Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

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

H. Zhong,[a]* S.-H. Duan,[a] Y.-P. Hong,[a] M.-L. Li,[a] Y.-Q. Liu,[a] C.-J. Luo,[a] Q.-Y. Luo,[a] S.-Z. Xiao,[a] H.-L. Xie,[a] Y.-P. Xu,[a] X.-M. Yang,[b,a] X.-R. Zeng[a] and Q. Y. Zhong[c]

[a]College of Chemistry and Chemical Engineering, Provincial Key Laboratory of Coordination Chemistry, Jinggangshan University, Jian 343009, People's Republic of China, [b]Institute of Applied Materials, Jiangxi University of Finance and Economics, Nanchang 330032, People's Republic of China, and [c]Jian Training School, Jian 343000, People's Republic of China
Correspondence e-mail: huazhong06@126.com

Received 20 November 2009; accepted 15 December 2009

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^{2}N,O)cobalt(III) glyoxal hemisolvate monohydrate	Zhong, Zeng, Liu & Luo (2006*b*)	10.1107/S1600536806050240	MEQHEW
(8-Quinolinol-κ^{2}N,O)bis(8-quinolinolato-κ^{2}N,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^{2}N,O)-bis(8-quinolinolato-κ^{2}N,O)zinc(II) glyoxal hemisolvate monohydrate	Zhong, Zeng, Luo, Li & Xiao (2007)	10.1107/S1600536807001171	DEXTEG
(Dimethylglyoxime-κ^{2}N,N′)bis(1,10-phenanthroline-κ^{2}N,N′)nickel(II) dinitrate dihydrate	Zhong, Zeng, Yang, Luo & Li (2007*a*)	10.1107/S1600536807004102	YEYGOZ
(Dimethylglyoxime-κ^{2}N,N′)bis(1,10-phenanthroline-κ^{2}N,N′)zinc(II) dinitrate dihydrate	Zhong, Zeng, Yang, Luo & Li (2007*b*)	10.1107/S1600536807004096	YEYGUF
Chloridobis(1,10-phenanthroline-κN,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^{2}O,O′)bis(4-phenylpyridine-κN)cerium(IV)	Zhong, Zeng, Yang & Luo (2007*c*)	10.1107/S1600536807018831	CICDOI
Bis(4,4′-bipyridine-κ^{2}N,N′)tetrakis(nitrato-κ^{2}O,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^{2}N,N′)tris(phenoxyacetato)-κO;κO;κO,O′-neodymium(III)	Zhong, Yang, Luo & Xu (2007*c*)	10.1107/S1600536807030371	UDUMEM
Bis(2,2′-bipyridyl-κ^{2}N,N′)bis(thiocyanato-κN)nickel(II)	Zhong, Yang, Luo & Xu (2007*d*)	10.1107/S1600536807031613	YEJGOJ01
Bis(2,2′-bipyridyl-κ^{2}N,N′)bis(isothiocyanato-κN)copper(II)	Zhong, Yang, Luo & Xu (2007*e*)	10.1107/S1600536807033181	UFAPOH
Bis(2,2′-bipyridyl-κ^{2}N,N′)bis(thiocyanato-κN)zinc(II)	Zhong, Yang, Luo & Xu (2007*f*)	10.1107/S1600536807035337	TIGFAR
(1,10-Phenanthroline-κ^{2}N,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-κ^{2}O:O′)bis(μ-anilinoacetato-κ^{3}O,O′:O)bis[(1,10-phenanthroline-κ^{2}N,N′)samarium(III)]-μ-anilino-acetato-κ^{2}O: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-κ²N,N′)cobalt(II)]-μ-acetato-κ²O: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-κ²N,N′)copper(II)]-μ-acetato-κ²O: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-κ²N,N′)nickel(II)]-μ-acetato-κ²O: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-κ²N,N′)bis(1,10-phenanthroline-κ²N,N′)copper(II) dinitrate dihydrate	Zhong, Yang, Luo & Li (2007)	10.1107/S1600536807061193	YIQNUI
catena-Poly[[(1,10-phenanthroline-κ²N,N′)praseodymium(III)]-di-μ-phenoxyacetato-κ⁴O:O′-[(1,10-phenanthroline-κ²N,N′)-praseodymium(III)]-di-μ-phenoxyacetato-κ⁴O:O′-di-μ-phenoxyacetato-κ³O,O′:O;κ³O: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.

Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

catena-Poly[[tetra-μ-anilinoacetato-bis(1,10-phenanthroline)dineodymium(III)]-di-μ-anilinoacetato]

H. Zhong,[a]* X.-M. Yang,[b] H.-L. Xie[a] and C.-J. Luo[a]

[a]College of Chemistry & Chemical Engineering, Provincial Key Laboratory of Coordination Chemistry, Jinggangshan University, Jian 343009, People's Republic of China, and [b]Institute of Applied Materials, Jiangxi University of Finance & Economics, Nanchang 330032, People's Republic of China
Correspondence e-mail: huazhong06@126.com

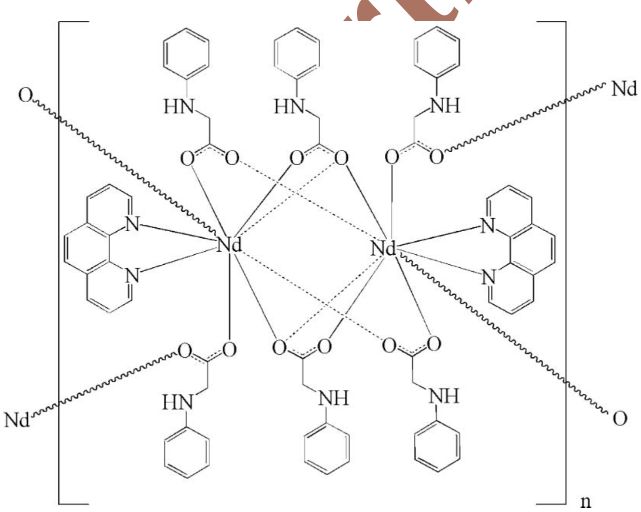
Received 28 September 2007; accepted 3 October 2007

Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.011 Å; R factor = 0.044; wR factor = 0.126; data-to-parameter ratio = 17.7.

In the crystal structure of the title compound, $[Nd_2(C_8H_8NO_2)_6(C_{12}H_8N_2)_2]_n$, the Nd^{III} atoms are bridged by two tridentate, two bidentate and four mondentate carboxylate groups with an inversion centre between the two Nd^{III} ions. Each Nd atom is nine-coordinated by two 1,10-phenanthroline N atoms 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 a related structure, see: Zhong *et al.* (2007). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$[Nd_2(C_8H_8NO_2)_6(C_{12}H_8N_2)_2]$
M_r = 1549.82
Monoclinic, $P2_1/n$
a = 19.9153 (14) Å
b = 8.488 (2) Å
c = 20.6617 (18) Å
β = 106.709 (3)°
V = 3345.0 (10) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.61 mm^{-1}
T = 273 (2) K
0.33 × 0.12 × 0.08 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.620, T_{max} = 0.884
26208 measured reflections
7191 independent reflections
4868 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.127
S = 0.97
7191 reflections
407 parameters
5 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.73 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Nd1—O1	2.554 (3)	Nd1—O5^{i}	2.517 (3)
Nd1—O2	2.811 (4)	Nd1—O6^{ii}	2.528 (3)
Nd1—O2^{i}	2.422 (3)	Nd1—N1	2.715 (4)
Nd1—O3	2.467 (3)	Nd1—N2	2.707 (4)
Nd1—O4	2.405 (3)		
O1—Nd1—O2	48.07 (9)	O3—Nd1—N1	127.07 (11)
O1—Nd1—O3	73.04 (10)	O4—Nd1—N1	77.34 (11)
O1—Nd1—O4	139.35 (11)	O1—Nd1—N2	74.25 (11)
O2—Nd1—O3	65.14 (10)	O2—Nd1—N2	118.37 (10)
O2—Nd1—O4	139.59 (10)	O3—Nd1—N2	80.78 (11)
O3—Nd1—O4	145.89 (11)	O4—Nd1—N2	96.73 (11)
O1—Nd1—N1	63.74 (11)	N1—Nd1—N2	59.77 (13)
O2—Nd1—N1	102.40 (11)		

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

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

D—H$\cdots$$A$	D—H	H$\cdots$$A$	$D\cdots A$	D—H$\cdots$$A$
C1—H1$\cdots$O5^{i}	0.93	2.41	3.106 (7)	132
C10—H10$\cdots$O1^{iii}	0.93	2.33	3.202 (7)	156
C12—H12$\cdots$O6^{ii}	0.93	2.46	3.049 (7)	122
C12—H12$\cdots$N5^{ii}	0.93	2.55	3.394 (7)	151
C22—H22$B$$\cdots$O4^{iv}	0.97	2.39	3.332 (6)	164
N3—H3$A$$\cdots$O5	0.86	2.26	2.616 (5)	105

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

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*.

The authors thank the Science and Technology Program of Jinggangshan University for financial support of this work (grant No. 2007).

  doi:10.1107/S1600536807048489 *Acta Cryst.* (2007). E**63**, m2680–m2681

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2416).

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.

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.

Zhong, H., Yang, X.-M., Xie, H.-L. & Luo, C.-J. (2007). *Acta Cryst.* E**63**, m2508–m2509.

supplementary materials

Acta Cryst. (2007). E**63**, m2680-m2681 [**doi:10.1107/S1600536807048489**]

catena-Poly[[tetra-μ-anilinoacetato-bis(1,10-phenanthroline)dineodymium(III)]-di-μ-anilino-acetato]

H. Zhong, X.-M. Yang, H.-L. Xie and C.-J. Luo

Comment

The crystal structure of *catena*-Poly[bisi(μ-anilinoacetato-κ^2*O*:*O*')bisi (μ-anilinoacetato-κ^3*O*,*O*':*O*)bis[(1,10-phenanthroline-κ^2*N*,*N*') samarium(III)]-μ-anilinoacetato-κ^2*O*:*O*'], (II), has previously been reported (Zhong *et al.*, 2007). The crystal structure determination of the title compound, (I), has been carried out in order to elucidate the molecular conformation and to compare it with that of (II). We report herein the crystal structure of (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, $[Nd_2(C_8H_8NO_2)_6(C_{12}H_8N_2)_2]_n$, which are bridged by two terdentate, two bidentate and four mondentate carboxyl groups with an inversion centre between the two Nd^{III} ions. Each Nd 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 Nd—O bond lengths are in the range 2.405 (3) to 2.812 (4) Å. The Nd—N bond lengths are in the range 2.707 (4) to 2.715 (4) Å, as in (II).

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, as in (II).

The both compounds, (I) and (II), are isostructural.

Experimental

Crystals of the title compound were synthesized using hydrothermal method in a 23 ml Teflon-lined Parr bomb, which was then sealed. Neodymium (III) nitrate hexahydrate (215.9 mg, 0.5 mmol), phen (198 mg, 1 mmol), anilinoacetic acid (292.4 mg, 2 mmol), ammonia (0.5 mol/l, 4 ml) and distilled water (10 g) were placed into the bomb and sealed. The bomb was then heated under autogenous pressure up to 453 K over the course of 7 d and allowed to cool at room temperature for 24 h. Upon opening the bomb, a clear colorless solution was decanted from small colourless crystals. These crystals were washed with distilled water followed by ethanol, and allowed to air-dry at room temperature.

Refinement

H5 (for NH) were located in difference syntheses and refined isotropically [N—H = 0.82 (4) Å, U_{iso}(H) = 0.07 (2) Å^2]. 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

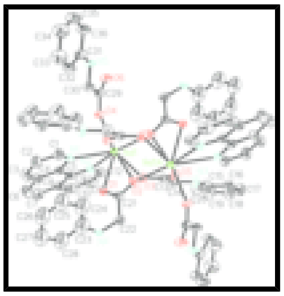


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level [symmetry code (A): 2 − x, −y, 2 − z]. All H atoms have been omitted for clarity.

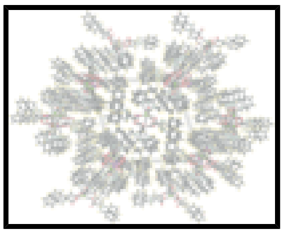


Fig. 2. A packing diagram of (I). Hydrogen bonds are shown as dashed lines.

catena-Poly[[tetra-μ-anilinoacetato-bis(1,10-\ phenanthroline)dineodymium(III)]-di-μ-anilinoacetato]

Crystal data

$[Nd_2(C_8H_8NO_2)_6(C_{12}H_8N_2)_2]$	F_{000} = 1564
M_r = 1549.82	D_x = 1.539 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 9024 reflections
a = 19.9153 (14) Å	θ = 2.4–26.7°
b = 8.488 (2) Å	μ = 1.61 mm^{-1}
c = 20.6617 (18) Å	T = 273 (2) K
β = 106.709 (3)°	Plane, colourless
V = 3345.0 (10) Å^3	0.33 × 0.12 × 0.08 mm
Z = 2	

Data collection

Bruker APEXII area-detector diffractometer	7191 independent reflections
Radiation source: fine-focus sealed tube	4868 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.042
T = 273(2) K	θ_{max} = 27.1°
φ and ω scans	θ_{min} = 2.1°
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −25→24
T_{min} = 0.620, T_{max} = 0.884	k = −10→10
26208 measured reflections	l = −26→26

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.044$

$wR(F^2) = 0.127$

$S = 0.97$

7191 reflections

407 parameters

5 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

$w = 1/[\sigma^2(F_o^2) + (0.0802P)^2 + 0.285P]$
where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{max} = 1.48$ e Å^{-3}

$\Delta\rho_{min} = -0.72$ 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}
Nd1	0.931205 (12)	0.19065 (3)	0.964283 (11)	0.03914 (10)
O1	0.84634 (15)	−0.0358 (4)	0.91879 (15)	0.0445 (7)
O2	0.94685 (16)	−0.1380 (4)	0.97732 (16)	0.0497 (8)
O3	0.97062 (17)	0.0612 (4)	0.87468 (15)	0.0476 (8)
O4	0.94003 (17)	0.4208 (4)	1.03416 (15)	0.0476 (8)
O5	1.06693 (17)	−0.0829 (4)	0.92169 (15)	0.0497 (8)
O6	1.00739 (19)	0.6127 (4)	1.09101 (15)	0.0563 (9)
N1	0.7969 (2)	0.2338 (5)	0.9669 (2)	0.0470 (9)
N2	0.8341 (2)	0.3070 (4)	0.85465 (19)	0.0481 (10)
N3	1.1178 (2)	−0.0165 (5)	0.82143 (19)	0.0506 (10)
H3A	1.1391	−0.0749	0.8551	0.061*
N4	0.7855 (2)	−0.3276 (4)	0.8985 (2)	0.0467 (10)
H4	0.7629	−0.3427	0.8567	0.056*
N5	0.9878 (2)	0.5258 (5)	1.20645 (18)	0.0451 (10)
C1	0.7784 (3)	0.1909 (6)	1.0197 (3)	0.0635 (15)
H1	0.8135	0.1671	1.0591	0.076*

C2	0.7094 (3)	0.1786 (8)	1.0207 (4)	0.084 (2)
H2	0.6981	0.1506	1.0598	0.101*
C3	0.6580 (4)	0.2097 (9)	0.9612 (5)	0.090 (2)
H3	0.6111	0.1970	0.9595	0.108*
C4	0.6745 (3)	0.2580 (9)	0.9056 (4)	0.0764 (18)
C5	0.7464 (3)	0.2672 (6)	0.9093 (3)	0.0532 (13)
C6	0.6218 (4)	0.2942 (11)	0.8390 (5)	0.113 (3)
H6	0.5743	0.2814	0.8345	0.136*
C7	0.6413 (4)	0.3429 (10)	0.7878 (4)	0.100 (3)
H7	0.6073	0.3715	0.7483	0.120*
C8	0.7135 (3)	0.3538 (8)	0.7905 (3)	0.0701 (17)
C9	0.7664 (3)	0.3102 (5)	0.8509 (3)	0.0525 (13)
C10	0.7358 (4)	0.4036 (8)	0.7368 (3)	0.087 (2)
H10	0.7034	0.4392	0.6976	0.104*
C11	0.8044 (4)	0.4011 (8)	0.7409 (3)	0.081 (2)
H11	0.8196	0.4332	0.7044	0.097*
C12	0.8526 (3)	0.3494 (7)	0.8007 (3)	0.0636 (15)
H12	0.8997	0.3448	0.8026	0.076*
C13	1.0288 (2)	0.0027 (5)	0.8771 (2)	0.0432 (10)
C14	1.0523 (3)	0.0517 (7)	0.8173 (2)	0.0544 (12)
H14A	1.0180	0.0180	0.7760	0.065*
H14B	1.0559	0.1656	0.8163	0.065*
C15	1.1462 (3)	0.0138 (7)	0.7699 (3)	0.0635 (14)
C16	1.2074 (3)	−0.0573 (8)	0.7760 (3)	0.0774 (18)
H16	1.2277	−0.1197	0.8136	0.093*
C17	1.2400 (4)	−0.0381 (9)	0.7270 (5)	0.093 (2)
H17	1.2830	−0.0861	0.7312	0.111*
C18	1.2094 (5)	0.0519 (9)	0.6714 (5)	0.107 (3)
H18	1.2317	0.0636	0.6379	0.129*
C19	1.1477 (5)	0.1236 (11)	0.6644 (4)	0.109 (3)
H19	1.1269	0.1832	0.6261	0.131*
C20	1.1151 (4)	0.1073 (9)	0.7158 (3)	0.083 (2)
H20	1.0732	0.1589	0.7132	0.099*
C21	0.8840 (3)	−0.1516 (6)	0.9390 (2)	0.0440 (11)
C22	0.8574 (3)	−0.3149 (6)	0.9196 (3)	0.0564 (13)
H22A	0.8758	−0.3516	0.8836	0.068*
H22B	0.8754	−0.3840	0.9581	0.068*
C23	0.7534 (6)	−0.3151 (9)	0.9459 (7)	0.1243 (15)
C24	0.7835 (6)	−0.2774 (9)	1.0119 (6)	0.1243 (15)
H24	0.8314	−0.2578	1.0284	0.149*
C25	0.7405 (6)	−0.2696 (10)	1.0531 (6)	0.1243 (15)
H25	0.7593	−0.2467	1.0988	0.149*
C26	0.6732 (6)	−0.2943 (9)	1.0284 (6)	0.1243 (15)
H26	0.6460	−0.2833	1.0579	0.149*
C27	0.6382 (6)	−0.3359 (10)	0.9615 (6)	0.1243 (15)
H27	0.5904	−0.3576	0.9468	0.149*
C28	0.6795 (5)	−0.3416 (10)	0.9204 (6)	0.1243 (15)
H28	0.6599	−0.3632	0.8747	0.149*
C29	0.9695 (3)	0.4991 (5)	1.0865 (2)	0.0439 (11)

C30	0.9485 (3)	0.4456 (7)	1.1471 (2)	0.0559 (13)
H30A	0.8989	0.4657	1.1398	0.067*
H30B	0.9562	0.3330	1.1531	0.067*
C31	0.9743 (3)	0.4886 (6)	1.2654 (2)	0.0555 (13)
C32	0.9277 (3)	0.3793 (8)	1.2718 (3)	0.0707 (17)
H32	0.9014	0.3245	1.2340	0.085*
C33	0.9192 (5)	0.3488 (11)	1.3340 (4)	0.105 (3)
H33	0.8881	0.2709	1.3388	0.126*
C34	0.9573 (4)	0.4354 (11)	1.3905 (3)	0.103 (3)
H34	0.9499	0.4188	1.4325	0.123*
C35	1.0044 (4)	0.5422 (9)	1.3835 (3)	0.088 (2)
H35	1.0307	0.5973	1.4212	0.106*
C36	1.0143 (3)	0.5709 (8)	1.3221 (3)	0.0724 (16)
H36	1.0473	0.6446	1.3179	0.087*
H5	0.958 (2)	0.593 (5)	1.206 (3)	0.07 (2)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Nd1	0.04549 (16)	0.03362 (16)	0.03377 (15)	−0.00155 (11)	0.00415 (10)	0.00057 (10)
O1	0.0449 (17)	0.0346 (18)	0.0471 (18)	−0.0001 (14)	0.0022 (13)	−0.0044 (14)
O2	0.0465 (19)	0.050 (2)	0.0452 (18)	−0.0024 (15)	0.0011 (14)	0.0080 (15)
O3	0.0568 (19)	0.048 (2)	0.0389 (17)	0.0054 (17)	0.0151 (14)	0.0019 (15)
O4	0.067 (2)	0.0340 (17)	0.0406 (17)	−0.0052 (16)	0.0144 (15)	−0.0059 (14)
O5	0.061 (2)	0.048 (2)	0.0420 (18)	0.0083 (16)	0.0170 (15)	0.0110 (15)
O6	0.082 (2)	0.050 (2)	0.0379 (18)	−0.0256 (19)	0.0183 (17)	−0.0029 (15)
N1	0.047 (2)	0.042 (2)	0.046 (2)	0.0036 (18)	0.0034 (18)	−0.0079 (18)
N2	0.059 (3)	0.039 (2)	0.037 (2)	0.0030 (18)	−0.0009 (17)	0.0007 (17)
N3	0.051 (2)	0.066 (3)	0.040 (2)	0.018 (2)	0.0224 (18)	0.0220 (19)
N4	0.043 (2)	0.033 (2)	0.054 (2)	−0.0128 (16)	−0.0041 (18)	−0.0071 (17)
N5	0.065 (3)	0.043 (2)	0.0293 (19)	−0.021 (2)	0.0163 (18)	−0.0063 (16)
C1	0.055 (3)	0.073 (4)	0.061 (3)	0.006 (3)	0.014 (3)	−0.002 (3)
C2	0.058 (4)	0.109 (6)	0.089 (5)	0.005 (4)	0.029 (4)	−0.010 (4)
C3	0.049 (3)	0.103 (6)	0.117 (7)	−0.004 (3)	0.018 (4)	−0.014 (5)
C4	0.053 (3)	0.087 (5)	0.075 (4)	0.006 (3)	−0.005 (3)	−0.020 (4)
C5	0.052 (3)	0.037 (3)	0.062 (3)	0.008 (2)	0.002 (2)	−0.010 (2)
C6	0.055 (4)	0.153 (9)	0.104 (7)	0.020 (5)	−0.021 (4)	−0.029 (6)
C7	0.080 (5)	0.110 (6)	0.078 (5)	0.039 (4)	−0.028 (4)	−0.016 (5)
C8	0.073 (4)	0.062 (4)	0.052 (3)	0.018 (3)	−0.019 (3)	−0.011 (3)
C9	0.060 (3)	0.034 (3)	0.048 (3)	0.006 (2)	−0.008 (2)	−0.004 (2)
C10	0.118 (6)	0.068 (4)	0.047 (4)	0.017 (4)	−0.017 (4)	0.001 (3)
C11	0.121 (6)	0.073 (5)	0.037 (3)	−0.001 (4)	0.003 (3)	0.012 (3)
C12	0.082 (4)	0.052 (3)	0.048 (3)	−0.003 (3)	0.003 (3)	0.009 (2)
C13	0.054 (3)	0.036 (3)	0.039 (2)	−0.006 (2)	0.011 (2)	−0.0032 (19)
C14	0.064 (3)	0.054 (3)	0.048 (3)	0.005 (3)	0.020 (2)	0.011 (2)
C15	0.069 (4)	0.071 (4)	0.058 (3)	−0.009 (3)	0.029 (3)	0.000 (3)
C16	0.077 (4)	0.094 (5)	0.071 (4)	0.006 (4)	0.037 (3)	−0.003 (4)
C17	0.086 (5)	0.097 (6)	0.112 (6)	−0.006 (4)	0.057 (4)	−0.006 (5)

C18	0.139 (7)	0.084 (5)	0.139 (8)	−0.014 (5)	0.104 (6)	−0.003 (5)
C19	0.153 (8)	0.105 (6)	0.095 (6)	0.017 (6)	0.077 (6)	0.031 (5)
C20	0.101 (5)	0.088 (5)	0.077 (4)	0.003 (4)	0.055 (4)	0.023 (4)
C21	0.047 (3)	0.048 (3)	0.032 (2)	−0.003 (2)	0.0035 (19)	−0.0038 (19)
C22	0.062 (3)	0.044 (3)	0.057 (3)	0.004 (2)	0.008 (3)	−0.006 (2)
C23	0.135 (4)	0.089 (3)	0.172 (4)	0.015 (3)	0.079 (4)	0.029 (3)
C24	0.135 (4)	0.089 (3)	0.172 (4)	0.015 (3)	0.079 (4)	0.029 (3)
C25	0.135 (4)	0.089 (3)	0.172 (4)	0.015 (3)	0.079 (4)	0.029 (3)
C26	0.135 (4)	0.089 (3)	0.172 (4)	0.015 (3)	0.079 (4)	0.029 (3)
C27	0.135 (4)	0.089 (3)	0.172 (4)	0.015 (3)	0.079 (4)	0.029 (3)
C28	0.135 (4)	0.089 (3)	0.172 (4)	0.015 (3)	0.079 (4)	0.029 (3)
C29	0.058 (3)	0.033 (3)	0.039 (2)	−0.002 (2)	0.012 (2)	0.0019 (19)
C30	0.074 (3)	0.053 (3)	0.041 (3)	−0.020 (3)	0.018 (2)	−0.006 (2)
C31	0.076 (3)	0.054 (3)	0.035 (3)	−0.002 (3)	0.014 (2)	0.004 (2)
C32	0.075 (4)	0.089 (4)	0.050 (3)	−0.033 (3)	0.021 (3)	−0.005 (3)
C33	0.125 (6)	0.130 (7)	0.075 (5)	−0.045 (6)	0.052 (5)	0.001 (5)
C34	0.122 (6)	0.144 (7)	0.048 (4)	−0.030 (6)	0.034 (4)	0.006 (4)
C35	0.113 (5)	0.104 (6)	0.042 (3)	−0.018 (5)	0.013 (3)	−0.006 (3)
C36	0.085 (4)	0.076 (4)	0.053 (3)	−0.019 (3)	0.014 (3)	−0.012 (3)

Geometric parameters (Å, °)

Nd1—O1	2.554 (3)	C10—H10	0.9300
Nd1—O2	2.811 (4)	C11—C12	1.400 (8)
Nd1—O2^{i}	2.422 (3)	C11—H11	0.9300
Nd1—O3	2.467 (3)	C12—H12	0.9300
Nd1—O4	2.405 (3)	C13—C14	1.500 (6)
Nd1—O5^{i}	2.517 (3)	C14—H14A	0.9700
Nd1—O6^{ii}	2.528 (3)	C14—H14B	0.9700
Nd1—N1	2.715 (4)	C15—C16	1.333 (8)
Nd1—N2	2.707 (4)	C15—C20	1.364 (8)
O1—C21	1.234 (6)	C16—C17	1.362 (9)
O2—C21	1.279 (5)	C16—H16	0.9300
O2—Nd1^{i}	2.422 (3)	C17—C18	1.368 (11)
O3—C13	1.248 (5)	C17—H17	0.9300
O4—C29	1.261 (5)	C18—C19	1.340 (11)
O5—C13	1.245 (5)	C18—H18	0.9300
O5—Nd1^{i}	2.517 (3)	C19—C20	1.404 (9)
O6—C29	1.212 (5)	C19—H19	0.9300
O6—Nd1^{ii}	2.528 (3)	C20—H20	0.9300
N1—C1	1.300 (7)	C21—C22	1.497 (7)
N1—C5	1.349 (6)	C22—H22A	0.9700
N2—C12	1.320 (7)	C22—H22B	0.9700
N2—C9	1.327 (7)	C23—C24	1.360 (15)
N3—C15	1.367 (6)	C23—C28	1.430 (14)
N3—C14	1.408 (6)	C24—C25	1.373 (12)
N3—H3A	0.8600	C24—H24	0.9300
N4—C23	1.320 (11)	C25—C26	1.307 (14)

N4—C22	1.374 (6)	C25—H25	0.9300
N4—H4	0.8600	C26—C27	1.403 (14)
N5—C31	1.359 (6)	C26—H26	0.9300
N5—C30	1.424 (6)	C27—C28	1.342 (12)
N5—H5	0.82 (4)	C27—H27	0.9300
C1—C2	1.384 (8)	C28—H28	0.9300
C1—H1	0.9300	C29—C30	1.500 (6)
C2—C3	1.379 (10)	C30—H30A	0.9700
C2—H2	0.9300	C30—H30B	0.9700
C3—C4	1.347 (10)	C31—C32	1.344 (7)
C3—H3	0.9300	C31—C36	1.399 (7)
C4—C5	1.415 (8)	C32—C33	1.369 (8)
C4—C6	1.503 (10)	C32—H32	0.9300
C5—C9	1.423 (8)	C33—C34	1.404 (10)
C6—C7	1.294 (12)	C33—H33	0.9300
C6—H6	0.9300	C34—C35	1.343 (10)
C7—C8	1.426 (11)	C34—H34	0.9300
C7—H7	0.9300	C35—C36	1.360 (8)
C8—C10	1.376 (10)	C35—H35	0.9300
C8—C9	1.431 (7)	C36—H36	0.9300
C10—C11	1.344 (9)		

O1—Nd1—O2	48.07 (9)	C10—C11—C12	119.1 (6)
O1—Nd1—O3	73.04 (10)	C10—C11—H11	120.5
O1—Nd1—O4	139.35 (11)	C12—C11—H11	120.5
O2—Nd1—O3	65.14 (10)	N2—C12—C11	123.0 (6)
O2—Nd1—O4	139.59 (10)	N2—C12—H12	118.5
O3—Nd1—O4	145.89 (11)	C11—C12—H12	118.5
O1—Nd1—N1	63.74 (11)	O5—C13—O3	128.6 (4)
O2—Nd1—N1	102.40 (11)	O5—C13—C14	120.2 (4)
O3—Nd1—N1	127.07 (11)	O3—C13—C14	111.2 (4)
O4—Nd1—N1	77.34 (11)	N3—C14—C13	109.8 (4)
O1—Nd1—N2	74.25 (11)	N3—C14—H14A	109.7
O2—Nd1—N2	118.37 (10)	C13—C14—H14A	109.7
O3—Nd1—N2	80.78 (11)	N3—C14—H14B	109.7
O4—Nd1—N2	96.73 (11)	C13—C14—H14B	109.7
N1—Nd1—N2	59.77 (13)	H14A—C14—H14B	108.2
O4—Nd1—O2^{i}	87.77 (12)	C16—C15—C20	122.0 (6)
O2^{i}—Nd1—O3	78.57 (11)	C16—C15—N3	114.3 (5)
O4—Nd1—O5^{i}	75.78 (10)	C20—C15—N3	123.7 (5)
O2^{i}—Nd1—O5^{i}	73.97 (11)	C15—C16—C17	119.5 (7)
O3—Nd1—O5^{i}	128.19 (11)	C15—C16—H16	120.2
O4—Nd1—O6^{ii}	76.92 (11)	C17—C16—H16	120.2
O2^{i}—Nd1—O6^{ii}	78.52 (12)	C16—C17—C18	119.9 (7)
O3—Nd1—O6^{ii}	69.83 (11)	C16—C17—H17	120.1
O5^{i}—Nd1—O6^{ii}	141.62 (11)	C18—C17—H17	120.1
O2^{i}—Nd1—O1	120.47 (12)	C19—C18—C17	121.2 (7)

O5^{i}—Nd1—O1	84.33 (11)	C19—C18—H18	119.4
O6^{ii}—Nd1—O1	133.28 (10)	C17—C18—H18	119.4
O2^{i}—Nd1—N2	148.98 (12)	C18—C19—C20	118.8 (8)
O5^{i}—Nd1—N2	136.90 (12)	C18—C19—H19	120.6
O6^{ii}—Nd1—N2	72.73 (12)	C20—C19—H19	120.6
O2^{i}—Nd1—N1	150.12 (12)	C15—C20—C19	118.5 (7)
O5^{i}—Nd1—N1	77.28 (12)	C15—C20—H20	120.8
O6^{ii}—Nd1—N1	121.82 (13)	C19—C20—H20	120.8
O2^{i}—Nd1—O2	72.64 (13)	O1—C21—O2	121.9 (4)
O5^{i}—Nd1—O2	65.08 (10)	O1—C21—C22	120.8 (4)
O6^{ii}—Nd1—O2	130.07 (11)	O2—C21—C22	117.3 (4)
C21—O1—Nd1	101.6 (3)	N4—C22—C21	114.4 (4)
C21—O2—Nd1^{i}	162.5 (3)	N4—C22—H22A	108.7
C21—O2—Nd1	88.2 (3)	C21—C22—H22A	108.7
Nd1^{i}—O2—Nd1	107.36 (12)	N4—C22—H22B	108.7
C13—O3—Nd1	129.7 (3)	C21—C22—H22B	108.7
C29—O4—Nd1	151.4 (3)	H22A—C22—H22B	107.6
C13—O5—Nd1^{i}	138.2 (3)	N4—C23—C24	126.4 (11)
C29—O6—Nd1^{ii}	149.6 (3)	N4—C23—C28	112.4 (11)
C1—N1—C5	118.7 (5)	C24—C23—C28	121.1 (10)
C1—N1—Nd1	119.9 (3)	C23—C24—C25	117.3 (12)
C5—N1—Nd1	120.0 (3)	C23—C24—H24	121.3
C12—N2—C9	118.0 (4)	C25—C24—H24	121.3
C12—N2—Nd1	120.0 (4)	C26—C25—C24	120.2 (12)
C9—N2—Nd1	121.7 (3)	C26—C25—H25	119.9
C15—N3—C14	117.4 (4)	C24—C25—H25	119.9
C15—N3—H3A	121.3	C25—C26—C27	126.0 (11)
C14—N3—H3A	121.3	C25—C26—H26	117.0
C23—N4—C22	116.2 (7)	C27—C26—H26	117.0
C23—N4—H4	121.9	C28—C27—C26	114.3 (11)
C22—N4—H4	121.9	C28—C27—H27	122.9
C31—N5—C30	117.3 (4)	C26—C27—H27	122.9
C31—N5—H5	81 (4)	C27—C28—C23	120.9 (12)
C30—N5—H5	96 (4)	C27—C28—H28	119.5
N1—C1—C2	123.8 (6)	C23—C28—H28	119.5
N1—C1—H1	118.1	O6—C29—O4	127.7 (4)
C2—C1—H1	118.1	O6—C29—C30	119.6 (4)
C3—C2—C1	117.3 (7)	O4—C29—C30	112.6 (4)
C3—C2—H2	121.4	N5—C30—C29	110.9 (4)
C1—C2—H2	121.4	N5—C30—H30A	109.5
C4—C3—C2	121.2 (6)	C29—C30—H30A	109.5
C4—C3—H3	119.4	N5—C30—H30B	109.5
C2—C3—H3	119.4	C29—C30—H30B	109.5
C3—C4—C5	117.5 (6)	H30A—C30—H30B	108.0
C3—C4—C6	124.5 (7)	C32—C31—N5	124.6 (5)
C5—C4—C6	117.9 (7)	C32—C31—C36	120.3 (5)

N1—C5—C4	121.5 (6)	N5—C31—C36	115.0 (5)
N1—C5—C9	118.9 (5)	C32—C31—H5	120 (2)
C4—C5—C9	119.6 (5)	C36—C31—H5	109 (2)
C7—C6—C4	121.2 (8)	C31—C32—C33	119.9 (6)
C7—C6—H6	119.4	C31—C32—H32	120.1
C4—C6—H6	119.4	C33—C32—H32	120.1
C6—C7—C8	121.7 (7)	C32—C33—C34	119.9 (7)
C6—C7—H7	119.2	C32—C33—H33	120.0
C8—C7—H7	119.2	C34—C33—H33	120.0
C10—C8—C7	123.1 (6)	C35—C34—C33	119.4 (6)
C10—C8—C9	117.0 (6)	C35—C34—H34	120.3
C7—C8—C9	119.9 (7)	C33—C34—H34	120.3
N2—C9—C5	118.2 (4)	C34—C35—C36	121.0 (6)
N2—C9—C8	122.5 (5)	C34—C35—H35	119.5
C5—C9—C8	119.3 (5)	C36—C35—H35	119.5
C11—C10—C8	120.2 (6)	C35—C36—C31	119.4 (6)
C11—C10—H10	119.9	C35—C36—H36	120.3
C8—C10—H10	119.9	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*
C1—H1···O5^{i}	0.93	2.41	3.106 (7)	132
C10—H10···O1^{iii}	0.93	2.33	3.202 (7)	156
C12—H12···O6^{ii}	0.93	2.46	3.049 (7)	122
C12—H12···N5^{ii}	0.93	2.55	3.394 (7)	151
C22—H22B···O4^{iv}	0.97	2.39	3.332 (6)	164
N3—H3A···O5	0.86	2.26	2.616 (5)	105

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

Fig. 1

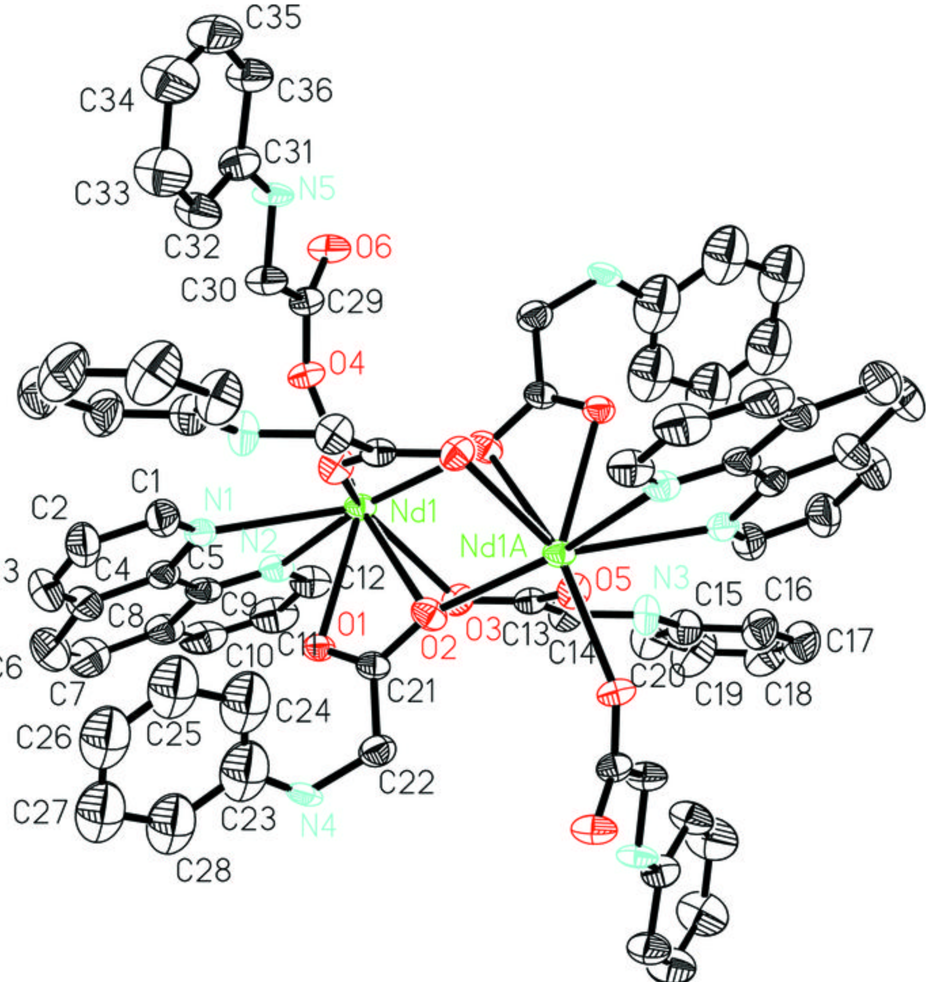

C35
C34
C36
C31
C33
N5
C32
O6
C30
C29
O4
C1
N1
C2
Nd1
N2
Nd1A
C3
C4
C5
C12
O5
N3
C15
C16
C8
C9
C6
C10
C11
O1
O2
O3
C13
C14
C17
C7
C21
C20
C19
C18
C24
C26
C25
C22
C27
C23
N4
C28

Fig. 2