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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

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

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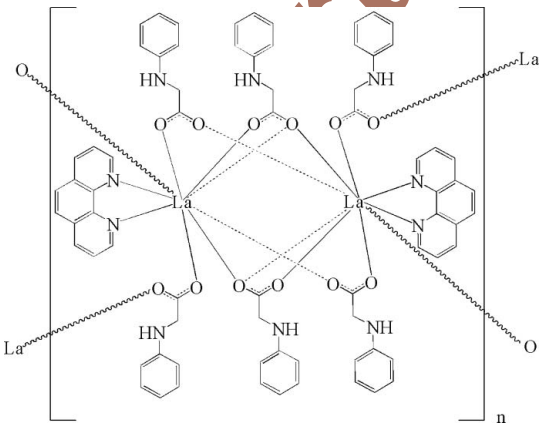
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.010 Å; R factor = 0.038; wR factor = 0.100; data-to-parameter ratio = 16.0.

In the crystal structure of the title compound, $[La_2(C_8H_8NO_2)_6(C_{12}H_8N_2)_2]_n$, the La^{III} atoms are bridged by two tridentate, two bidentate and four mondentate carboxylate groups with an inversion centre between the two La^{III} ions. Each La 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 sheet structure.

Related literature

For related structures, see: Zhong *et al.* (2007*a*,*b*). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$[La_2(C_8H_8NO_2)_6(C_{12}H_8N_2)_2]$
M_r = 1539.16
Monoclinic, $P2_1/n$
a = 20.2217 (15) Å
b = 8.5007 (18) Å
c = 20.449 (3) Å
β = 106.801 (3)°
V = 3365.1 (9) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.32 mm^{-1}
T = 273 (2) K
0.32 × 0.13 × 0.08 mm

Data collection

Bruker APEX-II area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.674, T_{max} = 0.900
24428 measured reflections
6591 independent reflections
4615 reflections with $I > 2\sigma(I)$
R_{int} = 0.040

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.100
S = 0.96
6591 reflections
411 parameters
5 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.54 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

La1—O1	2.568 (3)	La1—O5^{i}	2.497 (3)
La1—O2	2.815 (3)	La1—O6^{ii}	2.532 (3)
La1—O2^{i}	2.455 (3)	La1—N1	2.756 (4)
La1—O3	2.463 (3)	La1—N2	2.703 (3)
La1—O4	2.399 (3)		
O1—La1—O2	48.23 (8)	O3—La1—N1	127.37 (10)
O1—La1—O3	73.64 (9)	O4—La1—N1	77.38 (10)
O1—La1—O4	138.93 (10)	O1—La1—N2	73.99 (10)
O2—La1—O3	64.58 (9)	O2—La1—N2	118.24 (9)
O2—La1—O4	140.15 (9)	O3—La1—N2	81.95 (10)
O3—La1—O4	145.72 (10)	O4—La1—N2	96.14 (10)
O1—La1—N1	63.25 (10)	N1—La1—N2	58.89 (11)
O2—La1—N1	102.50 (10)		

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
C1—H1···O5^{i}	0.93	2.46	3.147 (6)	131
C10—H10···O1^{iii}	0.93	2.31	3.177 (6)	156
C12—H12···O6^{ii}	0.93	2.46	3.061 (6)	123
C12—H12···N4^{ii}	0.93	2.59	3.439 (7)	152
C22—H22*B*···O4^{iv}	0.97	2.38	3.328 (6)	165

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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2426).

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supplementary materials

Acta Cryst. (2007). E**63**, m2772-m2773 [**doi:10.1107/S1600536807051240**]

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

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

Comment

The crystal structure of *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'], (II), and *catena*- Poly[[tetra-μ-anilinoacetato-bis(1,10-phenanthroline) dineodymium(III)]-di-μ-anilinoacetato], (III), have previously been reported (Zhong *et al.*, 2007*a*,b). 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) and (III). 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, $[La_2(C_8H_8NO_2)_6(C_{12}H_8N_2)_2]_n$, which are bridged by two terdentate, two bidentate and four mondentate carboxyl groups with an inversion centre between the two La^{III} ions. Each La 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 La—O bond lengths are in the range 2.399 (3) to 2.815 (3) Å. The La—N bond lengths are in the range 2.703 (3) to 2.756 (4) Å, as in (II) and (III).

In the crystal structure, 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) and (III).

The three compounds, (I), (II) and (III), 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. Lanthanum (III) nitrate hexahydrate (213.2 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 colourless 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

H3A and H4A (for NH) were located in difference syntheses and refined isotropically [N—H = 0.771 (18) and 0.80 (4) Å, U_{iso}(H) = 0.072 (13) and 0.077 (16) Å^2]. The other 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

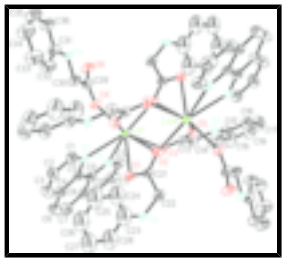

Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. [Ssymmetry code (A): 2 − *x*, −*y*, 2 − *z*]. All H atoms have been omitted for clarity.

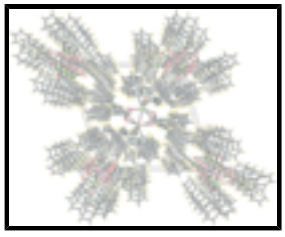

Fig. 2. A packing diagram of (I). Hydrogen bonds are shown as dashed lines.

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

Crystal data

$[La_2(C_8H_8NO_2)_6(C_{12}H_8N_2)_2]$	F_{000} = 1552
M_r = 1539.16	D_x = 1.519 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 9108 reflections
a = 20.2217 (15) Å	θ = 2.3–26.5°
b = 8.5007 (18) Å	μ = 1.32 mm^{-1}
c = 20.449 (3) Å	T = 273 (2) K
β = 106.801 (3)°	Plane, colourless
V = 3365.1 (9) Å^3	0.32 × 0.13 × 0.08 mm
Z = 2	

Data collection

Bruker APEX-II area-detector diffractometer	6591 independent reflections
Radiation source: fine-focus sealed tube	4615 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.040
T = 273(2) K	θ_{max} = 26.2°
φ and ω scans	θ_{min} = 2.1°
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −25→24
T_{min} = 0.674, T_{max} = 0.900	k = −10→10
24428 measured reflections	l = −25→25

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.038$

$wR(F^2) = 0.100$

$S = 0.96$

6591 reflections

411 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

$w = 1/[\sigma^2(F_o^2) + (0.058P)^2 + 1.1179P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.004$

$\Delta\rho_{max} = 1.36$ e Å^{-3}

$\Delta\rho_{min} = -0.54$ 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}
La1	0.931209 (11)	0.19062 (3)	0.964286 (10)	0.03914 (9)
O1	0.84636 (14)	−0.0359 (3)	0.91878 (14)	0.0506 (7)
O2	0.94664 (14)	−0.1380 (4)	0.97703 (14)	0.0556 (7)
O3	0.97057 (15)	0.0601 (3)	0.87468 (13)	0.0531 (7)
O4	0.93991 (15)	0.4210 (3)	1.03409 (13)	0.0535 (7)
O5	1.06690 (15)	−0.0828 (4)	0.92160 (14)	0.0557 (7)
O6	1.00768 (17)	0.6126 (4)	1.09102 (14)	0.0634 (8)
N1	0.79693 (18)	0.2346 (4)	0.96678 (19)	0.0533 (9)
N2	0.8342 (2)	0.3065 (4)	0.85460 (17)	0.0531 (9)
N3	1.1193 (2)	−0.0138 (5)	0.82285 (19)	0.0536 (9)
N5	0.78527 (18)	−0.3273 (4)	0.89864 (19)	0.0511 (9)
H5A	0.7629	−0.3436	0.8565	0.061*
N4	0.9879 (2)	0.5258 (5)	1.20644 (16)	0.0494 (9)
C1	0.7784 (3)	0.1913 (6)	1.0202 (3)	0.0688 (13)
H1	0.8127	0.1672	1.0602	0.083*
C2	0.7093 (3)	0.1794 (7)	1.0201 (3)	0.0902 (19)

H2	0.6985	0.1502	1.0597	0.108*
C3	0.6579 (3)	0.2110 (8)	0.9617 (4)	0.098 (2)
H3	0.6119	0.1995	0.9606	0.118*
C4	0.6745 (3)	0.2594 (8)	0.9051 (3)	0.0825 (17)
C5	0.7461 (2)	0.2673 (5)	0.9089 (2)	0.0577 (12)
C6	0.6230 (3)	0.2966 (9)	0.8392 (4)	0.114 (3)
H6	0.5762	0.2853	0.8351	0.137*
C7	0.6417 (4)	0.3442 (9)	0.7875 (4)	0.105 (2)
H7	0.6083	0.3729	0.7475	0.126*
C8	0.7136 (3)	0.3536 (7)	0.7910 (3)	0.0761 (16)
C9	0.7658 (2)	0.3102 (5)	0.8506 (2)	0.0577 (12)
C10	0.7356 (4)	0.4037 (7)	0.7369 (3)	0.093 (2)
H10	0.7035	0.4397	0.6974	0.112*
C11	0.8041 (4)	0.4012 (7)	0.7406 (3)	0.0897 (19)
H11	0.8186	0.4336	0.7035	0.108*
C12	0.8526 (3)	0.3493 (6)	0.8008 (2)	0.0703 (14)
H12	0.8990	0.3451	0.8025	0.084*
C13	1.0289 (2)	0.0032 (5)	0.8771 (2)	0.0476 (10)
C14	1.0525 (2)	0.0504 (6)	0.8173 (2)	0.0598 (12)
H14A	1.0198	0.0133	0.7756	0.072*
H14B	1.0545	0.1642	0.8151	0.072*
C15	1.1460 (3)	0.0147 (6)	0.7701 (3)	0.0692 (13)
C16	1.2079 (3)	−0.0558 (8)	0.7765 (3)	0.0866 (17)
H16	1.2284	−0.1173	0.8145	0.104*
C17	1.2398 (4)	−0.0358 (9)	0.7268 (4)	0.102 (2)
H17	1.2821	−0.0840	0.7306	0.122*
C18	1.2097 (5)	0.0543 (9)	0.6720 (4)	0.112 (2)
H18	1.2316	0.0685	0.6382	0.135*
C19	1.1478 (4)	0.1245 (9)	0.6656 (4)	0.114 (2)
H19	1.1273	0.1845	0.6270	0.137*
C20	1.1151 (3)	0.1078 (8)	0.7156 (3)	0.0910 (18)
H20	1.0734	0.1582	0.7123	0.109*
C21	0.8845 (2)	−0.1519 (5)	0.9392 (2)	0.0488 (10)
C22	0.8578 (3)	−0.3149 (5)	0.9190 (3)	0.0614 (12)
H22A	0.8748	−0.3501	0.8817	0.074*
H22B	0.8764	−0.3851	0.9573	0.074*
C23	0.7524 (5)	−0.3137 (9)	0.9450 (6)	0.1331 (14)
C24	0.7841 (5)	−0.2765 (8)	1.0120 (6)	0.1331 (14)
H24	0.8315	−0.2587	1.0280	0.160*
C25	0.7418 (5)	−0.2668 (9)	1.0547 (5)	0.1331 (14)
H25	0.7607	−0.2430	1.1008	0.160*
C26	0.6726 (5)	−0.2924 (9)	1.0290 (5)	0.1331 (14)
H26	0.6456	−0.2798	1.0585	0.160*
C27	0.6397 (5)	−0.3355 (9)	0.9627 (5)	0.1331 (14)
H27	0.5929	−0.3602	0.9482	0.160*
C28	0.6798 (5)	−0.3396 (9)	0.9199 (5)	0.1331 (14)
H28	0.6598	−0.3596	0.8736	0.160*
C29	0.9694 (2)	0.4992 (5)	1.0864 (2)	0.0496 (10)
C30	0.9490 (3)	0.4457 (6)	1.1472 (2)	0.0616 (12)

H30A	0.9002	0.4658	1.1401	0.074*
H30B	0.9566	0.3334	1.1533	0.074*
C31	0.9746 (3)	0.4884 (5)	1.2657 (2)	0.0601 (12)
C32	0.9278 (3)	0.3789 (7)	1.2719 (3)	0.0795 (16)
H32	0.9017	0.3240	1.2338	0.095*
C33	0.9198 (4)	0.3510 (9)	1.3347 (3)	0.112 (2)
H33	0.8889	0.2744	1.3398	0.135*
C34	0.9567 (4)	0.4341 (10)	1.3900 (3)	0.111 (2)
H34	0.9495	0.4173	1.4323	0.133*
C35	1.0043 (4)	0.5418 (8)	1.3836 (3)	0.097 (2)
H35	1.0304	0.5960	1.4220	0.117*
C36	1.0140 (3)	0.5705 (7)	1.3218 (2)	0.0781 (15)
H36	1.0464	0.6440	1.3173	0.094*
H4A	0.9596 (19)	0.594 (4)	1.201 (2)	0.077 (16)*
H3A	1.0989 (18)	−0.087 (3)	0.8058 (18)	0.072 (13)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
La1	0.04693 (14)	0.03354 (14)	0.03245 (13)	−0.00155 (10)	0.00435 (9)	0.00056 (9)
O1	0.0534 (16)	0.0401 (17)	0.0504 (16)	−0.0001 (14)	0.0028 (13)	−0.0038 (13)
O2	0.0527 (18)	0.0581 (19)	0.0478 (17)	−0.0034 (14)	0.0019 (13)	0.0077 (14)
O3	0.0655 (19)	0.0530 (18)	0.0415 (15)	0.0084 (16)	0.0167 (13)	0.0028 (13)
O4	0.0778 (19)	0.0390 (16)	0.0423 (15)	−0.0064 (15)	0.0149 (14)	−0.0069 (13)
O5	0.0693 (19)	0.0543 (19)	0.0450 (16)	0.0092 (16)	0.0190 (14)	0.0116 (14)
O6	0.094 (2)	0.054 (2)	0.0431 (16)	−0.0295 (18)	0.0207 (16)	−0.0028 (14)
N1	0.054 (2)	0.048 (2)	0.052 (2)	0.0035 (17)	0.0059 (17)	−0.0085 (17)
N2	0.068 (2)	0.043 (2)	0.0400 (19)	0.0015 (18)	0.0015 (16)	0.0007 (15)
N3	0.057 (2)	0.063 (3)	0.046 (2)	0.007 (2)	0.0236 (18)	0.012 (2)
N5	0.050 (2)	0.035 (2)	0.056 (2)	−0.0143 (15)	−0.0053 (16)	−0.0071 (15)
N4	0.074 (3)	0.045 (2)	0.0302 (17)	−0.019 (2)	0.0164 (17)	−0.0054 (15)
C1	0.065 (3)	0.081 (4)	0.060 (3)	0.007 (3)	0.017 (2)	−0.002 (3)
C2	0.065 (3)	0.120 (6)	0.092 (4)	0.006 (3)	0.033 (3)	−0.013 (4)
C3	0.055 (3)	0.118 (6)	0.117 (6)	−0.005 (3)	0.018 (4)	−0.017 (4)
C4	0.057 (3)	0.092 (4)	0.082 (4)	0.008 (3)	−0.006 (3)	−0.022 (3)
C5	0.058 (3)	0.043 (3)	0.062 (3)	0.006 (2)	0.003 (2)	−0.011 (2)
C6	0.058 (4)	0.147 (8)	0.113 (6)	0.015 (4)	−0.015 (4)	−0.024 (5)
C7	0.083 (5)	0.118 (6)	0.084 (5)	0.039 (4)	−0.025 (4)	−0.013 (4)
C8	0.084 (4)	0.067 (3)	0.054 (3)	0.017 (3)	−0.017 (3)	−0.009 (2)
C9	0.066 (3)	0.038 (2)	0.053 (3)	0.005 (2)	−0.008 (2)	−0.003 (2)
C10	0.123 (5)	0.076 (4)	0.054 (3)	0.017 (4)	−0.019 (3)	−0.001 (3)
C11	0.136 (6)	0.077 (4)	0.041 (3)	−0.005 (4)	0.001 (3)	0.010 (3)
C12	0.093 (4)	0.058 (3)	0.051 (3)	−0.002 (3)	0.006 (3)	0.009 (2)
C13	0.061 (3)	0.039 (2)	0.041 (2)	−0.004 (2)	0.0121 (19)	−0.0023 (18)
C14	0.072 (3)	0.059 (3)	0.050 (3)	0.005 (2)	0.020 (2)	0.011 (2)
C15	0.079 (3)	0.075 (4)	0.062 (3)	−0.006 (3)	0.034 (3)	0.000 (3)
C16	0.088 (4)	0.104 (5)	0.079 (4)	0.002 (4)	0.042 (3)	−0.003 (3)
C17	0.096 (5)	0.107 (6)	0.124 (6)	−0.006 (4)	0.067 (4)	−0.005 (5)

C18	0.155 (7)	0.089 (5)	0.131 (6)	−0.015 (5)	0.102 (6)	0.002 (5)
C19	0.162 (7)	0.109 (5)	0.100 (5)	0.013 (5)	0.082 (5)	0.032 (4)
C20	0.115 (5)	0.095 (5)	0.082 (4)	0.008 (4)	0.059 (4)	0.025 (3)
C21	0.053 (2)	0.052 (3)	0.036 (2)	−0.003 (2)	0.0041 (18)	−0.0030 (18)
C22	0.072 (3)	0.046 (3)	0.059 (3)	0.005 (2)	0.009 (2)	−0.005 (2)
C23	0.149 (3)	0.096 (2)	0.179 (4)	0.015 (2)	0.088 (3)	0.027 (3)
C24	0.149 (3)	0.096 (2)	0.179 (4)	0.015 (2)	0.088 (3)	0.027 (3)
C25	0.149 (3)	0.096 (2)	0.179 (4)	0.015 (2)	0.088 (3)	0.027 (3)
C26	0.149 (3)	0.096 (2)	0.179 (4)	0.015 (2)	0.088 (3)	0.027 (3)
C27	0.149 (3)	0.096 (2)	0.179 (4)	0.015 (2)	0.088 (3)	0.027 (3)
C28	0.149 (3)	0.096 (2)	0.179 (4)	0.015 (2)	0.088 (3)	0.027 (3)
C29	0.067 (3)	0.037 (2)	0.043 (2)	−0.002 (2)	0.014 (2)	0.0020 (18)
C30	0.081 (3)	0.059 (3)	0.045 (2)	−0.020 (3)	0.020 (2)	−0.006 (2)
C31	0.081 (3)	0.059 (3)	0.040 (2)	−0.002 (2)	0.017 (2)	0.003 (2)
C32	0.088 (4)	0.099 (4)	0.055 (3)	−0.037 (3)	0.027 (3)	−0.004 (3)
C33	0.134 (6)	0.141 (6)	0.074 (4)	−0.054 (5)	0.048 (4)	0.002 (4)
C34	0.142 (6)	0.147 (7)	0.051 (3)	−0.036 (5)	0.041 (4)	0.003 (4)
C35	0.127 (5)	0.115 (5)	0.044 (3)	−0.019 (4)	0.015 (3)	−0.007 (3)
C36	0.097 (4)	0.080 (4)	0.053 (3)	−0.019 (3)	0.015 (3)	−0.010 (3)

Geometric parameters (Å, °)

La1—O1	2.568 (3)	C10—H10	0.9300
La1—O2	2.815 (3)	C11—C12	1.404 (7)
La1—O2^{i}	2.455 (3)	C11—H11	0.9300
La1—O3	2.463 (3)	C12—H12	0.9300
La1—O4	2.399 (3)	C13—C14	1.490 (6)
La1—O5^{i}	2.497 (3)	C14—H14A	0.9700
La1—O6^{ii}	2.532 (3)	C14—H14B	0.9700
La1—N1	2.756 (4)	C15—C16	1.361 (7)
La1—N2	2.703 (3)	C15—C20	1.362 (7)
O1—C21	1.247 (5)	C16—C17	1.362 (8)
O2—C21	1.276 (5)	C16—H16	0.9300
O2—La1^{i}	2.455 (3)	C17—C18	1.348 (10)
O3—C13	1.263 (5)	C17—H17	0.9300
O4—C29	1.254 (5)	C18—C19	1.359 (9)
O5—C13	1.245 (5)	C18—H18	0.9300
O5—La1^{i}	2.497 (3)	C19—C20	1.377 (8)
O6—C29	1.223 (5)	C19—H19	0.9300
O6—La1^{ii}	2.532 (3)	C20—H20	0.9300
N1—C1	1.307 (6)	C21—C22	1.502 (6)
N1—C5	1.353 (6)	C22—H22A	0.9700
N2—C12	1.311 (6)	C22—H22B	0.9700
N2—C9	1.361 (6)	C23—C24	1.372 (13)
N3—C15	1.359 (6)	C23—C28	1.424 (13)
N3—C14	1.430 (6)	C24—C25	1.391 (11)
N3—H3A	0.771 (18)	C24—H24	0.9300
N5—C23	1.310 (10)	C25—C26	1.363 (12)

N5—C22	1.408 (6)	C25—H25	0.9300
N5—H5A	0.8600	C26—C27	1.377 (12)
N4—C31	1.352 (5)	C26—H26	0.9300
N4—C30	1.413 (5)	C27—C28	1.356 (10)
N4—H4A	0.80 (4)	C27—H27	0.9300
C1—C2	1.400 (7)	C28—H28	0.9300
C1—H1	0.9300	C29—C30	1.491 (6)
C2—C3	1.365 (9)	C30—H30A	0.9700
C2—H2	0.9300	C30—H30B	0.9700
C3—C4	1.360 (9)	C31—C32	1.359 (7)
C3—H3	0.9300	C31—C36	1.382 (7)
C4—C5	1.428 (7)	C32—C33	1.361 (7)
C4—C6	1.479 (9)	C32—H32	0.9300
C5—C9	1.410 (7)	C33—C34	1.359 (9)
C6—C7	1.287 (10)	C33—H33	0.9300
C6—H6	0.9300	C34—C35	1.361 (9)
C7—C8	1.437 (9)	C34—H34	0.9300
C7—H7	0.9300	C35—C36	1.357 (7)
C8—C10	1.375 (8)	C35—H35	0.9300
C8—C9	1.412 (6)	C36—H36	0.9300
C10—C11	1.366 (8)		
O1—La1—O2	48.23 (8)	C12—C11—H11	120.2
O1—La1—O3	73.64 (9)	N2—C12—C11	121.8 (6)
O1—La1—O4	138.93 (10)	N2—C12—H12	119.1
O2—La1—O3	64.58 (9)	C11—C12—H12	119.1
O2—La1—O4	140.15 (9)	O5—C13—O3	128.7 (4)
O3—La1—O4	145.72 (10)	O5—C13—C14	118.8 (4)
O1—La1—N1	63.25 (10)	O3—C13—C14	112.5 (4)
O2—La1—N1	102.50 (10)	N3—C14—C13	110.6 (4)
O3—La1—N1	127.37 (10)	N3—C14—H14A	109.5
O4—La1—N1	77.38 (10)	C13—C14—H14A	109.5
O1—La1—N2	73.99 (10)	N3—C14—H14B	109.5
O2—La1—N2	118.24 (9)	C13—C14—H14B	109.5
O3—La1—N2	81.95 (10)	H14A—C14—H14B	108.1
O4—La1—N2	96.14 (10)	C13—C14—H3A	105.8 (14)
N1—La1—N2	58.89 (11)	H14A—C14—H3A	84.9
O4—La1—O2^{i}	88.13 (10)	H14B—C14—H3A	134.9
O2^{i}—La1—O3	77.63 (10)	N3—C15—C16	114.3 (5)
O4—La1—O5^{i}	76.40 (9)	N3—C15—C20	124.0 (5)
O2^{i}—La1—O5^{i}	74.63 (9)	C16—C15—C20	121.7 (5)
O3—La1—O5^{i}	127.52 (10)	C15—C16—C17	119.7 (6)
O4—La1—O6^{ii}	76.42 (10)	C15—C16—H16	120.1
O2^{i}—La1—O6^{ii}	77.68 (10)	C17—C16—H16	120.1
O3—La1—O6^{ii}	70.18 (10)	C18—C17—C16	119.5 (7)
O5^{i}—La1—O6^{ii}	141.46 (10)	C18—C17—H17	120.2
O2^{i}—La1—O1	120.86 (10)	C16—C17—H17	120.2

O5^{i}—La1—O1	83.77 (9)	C17—C18—C19	120.8 (6)
O6^{ii}—La1—O1	134.00 (9)	C17—C18—H18	119.6
O2^{i}—La1—N2	149.12 (11)	C19—C18—H18	119.6
O5^{i}—La1—N2	136.11 (11)	C18—C19—C20	120.7 (7)
O6^{ii}—La1—N2	73.70 (11)	C18—C19—H19	119.7
O2^{i}—La1—N1	150.82 (10)	C20—C19—H19	119.7
O5^{i}—La1—N1	77.38 (10)	C15—C20—C19	117.5 (6)
O6^{ii}—La1—N1	121.95 (12)	C15—C20—H20	121.2
O2^{i}—La1—O2	72.85 (11)	C19—C20—H20	121.2
O5^{i}—La1—O2	65.03 (9)	O1—C21—O2	122.4 (4)
O6^{ii}—La1—O2	129.92 (10)	O1—C21—C22	119.9 (4)
C21—O1—La1	100.8 (2)	O2—C21—C22	117.7 (4)
C21—O2—La1^{i}	162.7 (3)	N5—C22—C21	114.3 (4)
C21—O2—La1	88.4 (2)	N5—C22—H22A	108.7
La1^{i}—O2—La1	107.15 (11)	C21—C22—H22A	108.7
C13—O3—La1	130.0 (2)	N5—C22—H22B	108.7
C29—O4—La1	151.1 (3)	C21—C22—H22B	108.7
C13—O5—La1^{i}	137.6 (3)	H22A—C22—H22B	107.6
C29—O6—La1^{ii}	150.0 (3)	N5—C23—C24	123.6 (10)
C1—N1—C5	117.4 (4)	N5—C23—C28	114.3 (10)
C1—N1—La1	120.0 (3)	C24—C23—C28	122.1 (9)
C5—N1—La1	121.0 (3)	C23—C24—C25	116.5 (10)
C12—N2—C9	118.2 (4)	C23—C24—H24	121.7
C12—N2—La1	118.9 (3)	C25—C24—H24	121.7
C9—N2—La1	122.6 (3)	C26—C25—C24	119.9 (10)
C15—N3—C14	116.8 (4)	C26—C25—H25	120.1
C15—N3—H3A	94 (3)	C24—C25—H25	120.1
C14—N3—H3A	84 (3)	C25—C26—C27	124.9 (9)
C23—N5—C22	118.8 (6)	C25—C26—H26	117.5
C23—N5—H5A	120.6	C27—C26—H26	117.5
C22—N5—H5A	120.6	C28—C27—C26	115.7 (10)
C31—N4—C30	116.6 (4)	C28—C27—H27	122.1
C31—N4—H4A	89 (3)	C26—C27—H27	122.1
C30—N4—H4A	92 (3)	C27—C28—C23	120.7 (10)
N1—C1—C2	123.2 (5)	C27—C28—H28	119.7
N1—C1—H1	118.4	C23—C28—H28	119.7
C2—C1—H1	118.4	O6—C29—O4	128.2 (4)
C3—C2—C1	119.6 (6)	O6—C29—C30	119.8 (4)
C3—C2—H2	120.2	O4—C29—C30	111.8 (4)
C1—C2—H2	120.2	N4—C30—C29	110.4 (4)
C4—C3—C2	119.5 (6)	N4—C30—H30A	109.6
C4—C3—H3	120.3	C29—C30—H30A	109.6
C2—C3—H3	120.3	N4—C30—H30B	109.6
C3—C4—C5	117.6 (5)	C29—C30—H30B	109.6
C3—C4—C6	123.9 (6)	H30A—C30—H30B	108.1
C5—C4—C6	118.5 (6)	N4—C31—C32	124.7 (4)

N1—C5—C9	117.6 (4)	N4—C31—C36	114.1 (4)
N1—C5—C4	122.7 (5)	C32—C31—C36	121.2 (5)
C9—C5—C4	119.7 (5)	C32—C31—H4A	120.4 (18)
C7—C6—C4	121.2 (7)	C36—C31—H4A	109.8 (18)
C7—C6—H6	119.4	C31—C32—C33	118.9 (5)
C4—C6—H6	119.4	C31—C32—H32	120.5
C6—C7—C8	120.6 (6)	C33—C32—H32	120.5
C6—C7—H7	119.7	C34—C33—C32	120.5 (6)
C8—C7—H7	119.7	C34—C33—H33	119.7
C10—C8—C9	116.1 (6)	C32—C33—H33	119.7
C10—C8—C7	122.4 (6)	C33—C34—C35	120.2 (5)
C9—C8—C7	121.5 (6)	C33—C34—H34	119.9
N2—C9—C5	118.3 (4)	C35—C34—H34	119.9
N2—C9—C8	123.5 (5)	C36—C35—C34	120.4 (6)
C5—C9—C8	118.2 (5)	C36—C35—H35	119.8
C11—C10—C8	120.6 (5)	C34—C35—H35	119.8
C11—C10—H10	119.7	C35—C36—C31	118.7 (5)
C8—C10—H10	119.7	C35—C36—H36	120.7
C10—C11—C12	119.6 (6)	C31—C36—H36	120.7
C10—C11—H11	120.2		

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	2.46	3.147 (6)	131
C10—H10···O1^{iii}	0.93	2.31	3.177 (6)	156
C12—H12···O6^{ii}	0.93	2.46	3.061 (6)	123
C12—H12···N4^{ii}	0.93	2.59	3.439 (7)	152
C22—H22B···O4^{iv}	0.97	2.38	3.328 (6)	165

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

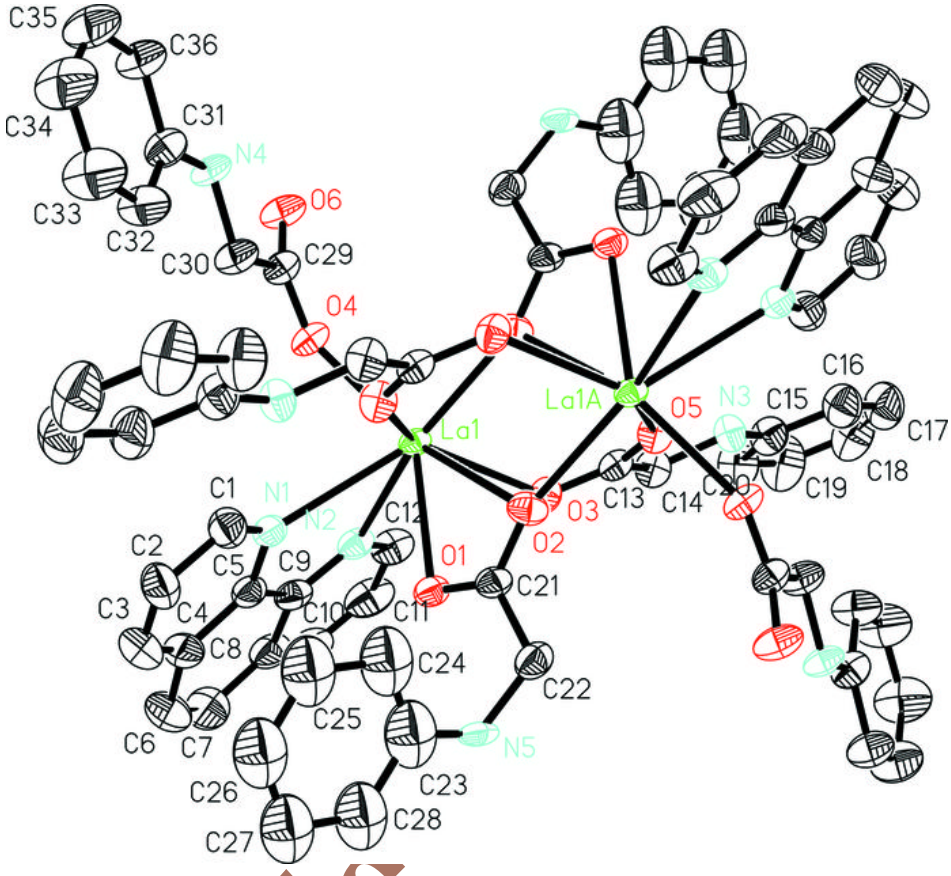

Fig. 2