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Poly[diaqua(μ_6-benzene-1,2,4,5-tetracarboxylato)(μ_6-2,5-dicarboxybenzene-1,4-dicarboxylato)dilanthanum(III)]

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Key indicators

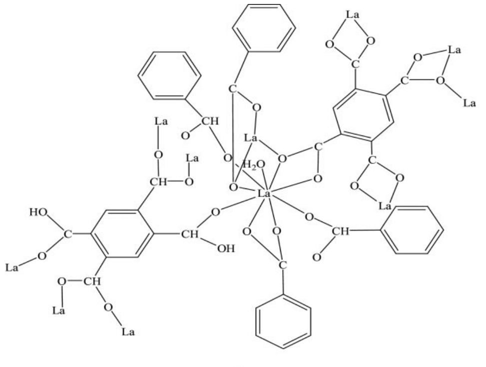
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.008 Å
R factor = 0.029
wR factor = 0.078
Data-to-parameter ratio = 9.9

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

The title compound, $[La_2(betc)(H_2betc)(H_2O)_2]_n$ (betc = benzene-1,2,4,5-tetracarboxylate, $C_{10}H_2O_4$, and H_2betc is 2,5-dicarboxybenzene-1,4-dicarboxylate, $C_{10}H_4O_4$) was obtained by hydrothermal reaction. The compound possesses an infinite three-dimensional network structure. The central La^{III} atom is nine-coordinate by eight carboxylate O atoms from six different organic ligands derived from H_4betc (1,2,4,5-benzenetetracarboxylic acid), with La—O distances ranging from 2.439 (4) to 2.658 (4) Å, and one water molecule, with La—OW1 = 2.503 (5) Å.

Comment

Chemists have devoted great effort to the research of novel coordination materials by using multidentate organic ligands to coordinate to transition metal centers (Fujita *et al.*, 1994; Desiraju, 1995). In particular, benzenepolycarboxylate ligands have been shown to be good building blocks in the design of metal–organic materials having the desired topologies owing to their rich variety of coordination modes. 1,2,4,5-Benzenetetracarboxylic acid (H_4btec) may be a good choice for the construction of coordination polymers through full or partial deprotonation of its carboxylic groups and a considerable number of complexes of metal ions with H_4btec have been determined in recent years (Sun *et al.*, 2002; Wu *et al.*, 2001).


(I)

We describe here the hydrothermal synthesis and structural characterization of the title compound, (I), with a three-dimensional network structure, as shown in Fig. 1. X-ray diffraction analysis shows that each 1,2,4,5-benzenetetracarboxylate ligand ($betc^{4-}$ and H_2betc^{2-}) adopts a μ_6-bridging mode, linking six La^{III} atoms through its carboxylic acid O atoms, and each lanthanum(III) center links six 1,2,4,5-benzenetetracarboxylate ligands, giving rise to a three-dimensional network structure. Furthermore, there are O—H···O hydrogen-bonding interactions between ligated water

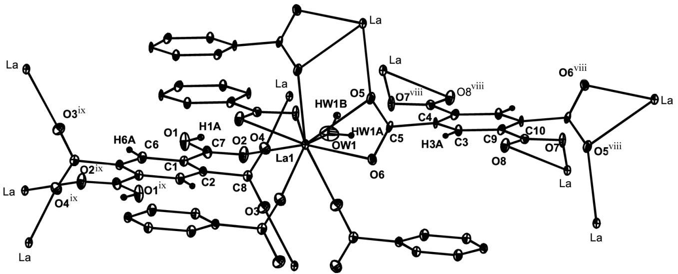


Figure 1

The structure of (I). Displacement ellipsoids are plotted at the 30% probability level [symmetry codes: (viii) $-x$, $3-y$, $1-z$; (ix) $2-x$, $1-y$, $2-z$].

molecules and carboxylic acid O atoms or between non-coordinated carboxylate and adjacent carboxylic acid O atoms. It is noteworthy that the benzenecarboxylate ligands have two different coordination modes. The first has all eight carboxylic O atoms of betc^{4-} ligands coordinated to La^{III} atoms with two O atoms bonded to one La^{III} atom [O5 and O6, O7 and O8, O5^{viii} and O6^{viii}, O7^{viii} and O8^{viii}; symmetry code: (viii) $-x$, $3-y$, $1-z$] or one O atom linking two La^{III} atoms (O5 and O5^{viii}). The second has only six carboxylic acid O atoms of H_2betc^{2-} ligands coordinated to La^{III} atoms with each O atom bonding to one La^{III}atom.

Experimental

A mixture of $La(NO_3)_3\cdot 3H_2O$ (0.22 g, 0.5 mmol), H_4betc (0.127 g, 0.5 mmol), 1,3-bis(4-pyridyl)propane (0.05 g, 0.025 mmol) and H_2O (18 ml) was sealed in a 25 ml stainless-steel reactor with a Telflon liner and was heated at 433 K for 3 d. On completion of the reaction, the reactor was cooled slowly to room temperature and the mixture was filtered, giving colorless single crystals suitable for X-ray analysis.

Crystal data

$[La_2(C_{10}H_2O_4)(C_{10}H_4O_4)(H_2O)_2]$
$M_r = 816.10$
Triclinic, $P\bar{1}$
$a = 6.441$ (1) Å
$b = 9.4467$ (3) Å
$c = 9.6323$ (1) Å
$\alpha = 88.518$ (2)°
$\beta = 74.744$ (2)°
$\gamma = 76.660$ (2)°
$V = 549.80$ (3) Å^3

$Z = 1$
$D_x = 2.465$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2449 reflections
$\theta = 2.2$–25.0°
$\mu = 3.93$ mm^{-1}
$T = 293$ (2) K
Prism, colorless
0.30 × 0.20 × 0.16 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.348$, $T_{max} = 0.533$
2896 measured reflections

1917 independent reflections
1793 reflections with $I > 2\sigma(I)$
$R_{int} = 0.023$
$\theta_{max} = 25.0°$
$h = -7 \rightarrow 7$
$k = -11 \rightarrow 11$
$l = -11 \rightarrow 7$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.029$
$wR(F^2) = 0.078$
$S = 1.00$
1917 reflections
193 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0509P)^2 + 2.7076P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.91$ e Å^{-3}
$\Delta\rho_{min} = -1.36$ e Å^{-3}

Table 1

Selected geometric parameters (Å, °).

La1—O4^{i}	2.439 (4)	La1—O2	2.579 (4)
La1—O3^{ii}	2.478 (4)	La1—O8^{iv}	2.598 (4)
La1—O*W*1	2.503 (5)	La1—O7^{iv}	2.609 (4)
La1—O5^{iii}	2.563 (4)	La1—O5	2.658 (4)
La1—O6	2.564 (4)		
O4^{i}—La1—O3^{ii}	77.72 (14)	O5^{iii}—La1—O7^{iv}	80.26 (12)
O4^{i}—La1—O*W*1	140.14 (18)	O6—La1—O7^{iv}	73.82 (12)
O3^{ii}—La1—O*W*1	66.59 (18)	O2—La1—O7^{iv}	119.80 (12)
O4^{i}—La1—O5^{iii}	144.77 (13)	O8^{iv}—La1—O7^{iv}	50.01 (11)
O3^{ii}—La1—O5^{iii}	136.51 (13)	O4^{i}—La1—O5	127.32 (13)
O*W*1—La1—O5^{iii}	70.31 (17)	O3^{ii}—La1—O5	101.14 (13)
O4^{i}—La1—O6	81.64 (13)	O*W*1—La1—O5	78.40 (18)
O3^{ii}—La1—O6	72.51 (13)	O5^{iii}—La1—O5	63.99 (13)
O*W*1—La1—O6	103.0 (2)	O6—La1—O5	49.70 (12)
O5^{iii}—La1—O6	112.76 (11)	O2—La1—O5	143.38 (13)
O4^{i}—La1—O2	89.14 (15)	O8^{iv}—La1—O5	114.33 (12)
O3^{ii}—La1—O2	88.89 (13)	O7^{iv}—La1—O5	74.67 (12)
O*W*1—La1—O2	73.5 (2)	La1—O*W*1—H*W*1*B*	138 (5)
O5^{iii}—La1—O2	84.46 (13)	La1—O*W*1—H*W*1*A*	99 (6)
O6—La1—O2	160.58 (13)	C7—O2—La1	142.3 (4)
O4^{i}—La1—O8^{iv}	71.89 (14)	C8—O3—La1^{ii}	139.0 (3)
O3^{ii}—La1—O8^{iv}	142.69 (13)	C8—O4—La1^{v}	169.9 (4)
O*W*1—La1—O8^{iv}	130.00 (19)	C5—O5—La1^{iii}	151.3 (3)
O5^{iii}—La1—O8^{iv}	73.38 (13)	C5—O5—La1	91.6 (3)
O6—La1—O8^{iv}	122.39 (12)	La1^{iii}—O5—La1	116.01 (13)
O2—La1—O8^{iv}	69.81 (12)	C5—O6—La1	96.6 (3)
O4^{i}—La1—O7^{iv}	73.08 (14)	C10—O7—La1^{vi}	93.9 (3)
O3^{ii}—La1—O7^{iv}	137.92 (13)	C10—O8—La1^{vi}	94.0 (3)
O*W*1—La1—O7^{iv}	146.62 (17)		

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

Table 2

Hydrogen-bonding geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···O8^{iv}	0.78 (7)	1.82 (7)	2.592 (5)	170 (7)
O*W*1—H*W*1*B*···O6^{v}	0.79 (8)	2.22 (8)	2.824 (6)	134 (7)
O*W*1—H*W*1*B*···O7^{vii}	0.79 (8)	2.32 (8)	2.975 (7)	141 (7)

Symmetry codes: (iv) $x, y-1, z$; (v) $1+x, y, z$; (vii) $1-x, 3-y, 1-z$.

H atoms bonded to C atoms were placed at calculated positions (C—H = 0.93 Å) and refined with isotropic displacement parameters [$U_{iso} = 1.2U_{eq}(C)$], using a riding model. H atoms associated with the water molecules and O atoms were located in difference maps and refined freely. The deepest hole is located 0.98 Å from atom La1.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SMART* and *SAINT* (Siemens, 1994); data reduction: *SAINT* and *XPREP* in *SHELXTL* (Siemens, 1994); program(s) used to solve structure: *SHELXTL*; program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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References

Desiraju, G. R. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 2311–2327.

m536 Yi-Hang Wen *et al.* • $[La_2(C_{10}H_2O_4)(C_{10}H_4O_4)(H_2O)_2]$ *Acta Cryst.* (2004). E**60**, m535–m537

Fujita, M., Kwon, Y. J., Washizu, S. & Ogura, K. (1994). *J. Am. Chem. Soc.* **116**, 1151–1152.

Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.

Siemens (1994). *SAINT* and *SHELXTL*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

Siemens (1996). *SMART*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

Sun, D., Cao, R., Liang, Y., Shi, Q. & Hong, M. (2002). *J. Chem. Soc. Dalton Trans.* pp. 1847–1851.

Wu, C.-D., Lu, C.-Z., Lu, S.-F., Zhuang, H.-H. & Huang, J.-S. (2001). *Inorg. Chem. Commun.* **5**, 171–174.

Acta Cryst. (2004). E**60**, m535–m537 Yi-Hang Wen *et al.* • $[La_2(C_{10}H_2O_4)(C_{10}H_4O_4)(H_2O)_2]$ **m537**