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catena-Poly[[[μ-benzene-1,4-dicarboxylato-bis[tetraaqualutetium(III)]]-di-μ-benzene-1,4-dicarboxylato] dihydrate]

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Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.006 Å
R factor = 0.027
wR factor = 0.065
Data-to-parameter ratio = 19.8

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

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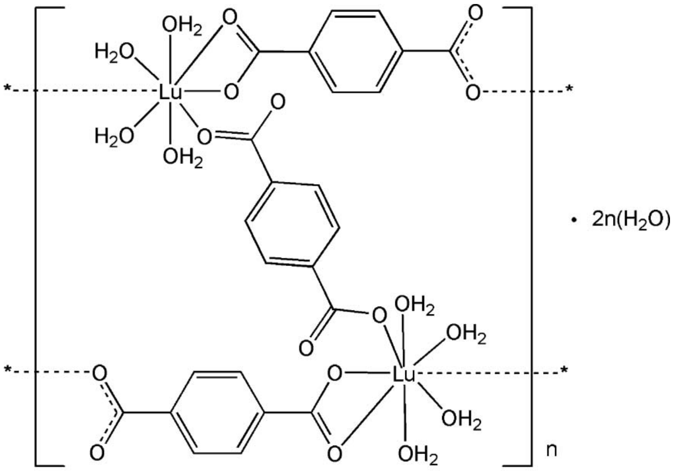
The title lanthanide–bdc complex, $\{[Lu_2(C_8H_4O_4)_3(H_2O)_8]\cdot 2H_2O\}_n$ (bdc is benzene-1,4-dicarboxylate), was synthesized under hydrothermal conditions. In this complex, the Lu^{III} centers are eight-coordinated by four O atoms from three benzene-1,4-dicarboxylate ligands and four from water molecules. Lu^{III} ions are bridged by benzene-1,4-dicarboxylate anions in two modes, forming polymeric chains. These chains are further assembled into a three-dimensional supramolecular network by O—H···O hydrogen-bonding interactions.

Comment

Research on metal-directed supramolecular compounds has rapidly been expanding because of their interesting topologies and potential applications as functional materials (Eddaoudi *et al.*, 2001; Hagrman *et al.*, 1999). A variety of organic molecules, including bi-, tri- and tetradentate ligands, have been used in the construction of many fascinating structures (Blake *et al.*, 1997; Gardner *et al.*, 1995). 1,4-Benzenedicarboxylic acid (H_2bdc), a rod-like bifunctional ligand, has afforded a number of extended structures by virtue of an exodentate coordination modes (Fun *et al.*, 1999; Groeneman *et al.*, 1999; Reineke *et al.*, 1999). We report here a new lanthanide–bdc complex, $[Lu_2(bdc)_3(H_2O)_8]\cdot 2H_2O$, (I).



(I)

As depicted in Fig. 1, the local coordination geometry around the Lu^{III} ions is dodecahedral, consisting of four O atoms from three bdc ligands [the Lu—O bond distances range from 2.178 (3) to 2.512 (3) Å] and four from water molecules [the Lu—O bond distances vary from 2.249 (3) to 2.373 (3) Å; Table 1]. Two types of coordination modes of the

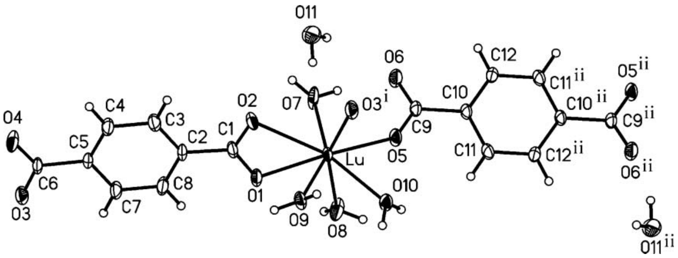


Figure 1
The coordination environment of the Lu atom, with the atom-numbering scheme, showing displacement ellipsoids at the 45% probability level [symmetry codes: (i) $x, y, z + 1$; (ii) $1 - x, -y, 2 - z$].

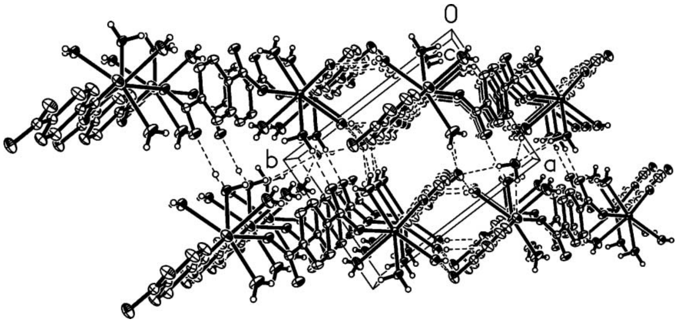


Figure 2
The three-dimensional structure of the title compound. Dashed lines illustrate the hydrogen bonds (only those H atoms that are involved in hydrogen-bonding interactions are shown).

bdc ligands exist in the complex: (i) chelating bidentate and monodentate, with the Lu^{III} cations bridged to form a one-dimensional chain along the [001] direction by the bdc anions in this mode; (ii) bis-monodentate, the bdc anions being centrosymmetric and bonded in this mode to two adjacent Lu–bdc chains. Thus, a one-dimensional double polymeric chain is formed *via* bridging bdc ligands.

Extensive hydrogen-bonding interactions exist between the water molecules and the carboxylate O atoms (Table 2). The uncoordinated carboxylate atom O6 forms hydrogen bonds with the coordinated water molecules (O7, O8 and O9), and the uncoordinated carboxylate atom O4 forms hydrogen bonds with the coordinated water (O7 and O9) and uncoordinated water molecules (O11). The coordinated carboxylate atom O1 is hydrogen bonded to the uncoordinated water molecule (O11), as is O2 to O9. The uncoordinated water molecule (O11) also accepts H atoms from the water molecules O8 and O10. Because of the extensive hydrogen-bonding interactions, the chains are interlinked into a three-dimensional framework.

Experimental

The title complex was hydrothermally synthesized from a mixture of lutetium(III) chloride hexahydrate, 1,4-benzenedicarboxylic acid, potassium hydroxide and water in the molar ratio 1:1:1:60. The starting mixture was heated for 12 h at 453 K under autogenous pressure (final pH = 5). The resulting solid phase, consisting of colourless blocks of the title complex, was filtered off and dried at room temperature.

Crystal data

$[Lu_2(C_8H_4O_4)_3(H_2O)_8]\cdot 2H_2O$
$M_r = 1022.44$
Triclinic, $P\overline{1}$
$a = 7.5264$ (4) Å
$b = 10.0492$ (6) Å
$c = 10.4543$ (5) Å
$\alpha = 87.806$ (4)°
$\beta = 82.513$ (3)°
$\gamma = 86.215$ (3)°
$V = 781.90$ (7) Å^3
$Z = 1$
$D_x = 2.171$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 156 reflections
$\theta = 3.3$–26.7°
$\mu = 6.37$ mm^{-1}
$T = 292$ (2) K
Block, colourless
0.09 × 0.07 × 0.05 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.586$, $T_{max} = 0.725$
10175 measured reflections
4327 independent reflections
3777 reflections with $I > 2\sigma(I)$
$R_{int} = 0.087$
$\theta_{max} = 29.8°$
$h = -10 \rightarrow 10$
$k = -14 \rightarrow 13$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.027$
$wR(F^2) = 0.065$
$S = 0.97$
4327 reflections
218 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0181P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 1.81$ e Å^{-3}
$\Delta\rho_{min} = -1.35$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0012 (3)

Table 1
Selected bond lengths (Å).

Lu—O3^i	2.178 (3)	Lu—O9	2.331 (3)
Lu—O7	2.248 (3)	Lu—O1	2.345 (3)
Lu—O5	2.294 (3)	Lu—O10	2.373 (3)
Lu—O8	2.304 (3)	Lu—O2	2.512 (3)

Symmetry code: (i) $x, y, z + 1$.

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

D—H···A	D—H	H···A	D···A	D—H···A
O7—H7A···O6	0.82	1.84	2.655 (4)	171
O7—H7B···O4^{iii}	0.82	1.99	2.776 (5)	159
O8—H8A···O11^{iv}	0.82	1.98	2.797 (5)	171
O8—H8B···O6^{v}	0.82	2.04	2.826 (4)	162
O9—H9A···O2^{vi}	0.82	2.06	2.712 (4)	136
O9—H9B···O4^{vii}	0.82	2.07	2.866 (5)	164
O10—H10A···O11^{iv}	0.82	2.07	2.840 (4)	158
O10—H10B···O6^{viii}	0.82	1.94	2.747 (4)	170
O11—H11A···O4^{i}	0.82	2.01	2.792 (4)	158
O11—H11B···O1^{vi}	0.82	2.00	2.802 (4)	166

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

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 = 0.82 Å) and refined as riding with $U_{iso}(H) = 1.2U_{eq}(O)$. The highest density peak and deepest hole are located 0.88 and 0.83 Å, respectively, from atom Lu.

Data collection: *SMART* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); 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, 2004); software used to prepare material for publication: *SHELXTL*.

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