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-$\kappa^2N,O$)cobalt(III) glyoxal hemisolvate monohydrate* | Zhong, Zeng, Liu & Luo (2006*b*) | 10.1107/S1600536806050240 | MEQHEW |
| *(8-Quinolinol-$\kappa^2N,O$)bis(8-quinolinolato-$\kappa^2N,O$)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-$\kappa^2N,O$)-bis(8-quinolinolato-$\kappa^2N,O$)zinc(II) glyoxal hemisolvate monohydrate* | Zhong, Zeng, Luo, Li & Xiao (2007) | 10.1107/S1600536807001171 | DEXTEG |
| *(Dimethylglyoxime-$\kappa^2N,N'$)bis(1,10-phenanthroline-$\kappa^2N,N'$)nickel(II) dinitrate dihydrate* | Zhong, Zeng, Yang, Luo & Li (2007*a*) | 10.1107/S1600536807004102 | YEYGOZ |
| *(Dimethylglyoxime-$\kappa^2N,N'$)bis(1,10-phenanthroline-$\kappa^2N,N'$)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-$\kappa N$)bis(thiocyanato-$\kappa N$)cobalt(II)* | Zhong, Zeng, Yang & Luo (2007*a*) | 10.1107/S1600536807017461 | ITCPCO01 |
| *Tetrakis(pyridine-$\kappa N$)bis(thiocyanato-$\kappa N$)copper(II)* | Zhong, Zeng, Yang & Luo (2007*b*) | 10.1107/S160053680701879X | AVUJEG02 |
| *Tetrakis(nitrato-$\kappa^2O,O'$)bis(4-phenylpyridine-$\kappa N$)cerium(IV)* | Zhong, Zeng, Yang & Luo (2007*c*) | 10.1107/S1600536807018831 | CICDOI |
| *Bis(4,4′-bipyridine-$\kappa^2N,N'$)tetrakis(nitrato-$\kappa^2O,O'$)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-$\kappa^2N,N'$)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-$\kappa^2N,N'$)bis(thiocyanato-$\kappa N$)nickel(II)* | Zhong, Yang, Luo & Xu (2007*d*) | 10.1107/S1600536807031613 | YEJGOJ01 |
| *Bis(2,2′-bipyridyl-$\kappa^2N,N'$)bis(isothiocyanato-$\kappa N$)copper(II)* | Zhong, Yang, Luo & Xu (2007*e*) | 10.1107/S1600536807033181 | UFAPOH |
| *Bis(2,2′-bipyridyl-$\kappa^2N,N'$)bis(thiocyanato-$\kappa N$)zinc(II)* | Zhong, Yang, Luo & Xu (2007*f*) | 10.1107/S1600536807035337 | TIGFAR |
| *(1,10-Phenanthroline-$\kappa^2N,N'$)tris(3-phenylpropanoato-$\kappa O$)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-$\kappa^2N,N'$)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-$\kappa^2N,N'$)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-$\kappa^2N,N'$)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-$\kappa^2N,N'$)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-$\kappa^2N,N'$)bis(1,10-phenanthroline-$\kappa^2N,N'$)copper(II) dinitrate dihydrate* | Zhong, Yang, Luo & Li (2007) | 10.1107/S1600536807061193 | YIQNUI |
| *catena-Poly[[(1,10-phenanthroline-$\kappa^2N,N'$)praseodymium(III)]-di-μ-phenoxyacetato-$\kappa^4O:O'$-[(1,10-phenanthroline-$\kappa^2N,N'$)-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.

Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# (1,10-Phenanthroline)tris(phenoxyacetato)lanthanum(III)

**H. Zhong,[a]* X.-R. Zeng,[a] X.-M. Yang,[b] Q.-Y. Luo[a] and Y.-P. Xu[a]**

[a]College of Chemistry and 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 and Economics, Nanchang 330032, People's Republic of China
Correspondence e-mail: huazhong06@126.com

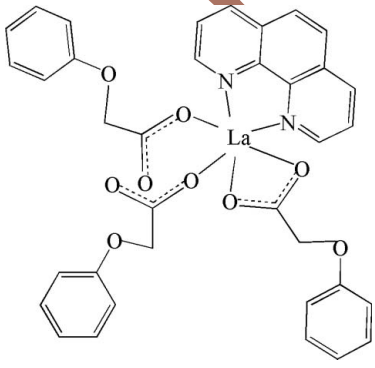
Received 5 May 2007; accepted 4 June 2007

Key indicators: single-crystal X-ray study; $T$ = 273 K; mean $\sigma$(C–C) = 0.009 Å; $R$ factor = 0.036; $wR$ factor = 0.090; data-to-parameter ratio = 16.5.

The $La^{III}$ atom in the title complex, $[La(C_8H_7O_3)_3(C_{12}H_8N_2)]$, is coordinated by two N atoms of the 1,10-phenanthroline ligand and four O atoms of three phenoxyacetate ligands. This mononuclear complex is further extended into a supramolecular network structure *via* nonclassical hydrogen bonds between CH groups of 1,10-phenanthroline and phenoxyacetate and O atoms of neighbouring phenoxyacetate ligands.

## Related literature

For related literature, see: Allen *et al.* (1987); 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

$[La(C_8H_7O_3)_3(C_{12}H_8N_2)]$
$M_r$ = 772.52
Monoclinic, $P2_1/n$
$a$ = 20.182 (3) Å
$b$ = 8.5307 (11) Å
$c$ = 20.833 (3) Å
$\beta$ = 107.779 (2)°
$V$ = 3415.5 (8) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 1.31 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)
$T_{min}$ = 0.674, $T_{max}$ = 0.903
24692 measured reflections
6634 independent reflections
4671 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.040

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.090
$S$ = 1.07
6634 reflections
403 parameters
3 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.43 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.59 e Å$^{-3}$

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| La1—O1 | 2.501 (3) | La1—O8 | 2.826 (3) |
| La1—O4 | 2.417 (3) | La1—N1 | 2.750 (3) |
| La1—O7 | 2.564 (2) | La1—N2 | 2.707 (3) |

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C10—H10···O7$^{i}$ | 0.93 | 2.33 | 3.196 (5) | 156 |
| C30—H30$B$···O4$^{ii}$ | 0.97 | 2.39 | 3.339 (5) | 166 |
| C12—H12···O5$^{iii}$ | 0.93 | 2.45 | 3.039 (5) | 122 |
| C1—H1···O2$^{iv}$ | 0.93 | 2.45 | 3.132 (5) | 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: *APEX2* (Bruker, 2004); 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*.

This work was supported by the Science and Technology Bureau of Jian, Jiangxi Province of China (grant No. 20052817).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BQ2017).

## 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 (2004). *APEX2*. Bruker AXS Inc., Madison, Wisconsin, USA.
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**, m1868-m1869 [ **doi:10.1107/S1600536807027171** ]

# (1,10-Phenanthroline)tris(phenoxyacetato)lanthanum(III)

**H. Zhong, X.-R. Zeng, X.-M. Yang, Q.-Y. Luo and Y.-P. Xu**

## 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 (Deborah *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).

In the molecule of (I) (Fig. 1), the ligand bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The six-coordinate environment of the La atom is completed by the two N atoms of 1,10-phenanthroline ligand and four O atoms of three phenoxyacetic acid ligands (Table 1). The La—O bond lengths are in the range 2.4175 (19) to 2.827 (2) Å. The La—N bond lengths are in the range 2.707 (2) to 2.750 (3) Å. C—H···O non-classica hydrogen bonds between C—H groups of 1,10-phenanthroline or phenoxyacetic acid and O atoms of neighbouring phenoxyacetic acid molecules, with an average C···O distances of 3.179 (9) Å, generate a layered hydrogen-bonded network (Fig. 2 and Table 2). The non-classical hydrogen-bonding interactions link the mononuclear complex into a supramolecular network structure.

## 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) chloride hexahydrate (70.7 mg, 0.2 mmol), phen (39.6 mg, 0.2 mmol), phenoxyacetic acid (91.3 mg, 0.6 mmol) and distilled water (4 g) were placed into the bomb and sealed. The bomb was then heated under autogenous pressure up to 413 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 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 − 0.97 Å, and constrained to ride on their parent atoms, with $U_{iso}$(H) = 1.2$U_{eq}$(C). FLAT and EADP restrains of *SHELXS* applied for C31/C36.

## Figures

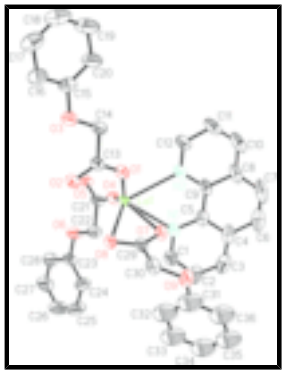


Fig. 1. View of the molecule of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. All H atoms have been omitted for clarity.

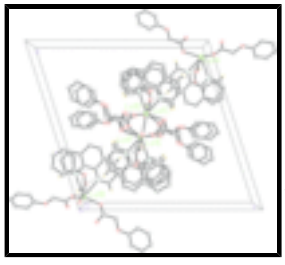


Fig. 2. A packing diagram of (I) wieved down to *b* axis. Hydrogen bonds are shown as dashed lines. Part H atoms have been omitted for clarity. [Symmetry code: (A) 2 − *x*, −*y*, 2 − *z*; (B) 1 − *x*, 1 − *y*, 1 − *z*; (C) *x* − 1, 1/2 − *y*, *z* − 1/2; (D) 1 − *x*, 1/2 + *y*, 3/2 − *z*; (E) *x*, *y*, *z*; (F) 2 − *x*, 1 − *y*, 2 − *z*]



## (1,10-Phenanthroline)tris(phenoxyacetato)lanthanum(III)

*Crystal data*

| | |
|---|---|
| $[La(C_8H_7O_3)_3(C_{12}H_8N_2)]$ | $F_{000}$ = 1552 |
| $M_r$ = 772.52 | $D_x$ = 1.502 Mg m$^{-3}$ |
| Monoclinic, $P2_1/n$ | Mo $K\alpha$ radiation |
| Hall symbol: -P 2yn | λ = 0.71073 Å |
| $a$ = 20.182 (3) Å | Cell parameters from 9081 reflections |
| $b$ = 8.5307 (11) Å | θ = 2.5–27.0º |
| $c$ = 20.833 (3) Å | μ = 1.31 mm$^{-1}$ |
| β = 107.779 (2)º | $T$ = 273 (2) K |
| $V$ = 3415.5 (8) Å$^3$ | Plane, colorless |
| $Z$ = 4 | 0.33 × 0.12 × 0.08 mm |

*Data collection*

| | |
|---|---|
| Bruker APEX II area-detector diffractometer | 6634 independent reflections |
| Radiation source: fine-focus sealed tube | 4671 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.040 |
| $T$ = 273(2) K | $\theta_{max}$ = 26.0º |
| φ and ω scans | $\theta_{min}$ = 2.1º |
| Absorption correction: multi-scan (SADABS; Sheldrick, 1996) | $h$ = −24→24 |

$T_{min}$ = 0.674, $T_{max}$ = 0.903
24692 measured reflections

$k$ = −10→10
$l$ = −25→25

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.090
$S$ = 1.07
6634 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
$w = 1/[\sigma^2(F_o^2) + (0.0436P)^2 + 0.615P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.43 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.59 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 $F^2 > 2\text{sigma}(F^2)$ 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 | 0.931205 (11) | 0.19064 (2) | 0.964291 (10) | 0.03933 (9) |
| O1 | 0.97062 (14) | 0.0601 (3) | 0.87477 (12) | 0.0530 (7) |
| O2 | 1.06694 (14) | −0.0829 (3) | 0.92161 (13) | 0.0557 (7) |
| O3 | 1.11837 (16) | −0.0162 (4) | 0.82201 (15) | 0.0735 (9) |
| O4 | 0.94007 (14) | 0.4209 (3) | 1.03406 (12) | 0.0535 (7) |
| O5 | 1.00792 (16) | 0.6128 (3) | 1.09095 (13) | 0.0635 (8) |
| O6 | 0.98698 (16) | 0.5279 (3) | 1.20623 (13) | 0.0681 (9) |
| O7 | 0.84638 (13) | −0.0360 (3) | 0.91880 (13) | 0.0505 (7) |
| O8 | 0.94658 (13) | −0.1382 (4) | 0.97709 (13) | 0.0555 (7) |
| O9 | 0.78443 (16) | −0.3265 (3) | 0.89809 (16) | 0.0696 (9) |
| N1 | 0.79701 (17) | 0.2347 (4) | 0.96669 (17) | 0.0533 (8) |
| N2 | 0.83407 (18) | 0.3069 (4) | 0.85438 (16) | 0.0535 (8) |
| C1 | 0.7780 (2) | 0.1918 (5) | 1.0201 (2) | 0.0688 (13) |
| H1 | 0.8127 | 0.1685 | 1.0600 | 0.083* |
| C2 | 0.7092 (3) | 0.1804 (7) | 1.0191 (3) | 0.0892 (17) |

| | | | | |
|---|---|---|---|---|
| H2 | 0.6984 | 0.1506 | 1.0577 | 0.107* |
| C3 | 0.6582 (3) | 0.2128 (7) | 0.9617 (4) | 0.099 (2) |
| H3 | 0.6119 | 0.2044 | 0.9605 | 0.119* |
| C4 | 0.6745 (3) | 0.2591 (7) | 0.9041 (3) | 0.0810 (16) |
| C5 | 0.7460 (2) | 0.2676 (5) | 0.9087 (2) | 0.0573 (11) |
| C6 | 0.6233 (3) | 0.2982 (8) | 0.8400 (4) | 0.116 (2) |
| H6 | 0.5762 | 0.2901 | 0.8357 | 0.139* |
| C7 | 0.6424 (3) | 0.3453 (8) | 0.7875 (3) | 0.109 (2) |
| H7 | 0.6084 | 0.3728 | 0.7478 | 0.131* |
| C8 | 0.7134 (3) | 0.3547 (6) | 0.7905 (2) | 0.0764 (15) |
| C9 | 0.7659 (2) | 0.3100 (5) | 0.8504 (2) | 0.0571 (11) |
| C10 | 0.7354 (4) | 0.4029 (7) | 0.7366 (3) | 0.0936 (19) |
| H10 | 0.7028 | 0.4371 | 0.6971 | 0.112* |
| C11 | 0.8036 (3) | 0.4011 (6) | 0.7406 (2) | 0.0872 (17) |
| H11 | 0.8179 | 0.4335 | 0.7043 | 0.105* |
| C12 | 0.8526 (3) | 0.3489 (5) | 0.8009 (2) | 0.0692 (13) |
| H12 | 0.8993 | 0.3438 | 0.8033 | 0.083* |
| C13 | 1.0287 (2) | 0.0035 (5) | 0.87698 (19) | 0.0473 (9) |
| C14 | 1.0525 (2) | 0.0507 (5) | 0.8173 (2) | 0.0608 (11) |
| H14A | 1.0185 | 0.0161 | 0.7759 | 0.073* |
| H14B | 1.0557 | 0.1640 | 0.8157 | 0.073* |
| C15 | 1.1456 (3) | 0.0146 (6) | 0.7704 (2) | 0.0679 (13) |
| C16 | 1.2080 (3) | −0.0552 (7) | 0.7767 (3) | 0.0873 (16) |
| H16 | 1.2293 | −0.1162 | 0.8144 | 0.105* |
| C17 | 1.2400 (3) | −0.0352 (8) | 0.7268 (4) | 0.1020 (19) |
| H17 | 1.2824 | −0.0835 | 0.7309 | 0.122* |
| C18 | 1.2094 (4) | 0.0543 (8) | 0.6722 (4) | 0.110 (2) |
| H18 | 1.2307 | 0.0669 | 0.6387 | 0.132* |
| C19 | 1.1481 (4) | 0.1252 (8) | 0.6664 (3) | 0.113 (2) |
| H19 | 1.1277 | 0.1876 | 0.6289 | 0.136* |
| C20 | 1.1149 (3) | 0.1063 (7) | 0.7158 (3) | 0.0902 (17) |
| H20 | 1.0726 | 0.1553 | 0.7114 | 0.108* |
| C21 | 0.9692 (2) | 0.4993 (5) | 1.08630 (19) | 0.0490 (10) |
| C22 | 0.9490 (2) | 0.4462 (5) | 1.14728 (19) | 0.0618 (11) |
| H22A | 0.8996 | 0.4638 | 1.1391 | 0.074* |
| H22B | 0.9577 | 0.3346 | 1.1540 | 0.074* |
| C23 | 0.9748 (2) | 0.4889 (5) | 1.2657 (2) | 0.0598 (11) |
| C24 | 0.9277 (3) | 0.3797 (7) | 1.2719 (2) | 0.0801 (15) |
| H24 | 0.9014 | 0.3240 | 1.2345 | 0.096* |
| C25 | 0.9197 (4) | 0.3526 (9) | 1.3349 (3) | 0.113 (2) |
| H25 | 0.8883 | 0.2768 | 1.3394 | 0.136* |
| C26 | 0.9566 (4) | 0.4343 (9) | 1.3897 (3) | 0.110 (2) |
| H26 | 0.9496 | 0.4173 | 1.4312 | 0.132* |
| C27 | 1.0043 (3) | 0.5416 (7) | 1.3837 (2) | 0.0969 (18) |
| H27 | 1.0305 | 0.5964 | 1.4215 | 0.116* |
| C28 | 1.0142 (3) | 0.5702 (6) | 1.3219 (2) | 0.0778 (14) |
| H28 | 1.0471 | 0.6432 | 1.3181 | 0.093* |
| C29 | 0.8843 (2) | −0.1515 (5) | 0.93930 (19) | 0.0489 (10) |
| C30 | 0.8575 (2) | −0.3151 (5) | 0.9191 (2) | 0.0610 (11) |

| | | | | |
|---|---|---|---|---|
| H30A | 0.8745 | −0.3503 | 0.8827 | 0.073* |
| H30B | 0.8763 | −0.3849 | 0.9571 | 0.073* |
| C31 | 0.7516 (5) | −0.3130 (8) | 0.9450 (5) | 0.1338 (13) |
| C32 | 0.7850 (5) | −0.2767 (8) | 1.0120 (5) | 0.1338 (13) |
| H32 | 0.8329 | −0.2613 | 1.0275 | 0.161* |
| C33 | 0.7437 (4) | −0.2637 (8) | 1.0562 (5) | 0.1338 (13) |
| H33 | 0.7638 | −0.2385 | 1.1015 | 0.161* |
| C34 | 0.6746 (5) | −0.2888 (8) | 1.0310 (5) | 0.1338 (13) |
| H34 | 0.6477 | −0.2755 | 1.0598 | 0.161* |
| C35 | 0.6406 (5) | −0.3336 (8) | 0.9643 (5) | 0.1338 (13) |
| H35 | 0.5936 | −0.3594 | 0.9501 | 0.161* |
| C36 | 0.6801 (4) | −0.3378 (8) | 0.9205 (4) | 0.1338 (13) |
| H36 | 0.6589 | −0.3572 | 0.8749 | 0.161* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| La1 | 0.04562 (13) | 0.03362 (13) | 0.03345 (12) | −0.00164 (10) | 0.00420 (8) | 0.00052 (10) |
| O1 | 0.0624 (17) | 0.0522 (17) | 0.0435 (15) | 0.0088 (15) | 0.0148 (13) | 0.0025 (13) |
| O2 | 0.0667 (17) | 0.0541 (18) | 0.0462 (16) | 0.0083 (15) | 0.0173 (13) | 0.0111 (14) |
| O3 | 0.074 (2) | 0.091 (2) | 0.0632 (19) | 0.0191 (18) | 0.0323 (16) | 0.0229 (17) |
| O4 | 0.0757 (18) | 0.0386 (16) | 0.0436 (15) | −0.0067 (14) | 0.0140 (13) | −0.0063 (13) |
| O5 | 0.092 (2) | 0.0529 (19) | 0.0445 (16) | −0.0291 (17) | 0.0192 (15) | −0.0019 (13) |
| O6 | 0.096 (2) | 0.066 (2) | 0.0420 (16) | −0.0290 (17) | 0.0206 (15) | −0.0074 (14) |
| O7 | 0.0510 (15) | 0.0388 (16) | 0.0524 (16) | 0.0003 (13) | 0.0021 (12) | −0.0032 (12) |
| O8 | 0.0492 (16) | 0.0594 (18) | 0.0477 (16) | −0.0039 (13) | −0.0005 (13) | 0.0073 (13) |
| O9 | 0.065 (2) | 0.050 (2) | 0.078 (2) | −0.0146 (15) | −0.0026 (16) | −0.0072 (16) |
| N1 | 0.053 (2) | 0.047 (2) | 0.051 (2) | 0.0039 (16) | 0.0044 (17) | −0.0078 (16) |
| N2 | 0.067 (2) | 0.040 (2) | 0.0426 (19) | 0.0027 (17) | 0.0014 (16) | 0.0006 (15) |
| C1 | 0.063 (3) | 0.083 (4) | 0.059 (3) | 0.008 (3) | 0.017 (2) | −0.002 (3) |
| C2 | 0.061 (3) | 0.126 (5) | 0.085 (4) | 0.005 (3) | 0.030 (3) | −0.015 (3) |
| C3 | 0.054 (3) | 0.120 (6) | 0.119 (5) | −0.003 (3) | 0.020 (3) | −0.019 (4) |
| C4 | 0.053 (3) | 0.091 (4) | 0.082 (4) | 0.008 (3) | −0.005 (3) | −0.021 (3) |
| C5 | 0.054 (3) | 0.043 (3) | 0.065 (3) | 0.0060 (19) | 0.003 (2) | −0.011 (2) |
| C6 | 0.063 (4) | 0.147 (7) | 0.111 (5) | 0.014 (4) | −0.014 (4) | −0.028 (5) |
| C7 | 0.081 (4) | 0.120 (6) | 0.089 (5) | 0.038 (4) | −0.030 (3) | −0.015 (4) |
| C8 | 0.081 (4) | 0.066 (3) | 0.057 (3) | 0.018 (3) | −0.016 (3) | −0.009 (2) |
| C9 | 0.062 (3) | 0.040 (2) | 0.051 (2) | 0.005 (2) | −0.011 (2) | −0.005 (2) |
| C10 | 0.119 (5) | 0.076 (4) | 0.053 (3) | 0.019 (4) | −0.022 (3) | 0.001 (3) |
| C11 | 0.125 (5) | 0.076 (4) | 0.044 (3) | −0.002 (4) | 0.001 (3) | 0.011 (3) |
| C12 | 0.090 (3) | 0.058 (3) | 0.050 (3) | −0.003 (2) | 0.006 (2) | 0.008 (2) |
| C13 | 0.061 (3) | 0.037 (2) | 0.042 (2) | −0.004 (2) | 0.0124 (19) | −0.0016 (17) |
| C14 | 0.070 (3) | 0.061 (3) | 0.054 (3) | 0.007 (2) | 0.022 (2) | 0.012 (2) |
| C15 | 0.076 (3) | 0.073 (3) | 0.065 (3) | −0.006 (3) | 0.037 (3) | 0.001 (2) |
| C16 | 0.086 (4) | 0.107 (5) | 0.081 (4) | 0.002 (3) | 0.043 (3) | 0.001 (3) |
| C17 | 0.098 (4) | 0.107 (5) | 0.123 (5) | −0.006 (4) | 0.066 (4) | −0.008 (4) |
| C18 | 0.148 (6) | 0.090 (5) | 0.126 (6) | −0.017 (5) | 0.095 (5) | 0.000 (4) |
| C19 | 0.159 (6) | 0.108 (5) | 0.101 (5) | 0.016 (5) | 0.082 (5) | 0.031 (4) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C20 | 0.109 (4) | 0.097 (4) | 0.082 (4) | 0.010 (4) | 0.056 (3) | 0.026 (3) |
| C21 | 0.064 (3) | 0.038 (2) | 0.043 (2) | −0.002 (2) | 0.0134 (19) | 0.0020 (18) |
| C22 | 0.080 (3) | 0.059 (3) | 0.047 (2) | −0.020 (2) | 0.020 (2) | −0.006 (2) |
| C23 | 0.077 (3) | 0.060 (3) | 0.042 (2) | −0.003 (2) | 0.017 (2) | 0.003 (2) |
| C24 | 0.088 (4) | 0.096 (4) | 0.060 (3) | −0.034 (3) | 0.027 (3) | −0.003 (3) |
| C25 | 0.133 (5) | 0.148 (6) | 0.070 (4) | −0.062 (5) | 0.047 (4) | −0.002 (4) |
| C26 | 0.138 (5) | 0.144 (6) | 0.055 (3) | −0.030 (5) | 0.042 (3) | 0.008 (4) |
| C27 | 0.125 (5) | 0.113 (5) | 0.045 (3) | −0.022 (4) | 0.015 (3) | −0.009 (3) |
| C28 | 0.095 (4) | 0.081 (4) | 0.053 (3) | −0.022 (3) | 0.017 (2) | −0.010 (3) |
| C29 | 0.053 (2) | 0.052 (3) | 0.037 (2) | −0.004 (2) | 0.0066 (18) | −0.0027 (18) |
| C30 | 0.066 (3) | 0.047 (3) | 0.061 (3) | 0.003 (2) | 0.007 (2) | −0.006 (2) |
| C31 | 0.148 (3) | 0.098 (2) | 0.182 (4) | 0.017 (2) | 0.089 (3) | 0.031 (2) |
| C32 | 0.148 (3) | 0.098 (2) | 0.182 (4) | 0.017 (2) | 0.089 (3) | 0.031 (2) |
| C33 | 0.148 (3) | 0.098 (2) | 0.182 (4) | 0.017 (2) | 0.089 (3) | 0.031 (2) |
| C34 | 0.148 (3) | 0.098 (2) | 0.182 (4) | 0.017 (2) | 0.089 (3) | 0.031 (2) |
| C35 | 0.148 (3) | 0.098 (2) | 0.182 (4) | 0.017 (2) | 0.089 (3) | 0.031 (2) |
| C36 | 0.148 (3) | 0.098 (2) | 0.182 (4) | 0.017 (2) | 0.089 (3) | 0.031 (2) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| La1—O1 | 2.501 (3) | C11—C12 | 1.413 (6) |
| La1—O4 | 2.417 (3) | C11—H11 | 0.9300 |
| La1—O7 | 2.564 (2) | C12—H12 | 0.9300 |
| La1—O8 | 2.826 (3) | C13—C14 | 1.518 (5) |
| La1—N1 | 2.750 (3) | C14—H14A | 0.9700 |
| La1—N2 | 2.707 (3) | C14—H14B | 0.9700 |
| La1—O8$^{i}$ | 2.436 (3) | C15—C16 | 1.362 (7) |
| La1—O2$^{i}$ | 2.538 (2) | C15—C20 | 1.363 (7) |
| La1—O5$^{ii}$ | 2.551 (3) | C16—C17 | 1.392 (7) |
| O1—C13 | 1.255 (4) | C16—H16 | 0.9300 |
| O2—C13 | 1.251 (4) | C17—C18 | 1.351 (8) |
| O2—La1$^{i}$ | 2.538 (2) | C17—H17 | 0.9300 |
| O3—C15 | 1.375 (5) | C18—C19 | 1.349 (8) |
| O3—C14 | 1.422 (5) | C18—H18 | 0.9300 |
| O4—C21 | 1.259 (4) | C19—C20 | 1.398 (7) |
| O5—C21 | 1.230 (5) | C19—H19 | 0.9300 |
| O5—La1$^{ii}$ | 2.551 (3) | C20—H20 | 0.9300 |
| O6—C23 | 1.376 (5) | C21—C22 | 1.517 (5) |
| O6—C22 | 1.417 (4) | C22—H22A | 0.9700 |
| O7—C29 | 1.241 (5) | C22—H22B | 0.9700 |
| O8—C29 | 1.268 (5) | C23—C24 | 1.365 (6) |
| O8—La1$^{i}$ | 2.436 (3) | C23—C28 | 1.383 (6) |
| O9—C31 | 1.343 (8) | C24—C25 | 1.390 (7) |
| O9—C30 | 1.408 (5) | C24—H24 | 0.9300 |
| N1—C1 | 1.334 (5) | C25—C26 | 1.350 (8) |
| N1—C5 | 1.356 (5) | C25—H25 | 0.9300 |
| N2—C12 | 1.327 (5) | C26—C27 | 1.362 (8) |
| N2—C9 | 1.354 (5) | C26—H26 | 0.9300 |

| | | | |
|---|---|---|---|
| C1—C2 | 1.386 (6) | C27—C28 | 1.383 (7) |
| C1—H1 | 0.9300 | C27—H27 | 0.9300 |
| C2—C3 | 1.347 (8) | C28—H28 | 0.9300 |
| C2—H2 | 0.9300 | C29—C30 | 1.509 (5) |
| C3—C4 | 1.396 (8) | C30—H30A | 0.9700 |
| C3—H3 | 0.9300 | C30—H30B | 0.9700 |
| C4—C5 | 1.418 (6) | C31—C32 | 1.387 (11) |
| C4—C6 | 1.457 (8) | C31—C36 | 1.392 (11) |
| C5—C9 | 1.436 (6) | C32—C33 | 1.425 (9) |
| C6—C7 | 1.328 (9) | C32—H32 | 0.9300 |
| C6—H6 | 0.9300 | C33—C34 | 1.347 (10) |
| C7—C8 | 1.418 (8) | C33—H33 | 0.9300 |
| C7—H7 | 0.9300 | C34—C35 | 1.402 (11) |
| C8—C10 | 1.390 (8) | C34—H34 | 0.9300 |
| C8—C9 | 1.420 (6) | C35—C36 | 1.383 (9) |
| C10—C11 | 1.353 (7) | C35—H35 | 0.9300 |
| C10—H10 | 0.9300 | C36—H36 | 0.9300 |
| O1—La1—O4 | 145.89 (9) | C12—C11—H11 | 120.7 |
| O1—La1—O7 | 73.58 (9) | N2—C12—C11 | 122.1 (5) |
| O1—La1—O8 | 65.02 (8) | N2—C12—H12 | 118.9 |
| O4—La1—O7 | 138.87 (9) | C11—C12—H12 | 118.9 |
| O4—La1—O8 | 139.82 (8) | O2—C13—O1 | 127.7 (4) |
| O7—La1—O8 | 47.79 (7) | O2—C13—C14 | 119.2 (4) |
| O1—La1—N1 | 127.85 (9) | O1—C13—C14 | 113.1 (3) |
| O4—La1—N1 | 76.73 (9) | O3—C14—C13 | 111.1 (3) |
| O7—La1—N1 | 63.87 (9) | O3—C14—H14A | 109.4 |
| O8—La1—N1 | 102.38 (9) | C13—C14—H14A | 109.4 |
| O1—La1—N2 | 81.11 (9) | O3—C14—H14B | 109.4 |
| O4—La1—N2 | 96.46 (9) | C13—C14—H14B | 109.4 |
| O7—La1—N2 | 74.58 (9) | H14A—C14—H14B | 108.0 |
| O8—La1—N2 | 118.27 (8) | C16—C15—C20 | 120.2 (5) |
| N1—La1—N2 | 60.16 (11) | C16—C15—O3 | 114.8 (4) |
| O4—La1—O8$^{i}$ | 88.28 (10) | C20—C15—O3 | 125.0 (4) |
| O8$^{i}$—La1—O1 | 77.78 (9) | C15—C16—C17 | 119.9 (6) |
| O4—La1—O2$^{i}$ | 75.76 (9) | C15—C16—H16 | 120.0 |
| O8$^{i}$—La1—O2$^{i}$ | 74.99 (9) | C17—C16—H16 | 120.0 |
| O1—La1—O2$^{i}$ | 128.31 (9) | C18—C17—C16 | 120.1 (6) |
| O4—La1—O5$^{ii}$ | 77.28 (9) | C18—C17—H17 | 120.0 |
| O8$^{i}$—La1—O5$^{ii}$ | 78.07 (10) | C16—C17—H17 | 120.0 |
| O1—La1—O5$^{ii}$ | 69.48 (9) | C19—C18—C17 | 120.0 (6) |
| O2$^{i}$—La1—O5$^{ii}$ | 142.10 (9) | C19—C18—H18 | 120.0 |
| O8$^{i}$—La1—O7 | 120.43 (9) | C17—C18—H18 | 120.0 |
| O2$^{i}$—La1—O7 | 83.70 (9) | C18—C19—C20 | 120.9 (6) |
| O5$^{ii}$—La1—O7 | 133.46 (8) | C18—C19—H19 | 119.5 |
| O8$^{i}$—La1—N2 | 148.44 (10) | C20—C19—H19 | 119.5 |
| O2$^{i}$—La1—N2 | 136.43 (10) | C15—C20—C19 | 118.9 (6) |

| | | | |
|---|---|---|---|
| O5$^{ii}$—La1—N2 | 72.66 (10) | C15—C20—H20 | 120.6 |
| O8$^{i}$—La1—N1 | 150.22 (10) | C19—C20—H20 | 120.6 |
| O2$^{i}$—La1—N1 | 76.43 (9) | O5—C21—O4 | 127.2 (4) |
| O5$^{ii}$—La1—N1 | 122.08 (10) | O5—C21—C22 | 119.7 (4) |
| O8$^{i}$—La1—O8 | 72.87 (10) | O4—C21—C22 | 113.0 (4) |
| O2$^{i}$—La1—O8 | 65.31 (8) | O6—C22—C21 | 111.5 (3) |
| O5$^{ii}$—La1—O8 | 129.85 (9) | O6—C22—H22A | 109.3 |
| C13—O1—La1 | 130.5 (2) | C21—C22—H22A | 109.3 |
| C13—O2—La1$^{i}$ | 137.6 (3) | O6—C22—H22B | 109.3 |
| C15—O3—C14 | 117.3 (3) | C21—C22—H22B | 109.3 |
| C21—O4—La1 | 151.7 (3) | H22A—C22—H22B | 108.0 |
| C21—O5—La1$^{ii}$ | 149.8 (3) | C24—C23—O6 | 124.8 (4) |
| C23—O6—C22 | 117.6 (3) | C24—C23—C28 | 119.9 (4) |
| C29—O7—La1 | 101.5 (2) | O6—C23—C28 | 115.2 (4) |
| C29—O8—La1$^{i}$ | 162.7 (3) | C23—C24—C25 | 119.2 (5) |
| C29—O8—La1 | 88.3 (2) | C23—C24—H24 | 120.4 |
| La1$^{i}$—O8—La1 | 107.13 (10) | C25—C24—H24 | 120.4 |
| C31—O9—C30 | 118.1 (5) | C26—C25—C24 | 121.2 (5) |
| C1—N1—C5 | 117.8 (4) | C26—C25—H25 | 119.4 |
| C1—N1—La1 | 120.9 (3) | C24—C25—H25 | 119.4 |
| C5—N1—La1 | 119.8 (3) | C25—C26—C27 | 119.6 (5) |
| C12—N2—C9 | 119.0 (4) | C25—C26—H26 | 120.2 |
| C12—N2—La1 | 119.5 (3) | C27—C26—H26 | 120.2 |
| C9—N2—La1 | 121.3 (3) | C26—C27—C28 | 120.7 (5) |
| N1—C1—C2 | 123.3 (5) | C26—C27—H27 | 119.6 |
| N1—C1—H1 | 118.4 | C28—C27—H27 | 119.6 |
| C2—C1—H1 | 118.4 | C23—C28—C27 | 119.3 (5) |
| C3—C2—C1 | 119.4 (5) | C23—C28—H28 | 120.4 |
| C3—C2—H2 | 120.3 | C27—C28—H28 | 120.4 |
| C1—C2—H2 | 120.3 | O7—C29—O8 | 122.2 (4) |
| C2—C3—C4 | 120.3 (5) | O7—C29—C30 | 120.5 (4) |
| C2—C3—H3 | 119.9 | O8—C29—C30 | 117.3 (4) |
| C4—C3—H3 | 119.9 | O9—C30—C29 | 113.8 (3) |
| C3—C4—C5 | 117.3 (5) | O9—C30—H30A | 108.8 |
| C3—C4—C6 | 124.5 (6) | C29—C30—H30A | 108.8 |
| C5—C4—C6 | 118.2 (6) | O9—C30—H30B | 108.8 |
| N1—C5—C4 | 122.0 (5) | C29—C30—H30B | 108.8 |
| N1—C5—C9 | 118.2 (4) | H30A—C30—H30B | 107.7 |
| C4—C5—C9 | 119.8 (4) | O9—C31—C32 | 123.7 (8) |
| C7—C6—C4 | 121.5 (6) | O9—C31—C36 | 114.0 (9) |
| C7—C6—H6 | 119.3 | C32—C31—C36 | 122.3 (8) |
| C4—C6—H6 | 119.3 | C31—C32—C33 | 117.9 (9) |
| C6—C7—C8 | 121.6 (5) | C31—C32—H32 | 121.1 |
| C6—C7—H7 | 119.2 | C33—C32—H32 | 121.1 |
| C8—C7—H7 | 119.2 | C34—C33—C32 | 118.4 (9) |
| C10—C8—C7 | 123.3 (5) | C34—C33—H33 | 120.8 |
| C10—C8—C9 | 117.0 (5) | C32—C33—H33 | 120.8 |

| | | | |
|---|---|---|---|
| C7—C8—C9 | 119.7 (5) | C33—C34—C35 | 124.4 (8) |
| N2—C9—C8 | 122.0 (4) | C33—C34—H34 | 117.8 |
| N2—C9—C5 | 119.0 (3) | C35—C34—H34 | 117.8 |
| C8—C9—C5 | 119.0 (5) | C36—C35—C34 | 117.0 (9) |
| C11—C10—C8 | 121.1 (5) | C36—C35—H35 | 121.5 |
| C11—C10—H10 | 119.4 | C34—C35—H35 | 121.5 |
| C8—C10—H10 | 119.4 | C35—C36—C31 | 119.7 (9) |
| C10—C11—C12 | 118.7 (5) | C35—C36—H36 | 120.1 |
| C10—C11—H11 | 120.7 | C31—C36—H36 | 120.1 |

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···O7$^{iii}$ | 0.93 | 2.33 | 3.196 (5) | 156 |
| C30—H30B···O4$^{iv}$ | 0.97 | 2.39 | 3.339 (5) | 166 |
| C12—H12···O5$^{ii}$ | 0.93 | 2.45 | 3.039 (5) | 122 |
| C1—H1···O2$^{i}$ | 0.93 | 2.45 | 3.132 (5) | 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**

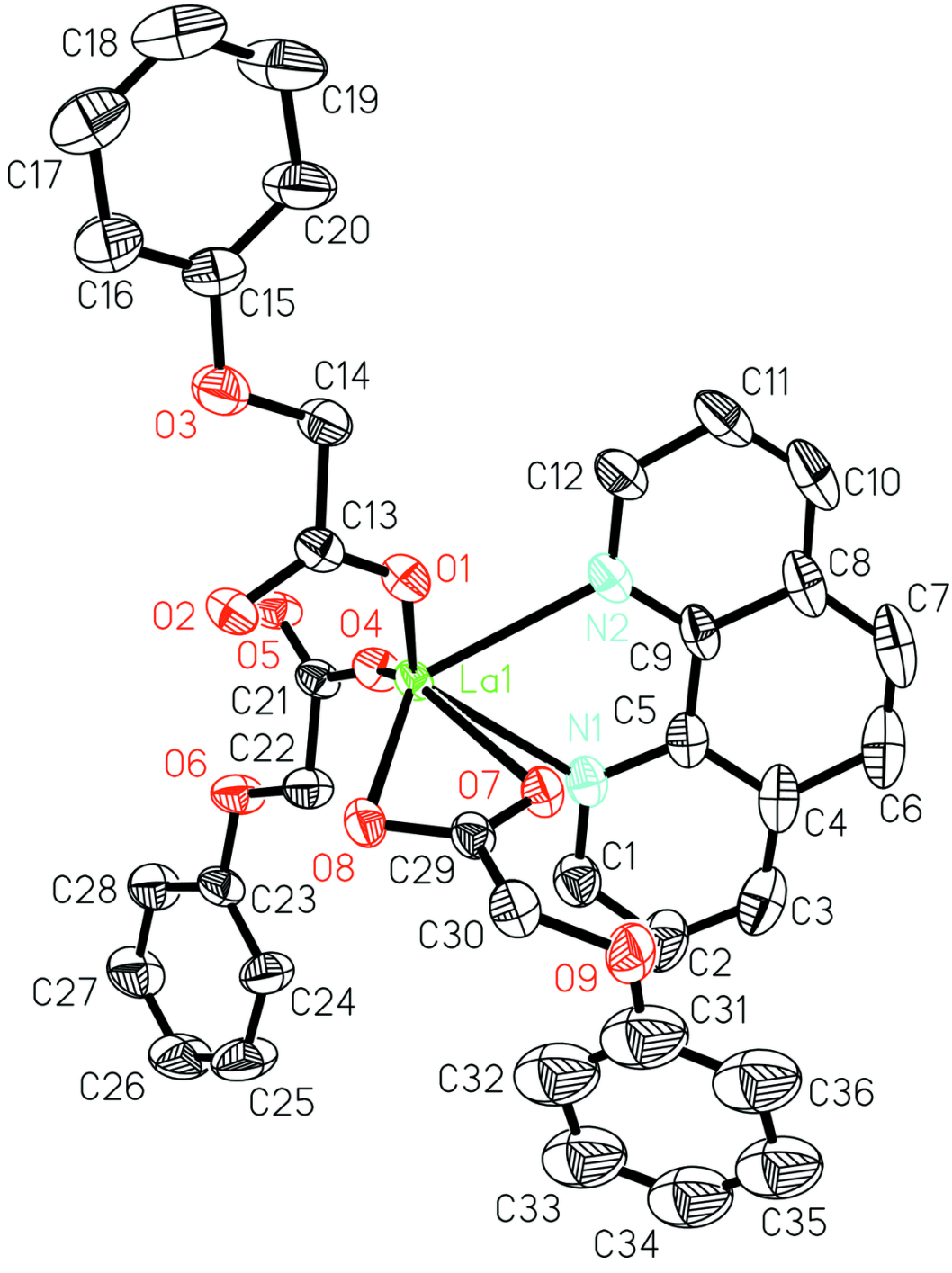

C18
C19
C17
C20
C16
C15
C14
O3
C11
C12
C10
C13
O1
C8
C7
O2
O4
N2
C9
O5
La1
C21
C5
N1
C22
O6
O7
C4
C6
O8
C29
C1
C28
C23
C30
C3
C27
C24
O9
C2
C31
C26
C25
C32
C36
C33
C35
C34

**Fig. 2**