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Key indicators

Single-crystal X-ray study
 $T = 173\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.005\text{ \AA}$
 R factor = 0.025
 wR factor = 0.064
Data-to-parameter ratio = 13.9For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.Poly[[diaquatrakis(μ -benzene-1,4-dioxydiacetato)dilanthanum(III)] dihydrate]

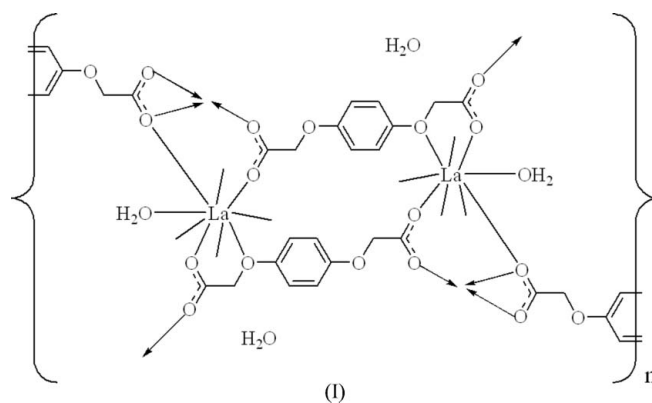
The title lanthanum coordination polymer, $\{[\text{La}_2(\text{C}_{10}\text{H}_8\text{O}_6)_3(\text{H}_2\text{O})_2] \cdot 2\text{H}_2\text{O}\}_n$, was synthesized by reacting lanthanum(III) chloride and the flexible ligand benzene-1,4-dioxydiacetic acid under hydrothermal conditions. Single-crystal X-ray studies reveal that self-assembly between the bridging ligands and metal ions results in a three-dimensional coordination polymer.

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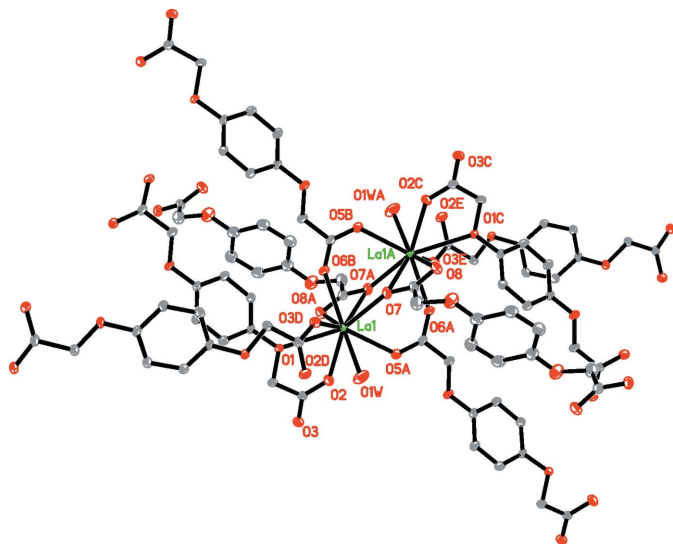
Comment

Benzene-1,4-dioxydiacetate acid (H_2 -pBDOA) is a potentially multidentate ligand with more flexibility than 1,4-benzenedicarboxylic acid and the latter can exhibit diverse coordination modes (Rosi *et al.*, 2003). Up to now, only a few simple d -block metal complexes with pBDOA^{2-} have been reported (Gao *et al.*, 2005), and no lanthanide complexes have been mentioned. We expected that this dicarboxylate ligand would lead to more complicated structures with $4f$ metal ions because of their potential for high and variable coordination numbers (Wan *et al.*, 2003). We report here the self-assembly of the lanthanum(III) ion with the pBDOA^{2-} ligand.

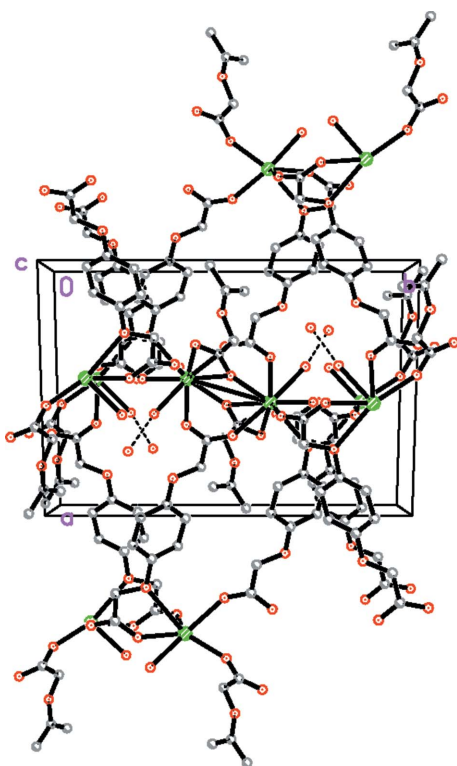


In the title complex, (I), each La^{III} ion is coordinated by nine O atoms, eight from four pBDOA^{2-} ligands and one from a water molecule. The coordination environment around the La^{III} ion can be described as tricapped trigonal-prismatic with $\text{O}-\text{La}-\text{O}$ bond angles ranging from $47.96(6)^\circ$ to $149.63(7)^\circ$. A pair of La^{III} atoms are bridged by the two ligands in different coordination modes. The $\text{La}\cdots\text{La}$ distance is $4.1804(4)\text{ \AA}$ (Fig. 1).

Along the b axis, the La^{III} units are bridged by the ligands to form a zigzag chain. Adjacent chains are further extended into a two-dimensional network *via* intercalation between the lateral ligands in a zipper-like fashion. In this zipper-like arrangement, the benzyl groups are arranged in an offset


Figure 1

The dinuclear unit of the polymeric complex, with displacement ellipsoids shown at the 30% probability level. All H atoms have been omitted for clarity and atom labels have been given suffixes with the following symmetry codes: (A) $1 + x, y, 1 + z$; (B) $-x, -y, 1 - z$; (C) $1 - x, -y, 2 - z$; (D) $x, \frac{1}{2} - y, -\frac{1}{2} + z$; (E) $1 - x, -\frac{1}{2} + y, 2.5 - z$.


Figure 2

Perspective view of the three-dimensional network in the complex. H atoms are omitted for clarity. Hydrogen bonds are shown as dashed lines.

fashion with a face-to-face distance of 3.241 (5) Å, indicating strong π - π stacking interactions (Zhang *et al.*, 2003). Finally, these layers are cross-linked into a three-dimensional network through the bridging carboxylate groups (Fig. 2).

Experimental

A mixture of $\text{LaCl}_3 \cdot 6\text{H}_2\text{O}$ (0.5 mmol), H_2 -pBDOA (0.75 mmol), NaOH (1.5 mmol) and H_2O (15 ml) was placed in a 23 ml Teflon reactor, which was heated at 433 K for seven days and then cooled to room temperature at a rate of 5 K h^{-1} . Crystals were obtained after washing with water and drying in air.

Crystal data

$[\text{La}_2(\text{C}_{10}\text{H}_8\text{O}_6)_3(\text{H}_2\text{O})_2] \cdot 2\text{H}_2\text{O}$
 $M_r = 1022.38$
 Monoclinic, $P2_1/c$
 $a = 12.1493$ (8) Å
 $b = 16.9135$ (11) Å
 $c = 8.9264$ (6) Å
 $\beta = 108.918$ (1)°
 $V = 1735.2$ (2) Å³

$Z = 2$
 $D_x = 1.957$ Mg m⁻³
 Mo $K\alpha$ radiation
 $\mu = 2.52$ mm⁻¹
 $T = 173$ (2) K
 Block, colorless
 $0.36 \times 0.27 \times 0.21$ mm

Data collection

Bruker SMART APEX area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.465$, $T_{\max} = 0.614$

9349 measured reflections
 3393 independent reflections
 3160 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.025$
 $\theta_{\text{max}} = 26.0^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.026$
 $wR(F^2) = 0.065$
 $S = 1.01$
 3393 reflections
 244 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0342P)^2 + 1.6475P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.64$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.61$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$\text{O1W}-\text{H1WA} \cdots \text{O2}^i$	0.85	2.24	2.716 (3)	115
$\text{O1W}-\text{H1WB} \cdots \text{O5}^{ii}$	0.85	2.08	2.926 (3)	180
$\text{O2W}-\text{H2WA} \cdots \text{O1W}^i$	0.85	2.33	3.179 (5)	180
$\text{O2W}-\text{H2WB} \cdots \text{O4}^{iii}$	0.85	2.50	3.240 (4)	146

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

The carbon-bound H atoms were placed in calculated positions [methylene C-H = 0.97 Å, aromatic C-H = 0.93 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$] and were included in the refinement in the riding-model approximation. The water H atoms were located in difference Fourier maps and were then refined as riding, with O-H = 0.85 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{O})$.

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: ORTEPIII (Johnson, 1976); software used to prepare material for publication: SHELXL97.

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