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Tetra-μ-benzoato-*O*:*O*′-bis[(benzoato-*O*,*O*′)-(1,10-phenanthroline-*N*,*N*′)lanthanum(III)]

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.024
wR factor = 0.060
Data-to-parameter ratio = 12.9

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

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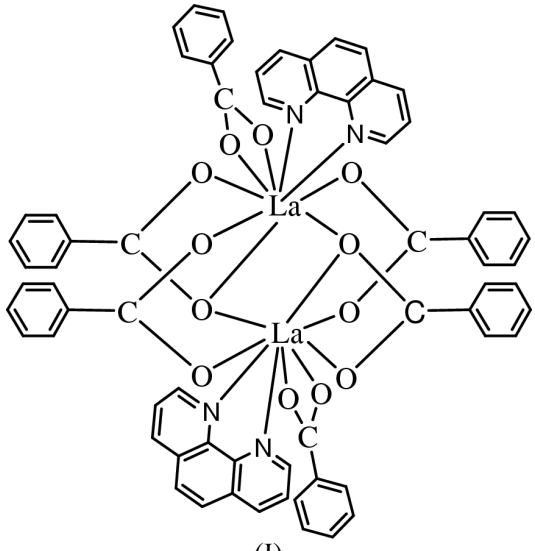
The title complex, $[La_2(C_{12}H_8N_2)_2(C_6H_5CO_2)_6]$, has a binuclear cage structure in which two La atoms are bridged by four benzoate ions with an La···La distance of 4.1143 (3) Å. The complex has a center of symmetry. The benzoate groups coordinate each La^{III} atom in three different ways.

Comment

Lanthanide complexes play an important role in special materials having optical, electronic, magnetic and biological importance (Deborah *et al.*, 2000; Farrugia *et al.*, 2000). The varied coordination modes of lanthanide elements and carboxylate groups also stimulated our interest in this work.



(I)

In the title compound, (I), two La atoms are bridged by four benzoate groups, forming a binuclear cage structure with C_i symmetry. Among them, two benzoate groups also behave as chelating ligands to the La atoms. Another benzoate ion and a 1,10-phenanthroline (phen) molecule chelate with each La atom in the terminal position of the cage. The irregular nine-coordinate environment of the La atom is completed by seven O and two N atoms. The La—O bond lengths are in the range 2.4460 (19) to 2.860 (2) Å (Table 1). The La—N1 and La—N2 bond lengths are 2.704 (2) and 2.756 (2) Å, respectively. The distance between the two La atoms is 4.1143 (3) Å. These values are slightly larger than in the Sm^{III}–benzoate complex $Sm_2(C_{12}H_8N_2)_2(C_6H_5CO_2)_6$ (Niu *et al.*, 1999) due to the effect of the lanthanide contraction.

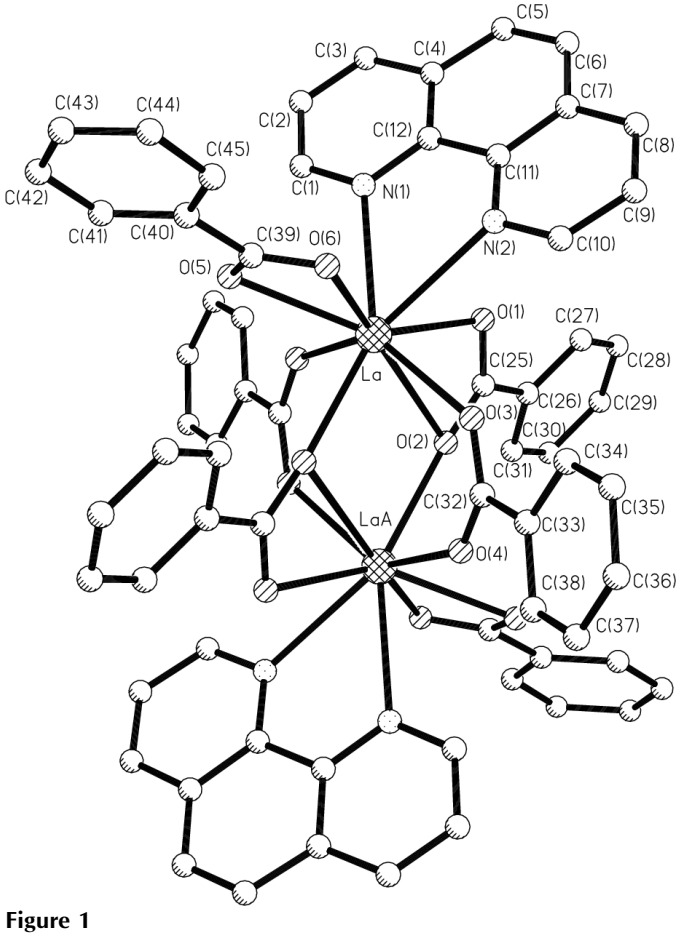


Figure 1
A view of (I) with the atomic numbering scheme. H atoms have been omitted for clarity.

Experimental

$La(NO_3)_3$ (0.5 mmol) in methanol (30 ml) was added dropwise to a solution (methanol–H_2O, 1:1, 30 ml) of phen (0.5 mmol) and benzoic acid (1.5 mmol). The mixture was heated and refluxed for 10 h to give a pink solution. The solution was filtered at room temperature and crystals of (I) were obtained after 6 d.

Crystal data

$[La_2(C_7H_5O_2)_6(C_{12}H_8N_2)_2]$	$Z = 1$
$M_r = 1364.92$	$D_x = 1.585$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 10.9356$ (2) Å	Cell parameters from 120 reflections
$b = 11.9818$ (2) Å	$\theta = 1.7$–$25.0°$
$c = 12.4945$ (3) Å	$\mu = 1.54$ mm^{-1}
$\alpha = 104.888$ (1)°	$T = 293$ (2) K
$\beta = 93.268$ (1)°	Plane, pink
$\gamma = 113.402$ (1)°	0.31 × 0.21 × 0.20 mm
$V = 1428.48$ (5) Å^3	

Data collection

Siemens Smart CCD diffractometer	4427 reflections with $I > 2\sigma(I)$
ω scans	$R_{int} = 0.019$
Absorption correction: empirical (*SADABS*; Sheldrick, 1996)	$\theta_{max} = 25.0°$
$T_{min} = 0.546$, $T_{max} = 0.734$	$h = -13 \rightarrow 13$
7321 measured reflections	$k = -13 \rightarrow 14$
4901 independent reflections	$l = -14 \rightarrow 9$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0302P)^2 + 0.0941P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.024$	$(\Delta/\sigma)_{max} = 0.017$
$wR(F^2) = 0.060$	$\Delta\rho_{max} = 0.61$ e Å^{-3}
$S = 1.04$	$\Delta\rho_{min} = -0.59$ e Å^{-3}
4901 reflections	Extinction correction: *SHELXL*97
380 parameters	Extinction coefficient: 0.0022 (4)
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

La—O2^i	2.4460 (19)	La—O5	2.6048 (19)
La—O3	2.4685 (19)	La—N1	2.704 (2)
La—O4^i	2.4756 (18)	La—N2	2.756 (2)
La—O6	2.5173 (19)	La—O2	2.860 (2)
La—O1	2.542 (2)		
O2^i—La—O3	72.52 (7)	O1—La—N1	72.91 (7)
O2^i—La—O4^i	79.10 (7)	O5—La—N1	72.40 (7)
O3—La—O4^i	134.26 (7)	O2^i—La—N2	148.23 (7)
O2^i—La—O6	91.19 (7)	O3—La—N2	78.28 (7)
O3—La—O6	87.38 (7)	O4^i—La—N2	131.77 (7)
O4^i—La—O6	128.87 (6)	O6—La—N2	75.01 (7)
O2^i—La—O1	126.03 (7)	O1—La—N2	63.59 (7)
O3—La—O1	87.45 (7)	O5—La—N2	110.24 (7)
O4^i—La—O1	81.04 (7)	N1—La—N2	60.11 (7)
O6—La—O1	138.47 (7)	O2^i—La—O2	78.60 (6)
O2^i—La—O5	80.24 (7)	O3—La—O2	73.34 (6)
O3—La—O5	129.53 (7)	O4^i—La—O2	66.31 (6)
O4^i—La—O5	77.79 (6)	O6—La—O2	160.12 (7)
O6—La—O5	51.07 (6)	O1—La—O2	47.49 (6)
O1—La—O5	141.97 (7)	O5—La—O2	141.02 (6)
O2^i—La—N1	148.16 (7)	N1—La—O2	113.37 (6)
O3—La—N1	138.33 (7)	N2—La—O2	104.95 (6)
O4^i—La—N1	79.48 (7)	La^i—O2—La	101.40 (6)
O6—La—N1	84.22 (7)		

Symmetry code: (i) $-x, -y, -z$.

The positions of all H atoms were generated geometrically (C—H distance fixed at 0.96 Å), and allowed to ride on their respective parent C atoms.

Data collection: *SMART* (Siemens, 1994); cell refinement: *SMART*; data reduction: *SMART*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXL*97; software used to prepare material for publication: *SHELXL*97.

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References

Deborah, L. B., David, L. C., Robert, J. D., John, C. G., Pamela, L. G., Webster, K., Brian, L. S., Drew, T. & John, G. W. (2000). *Inorg. Chim. Acta*, **304**, 161–169.
Farrugia, L. J., Peacock, R. D. & Stewart, B. (2000). *Acta Cryst.* C**56**, 435–436.
Niu, Sh. Y., Jin, J., Bu, W. M., Yang, G. D., Cao, J. Q. & Yang, B. (1999). *Chin. J. Struct. Chem.* **18**, 245–248.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXTL*. Version 5.10. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Siemens (1994). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.