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Key indicators

Single-crystal X-ray study
T = 193 K
Mean $\sigma(C-C)$ = 0.004 Å
R factor = 0.023
wR factor = 0.054
Data-to-parameter ratio = 14.0

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

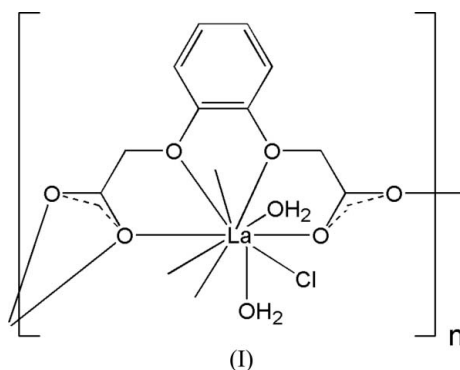
Poly[di-aqua-chloro(μ_3 -*p*-phenylenedioxy-diacetato)lanthanum(III)]

The title compound, $[La(C_{10}H_8O_6)Cl(H_2O)_2]_n$, was synthesized from lanthanum(III) chloride and *p*-phenylenedioxy-diacetic acid under hydrothermal conditions. The ligands are bridging through carboxylate groups, forming a coordination polymer with ten-coordinate lanthanum(III) ions.

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Comment

p-Phenylenedioxydiacetic acid (H₂oBDOA) is a potential multidentate ligand. Several types of complexes of oBDOA²⁻ and transition metal ions have been studied (McCann *et al.*, 1996). Up to now, however, only a few crystallographic studies of *f*-block metal complexes of oBDOA²⁻ have been reported (Kerfoot *et al.*, 1979). We expected this dicarboxylate ligand would lead to more complicated structures for the high and variable coordination numbers of the 4*f* metal ions. In this work, the oBDOA²⁻ ligand reacted with lanthanum(III) under hydrothermal conditions.



In the resulting complex (Fig. 1), each La^{III} is coordinated by a chloride ion and nine O atoms, among which two O atoms are from water molecules, two are ether O atoms of the ligand, and five are from the carboxylate groups of three different ligands. The total coordination number of La is ten.

A pair of La centres are bridged by two carboxylate O atoms (O3 and O3ⁱ; symmetry code in Table 1), with an La...La distance of 4.593 (2) Å. Dinuclear units are further bridged by other carboxylate O atoms, giving a chain polymer structure (Fig. 2).

Experimental

A mixture of LaCl₃·6H₂O (0.5 mmol), H₂oBDOA (0.5 mmol), NaOH (1.5 mmol) and ethanol (15 ml) was placed in a 23 ml Teflon reactor, which was heated at 393 K for 7 d and then cooled to room temperature at a rate of 5 K h⁻¹. The resulting crystals were washed with ethanol and dried in air.

Crystal data

$C_{10}H_{12}ClLaO_8$
 $M_r = 434.56$
 Monoclinic, $P2_1/c$
 $a = 13.8892$ (11) Å
 $b = 6.2703$ (5) Å
 $c = 14.9800$ (11) Å
 $\beta = 95.151$ (1)°
 $V = 1299.33$ (17) Å³

$Z = 4$
 $D_x = 2.221$ Mg m⁻³
 Mo $K\alpha$ radiation
 $\mu = 3.53$ mm⁻¹
 $T = 193$ (2) K
 Block, colorless
 $0.37 \times 0.23 \times 0.21$ mm

Data collection

Bruker APEX CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.356$, $T_{\max} = 0.519$
 (expected range = 0.327–0.477)

6619 measured reflections
 2532 independent reflections
 2379 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.024$
 $\theta_{\text{max}} = 26.0^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.023$
 $wR(F^2) = 0.054$
 $S = 1.06$
 2532 reflections
 181 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0272P)^2 + 0.4094P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.71$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.79$ e Å⁻³

Table 1

Selected bond lengths (Å).

La–O6 ⁱ	2.488 (2)	La–O3	2.744 (2)
La–O3 ⁱ	2.541 (2)	La–O1 ⁱ	2.771 (2)
La–O5 ⁱⁱ	2.578 (2)	La–O1W	2.600 (2)
La–O4 ⁱ	2.622 (2)	La–O2W	2.563 (2)
La–O2	2.688 (2)	La–Cl1	2.8892 (8)

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

Table 2

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O1W–H1WA \cdots O2W ⁱ	0.84	1.91	2.738 (3)	166
O1W–H1WB \cdots Cl1 ⁱⁱⁱ	0.84	2.43	3.223 (2)	156
O2W–H2WA \cdots O2 ^{iv}	0.85	1.81	2.663 (3)	176
O2W–H2WB \cdots O6 ⁱⁱ	0.85	1.82	2.668 (3)	173
O2W–H2WB \cdots O5 ⁱⁱ	0.85	2.52	2.995 (3)	116

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

H atoms were placed at calculated positions and refined as riding, with C–H = 0.93 or 0.97 Å, O–H = 0.84–0.85 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{O}, \text{C})$.

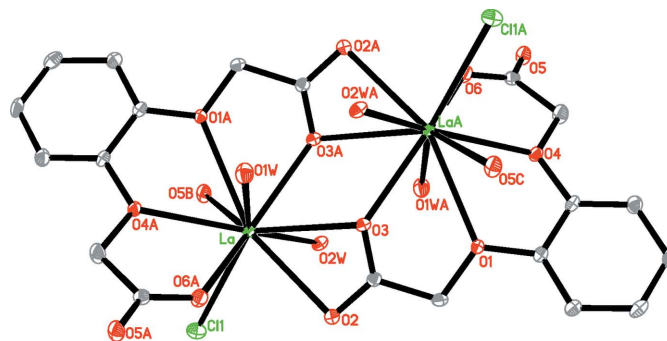


Figure 1

Part of the title polymeric structure, showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity. [Symmetry codes: (A) $2 - x, 2 - y, 1 - z$; (B) $2 - x, 1 - y, 1 - z$.]

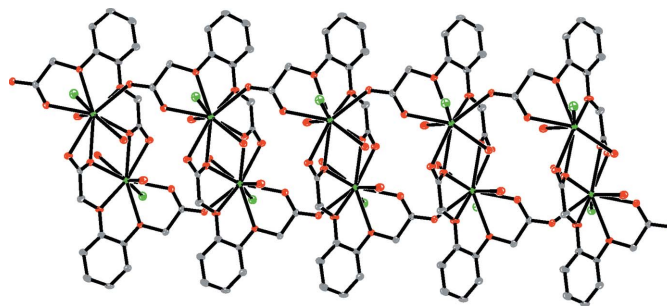


Figure 2

Chain-like polymer structure of the complex. H atoms have been omitted for clarity.

Data collection: SMART (Bruker, 2001); cell refinement: SAINT (Bruker, 2001); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 2001); software used to prepare material for publication: SHELXTL.

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