (10)
N1	0.7968 (2)	0.2338 (6)	0.9669 (2)	0.0444 (10)
N2	0.8342 (3)	0.3067 (5)	0.8547 (2)	0.0451 (11)
N3	1.1177 (2)	−0.0164 (5)	0.8215 (2)	0.0481 (11)
H3A	1.1390	−0.0746	0.8551	0.058*
N4	0.7857 (2)	−0.3269 (5)	0.8983 (2)	0.0447 (11)
H4	0.7628	−0.3419	0.8568	0.054*
N5	0.9861 (2)	0.5266 (5)	1.20625 (19)	0.0436 (11)
H5	1.0160	0.5982	1.2047	0.052*
C1	0.7787 (3)	0.1908 (7)	1.0198 (3)	0.0606 (17)
H1	0.8137	0.1676	1.0592	0.073*

C2	0.7093 (4)	0.1781 (9)	1.0197 (4)	0.080 (2)
H2	0.6981	0.1487	1.0584	0.097*
C3	0.6582 (4)	0.2099 (9)	0.9616 (5)	0.086 (3)
H3	0.6115	0.1989	0.9603	0.103*
C4	0.6742 (4)	0.2571 (10)	0.9056 (4)	0.0717 (19)
C5	0.7467 (3)	0.2673 (7)	0.9095 (3)	0.0508 (14)
C6	0.6212 (5)	0.2936 (13)	0.8394 (6)	0.115 (4)
H6	0.5738	0.2819	0.8348	0.137*
C7	0.6416 (5)	0.3427 (12)	0.7869 (5)	0.098 (3)
H7	0.6080	0.3702	0.7471	0.118*
C8	0.7132 (4)	0.3537 (9)	0.7906 (3)	0.0653 (18)
C9	0.7671 (3)	0.3102 (6)	0.8507 (3)	0.0499 (14)
C10	0.7358 (5)	0.4034 (9)	0.7370 (3)	0.086 (2)
H10	0.7034	0.4381	0.6977	0.103*
C11	0.8045 (5)	0.4019 (9)	0.7413 (3)	0.078 (2)
H11	0.8197	0.4354	0.7054	0.094*
C12	0.8524 (4)	0.3491 (7)	0.8008 (3)	0.0611 (17)
H12	0.8994	0.3434	0.8026	0.073*
C13	1.0287 (3)	0.0024 (6)	0.8770 (2)	0.0408 (12)
C14	1.0520 (3)	0.0521 (7)	0.8172 (3)	0.0525 (14)
H14A	1.0178	0.0188	0.7760	0.063*
H14B	1.0557	0.1658	0.8164	0.063*
C15	1.1463 (3)	0.0134 (8)	0.7697 (3)	0.0604 (16)
C16	1.2074 (4)	−0.0576 (10)	0.7761 (4)	0.074 (2)
H16	1.2277	−0.1203	0.8134	0.089*
C17	1.2401 (4)	−0.0366 (11)	0.7264 (5)	0.090 (2)
H17	1.2833	−0.0832	0.7308	0.108*
C18	1.2091 (6)	0.0522 (10)	0.6712 (5)	0.104 (3)
H18	1.2311	0.0634	0.6376	0.125*
C19	1.1481 (6)	0.1232 (12)	0.6642 (5)	0.106 (3)
H19	1.1275	0.1836	0.6263	0.128*
C20	1.1148 (4)	0.1056 (10)	0.7154 (4)	0.082 (2)
H20	1.0725	0.1555	0.7122	0.098*
C21	0.8834 (3)	−0.1514 (7)	0.9387 (2)	0.0417 (12)
C22	0.8569 (3)	−0.3142 (6)	0.9196 (3)	0.0534 (15)
H22A	0.8754	−0.3514	0.8841	0.064*
H22B	0.8748	−0.3826	0.9582	0.064*
C23	0.7543 (7)	−0.3144 (10)	0.9466 (8)	0.1220 (17)
C24	0.7823 (7)	−0.2775 (10)	1.0106 (7)	0.1220 (17)
H24	0.8300	−0.2575	1.0267	0.146*
C25	0.7405 (6)	−0.2680 (12)	1.0550 (7)	0.1220 (17)
H25	0.7600	−0.2440	1.1003	0.146*
C26	0.6741 (7)	−0.2941 (11)	1.0303 (7)	0.1220 (17)
H26	0.6472	−0.2847	1.0597	0.146*
C27	0.6369 (7)	−0.3372 (11)	0.9601 (7)	0.1220 (17)
H27	0.5893	−0.3591	0.9448	0.146*
C28	0.6792 (6)	−0.3411 (12)	0.9210 (7)	0.1220 (17)
H28	0.6599	−0.3618	0.8754	0.146*
C29	0.9695 (3)	0.4988 (6)	1.0865 (3)	0.0414 (12)

C30	0.9487 (3)	0.4451 (7)	1.1472 (3)	0.0536 (14)
H30A	0.8990	0.4623	1.1392	0.064*
H30B	0.9576	0.3331	1.1537	0.064*
C31	0.9739 (3)	0.4896 (7)	1.2654 (3)	0.0531 (14)
C32	0.9277 (4)	0.3796 (9)	1.2718 (3)	0.0679 (19)
H32	0.9015	0.3244	1.2342	0.081*
C33	0.9192 (6)	0.3492 (13)	1.3339 (5)	0.106 (3)
H33	0.8883	0.2713	1.3385	0.127*
C34	0.9573 (5)	0.4356 (12)	1.3906 (4)	0.099 (3)
H34	0.9497	0.4199	1.4322	0.119*
C35	1.0045 (4)	0.5409 (10)	1.3836 (3)	0.086 (2)
H35	1.0312	0.5954	1.4212	0.103*
C36	1.0143 (4)	0.5699 (9)	1.3219 (3)	0.0692 (18)
H36	1.0477	0.6425	1.3179	0.083*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sm1	0.04626 (18)	0.03404 (18)	0.03452 (17)	−0.00154 (11)	0.00400 (11)	0.00062 (11)
O1	0.0414 (18)	0.0306 (19)	0.045 (2)	0.0002 (15)	0.0011 (15)	−0.0031 (15)
O2	0.046 (2)	0.047 (2)	0.043 (2)	−0.0021 (18)	0.0004 (16)	0.0087 (17)
O3	0.054 (2)	0.043 (2)	0.0378 (19)	0.0038 (18)	0.0138 (16)	0.0029 (16)
O4	0.057 (2)	0.046 (2)	0.040 (2)	0.0070 (18)	0.0157 (17)	0.0103 (17)
O5	0.063 (2)	0.0307 (19)	0.0391 (19)	−0.0050 (17)	0.0125 (16)	−0.0051 (15)
O6	0.077 (3)	0.049 (2)	0.0344 (19)	−0.024 (2)	0.0176 (18)	−0.0038 (17)
N1	0.043 (2)	0.038 (2)	0.045 (3)	0.003 (2)	0.002 (2)	−0.008 (2)
N2	0.057 (3)	0.038 (3)	0.032 (2)	0.002 (2)	−0.0015 (19)	0.0013 (18)
N3	0.048 (2)	0.063 (3)	0.039 (2)	0.018 (2)	0.022 (2)	0.023 (2)
N4	0.040 (2)	0.032 (3)	0.051 (3)	−0.0124 (18)	−0.003 (2)	−0.0068 (19)
N5	0.063 (3)	0.041 (3)	0.028 (2)	−0.028 (2)	0.0153 (19)	−0.0057 (17)
C1	0.052 (3)	0.072 (5)	0.056 (4)	0.007 (3)	0.014 (3)	−0.004 (3)
C2	0.057 (4)	0.108 (7)	0.081 (5)	0.001 (4)	0.029 (4)	−0.014 (4)
C3	0.046 (4)	0.090 (7)	0.118 (8)	−0.004 (4)	0.018 (4)	−0.013 (5)
C4	0.052 (4)	0.080 (5)	0.070 (5)	0.005 (4)	−0.002 (3)	−0.017 (4)
C5	0.051 (3)	0.033 (3)	0.059 (4)	0.008 (2)	0.001 (3)	−0.009 (3)
C6	0.052 (5)	0.152 (11)	0.109 (8)	0.019 (5)	−0.024 (5)	−0.037 (7)
C7	0.080 (6)	0.110 (7)	0.073 (6)	0.037 (5)	−0.027 (4)	−0.012 (5)
C8	0.067 (4)	0.063 (4)	0.045 (4)	0.018 (3)	−0.016 (3)	−0.008 (3)
C9	0.057 (3)	0.032 (3)	0.045 (3)	0.005 (2)	−0.009 (3)	−0.004 (2)
C10	0.119 (7)	0.065 (5)	0.046 (4)	0.015 (5)	−0.019 (4)	−0.002 (3)
C11	0.114 (6)	0.075 (5)	0.034 (3)	−0.001 (5)	0.003 (4)	0.011 (3)
C12	0.076 (4)	0.049 (4)	0.048 (4)	−0.003 (3)	0.003 (3)	0.008 (3)
C13	0.050 (3)	0.033 (3)	0.038 (3)	−0.008 (2)	0.010 (2)	−0.002 (2)
C14	0.063 (3)	0.053 (4)	0.043 (3)	0.005 (3)	0.019 (3)	0.010 (3)
C15	0.066 (4)	0.066 (4)	0.055 (4)	−0.009 (3)	0.027 (3)	0.002 (3)
C16	0.075 (5)	0.092 (5)	0.067 (4)	0.005 (4)	0.037 (4)	−0.001 (4)
C17	0.082 (5)	0.094 (7)	0.109 (7)	−0.009 (5)	0.053 (5)	−0.011 (5)
C18	0.138 (8)	0.077 (6)	0.138 (9)	−0.014 (6)	0.104 (7)	−0.002 (6)

C19	0.153 (9)	0.103 (7)	0.089 (6)	0.015 (7)	0.077 (6)	0.031 (5)
C20	0.098 (6)	0.087 (6)	0.077 (5)	0.001 (5)	0.053 (4)	0.020 (4)
C21	0.044 (3)	0.047 (3)	0.029 (2)	−0.006 (2)	0.004 (2)	−0.004 (2)
C22	0.059 (4)	0.045 (4)	0.052 (3)	0.003 (3)	0.010 (3)	−0.007 (3)
C23	0.134 (4)	0.086 (3)	0.169 (5)	0.015 (3)	0.079 (4)	0.031 (3)
C24	0.134 (4)	0.086 (3)	0.169 (5)	0.015 (3)	0.079 (4)	0.031 (3)
C25	0.134 (4)	0.086 (3)	0.169 (5)	0.015 (3)	0.079 (4)	0.031 (3)
C26	0.134 (4)	0.086 (3)	0.169 (5)	0.015 (3)	0.079 (4)	0.031 (3)
C27	0.134 (4)	0.086 (3)	0.169 (5)	0.015 (3)	0.079 (4)	0.031 (3)
C28	0.134 (4)	0.086 (3)	0.169 (5)	0.015 (3)	0.079 (4)	0.031 (3)
C29	0.055 (3)	0.030 (3)	0.038 (3)	−0.001 (2)	0.012 (2)	0.003 (2)
C30	0.073 (4)	0.049 (3)	0.040 (3)	−0.021 (3)	0.018 (3)	−0.005 (2)
C31	0.072 (4)	0.052 (4)	0.033 (3)	−0.001 (3)	0.014 (3)	0.003 (2)
C32	0.071 (4)	0.088 (5)	0.046 (3)	−0.034 (4)	0.019 (3)	−0.006 (3)
C33	0.124 (8)	0.134 (8)	0.075 (6)	−0.049 (7)	0.053 (6)	0.002 (5)
C34	0.118 (7)	0.143 (8)	0.044 (4)	−0.029 (6)	0.034 (4)	0.005 (5)
C35	0.112 (6)	0.100 (6)	0.040 (4)	−0.020 (5)	0.013 (4)	−0.008 (4)
C36	0.079 (4)	0.073 (5)	0.052 (4)	−0.018 (4)	0.013 (3)	−0.012 (3)

Geometric parameters (Å, °)

Sm1—O1	2.559 (3)	C10—H10	0.9300
Sm1—O2	2.822 (4)	C11—C12	1.398 (9)
Sm1—O2^{i}	2.421 (4)	C11—H11	0.9300
Sm1—O3	2.480 (3)	C12—H12	0.9300
Sm1—O4^{i}	2.533 (3)	C13—C14	1.509 (7)
Sm1—O5	2.414 (3)	C14—H14A	0.9700
Sm1—O6^{ii}	2.537 (4)	C14—H14B	0.9700
Sm1—N1	2.728 (4)	C15—C16	1.334 (9)
Sm1—N2	2.710 (4)	C15—C20	1.366 (10)
O1—C21	1.225 (6)	C16—C17	1.386 (11)
O2—C21	1.297 (6)	C16—H16	0.9300
O2—Sm1^{i}	2.421 (4)	C17—C18	1.363 (13)
O3—C13	1.252 (6)	C17—H17	0.9300
O4—C13	1.247 (6)	C18—C19	1.331 (12)
O4—Sm1^{i}	2.533 (3)	C18—H18	0.9300
O5—C29	1.260 (6)	C19—C20	1.419 (10)
O6—C29	1.215 (6)	C19—H19	0.9300
O6—Sm1^{ii}	2.537 (4)	C20—H20	0.9300
N1—C1	1.307 (8)	C21—C22	1.493 (8)
N1—C5	1.345 (7)	C22—H22A	0.9700
N2—C9	1.321 (8)	C22—H22B	0.9700
N2—C12	1.326 (8)	C23—C24	1.320 (17)
N3—C15	1.383 (7)	C23—C28	1.457 (17)
N3—C14	1.415 (7)	C24—C25	1.418 (14)
N3—H3A	0.8600	C24—H24	0.9300
N4—C23	1.337 (13)	C25—C26	1.293 (16)
N4—C22	1.365 (7)	C25—H25	0.9300

N4—H4	0.8600	C26—C27	1.478 (17)
N5—C31	1.359 (7)	C26—H26	0.9300
N5—C30	1.418 (6)	C27—C28	1.332 (14)
N5—H5	0.8600	C27—H27	0.9300
C1—C2	1.390 (9)	C28—H28	0.9300
C1—H1	0.9300	C29—C30	1.511 (7)
C2—C3	1.363 (12)	C30—H30A	0.9700
C2—H2	0.9300	C30—H30B	0.9700
C3—C4	1.354 (12)	C31—C32	1.347 (8)
C3—H3	0.9300	C31—C36	1.395 (8)
C4—C5	1.431 (9)	C32—C33	1.375 (10)
C4—C6	1.504 (12)	C32—H32	0.9300
C5—C9	1.443 (9)	C33—C34	1.407 (12)
C6—C7	1.338 (14)	C33—H33	0.9300
C6—H6	0.9300	C34—C35	1.340 (11)
C7—C8	1.414 (12)	C34—H34	0.9300
C7—H7	0.9300	C35—C36	1.374 (10)
C8—C10	1.385 (11)	C35—H35	0.9300
C8—C9	1.440 (8)	C36—H36	0.9300
C10—C11	1.350 (11)		
O1—Sm1—O2	48.11 (10)	C8—C10—H10	119.7
O1—Sm1—O3	73.35 (12)	C10—C11—C12	118.9 (7)
O1—Sm1—O5	139.14 (12)	C10—C11—H11	120.5
O2—Sm1—O3	65.25 (11)	C12—C11—H11	120.5
O2—Sm1—O5	139.49 (11)	N2—C12—C11	123.2 (7)
O3—Sm1—O5	145.83 (12)	N2—C12—H12	118.4
O1—Sm1—N1	63.68 (12)	C11—C12—H12	118.4
O2—Sm1—N1	102.42 (13)	O4—C13—O3	128.3 (5)
O3—Sm1—N1	127.29 (13)	O4—C13—C14	120.2 (5)
O5—Sm1—N1	77.22 (13)	O3—C13—C14	111.4 (4)
O1—Sm1—N2	74.31 (12)	N3—C14—C13	109.8 (4)
O2—Sm1—N2	118.35 (11)	N3—C14—H14A	109.7
O3—Sm1—N2	80.65 (13)	C13—C14—H14A	109.7
O5—Sm1—N2	96.87 (12)	N3—C14—H14B	109.7
N1—Sm1—N2	60.01 (14)	C13—C14—H14B	109.7
O5—Sm1—O2^{i}	87.71 (14)	H14A—C14—H14B	108.2
O2^{i}—Sm1—O3	78.49 (12)	C16—C15—C20	122.1 (6)
O5—Sm1—O4^{i}	75.58 (12)	C16—C15—N3	114.5 (6)
O2^{i}—Sm1—O4^{i}	74.21 (12)	C20—C15—N3	123.4 (6)
O3—Sm1—O4^{i}	128.43 (12)	C15—C16—C17	119.0 (8)
O5—Sm1—O6^{ii}	77.15 (12)	C15—C16—H16	120.5
O2^{i}—Sm1—O6^{ii}	78.27 (13)	C17—C16—H16	120.5
O3—Sm1—O6^{ii}	69.53 (12)	C18—C17—C16	120.2 (8)
O4^{i}—Sm1—O6^{ii}	141.66 (12)	C18—C17—H17	119.9
O2^{i}—Sm1—O1	120.60 (13)	C16—C17—H17	119.9
O4^{i}—Sm1—O1	84.19 (12)	C19—C18—C17	121.2 (8)

O6^{ii}—Sm1—O1	133.38 (11)	C19—C18—H18	119.4
O2^{i}—Sm1—N2	148.76 (14)	C17—C18—H18	119.4
O4^{i}—Sm1—N2	136.88 (14)	C18—C19—C20	119.2 (9)
O6^{ii}—Sm1—N2	72.75 (14)	C18—C19—H19	120.4
O2^{i}—Sm1—N1	150.06 (13)	C20—C19—H19	120.4
O4^{i}—Sm1—N1	77.01 (13)	C15—C20—C19	118.3 (8)
O6^{ii}—Sm1—N1	122.05 (14)	C15—C20—H20	120.8
O2^{i}—Sm1—O2	72.71 (14)	C19—C20—H20	120.8
O4^{i}—Sm1—O2	65.20 (11)	O1—C21—O2	122.0 (5)
O6^{ii}—Sm1—O2	129.87 (12)	O1—C21—C22	121.3 (5)
C21—O1—Sm1	102.0 (3)	O2—C21—C22	116.7 (5)
C21—O2—Sm1^{i}	163.1 (4)	N4—C22—C21	114.5 (5)
C21—O2—Sm1	87.7 (3)	N4—C22—H22A	108.6
Sm1^{i}—O2—Sm1	107.29 (14)	C21—C22—H22A	108.6
C13—O3—Sm1	130.2 (3)	N4—C22—H22B	108.6
C13—O4—Sm1^{i}	138.1 (3)	C21—C22—H22B	108.6
C29—O5—Sm1	151.4 (3)	H22A—C22—H22B	107.6
C29—O6—Sm1^{ii}	149.8 (3)	C24—C23—N4	128.4 (13)
C1—N1—C5	119.1 (5)	C24—C23—C28	119.6 (12)
C1—N1—Sm1	119.8 (4)	N4—C23—C28	112.0 (13)
C5—N1—Sm1	119.6 (4)	C23—C24—C25	120.7 (13)
C9—N2—C12	117.8 (5)	C23—C24—H24	119.6
C9—N2—Sm1	121.7 (4)	C25—C24—H24	119.6
C12—N2—Sm1	120.2 (4)	C26—C25—C24	117.7 (14)
C15—N3—C14	117.7 (5)	C26—C25—H25	121.2
C15—N3—H3A	121.2	C24—C25—H25	121.2
C14—N3—H3A	121.2	C25—C26—C27	126.6 (12)
C23—N4—C22	115.1 (8)	C25—C26—H26	116.7
C23—N4—H4	122.4	C27—C26—H26	116.7
C22—N4—H4	122.4	C28—C27—C26	112.5 (12)
C31—N5—C30	118.7 (4)	C28—C27—H27	123.8
C31—N5—H5	120.7	C26—C27—H27	123.8
C30—N5—H5	120.7	C27—C28—C23	122.9 (14)
N1—C1—C2	122.9 (7)	C27—C28—H28	118.6
N1—C1—H1	118.5	C23—C28—H28	118.6
C2—C1—H1	118.5	O6—C29—O5	127.3 (5)
C3—C2—C1	118.4 (7)	O6—C29—C30	119.7 (5)
C3—C2—H2	120.8	O5—C29—C30	112.8 (5)
C1—C2—H2	120.8	N5—C30—C29	111.7 (4)
C4—C3—C2	121.0 (7)	N5—C30—H30A	109.3
C4—C3—H3	119.5	C29—C30—H30A	109.3
C2—C3—H3	119.5	N5—C30—H30B	109.3
C3—C4—C5	117.4 (7)	C29—C30—H30B	109.3
C3—C4—C6	124.6 (8)	H30A—C30—H30B	107.9
C5—C4—C6	118.0 (8)	C32—C31—N5	124.0 (5)
N1—C5—C4	121.2 (6)	C32—C31—C36	120.2 (6)

N1—C5—C9	118.8 (5)	N5—C31—C36	115.8 (6)
C4—C5—C9	120.0 (6)	C31—C32—C33	119.9 (7)
C7—C6—C4	120.6 (8)	C31—C32—H32	120.1
C7—C6—H6	119.7	C33—C32—H32	120.1
C4—C6—H6	119.7	C32—C33—C34	120.2 (8)
C6—C7—C8	121.4 (7)	C32—C33—H33	119.9
C6—C7—H7	119.3	C34—C33—H33	119.9
C8—C7—H7	119.3	C35—C34—C33	118.9 (7)
C10—C8—C7	122.7 (7)	C35—C34—H34	120.5
C10—C8—C9	116.1 (7)	C33—C34—H34	120.5
C7—C8—C9	121.2 (7)	C34—C35—C36	121.2 (7)
N2—C9—C8	123.3 (6)	C34—C35—H35	119.4
N2—C9—C5	118.3 (5)	C36—C35—H35	119.4
C8—C9—C5	118.4 (6)	C35—C36—C31	119.5 (7)
C11—C10—C8	120.5 (6)	C35—C36—H36	120.3
C11—C10—H10	119.7	C31—C36—H36	120.3

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N5—H5···O6	0.86	2.32	2.658 (5)	103
N3—H3A···O4	0.86	2.27	2.628 (5)	105
C22—H22B···O5^{iii}	0.97	2.40	3.345 (7)	163
C12—H12···N5^{ii}	0.93	2.60	3.441 (8)	151
C12—H12···O6^{ii}	0.93	2.47	3.059 (8)	121
C10—H10···O1^{iv}	0.93	2.35	3.218 (7)	156
C1—H1···O4^{i}	0.93	2.41	3.108 (8)	132

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

Fig. 1

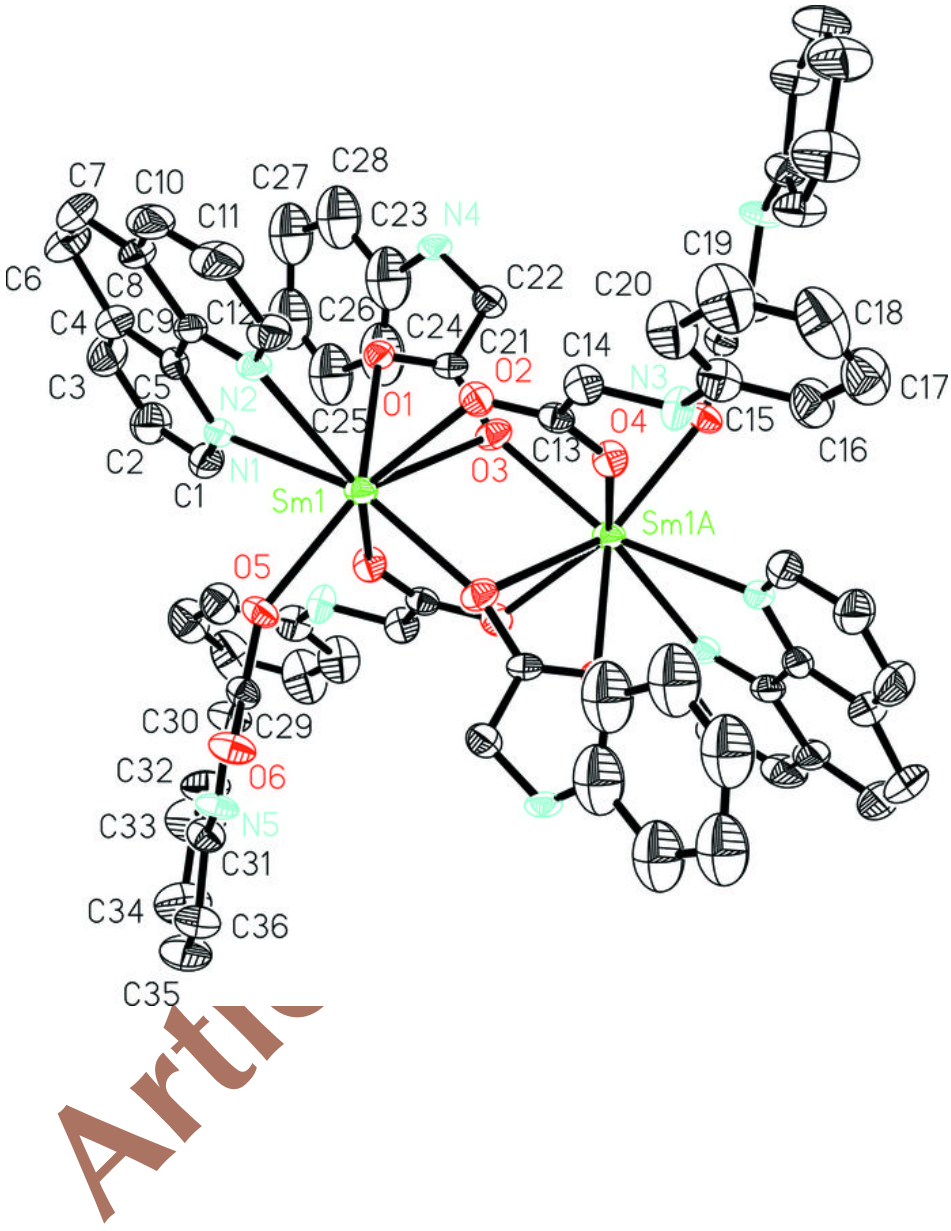
C7
C10
C27
C28
C11
C23
N4
C19
C6
C8
C22
C20
C18
C4
C9
C12
C26
C24
C21
C14
C3
C5
N2
O2
N3
C17
C25
O1
O4
C15
C2
N1
C13
C16
C1
Sm1
O3
Sm1A
O5
C30
C29
C32
O6
C33
N5
C31
C34
C36
C35

Fig. 2