Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Diaquatris(nicotinato-κO)bis(1,10-phenanthroline-$\kappa^2 N,N'$)lanthanum(III) trihydrate

Ping Wang,* Yong Xiao and Zhi-Feng Li

School of Materials and Chemical Engineering, Jiangxi University of Science and Technology, Ganzhou 341000, People's Republic of China

Correspondence e-mail: wangp520@yahoo.com.cn

Key indicators

Single-crystal X-ray study
T = 290 K
Mean σ(C–C) = 0.003 Å
R factor = 0.020
wR factor = 0.054
Data-to-parameter ratio = 22.5

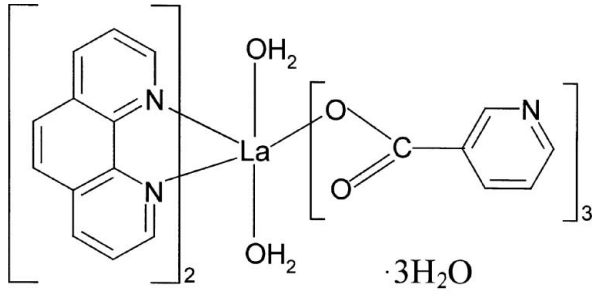
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, $[La(C_6H_4NO_2)_3(C_{12}H_8N_2)_2(H_2O)_2]\cdot 3H_2O$, consists of a mononuclear complex and three non-coordinated water molecules. The La atom is coordinated by five O atoms of three nicotinate groups and two coordinated water molecules, and four N atoms of two bidentate phenanthroline molecules, in a tricapped trigonal–prismatic coordination geometry. The complex molecule and water molecules are linked into layers through O—H···O and O—H···N hydrogen bonds.

Received 23 August 2005
Accepted 30 August 2005
Online 7 September 2005

Comment

The title compound, (I), is isostructural with its $[M(C_6H_4NO_2)_3(C_{12}H_8N_2)_2(H_2O)_2]\cdot 3H_2O$ [M = Pr (Yue *et al.*, 2004), Nd (Liu & Wang, 2004) and Ce (Liu *et al.*, 2005)] analogues. It consists of a mononuclear $[La(C_6H_4NO_2)_3(C_{12}H_8N_2)_2(H_2O)_2]$ neutral molecule and three uncoordinated water molecules (Fig. 1). The La atom possesses trigonal prismatic coordination geometry (Table 1), in which the La—O bond distances range from 2.4199 (10) to 2.5416 (10) Å and the La—N bond distances range from 2.7565 (12) to 2.7757 (11) Å, which are similar to those in the previously reported isostructural complexes. In (I), the uncoordinated water molecules participate in the extensive hydrogen-bonding interactions formed between the water molecules and the N and O atoms of the nicotinate groups (Table 2), resulting in a layered structure.



(I)

Experimental

1,10-Phenanthroline monohydrate (0.0198 g, 0.10 mmol) and nicotinic acid (0.0123 g, 0.10 mmol) were completely dissolved in CH_3OH/H_2O (30 ml, 1:1 v/v); $La(CH_3COO)_3\cdot 3H_2O$ (0.0158 g) was added and the mixture was stirred for 40 min. The resulting white slurry was filtered and the filtrate was left to stand at room temperature. Crystals of (I) suitable for X-ray analysis were obtained after two weeks (yield *ca* 35%).

Crystal data

$[La(C_6H_4NO_2)_3(C_{12}H_8N_2)_2(H_2O)_2]\cdot 3H_2O$
$M_r = 955.70$
Triclinic, $P\overline{1}$
$a = 9.0676$ (1) Å
$b = 12.9618$ (2) Å
$c = 17.9351$ (3) Å
$\alpha = 84.998$ (1)°
$\beta = 80.800$ (1)°
$\gamma = 84.190$ (1)°
$V = 2064.73$ (5) Å^3
$Z = 2$
$D_x = 1.537$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 985 reflections
$\theta = 3.3$–$26.7°$
$\mu = 1.10$ mm^{-1}
$T = 290$ (2) K
Block, colorless
0.20 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.791$, $T_{max} = 0.811$
45880 measured reflections
12414 independent reflections
11284 reflections with $I > 2\sigma(I)$
$R_{int} = 0.020$
$\theta_{max} = 30.7°$
$h = -12 \rightarrow 12$
$k = -18 \rightarrow 17$
$l = -25 \rightarrow 23$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.020$
$wR(F^2) = 0.054$
$S = 1.04$
12414 reflections
552 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0318P)^2 + 0.2509P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.005$
$\Delta\rho_{max} = 0.50$ e Å^{-3}
$\Delta\rho_{min} = -0.26$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0010 (2)

Table 1
Selected interatomic distances (Å).

La—O4	2.4199 (10)	La—N2	2.7565 (12)
La—O6	2.5200 (10)	La—N3	2.7566 (12)
La—O2	2.5355 (10)	La—N4	2.7678 (11)
La—O7	2.5367 (10)	La—N1	2.7757 (11)
La—O8	2.5416 (10)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O7—H7A···O1^{i}	0.85	1.77	2.612 (2)	172
O7—H7B···O9^{ii}	0.85	1.85	2.701 (2)	178
O8—H8A···O5^{i}	0.85	1.82	2.643 (2)	163
O8—H8B···O10^{i}	0.85	1.90	2.744 (2)	176
O9—H9A···O10^{iii}	0.85	1.96	2.786 (2)	164
O9—H9B···O11^{iv}	0.85	1.92	2.763 (2)	173
O10—H10A···O3^{iv}	0.85	1.89	2.731 (2)	172
O10—H10B···O2^{iv}	0.85	2.05	2.886 (2)	169
O11—H11A···N6^{i}	0.85	2.04	2.868 (2)	165
O11—H11B···N5^{v}	0.85	2.05	2.894 (2)	174

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

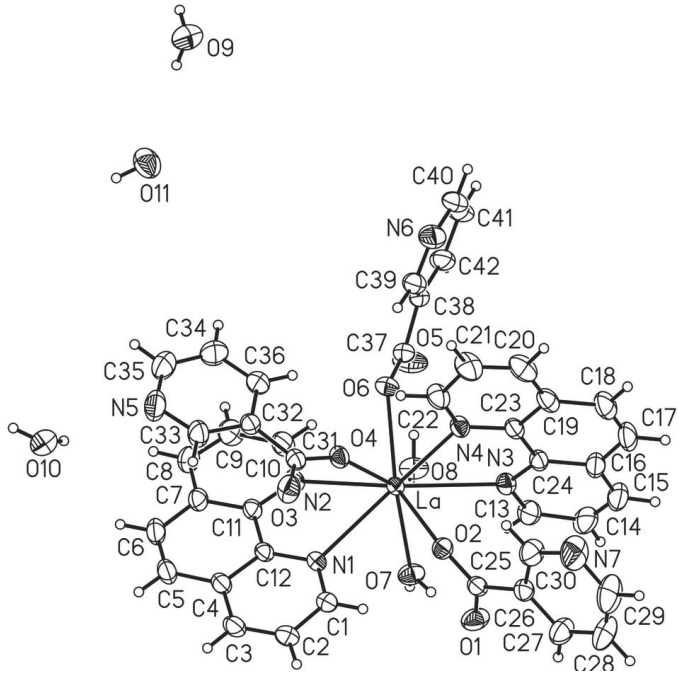


Figure 1
The asymmetric unit of (I), showing 35% probability displacement ellipsoids (arbitrary spheres for H atoms).

H atoms attached to C atoms were included at calculated positions and treated as riding atoms [C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$]. The water H atoms were found in a difference map, relocated in idealized positions (O—H = 0.85 Å) and refined as riding with $U_{iso}(H) = 1.2U_{eq}(O)$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1998); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

This work was supported by the Jiangxi Provincial Educational Foundation (2005-146) and the Jiangxi University of Science and Technology Doctoral Foundation (2003-1).

References

Bruker (1998). *SMART*, *SAINT* and *SHELXTL* (Versions 5.16). Bruker AXS Inc., Madison, Wisconsin, USA.
Liu, F.-C., Li, J.-R. & Ng, S. W. (2005). *Acta Cryst.* E**61**, m9–m10.
Liu, F.-C. & Wang, X.-L. (2004). *Acta Cryst.* E**60**, m1630–m1632.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Yue, Z.-Y., Jin, H.-J., Yan, P.-F. & Gao, P. (2004). *Acta Cryst.* E**60**, m890–m892.