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Retraction of articles by T. Liu *et al.*

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A series of 29 papers by Liu *et al.* are retracted.

As a result of problems with the data sets and incorrect atom assignments, 29 papers by Liu *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
Tetrakis(pyrazine-κN)bis(thiocyanato-κN)manganese(II)	Liu & Xie (2007*a*)	10.1107/S1600536807026852	EDUMAS
(Dihydroxyglyoxime-κ^2N,N')bis(1,10-phenanthroline-κ^2N,N')copper(II) dinitrate dihydrate	Liu, Wang, Wang & Xie (2007*b*)	10.1107/S1600536807028255	EDUVAB
Tetrakis(pyrazine-κN)bis(thiocyanato-κN)zinc(II)	Liu & Xie (2007*b*)	10.1107/S1600536807028735	RIGQAA
Tetrakis(μ-2-pyridyloxyacetato)bis[(1,10-phenanthroline)(2-pyridyloxyacetato)-lanthanum(III)]	Liu, Wang, Wang & Xie (2007*c*)	10.1107/S1600536807030917	UDUMIQ
Polymeric $KNOF_2$	Liu Wang, Wang & Xie (2007*a*)	10.1107/S1600536807027195	ICSD 240891
(Dihydroxyglyoxime-κ^2N,N')bis(1,10-phenanthroline-κ^2N,N')cobalt(II) dinitrate dihydrate	Liu, Wang, Wang & Xie (2007*d*)	10.1107/S1600536807031224	WIHJED
Tetrakis(μ-2-pyridyloxyacetato)bis[(1,10-phenanthroline)(2-pyridyloxyacetato)-praseodymium(III)]	Liu, Wang, Wang & Xie (2007*e*)	10.1107/S1600536807032679	WIHQEK
Tetrakis[μ-(2-pyridyloxy)acetato-$\kappa^2O:O'$]bis{(1,10-phenanthroline-κ^2N,N')-[(2-pyridyloxy)acetato-κO]neodymium(III)}	Liu, Wang, Wang & Xie (2007*f*)	10.1107/S1600536807035349	TIGDAP
(Dihydroxyglyoxime-κ^2N,N')bis(1,10-phenanthroline-κ^2N,N')manganese(II) dinitrate dihydrate	Liu, Wang, Wang & Xie (2007*g*)	10.1107/S1600536807035076	TIGDET
2-Amino-3,5-dinitrobenzoic acid–ammonia (1/1)	Liu & Zhu (2007*j*)	10.1107/S1600536807040068	KIKQAX
2-Hydroxy-3,5-dinitrobenzamide monohydrate	Liu & Zhu (2007*k*)	10.1107/S1600536807039712	KIKQEB
2-(1-Hydroxy-2-pyridyl)acetamide monohydrate	Liu & Zhu (2007*l*)	10.1107/S1600536807040652	CIKQOD
Bis(2,2′-bipyridine-κN,N′)bis(thiocyanato-κN)iron(II)	Liu & Zhu (2007*a*)	10.1107/S1600536807043486	XIFXOA
catena-Poly[hexakis(μ_2-anilinoacetamide)bis(1,10-phenanthroline)disamarium(III]	Liu & Zhu (2007*b*)	10.1107/S1600536807045485	XILNAI
3-Hydroxy-2,4,6-trinitropyridine monohydrate	Liu & Zhu (2007*m*)	10.1107/S1600536807045230	PILNOO
catena-Poly[hexakis(μ_2-anilinoacetamide)bis(1,10-phenanthroline)-dipraseodymium(III)]	Liu & Zhu (2007*c*)	10.1107/S1600536807047733	SILZET
catena-Poly[[tetra-μ-anilinoacetamidato-bis(1,10-phenanthroline)dicerium(III)]-di-μ-anilinoacetamidato]	Liu & Zhu (2007*d*)	10.1107/S1600536807050969	GIMZOS
Tetrakis(pyridine-κN)bis(thiocyanato-κN)chromium(II)	Liu & Zhu (2007*e*)	10.1107/S1600536807051756	WINFAB
2-Ammonio-3-carboxy-5-nitrobenzoate monohydrate	Liu & Zhu (2007*n*)	10.1107/S1600536807048477	GINFEP
2-(Benzoylhydrazinocarbonyl)benzoic acid	Liu & Zhu (2007*o*)	10.1107/S160053680705204X	TINZIA
Tetrakis(pyridine-κN)bis(thiocyanato-κN)vanadium(II)	Liu & Zhu (2007*f*)	10.1107/S1600536807054529	HIPZIQ
catena-Poly[[(nitrato-κO)(1,10-phenanthroline-κ^2N,N')nickel(II)]-μ-acetamido-$\kappa^2O:N$]	Liu & Zhu (2007*g*)	10.1107/S1600536807056504	XIRGIP
catena-Poly[[(nitrato-κO)(1,10-phenanthroline-κ^2N,N')copper(II)]-μ-acetamido-$\kappa^2O:N$]	Liu & Zhu (2007*h*)	10.1107/S1600536807059077	HIQROP
catena-Poly[[(nitrato-κO)(1,10-phenanthroline-κ^2N,N')cobalt(II)]-μ-acetamidato-$\kappa^2O:N$]	Liu & Zhu (2007*i*)	10.1107/S1600536807060631	YIQMER
N′-Benzoyl-4-nitronicotinohydrazide	Liu & Zhu (2007*p*)	10.1107/S1600536807053068	CIPVON
N′-(3-Nitro-4-pyridylcarbonyl)pyridine-4-carbohydrazide	Liu & Zhu (2007*q*)	10.1107/S1600536807054876	RIRWEV

 doi:10.1107/S1600536809049976

Table 1 (continued)

Title	Reference	DOI	Refcode
Ethylenediammonium sulfate	Liu & Zhu (2007*r*)	10.1107/S1600536807056280	ETDAMS03
Ethylenediammonium perchlorate	Liu & Zhu (2007*s*)	10.1107/S1600536807059909	HIRYEN
catena-Poly[[(nitrato-κO)(1,10-phenanthroline-κ^2N,N')manganese(II)]-μ-nitrato-$\kappa^2O:O'$]	Liu & Zhu (2008)	10.1107/S160053680706254X	MIRROV

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Liu, T., Wang, Z.-W., Wang, Y.-X. & Xie, Z.-P. (2007*g*). *Acta Cryst.* E**63**, m2198–m2199.
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Liu, T. & Xie, Z.-P. (2007*b*). *Acta Cryst.* E**63**, m1908.
Liu, T. & Zhu, J. Y. (2007*a*). *Acta Cryst.* E**63**, m2506–m2507.
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Liu, T. & Zhu, J. Y. (2007*h*). *Acta Cryst.* E**63**, m3108.
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Tetrakis(μ-2-pyridyloxyacetato)bis[(1,10-phenanthroline)(2-pyridyloxyacetato)-lanthanum(III)]

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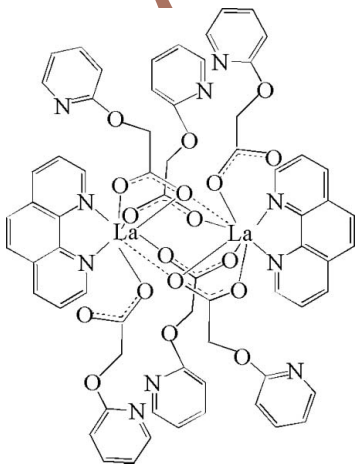
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.010 Å; R factor = 0.039; wR factor = 0.099; data-to-parameter ratio = 18.8.

The molecule of the title compound, $[La_2(C_7H_6NO_3)_6(C_{12}H_8N_2)_2]$, has an inversion centre midway between the two La^{III} ions, which are bridged by two terdentate and two bidentate carboxylate groups. Each La atom is seven-coordinated by two N atoms of a 1,10-phenanthroline ligand and five O atoms of 2-pyridyloxyacetate ligands. In the crystal structure, intermolecular C—H···O hydrogen bonds lead to a supramolecular network.

Related literature

For bond length data, see: Allen *et al.* (1987). For related literature, see: Braga & Grepioni (2000); Braga *et al.* (1998); Desiraju (1997); Hof *et al.* (2002); Johnson & Raymond (2001); Kay *et al.* (1972); Ma *et al.* (1999); Mao *et al.* (1998); Swiegers & Malefetse (2002); Tsukube & Shinoda (2002); Zaworotko (1997); Zhang *et al.* (2005).



Experimental

Crystal data

$[La_2(C_7H_6NO_3)_6(C_{12}H_8N_2)_2]$
M_r = 1551.00
Monoclinic, $P2_1/n$
a = 20.312 (3) Å
b = 8.721 (2) Å
c = 20.915 (3) Å
β = 107.332 (9)°
V = 3536.8 (11) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.26 mm^{-1}
T = 273 (2) K
0.33 × 0.13 × 0.08 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.682, T_{max} = 0.905
27369 measured reflections
7585 independent reflections
5008 reflections with $I > 2\sigma(I)$
R_{int} = 0.043

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.099
S = 1.00
7585 reflections
403 parameters
3 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.59 e Å^{-3}
$\Delta\rho_{min}$ = −0.59 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

La1—O1	2.608 (3)	La1—O4	2.517 (3)
La1—O2	2.887 (3)	La1—N1	2.769 (3)
La1—O3	2.457 (3)	La1—N2	2.739 (3)
O1—La1—O2	47.35 (8)	O3—La1—N1	76.96 (10)
O1—La1—O3	139.39 (9)	O4—La1—N1	127.54 (9)
O1—La1—O4	73.00 (9)	O1—La1—N2	75.05 (9)
O2—La1—O3	140.28 (8)	O2—La1—N2	118.42 (8)
O2—La1—O4	64.52 (8)	O3—La1—N2	95.92 (9)
O3—La1—O4	145.97 (9)	O4—La1—N2	81.57 (9)
O1—La1—N1	64.18 (9)	N1—La1—N2	59.76 (11)
O2—La1—N1	102.42 (9)		

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

D—H···A	D—H	H···A	D···A	D—H···A
C10—H10···O1^{i}	0.93	2.35	3.224 (6)	156
C14—H14B···O3^{ii}	0.97	2.45	3.394 (5)	165
C12—H12···O8^{iii}	0.93	2.48	3.076 (6)	122
C1—H1···O5^{iv}	0.93	2.48	3.163 (6)	130

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

Data collection: *SMART* (Siemens, 1996); 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: HK2279).

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supplementary materials

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Tetrakis(μ-2-pyridyloxyacetato)bis[(1,10-phenanthroline)(2-pyridyloxyacetato)lanthanum(III)]

T. Liu, Z.-W. Wang, Y.-X. Wang and Z.-P. Xie

Comment

There has been great interest in the design and synthesis of supramolecular metal organic frameworks with organic ligands and rare earth metals exhibiting novel properties such as optical, electronic, magnetic and biological (Swiegers & Malefetse, 2002; Johnson & Raymond, 2001; Hof *et al.*, 2002; Tsukube & Shinoda, 2002; Zhang *et al.*, 2005). In the synthesis of supramolecular metal organic frameworks by design, the assembly of molecular units in predefined arrangements is a key goal (Desiraju, 1997; Braga *et al.*, 1998). Directional intermolecular interactions are the primary tools in achieving this goal and hydrogen bonding is currently the best tool amongst them (Zaworotko, 1997; Braga & Grepioni, 2000). These compounds are usually prepared by the reaction of rare-earth metal ions with bi- or multidentate ligands (Kay *et al.*, 1972; Ma *et al.*, 1999; 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). It has an inversion centre between the two La^{III} ions, in which they are bridged by the two terdentate and the two bidentate carboxylate groups. Each La atom is seven-coordinated by the two N atoms of 1,10-phenanthroline (phen) ligand and the five O atoms of 2-pyridyloxyacetic acid ligands (Table 1). The La—O and La—N bonds are in the range of [2.457 (3)–2.887 (3) Å] and [2.739 (3)–2.769 (3) Å], respectively.

In the crystal structure, intermolecular C—H···O hydrogen bonds (Table 2) lead to a supramolecular network structure (Fig. 2), in which they may be effective in the stabilization of the structure.

Experimental

Crystals of the title compound were synthesized using hydrothermal method in a 23 ml Teflon-lined Parr bomb. Lanthanum (III) chloride hexahydrate (143 mg, 0.4 mmol), phen (79.2 mg, 0.4 mmol), phenoxyacetic acid (182.6 mg, 1.2 mmol) and distilled water (6 g) were placed into the bomb and sealed. The bomb was then heated under autogenous pressure for 7 d at 433 K and allowed to cool at room temperature for 24 h. Upon opening the bomb, a clear colorless 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

H atoms were positioned geometrically, with C—H = 0.93 and 0.97 Å for aromatic and methylene H atoms, and constrained to ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

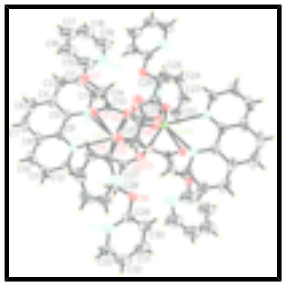

Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level [symmetry code (A): 2 − *x*, −*y*, 2 − *z*].

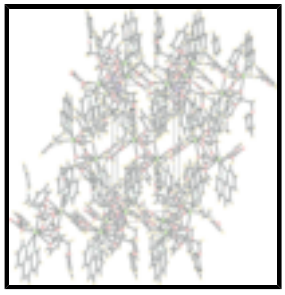

Fig. 2. A packing diagram for (I). Hydrogen bonds are shown as dashed lines.

Tetrakis(μ-2-pyridyloxyacetato)bis[(1,10-phenanthroline)(2-pyridyloxyacetato)lanthanum(III)]

Crystal data

$[La_2(C_7H_6NO_3)_6(C_{12}H_8N_2)_2]$	F_{000} = 1552
M_r = 1551.00	D_x = 1.456 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
	λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 9025 reflections
a = 20.312 (3) Å	θ = 2.4–26.7º
b = 8.721 (2) Å	μ = 1.27 mm^{-1}
c = 20.915 (3) Å	T = 273 (2) K
β = 107.332 (9)º	Plate, colorless
V = 3536.8 (11) Å^3	0.33 × 0.13 × 0.08 mm
Z = 2	

Data collection

Bruker SMART CCD area-detector diffractometer	7585 independent reflections
Radiation source: fine-focus sealed tube	5008 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.043
T = 273(2) K	θ_{max} = 27.0º
φ and ω scans	θ_{min} = 2.0º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −25→25
T_{min} = 0.682, T_{max} = 0.905	k = −10→11
27369 measured reflections	l = −26→26

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.039$	H-atom parameters constrained
$wR(F^2) = 0.099$	$w = 1/[\sigma^2(F_o^2) + (0.05P)^2 + 0.9707P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{max} = 0.001$
7585 reflections	$\Delta\rho_{max} = 0.59$ e Å^{-3}
403 parameters	$\Delta\rho_{min} = -0.59$ e Å^{-3}
3 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
La1	0.931204 (11)	0.19063 (2)	0.964291 (10)	0.04055 (9)
O1	0.84640 (13)	−0.0360 (3)	0.91884 (13)	0.0525 (7)
O2	0.94651 (13)	−0.1380 (4)	0.97709 (13)	0.0578 (7)
O3	0.94005 (14)	0.4208 (3)	1.03412 (12)	0.0560 (7)
O4	0.97065 (14)	0.0599 (3)	0.87485 (12)	0.0558 (7)
O5	1.06702 (14)	−0.0831 (3)	0.92168 (13)	0.0577 (7)
O6	1.11841 (16)	−0.0166 (4)	0.82197 (15)	0.0765 (9)
O7	0.78448 (16)	−0.3265 (3)	0.89795 (17)	0.0721 (9)
O8	1.00778 (16)	0.6128 (4)	1.09096 (13)	0.0656 (8)
O9	0.98699 (16)	0.5278 (4)	1.20622 (13)	0.0711 (9)
N1	0.79696 (17)	0.2345 (4)	0.96667 (17)	0.0554 (9)
N2	0.83402 (19)	0.3068 (4)	0.85441 (16)	0.0557 (9)
N3	1.1133 (3)	0.1077 (7)	0.7156 (3)	0.129 (2)
N4	0.7868 (4)	−0.2775 (7)	1.0123 (4)	0.1454 (13)
N5	0.9271 (3)	0.3777 (7)	1.2705 (2)	0.1130 (17)
C1	0.7780 (2)	0.1921 (5)	1.0201 (2)	0.0710 (13)
H1	0.8122	0.1690	1.0597	0.085*

C2	0.7091 (3)	0.1811 (7)	1.0189 (3)	0.0924 (18)
H2	0.6981	0.1515	1.0572	0.111*
C3	0.6578 (3)	0.2138 (8)	0.9613 (4)	0.101 (2)
H3	0.6118	0.2060	0.9603	0.122*
C4	0.6742 (3)	0.2588 (7)	0.9043 (3)	0.0846 (16)
C5	0.7460 (2)	0.2676 (5)	0.9088 (2)	0.0595 (11)
C6	0.6238 (3)	0.2977 (9)	0.8398 (4)	0.120 (3)
H6	0.5770	0.2888	0.8354	0.144*
C7	0.6427 (3)	0.3450 (8)	0.7875 (3)	0.112 (2)
H7	0.6090	0.3726	0.7482	0.135*
C8	0.7133 (3)	0.3542 (6)	0.7904 (3)	0.0787 (15)
C9	0.7658 (2)	0.3096 (5)	0.8505 (2)	0.0588 (11)
C10	0.7356 (4)	0.4030 (7)	0.7365 (3)	0.0950 (19)
H10	0.7034	0.4371	0.6975	0.114*
C11	0.8032 (4)	0.4012 (6)	0.7407 (2)	0.0903 (17)
H11	0.8177	0.4336	0.7046	0.108*
C12	0.8524 (3)	0.3489 (5)	0.8009 (2)	0.0711 (13)
H12	0.8987	0.3441	0.8028	0.085*
C13	0.8843 (2)	−0.1512 (5)	0.93930 (19)	0.0505 (10)
C14	0.8576 (2)	−0.3145 (5)	0.9191 (2)	0.0623 (11)
H14A	0.8749	−0.3490	0.8830	0.075*
H14B	0.8761	−0.3824	0.9569	0.075*
C15	0.7509 (6)	−0.3132 (8)	0.9433 (5)	0.1454 (13)
C16	0.6798 (5)	−0.3380 (8)	0.9209 (5)	0.1454 (13)
H16	0.6584	−0.3580	0.8758	0.174*
C17	0.6412 (5)	−0.3333 (8)	0.9649 (5)	0.1454 (13)
H17	0.5945	−0.3582	0.9510	0.174*
C18	0.6736 (5)	−0.2903 (8)	1.0307 (5)	0.1454 (13)
H18	0.6464	−0.2789	1.0591	0.174*
C19	0.7428 (5)	−0.2636 (9)	1.0565 (5)	0.1454 (13)
H19	0.7616	−0.2371	1.1013	0.174*
C20	0.9691 (2)	0.4992 (5)	1.08642 (19)	0.0505 (10)
C21	0.9490 (2)	0.4459 (5)	1.14740 (19)	0.0650 (12)
H21A	0.9000	0.4623	1.1397	0.078*
H21B	0.9581	0.3370	1.1541	0.078*
C22	0.9751 (2)	0.4892 (5)	1.2657 (2)	0.0617 (11)
C23	1.0144 (3)	0.5693 (6)	1.3220 (2)	0.0795 (15)
H23	1.0469	0.6408	1.3180	0.095*
C24	1.0047 (3)	0.5416 (8)	1.3834 (2)	0.1020 (19)
H24	1.0304	0.5954	1.4210	0.122*
C25	0.9566 (4)	0.4332 (9)	1.3894 (3)	0.115 (2)
H25	0.9494	0.4167	1.4308	0.138*
C26	0.9201 (4)	0.3518 (9)	1.3352 (3)	0.119 (3)
H26	0.8895	0.2768	1.3405	0.142*
C27	1.0287 (2)	0.0032 (5)	0.87717 (19)	0.0491 (9)
C28	1.0526 (2)	0.0503 (5)	0.8173 (2)	0.0637 (12)
H28B	1.0190	0.0170	0.7761	0.076*
H28A	1.0560	0.1611	0.8159	0.076*
C29	1.1458 (3)	0.0143 (6)	0.7707 (2)	0.0697 (13)

C30	1.2082 (3)	−0.0548 (7)	0.7764 (3)	0.0895 (16)
H30	1.2292	−0.1148	0.8136	0.107*
C31	1.2398 (3)	−0.0351 (8)	0.7264 (4)	0.106 (2)
H31	1.2817	−0.0831	0.7300	0.127*
C32	1.2096 (4)	0.0547 (8)	0.6720 (4)	0.114 (2)
H32	1.2312	0.0679	0.6389	0.136*
C33	1.1486 (4)	0.1242 (8)	0.6661 (3)	0.119 (2)
H33	1.1290	0.1847	0.6286	0.142*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
La1	0.04671 (13)	0.03586 (13)	0.03402 (12)	−0.00164 (11)	0.00427 (8)	0.00055 (10)
O1	0.0531 (15)	0.0420 (17)	0.0535 (16)	0.0007 (13)	0.0023 (12)	−0.0036 (12)
O2	0.0511 (17)	0.0636 (19)	0.0493 (16)	−0.0041 (13)	0.0005 (13)	0.0072 (13)
O3	0.0775 (19)	0.0429 (16)	0.0449 (15)	−0.0070 (15)	0.0142 (13)	−0.0061 (13)
O4	0.0648 (18)	0.0573 (18)	0.0446 (15)	0.0085 (15)	0.0152 (13)	0.0023 (13)
O5	0.0684 (18)	0.0585 (19)	0.0466 (16)	0.0088 (15)	0.0178 (13)	0.0117 (14)
O6	0.077 (2)	0.096 (3)	0.064 (2)	0.0207 (19)	0.0335 (17)	0.0231 (18)
O7	0.067 (2)	0.055 (2)	0.079 (2)	−0.0157 (15)	−0.0016 (16)	−0.0073 (16)
O8	0.094 (2)	0.0575 (19)	0.0445 (16)	−0.0287 (18)	0.0195 (15)	−0.0028 (14)
O9	0.099 (2)	0.072 (2)	0.0426 (16)	−0.0303 (18)	0.0207 (15)	−0.0074 (14)
N1	0.055 (2)	0.051 (2)	0.053 (2)	0.0033 (16)	0.0047 (17)	−0.0081 (16)
N2	0.069 (2)	0.045 (2)	0.0430 (19)	0.0038 (17)	0.0015 (16)	0.0007 (16)
N3	0.166 (5)	0.136 (5)	0.106 (4)	−0.003 (4)	0.075 (4)	0.026 (4)
N4	0.171 (4)	0.110 (2)	0.186 (4)	0.018 (2)	0.100 (3)	0.030 (3)
N5	0.117 (4)	0.135 (5)	0.096 (4)	−0.033 (4)	0.046 (3)	0.008 (3)
C1	0.065 (3)	0.087 (4)	0.060 (3)	0.007 (3)	0.017 (2)	−0.003 (3)
C2	0.066 (3)	0.129 (5)	0.088 (4)	0.004 (3)	0.033 (3)	−0.014 (4)
C3	0.052 (3)	0.133 (6)	0.116 (5)	−0.002 (3)	0.020 (3)	−0.019 (4)
C4	0.052 (3)	0.097 (4)	0.085 (4)	0.008 (3)	−0.008 (3)	−0.021 (3)
C5	0.056 (3)	0.047 (3)	0.066 (3)	0.006 (2)	0.004 (2)	−0.011 (2)
C6	0.064 (4)	0.159 (8)	0.111 (5)	0.015 (4)	−0.012 (4)	−0.032 (5)
C7	0.082 (4)	0.128 (6)	0.090 (5)	0.041 (4)	−0.030 (3)	−0.018 (4)
C8	0.082 (4)	0.070 (3)	0.059 (3)	0.018 (3)	−0.018 (3)	−0.011 (2)
C9	0.064 (3)	0.042 (2)	0.052 (2)	0.005 (2)	−0.0114 (19)	−0.005 (2)
C10	0.118 (5)	0.082 (4)	0.055 (3)	0.020 (4)	−0.021 (3)	0.002 (3)
C11	0.130 (5)	0.081 (4)	0.044 (3)	0.001 (4)	0.001 (3)	0.012 (3)
C12	0.092 (4)	0.062 (3)	0.050 (3)	−0.003 (3)	0.006 (2)	0.009 (2)
C13	0.054 (2)	0.056 (3)	0.037 (2)	−0.003 (2)	0.0061 (17)	−0.0027 (18)
C14	0.067 (3)	0.051 (3)	0.062 (3)	0.004 (2)	0.007 (2)	−0.006 (2)
C15	0.171 (4)	0.110 (2)	0.186 (4)	0.018 (2)	0.100 (3)	0.030 (3)
C16	0.171 (4)	0.110 (2)	0.186 (4)	0.018 (2)	0.100 (3)	0.030 (3)
C17	0.171 (4)	0.110 (2)	0.186 (4)	0.018 (2)	0.100 (3)	0.030 (3)
C18	0.171 (4)	0.110 (2)	0.186 (4)	0.018 (2)	0.100 (3)	0.030 (3)
C19	0.171 (4)	0.110 (2)	0.186 (4)	0.018 (2)	0.100 (3)	0.030 (3)
C20	0.067 (3)	0.039 (2)	0.045 (2)	−0.004 (2)	0.0145 (19)	0.0012 (18)
C21	0.084 (3)	0.063 (3)	0.049 (2)	−0.021 (3)	0.021 (2)	−0.006 (2)

C22	0.078 (3)	0.063 (3)	0.045 (2)	−0.007 (2)	0.021 (2)	0.004 (2)
C23	0.098 (4)	0.086 (4)	0.052 (3)	−0.024 (3)	0.017 (2)	−0.010 (3)
C24	0.130 (5)	0.121 (5)	0.047 (3)	−0.024 (4)	0.013 (3)	−0.010 (3)
C25	0.144 (6)	0.154 (7)	0.057 (3)	−0.032 (5)	0.043 (4)	0.008 (4)
C26	0.140 (6)	0.160 (7)	0.067 (4)	−0.067 (5)	0.048 (4)	−0.002 (4)
C27	0.061 (3)	0.042 (2)	0.043 (2)	−0.003 (2)	0.0134 (19)	−0.0015 (18)
C28	0.073 (3)	0.065 (3)	0.055 (3)	0.007 (2)	0.023 (2)	0.014 (2)
C29	0.081 (3)	0.075 (3)	0.063 (3)	−0.004 (3)	0.038 (3)	0.005 (2)
C30	0.090 (4)	0.110 (5)	0.081 (4)	0.002 (4)	0.044 (3)	0.002 (3)
C31	0.101 (4)	0.114 (6)	0.126 (5)	−0.005 (4)	0.069 (4)	−0.009 (4)
C32	0.152 (6)	0.096 (5)	0.131 (6)	−0.015 (5)	0.100 (5)	0.001 (4)
C33	0.169 (7)	0.117 (5)	0.103 (5)	0.016 (5)	0.091 (5)	0.033 (4)

Geometric parameters (Å, °)

La1—O1	2.608 (3)	C6—H6	0.9300
La1—O2	2.887 (3)	C7—C8	1.420 (9)
La1—O3	2.457 (3)	C7—H7	0.9300
La1—O4	2.517 (3)	C8—C10	1.400 (8)
La1—N1	2.769 (3)	C8—C9	1.438 (6)
La1—N2	2.739 (3)	C10—C11	1.351 (8)
La1—O2^{i}	2.463 (3)	C10—H10	0.9300
La1—O5^{i}	2.553 (3)	C11—C12	1.429 (6)
La1—O8^{ii}	2.581 (3)	C11—H11	0.9300
O1—C13	1.260 (5)	C12—H12	0.9300
O2—C13	1.280 (5)	C13—C14	1.538 (6)
O2—La1^{i}	2.463 (3)	C14—H14A	0.9700
O3—C20	1.276 (4)	C14—H14B	0.9700
O4—C27	1.266 (4)	C15—C16	1.396 (12)
O5—C27	1.268 (4)	C16—C17	1.377 (10)
O5—La1^{i}	2.553 (3)	C16—H16	0.9300
O6—C29	1.373 (5)	C17—C18	1.388 (12)
O6—C28	1.435 (5)	C17—H17	0.9300
O7—C15	1.329 (9)	C18—C19	1.366 (11)
O7—C14	1.422 (5)	C18—H18	0.9300
O8—C20	1.251 (5)	C19—H19	0.9300
O8—La1^{ii}	2.581 (3)	C20—C21	1.523 (5)
O9—C22	1.377 (5)	C21—H21A	0.9700
O9—C21	1.433 (5)	C21—H21B	0.9700
N1—C1	1.338 (5)	C22—C23	1.397 (6)
N1—C5	1.369 (5)	C23—C24	1.378 (7)
N2—C12	1.333 (5)	C23—H23	0.9300
N2—C9	1.363 (6)	C24—C25	1.393 (8)
N3—C29	1.406 (7)	C24—H24	0.9300
N3—C33	1.432 (7)	C25—C26	1.357 (8)
N4—C15	1.444 (11)	C25—H25	0.9300
N4—C19	1.470 (9)	C26—H26	0.9300
N5—C22	1.403 (6)	C27—C28	1.529 (5)

N5—C26	1.420 (7)	C28—H28B	0.9700
C1—C2	1.396 (7)	C28—H28A	0.9700
C1—H1	0.9300	C29—C30	1.376 (7)
C2—C3	1.370 (8)	C30—C31	1.391 (7)
C2—H2	0.9300	C30—H30	0.9300
C3—C4	1.387 (8)	C31—C32	1.366 (9)
C3—H3	0.9300	C31—H31	0.9300
C4—C5	1.436 (7)	C32—C33	1.351 (9)
C4—C6	1.470 (8)	C32—H32	0.9300
C5—C9	1.441 (6)	C33—H33	0.9300
C6—C7	1.328 (9)		
O1—La1—O2	47.35 (8)	C8—C9—C5	119.1 (5)
O1—La1—O3	139.39 (9)	C11—C10—C8	120.8 (5)
O1—La1—O4	73.00 (9)	C11—C10—H10	119.6
O2—La1—O3	140.28 (8)	C8—C10—H10	119.6
O2—La1—O4	64.52 (8)	C10—C11—C12	119.4 (5)
O3—La1—O4	145.97 (9)	C10—C11—H11	120.3
O1—La1—N1	64.18 (9)	C12—C11—H11	120.3
O2—La1—N1	102.42 (9)	N2—C12—C11	122.0 (5)
O3—La1—N1	76.96 (10)	N2—C12—H12	119.0
O4—La1—N1	127.54 (9)	C11—C12—H12	119.0
O1—La1—N2	75.05 (9)	O1—C13—O2	121.9 (4)
O2—La1—N2	118.42 (8)	O1—C13—C14	121.0 (4)
O3—La1—N2	95.92 (9)	O2—C13—C14	117.1 (4)
O4—La1—N2	81.57 (9)	O7—C14—C13	113.8 (3)
N1—La1—N2	59.76 (11)	O7—C14—H14A	108.8
O3—La1—O2^{i}	88.40 (10)	C13—C14—H14A	108.8
O2^{i}—La1—O4	77.79 (9)	O7—C14—H14B	108.8
O3—La1—O5^{i}	76.50 (9)	C13—C14—H14B	108.8
O2^{i}—La1—O5^{i}	74.64 (9)	H14A—C14—H14B	107.7
O4—La1—O5^{i}	127.51 (9)	O7—C15—C16	116.5 (10)
O3—La1—O8^{ii}	76.33 (9)	O7—C15—N4	121.3 (9)
O2^{i}—La1—O8^{ii}	78.41 (10)	C16—C15—N4	122.2 (8)
O4—La1—O8^{ii}	70.52 (9)	C17—C16—C15	120.7 (10)
O5^{i}—La1—O8^{ii}	141.91 (9)	C17—C16—H16	119.7
O2^{i}—La1—O1	119.91 (10)	C15—C16—H16	119.7
O5^{i}—La1—O1	83.46 (9)	C16—C17—C18	118.2 (10)
O8^{ii}—La1—O1	133.88 (8)	C16—C17—H17	120.9
O2^{i}—La1—N2	148.68 (10)	C18—C17—H17	120.9
O5^{i}—La1—N2	136.54 (10)	C19—C18—C17	124.6 (9)
O8^{ii}—La1—N2	72.59 (10)	C19—C18—H18	117.7
O2^{i}—La1—N1	150.37 (10)	C17—C18—H18	117.7
O5^{i}—La1—N1	76.93 (10)	C18—C19—N4	118.9 (9)
O8^{ii}—La1—N1	121.53 (11)	C18—C19—H19	120.5
O2^{i}—La1—O2	72.79 (10)	N4—C19—H19	120.5

O5^{i}—La1—O2	65.01 (8)	O8—C20—O3	127.5 (4)
O8^{ii}—La1—O2	130.39 (9)	O8—C20—C21	119.8 (4)
C13—O1—La1	102.1 (2)	O3—C20—C21	112.6 (3)
C13—O2—La1^{i}	162.5 (3)	O9—C21—C20	110.9 (3)
C13—O2—La1	88.4 (2)	O9—C21—H21A	109.5
La1^{i}—O2—La1	107.21 (10)	C20—C21—H21A	109.5
C20—O3—La1	151.7 (3)	O9—C21—H21B	109.5
C27—O4—La1	130.4 (2)	C20—C21—H21B	109.5
C27—O5—La1^{i}	137.6 (3)	H21A—C21—H21B	108.0
C29—O6—C28	116.9 (3)	O9—C22—C23	115.4 (4)
C15—O7—C14	118.9 (6)	O9—C22—N5	123.2 (4)
C20—O8—La1^{ii}	150.1 (3)	C23—C22—N5	121.4 (4)
C22—O9—C21	117.3 (3)	C24—C23—C22	119.6 (5)
C1—N1—C5	117.9 (4)	C24—C23—H23	120.2
C1—N1—La1	120.4 (3)	C22—C23—H23	120.2
C5—N1—La1	120.1 (3)	C23—C24—C25	120.2 (5)
C12—N2—C9	118.6 (4)	C23—C24—H24	119.9
C12—N2—La1	119.6 (3)	C25—C24—H24	119.9
C9—N2—La1	121.5 (3)	C26—C25—C24	120.2 (5)
C29—N3—C33	116.0 (6)	C26—C25—H25	119.9
C15—N4—C19	115.2 (8)	C24—C25—H25	119.9
C22—N5—C26	116.7 (5)	C25—C26—N5	121.9 (6)
N1—C1—C2	122.7 (5)	C25—C26—H26	119.1
N1—C1—H1	118.6	N5—C26—H26	119.1
C2—C1—H1	118.6	O4—C27—O5	128.4 (4)
C3—C2—C1	119.9 (5)	O4—C27—C28	112.5 (3)
C3—C2—H2	120.1	O5—C27—C28	119.1 (4)
C1—C2—H2	120.1	O6—C28—C27	110.6 (3)
C2—C3—C4	120.1 (5)	O6—C28—H28B	109.5
C2—C3—H3	120.0	C27—C28—H28B	109.5
C4—C3—H3	120.0	O6—C28—H28A	109.5
C3—C4—C5	117.3 (5)	C27—C28—H28A	109.5
C3—C4—C6	125.0 (6)	H28B—C28—H28A	108.1
C5—C4—C6	117.7 (6)	O6—C29—C30	115.1 (4)
N1—C5—C4	122.1 (5)	O6—C29—N3	123.6 (5)
N1—C5—C9	118.3 (4)	C30—C29—N3	121.3 (5)
C4—C5—C9	119.5 (4)	C29—C30—C31	120.1 (6)
C7—C6—C4	122.3 (6)	C29—C30—H30	119.9
C7—C6—H6	118.8	C31—C30—H30	120.0
C4—C6—H6	118.8	C32—C31—C30	120.2 (6)
C6—C7—C8	121.2 (6)	C32—C31—H31	119.9
C6—C7—H7	119.4	C30—C31—H31	119.9
C8—C7—H7	119.4	C33—C32—C31	120.4 (6)
C10—C8—C7	123.2 (5)	C33—C32—H32	119.8
C10—C8—C9	116.8 (5)	C31—C32—H32	119.8
C7—C8—C9	120.0 (6)	C32—C33—N3	122.1 (6)
N2—C9—C8	122.3 (5)	C32—C33—H33	119.0
N2—C9—C5	118.6 (3)	N3—C33—H33	119.0

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*
C10—H10···O1^{iii}	0.93	2.35	3.224 (6)	156
C14—H14B···O3^{iv}	0.97	2.45	3.394 (5)	165
C12—H12···O8^{ii}	0.93	2.48	3.076 (6)	122
C1—H1···O5^{i}	0.93	2.48	3.163 (6)	130

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

Fig. 1

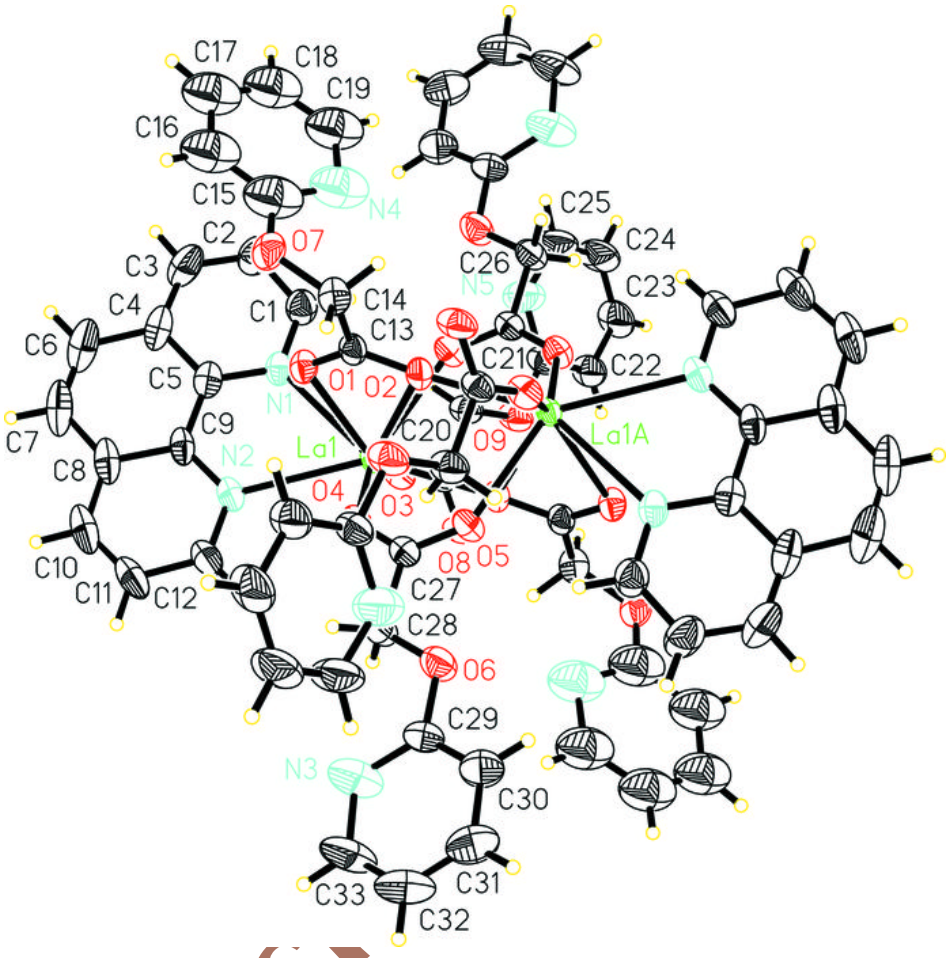
C17
C18
C19
C16
C15
N4
C2
O7
C3
C4
C1
C14
C13
C6
C5
O1
O2
N1
C9
C7
C8
N2
La1
C20
O9
La1A
O4
O3
O8
O5
C10
C11
C12
C27
C28
O6
C29
N3
C30
C33
C31
C32
C25
C24
C26
N5
C23
C21
C22

Fig. 2