

Poly[[hexaqua(μ_2 -oxalato- $\kappa^4 O^1, O^2$;- O^1', O^2')bis(μ_3 -pyridine-2,4-dicarboxylato- $\kappa^4 N, O^2': O^2': O^4$)dilanthanum(III)] monohydrate]

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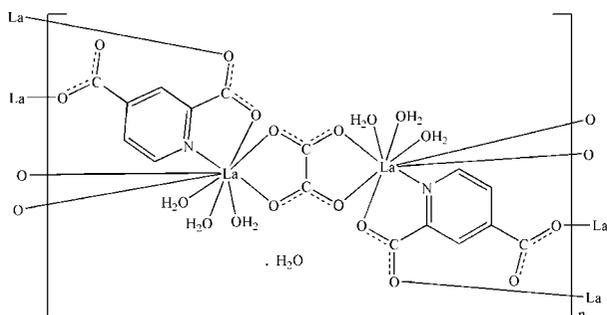
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Key indicators: single-crystal X-ray study; $T = 295$ K; mean $\sigma(C-C) = 0.008$ Å; disorder in solvent or counterion; R factor = 0.032; wR factor = 0.093; data-to-parameter ratio = 11.7.

In the polymeric title compound, $\{[La_2(C_7H_3NO_4)_2(C_2O_4)(H_2O)_6] \cdot (H_2O)_n\}$, the La^{3+} cation is nine-coordinated in a distorted $LaNO_8$ tricapped trigonal-prismatic geometry formed by three pyridinedicarboxylate anions, one oxalate anion and three water molecules. The oxalate anion is located on an inversion center. The oxalate and pyridinedicarboxylate anions bridge the La^{3+} cations, forming a two-dimensional polymeric complex parallel to (010). Intermolecular O—H...O hydrogen bonding and weak C—H...O hydrogen bonding is present in the crystal structure and π – π stacking [centroid–centroid distance = 3.571 (3) Å] is observed between parallel pyridine rings of adjacent molecules. The uncoordinated water molecule shows an occupancy of 0.5.

Related literature

For related structures, see: Aghabozorg *et al.* (2011); Li *et al.* (2007); Wang *et al.* (2009).



Experimental

Crystal data

$[La_2(C_7H_3NO_4)_2(C_2O_4)(H_2O)_6] \cdot H_2O$
 $M_r = 822.16$
 Triclinic, $P\bar{1}$
 $a = 6.4614$ (8) Å
 $b = 6.6844$ (8) Å
 $c = 14.0796$ (17) Å
 $\alpha = 89.735$ (2)°

$\beta = 85.266$ (2)°
 $\gamma = 73.135$ (2)°
 $V = 579.85$ (12) Å³
 $Z = 1$
 Mo $K\alpha$ radiation
 $\mu = 3.73$ mm⁻¹
 $T = 295$ K
 $0.30 \times 0.10 \times 0.10$ mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2001)
 $T_{min} = 0.686$, $T_{max} = 0.950$

5023 measured reflections
 2046 independent reflections
 1795 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.035$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.032$
 $wR(F^2) = 0.093$
 $S = 1.09$
 2046 reflections

175 parameters
 H-atom parameters constrained
 $\Delta\rho_{max} = 2.14$ e Å⁻³
 $\Delta\rho_{min} = -2.13$ e Å⁻³

Table 1

Selected bond lengths (Å).

La1—N1	2.726 (4)	La1—O6 ⁱⁱⁱ	2.550 (5)
La1—O1 ⁱ	2.454 (4)	La1—O7	2.604 (7)
La1—O3 ⁱⁱ	2.541 (5)	La1—O8	2.553 (5)
La1—O4	2.551 (5)	La1—O9	2.612 (7)
La1—O5	2.543 (4)		

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

Table 2

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O7—H7A...O4 ⁱⁱ	0.84	2.08	2.911 (8)	168
O7—H7B...O10 ^{iv}	0.83	1.71	2.533 (12)	168
O8—H8A...O2 ^v	0.83	1.83	2.660 (7)	173
O8—H8B...O6 ^{vi}	0.96	2.03	2.914 (7)	153
O9—H9A...O6 ^{vi}	0.88	2.27	2.987 (8)	138
O9—H9B...O10	0.85	1.73	2.390 (14)	133
O10—H10A...O5 ⁱⁱ	0.83	2.24	2.885 (12)	135
O10—H10A...O8 ⁱⁱ	0.83	2.29	2.924 (15)	133
O10—H10B...O9 ^{vii}	0.85	1.77	2.591 (17)	163
C5—H5A...O3 ⁱⁱⁱ	0.93	2.49	3.164 (7)	130

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

Data collection: SMART (Bruker, 2007); cell refinement: SAINT (Bruker, 2007); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 2008); program(s) used to refine structure: SHELXTL; molecular graphics: PLATON (Spek, 2009); software used to prepare material for publication: PLATON.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5376).

References

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supplementary materials

Acta Cryst. (2011). E67, m1731-m1732 [doi:10.1107/S160053681104668X]

Poly[[hexaaqua(μ_2 -oxalato- $\kappa^4 O^1, O^2:O^{1'}, O^{2'}$)bis(μ_3 -pyridine-2,4-dicarboxylato- $\kappa^4 N, O^2:O^{2'}:O^4$)dilanathanum(III)] monohydrate]

F. M. Shen and S. F. Lush

Comment

The pyridine-2,4-dicarboxylic acid (pdcH₂) has important coordination functions to metals by either carboxylate bridges between metal centers, to form dimeric complexes or tridentate (O, N, O') chelation to metal ions. Some pydc complexes have been reported (Li *et al.*, 2007; Wang *et al.*, 2009; Aghabozorg *et al.*, 2011).

The symmetric unit of the title compound, $\{[(LaC_7H_3NO_4)(C_2O_4)_{0.5}(H_2O)_3]_2 \cdot (H_2O)\}_n$, contains two La^{III} atoms, two pyridine-2,4-dicarboxylate(pydc) ligands, one oxalate ligand and six coordinated water molecules. The oxalate ligand are both chelating and bridging, forming an oxalate-bridged dinuclear complex. The La^{III} is nine-coordinated in a distorted tricapped trigonal prismatic geometry by N,O atom from a pydc ligand, two O atoms from two pydc ligands, two O atoms from one oxalate ligand and three O atoms from coordinated water molecules (shown as Fig. 1, Table 1). The geometric center of the dimer lies on an inversion center.

The crystal structure contains weak O—H \cdots O and non-classical C—H \cdots O hydrogen bonds. The π - π stacking between two pyridine rings of (pydc) anion fragments with distances of 3.570 (3) Å (1 - x, 1 - y, 1 - z) are observed (Fig. 3). The uncoordinated water molecule shows half-occupation.

Experimental

La(NO₃)₃·6H₂O (0.1096 g, 0.25 mmole), pyridine-2,4-dicarboxylic acid (0.0418 g, 0.25 mmol) and 4,4'-dipyridine (0.0464 g, 0.25 mmol) were mixed in 10 ml of deionized water. After stirring for 30 min, the mixture was placed in a 23 ml Teflon-lined reactor which was heated under autogenous pressure to 418 K for 48 h and then allowed to cool to room temperature. The brown transparent single crystals were obtained in 41.3% yield (based on La).

Refinement

The site occupancy factor of the lattice water O10 was refined to 0.509 (16), and was set as 0.5 at the final cycles of refinement. Water H atoms were fixed in chemically sensible positions, thermal parameters were fixed as 0.08 Å². Other H atoms were positioned geometrically with C—H = 0.93 Å (aromatic) and refined using a riding model with $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

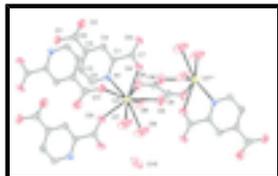


Fig. 1. View of the title compound with the atom numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 50% probability level. All H atoms have been omitted for clarity. [Symmetry code: (i) $-1 + x, y, z$; (ii) $1 - x, 1 - y, 1 - z$; (iv) $1 + x, y, z$.]

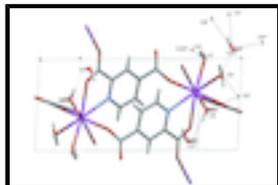


Fig. 2. The molecular packing for the title compound. Hydrogen bonds are shown as dashed lines.

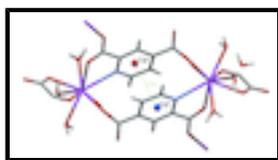


Fig. 3. π - π Stacking between pyridine rings [symmetry code: (ii) $1 - x, 1 - y, 1 - z$.]

Poly[[hexaaqua(μ_2 -oxalato- $\kappa^4 O^1, O^2:O^1, O^2$)bis(μ_3 -pyridine-2,4- dicarboxylato- $\kappa^4 N, O^2:O^2:O^4$) dilanthanum(III)] monohydrate]

Crystal data

$[\text{La}_2(\text{C}_7\text{H}_3\text{NO}_4)_2(\text{C}_2\text{O}_4)(\text{H}_2\text{O})_6]\cdot\text{H}_2\text{O}$

$M_r = 822.16$

Triclinic, $P\bar{1}$

Hall symbol: $-P\ 1$

$a = 6.4614\ (8)\ \text{\AA}$

$b = 6.6844\ (8)\ \text{\AA}$

$c = 14.0796\ (17)\ \text{\AA}$

$\alpha = 89.735\ (2)^\circ$

$\beta = 85.266\ (2)^\circ$

$\gamma = 73.135\ (2)^\circ$

$V = 579.85\ (12)\ \text{\AA}^3$

$Z = 1$

$F(000) = 396$

$D_x = 2.355\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 3390 reflections

$\theta = 2.5\text{--}25.0^\circ$

$\mu = 3.73\ \text{mm}^{-1}$

$T = 295\ \text{K}$

Columnar, brown

$0.30 \times 0.10 \times 0.10\ \text{mm}$

Data collection

Bruker SMART 1000 CCD area-detector diffractometer

Radiation source: fine-focus sealed tube graphite

Detector resolution: 9 pixels mm^{-1}

ϕ and ω scans

Absorption correction: multi-scan (*SADABS*; Bruker, 2001)

$T_{\min} = 0.686$, $T_{\max} = 0.950$

2046 independent reflections

1795 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.035$

$\theta_{\max} = 25.0^\circ$, $\theta_{\min} = 1.5^\circ$

$h = -7 \rightarrow 7$

$k = -7 \rightarrow 7$

$l = -16 \rightarrow 16$

5023 measured reflections

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.032$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.093$	H-atom parameters constrained
$S = 1.09$	$w = 1/[\sigma^2(F_o^2) + (0.0639P)^2]$
2046 reflections	where $P = (F_o^2 + 2F_c^2)/3$
175 parameters	$(\Delta/\sigma)_{\max} = 0.001$
0 restraints	$\Delta\rho_{\max} = 2.14 \text{ e } \text{\AA}^{-3}$
	$\Delta\rho_{\min} = -2.13 \text{ e } \text{\AA}^{-3}$

Special details

Geometry. Bond distances, angles *etc.* have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted R -factors wR and all goodnesses of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating $-R$ -factor-obs *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
La1	0.36051 (5)	0.32815 (5)	0.80389 (2)	0.0265 (1)	
O1	0.7674 (8)	0.3427 (7)	0.2806 (3)	0.0392 (16)	
O2	1.0913 (8)	0.2154 (8)	0.3384 (3)	0.0525 (19)	
O3	1.0788 (7)	0.2730 (8)	0.6993 (3)	0.0396 (16)	
O4	0.7592 (7)	0.3177 (9)	0.7799 (3)	0.0521 (18)	
O5	0.5103 (8)	0.2478 (6)	0.9657 (3)	0.0423 (14)	
O6	0.5841 (9)	0.3677 (7)	1.1030 (3)	0.0485 (18)	
O7	-0.0071 (10)	0.5171 (10)	0.8990 (5)	0.0863 (19)	
O8	0.5618 (9)	-0.0608 (7)	0.7835 (4)	0.0542 (19)	
O9	0.1731 (10)	0.0871 (10)	0.9025 (5)	0.0863 (19)	
N1	0.5725 (7)	0.2598 (7)	0.6261 (3)	0.0249 (14)	
C1	0.7769 (9)	0.2729 (9)	0.6137 (4)	0.0257 (17)	
C2	0.5722 (10)	0.2408 (9)	0.4559 (4)	0.0294 (17)	
C3	0.7801 (9)	0.2612 (8)	0.4439 (4)	0.0260 (17)	
C4	0.8843 (9)	0.2739 (9)	0.5250 (4)	0.0285 (17)	
C5	0.4771 (9)	0.2395 (9)	0.5474 (4)	0.0291 (17)	
C6	0.8914 (10)	0.2739 (9)	0.3464 (4)	0.0301 (17)	

supplementary materials

C7	0.8804 (10)	0.2893 (10)	0.7040 (4)	0.0341 (19)	
C8	0.5274 (10)	0.3885 (9)	1.0197 (4)	0.0288 (17)	
O10	-0.1015 (18)	-0.0885 (16)	0.9137 (11)	0.072 (5)	0.500
H2A	0.49810	0.22820	0.40340	0.0350*	
H4A	1.02570	0.28300	0.51960	0.0340*	
H5A	0.33850	0.22340	0.55470	0.0350*	
H7A	-0.08470	0.47740	0.86270	0.0800*	
H7B	-0.05250	0.64720	0.89900	0.0800*	
H8A	0.67010	-0.11890	0.74700	0.0800*	
H8B	0.55880	-0.18960	0.81340	0.0800*	
H9A	0.29540	-0.01320	0.89080	0.0800*	
H9B	0.07450	0.05280	0.87580	0.0800*	
H10A	-0.22390	-0.01980	0.89910	0.0800*	0.500
H10B	-0.11240	-0.06870	0.97360	0.0800*	0.500

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
La1	0.0283 (2)	0.0378 (2)	0.0187 (2)	-0.0182 (2)	-0.0020 (1)	0.0042 (1)
O1	0.043 (3)	0.047 (3)	0.025 (2)	-0.009 (2)	-0.004 (2)	0.0078 (19)
O2	0.033 (3)	0.074 (4)	0.039 (3)	-0.001 (2)	0.009 (2)	0.014 (2)
O3	0.028 (2)	0.060 (3)	0.038 (3)	-0.022 (2)	-0.0100 (19)	0.002 (2)
O4	0.037 (3)	0.112 (4)	0.023 (2)	-0.046 (3)	-0.005 (2)	0.007 (2)
O5	0.067 (3)	0.029 (2)	0.032 (2)	-0.013 (2)	-0.015 (2)	0.0013 (19)
O6	0.079 (4)	0.038 (2)	0.036 (3)	-0.022 (2)	-0.030 (3)	0.013 (2)
O7	0.059 (3)	0.072 (3)	0.113 (4)	-0.008 (2)	0.037 (3)	0.026 (3)
O8	0.071 (4)	0.034 (3)	0.053 (3)	-0.016 (2)	0.023 (3)	0.001 (2)
O9	0.059 (3)	0.072 (3)	0.113 (4)	-0.008 (2)	0.037 (3)	0.026 (3)
N1	0.020 (2)	0.029 (2)	0.027 (3)	-0.0093 (19)	-0.0018 (19)	0.002 (2)
C1	0.018 (3)	0.029 (3)	0.031 (3)	-0.008 (2)	-0.003 (2)	0.006 (2)
C2	0.030 (3)	0.037 (3)	0.023 (3)	-0.011 (3)	-0.009 (2)	0.002 (2)
C3	0.025 (3)	0.027 (3)	0.024 (3)	-0.005 (2)	-0.001 (2)	0.004 (2)
C4	0.019 (3)	0.039 (3)	0.027 (3)	-0.008 (2)	-0.002 (2)	0.008 (3)
C5	0.023 (3)	0.036 (3)	0.030 (3)	-0.011 (2)	-0.004 (2)	0.003 (2)
C6	0.033 (3)	0.032 (3)	0.023 (3)	-0.007 (3)	0.001 (2)	0.000 (2)
C7	0.030 (3)	0.046 (4)	0.033 (3)	-0.021 (3)	-0.006 (3)	0.011 (3)
C8	0.032 (3)	0.030 (3)	0.022 (3)	-0.006 (2)	0.000 (2)	0.003 (2)
O10	0.044 (6)	0.044 (6)	0.135 (12)	-0.014 (5)	-0.036 (7)	0.007 (7)

Geometric parameters (\AA , $^\circ$)

La1—N1	2.726 (4)	O8—H8B	0.9600
La1—O1 ⁱ	2.454 (4)	O9—H9B	0.8500
La1—O3 ⁱⁱ	2.541 (5)	O9—H9A	0.8800
La1—O4	2.551 (5)	O10—H10A	0.8300
La1—O5	2.543 (4)	O10—H10B	0.8500
La1—O6 ⁱⁱⁱ	2.550 (5)	N1—C5	1.338 (7)
La1—O7	2.604 (7)	N1—C1	1.346 (8)

La1—O8	2.553 (5)	C1—C4	1.379 (8)
La1—O9	2.612 (7)	C1—C7	1.503 (8)
O1—C6	1.271 (8)	C2—C3	1.386 (9)
O2—C6	1.232 (9)	C2—C5	1.382 (8)
O3—C7	1.251 (8)	C3—C6	1.510 (8)
O4—C7	1.253 (7)	C3—C4	1.388 (8)
O5—C8	1.247 (7)	C8—C8 ⁱⁱⁱ	1.541 (8)
O6—C8	1.253 (7)	C2—H2A	0.9300
O7—H7B	0.8300	C4—H4A	0.9300
O7—H7A	0.8400	C5—H5A	0.9300
O8—H8A	0.8300		
O4—La1—O5	73.91 (15)	La1—O5—C8	121.8 (4)
O4—La1—O7	143.20 (19)	La1 ⁱⁱⁱ —O6—C8	121.6 (4)
O4—La1—O8	76.08 (19)	La1—O7—H7B	119.00
O4—La1—O9	130.46 (19)	H7A—O7—H7B	105.00
O4—La1—N1	60.09 (14)	La1—O7—H7A	96.00
O3 ⁱⁱ —La1—O4	136.05 (14)	La1—O8—H8A	129.00
O1 ⁱ —La1—O4	94.15 (17)	H8A—O8—H8B	93.00
O4—La1—O6 ⁱⁱⁱ	71.03 (17)	La1—O8—H8B	138.00
O5—La1—O7	85.94 (19)	La1—O9—H9A	87.00
O5—La1—O8	78.78 (15)	H9A—O9—H9B	108.00
O5—La1—O9	68.31 (19)	La1—O9—H9B	116.00
O5—La1—N1	129.55 (15)	H10A—O10—H10B	102.00
O3 ⁱⁱ —La1—O5	143.58 (15)	La1—N1—C5	123.7 (4)
O1 ⁱ —La1—O5	131.93 (14)	La1—N1—C1	118.9 (3)
O5—La1—O6 ⁱⁱⁱ	62.98 (13)	C1—N1—C5	116.8 (5)
O7—La1—O8	130.39 (19)	N1—C1—C4	122.9 (5)
O7—La1—O9	64.2 (2)	N1—C1—C7	115.1 (5)
O7—La1—N1	143.97 (18)	C4—C1—C7	121.9 (6)
O3 ⁱⁱ —La1—O7	76.45 (18)	C3—C2—C5	118.7 (5)
O1 ⁱ —La1—O7	76.62 (19)	C2—C3—C6	122.0 (5)
O6 ⁱⁱⁱ —La1—O7	72.42 (19)	C4—C3—C6	120.1 (5)
O8—La1—O9	66.27 (19)	C2—C3—C4	117.9 (5)
O8—La1—N1	71.47 (16)	C1—C4—C3	119.6 (6)
O3 ⁱⁱ —La1—O8	88.67 (17)	N1—C5—C2	123.9 (6)
O1 ⁱ —La1—O8	144.45 (16)	O1—C6—O2	126.8 (6)
O6 ⁱⁱⁱ —La1—O8	134.78 (18)	O2—C6—C3	117.2 (5)
O9—La1—N1	128.72 (18)	O1—C6—C3	116.1 (6)
O3 ⁱⁱ —La1—O9	75.33 (18)	O4—C7—C1	116.7 (6)
O1 ⁱ —La1—O9	135.03 (19)	O3—C7—C1	119.0 (5)
O6 ⁱⁱⁱ —La1—O9	115.40 (18)	O3—C7—O4	124.3 (6)
O3 ⁱⁱ —La1—N1	76.02 (14)	O5—C8—O6	126.8 (5)
O1 ⁱ —La1—N1	74.06 (14)	O5—C8—C8 ⁱⁱⁱ	116.9 (5)
O6 ⁱⁱⁱ —La1—N1	114.76 (15)	O6—C8—C8 ⁱⁱⁱ	116.4 (5)

supplementary materials

O1 ⁱ —La1—O3 ⁱⁱ	74.77 (16)	C5—C2—H2A	121.00
O3 ⁱⁱ —La1—O6 ⁱⁱⁱ	136.50 (17)	C3—C2—H2A	121.00
O1 ⁱ —La1—O6 ⁱⁱⁱ	69.06 (15)	C1—C4—H4A	120.00
La1 ⁱ —O1—C6	137.1 (4)	C3—C4—H4A	120.00
La1 ^{iv} —O3—C7	139.6 (4)	N1—C5—H5A	118.00
La1—O4—C7	128.4 (4)	C2—C5—H5A	118.00
O5—La1—O4—C7	158.8 (6)	N1—La1—O1 ⁱ —C6 ⁱ	73.1 (6)
O7—La1—O4—C7	-141.7 (5)	O4—La1—O6 ⁱⁱⁱ —C8 ⁱⁱⁱ	-86.9 (5)
O8—La1—O4—C7	76.7 (6)	O5—La1—O6 ⁱⁱⁱ —C8 ⁱⁱⁱ	-5.7 (5)
O9—La1—O4—C7	117.6 (6)	O7—La1—O6 ⁱⁱⁱ —C8 ⁱⁱⁱ	88.8 (5)
N1—La1—O4—C7	0.3 (5)	O8—La1—O6 ⁱⁱⁱ —C8 ⁱⁱⁱ	-41.2 (6)
O3 ⁱⁱ —La1—O4—C7	3.7 (7)	O9—La1—O6 ⁱⁱⁱ —C8 ⁱⁱⁱ	39.8 (6)
O1 ⁱ —La1—O4—C7	-68.6 (6)	N1—La1—O6 ⁱⁱⁱ —C8 ⁱⁱⁱ	-129.2 (5)
O6 ⁱⁱⁱ —La1—O4—C7	-134.8 (6)	La1 ⁱ —O1—C6—C3	102.3 (6)
O4—La1—O5—C8	82.1 (5)	La1 ⁱ —O1—C6—O2	-78.5 (8)
O7—La1—O5—C8	-66.7 (5)	La1 ^{iv} —O3—C7—O4	-11.4 (11)
O8—La1—O5—C8	160.7 (5)	La1 ^{iv} —O3—C7—C1	169.0 (4)
O9—La1—O5—C8	-130.5 (5)	La1—O4—C7—C1	4.4 (9)
N1—La1—O5—C8	106.5 (5)	La1—O4—C7—O3	-175.2 (5)
O3 ⁱⁱ —La1—O5—C8	-127.3 (5)	La1—O5—C8—O6	174.5 (5)
O1 ⁱ —La1—O5—C8	1.2 (6)	La1—O5—C8—C8 ⁱⁱⁱ	-5.3 (8)
O6 ⁱⁱⁱ —La1—O5—C8	5.6 (5)	La1 ⁱⁱⁱ —O6—C8—O5	174.7 (5)
O4—La1—N1—C1	-5.7 (4)	La1 ⁱⁱⁱ —O6—C8—C8 ⁱⁱⁱ	-5.5 (8)
O4—La1—N1—C5	-177.0 (5)	C5—N1—C1—C4	2.4 (8)
O5—La1—N1—C1	-32.9 (5)	La1—N1—C1—C7	9.8 (6)
O5—La1—N1—C5	155.9 (4)	C1—N1—C5—C2	-3.0 (8)
O7—La1—N1—C1	135.5 (4)	C5—N1—C1—C7	-178.3 (5)
O7—La1—N1—C5	-35.7 (6)	La1—N1—C5—C2	168.4 (4)
O8—La1—N1—C1	-90.0 (4)	La1—N1—C1—C4	-169.4 (4)
O8—La1—N1—C5	98.8 (4)	N1—C1—C7—O3	170.2 (6)
O9—La1—N1—C1	-125.6 (4)	N1—C1—C7—O4	-9.4 (8)
O9—La1—N1—C5	63.2 (5)	C4—C1—C7—O3	-10.5 (9)
O3 ⁱⁱ —La1—N1—C1	176.7 (4)	C4—C1—C7—O4	169.9 (6)
O3 ⁱⁱ —La1—N1—C5	5.4 (4)	N1—C1—C4—C3	0.1 (9)
O1 ⁱ —La1—N1—C1	98.8 (4)	C7—C1—C4—C3	-179.1 (5)
O1 ⁱ —La1—N1—C5	-72.4 (4)	C5—C2—C3—C4	1.6 (8)
O6 ⁱⁱⁱ —La1—N1—C1	41.6 (4)	C3—C2—C5—N1	1.0 (9)
O6 ⁱⁱⁱ —La1—N1—C5	-129.7 (4)	C5—C2—C3—C6	-177.2 (5)
O4—La1—O3 ⁱⁱ —C7 ⁱⁱ	-173.4 (6)	C2—C3—C6—O1	25.5 (8)
O5—La1—O3 ⁱⁱ —C7 ⁱⁱ	49.4 (8)	C6—C3—C4—C1	176.7 (5)
O7—La1—O3 ⁱⁱ —C7 ⁱⁱ	-13.9 (7)	C4—C3—C6—O2	27.4 (8)
O8—La1—O3 ⁱⁱ —C7 ⁱⁱ	118.3 (7)	C2—C3—C6—O2	-153.9 (6)

O9—La1—O3 ⁱⁱ —C7 ⁱⁱ	52.5 (7)	C4—C3—C6—O1	-153.3 (5)
N1—La1—O3 ⁱⁱ —C7 ⁱⁱ	-170.5 (7)	C2—C3—C4—C1	-2.1 (8)
O4—La1—O1 ⁱ —C6 ⁱ	130.4 (6)	O5—C8—C8 ⁱⁱⁱ —O5 ⁱⁱⁱ	-180.0 (6)
O5—La1—O1 ⁱ —C6 ⁱ	-157.6 (6)	O5—C8—C8 ⁱⁱⁱ —O6 ⁱⁱⁱ	-0.2 (9)
O7—La1—O1 ⁱ —C6 ⁱ	-85.8 (6)	O6—C8—C8 ⁱⁱⁱ —O5 ⁱⁱⁱ	0.2 (9)
O8—La1—O1 ⁱ —C6 ⁱ	58.6 (7)	O6—C8—C8 ⁱⁱⁱ —O6 ⁱⁱⁱ	180.0 (6)
O9—La1—O1 ⁱ —C6 ⁱ	-56.3 (7)		

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

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
O7—H7A \cdots O4 ⁱⁱ	0.84	2.08	2.911 (8)	168
O7—H7B \cdots O10 ^v	0.83	1.71	2.533 (12)	168
O8—H8A \cdots O2 ^{vi}	0.83	1.83	2.660 (7)	173
O8—H8B \cdots O6 ^{vii}	0.96	2.03	2.914 (7)	153
O9—H9A \cdots O6 ^{vii}	0.88	2.27	2.987 (8)	138
O9—H9B \cdots O10	0.85	1.73	2.390 (14)	133
O10—H10A \cdots O5 ⁱⁱ	0.83	2.24	2.885 (12)	135
O10—H10A \cdots O8 ⁱⁱ	0.83	2.29	2.924 (15)	133
O10—H10B \cdots O9 ^{viii}	0.85	1.77	2.591 (17)	163
C5—H5A \cdots O3 ⁱⁱ	0.93	2.49	3.164 (7)	130

Symmetry codes: (ii) $x-1, y, z$; (v) $x, y+1, z$; (vi) $-x+2, -y, -z+1$; (vii) $-x+1, -y, -z+2$; (viii) $-x, -y, -z+2$.

Fig. 1

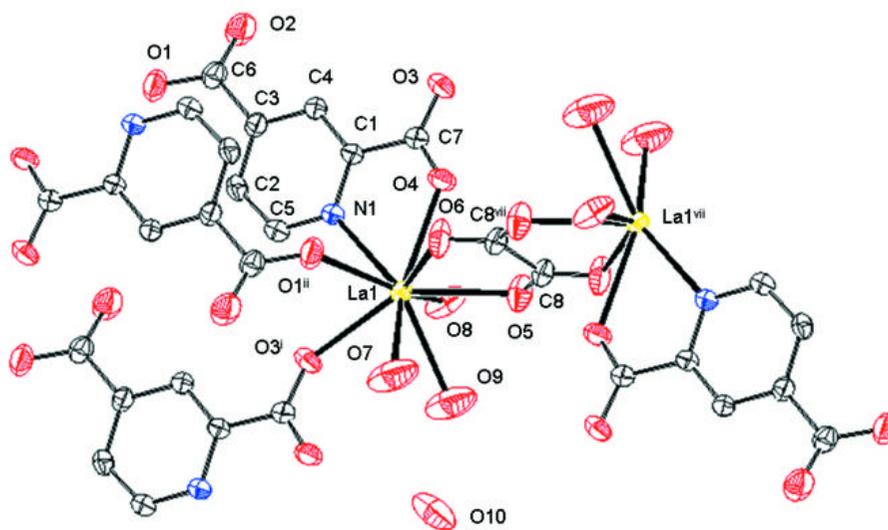


Fig. 2

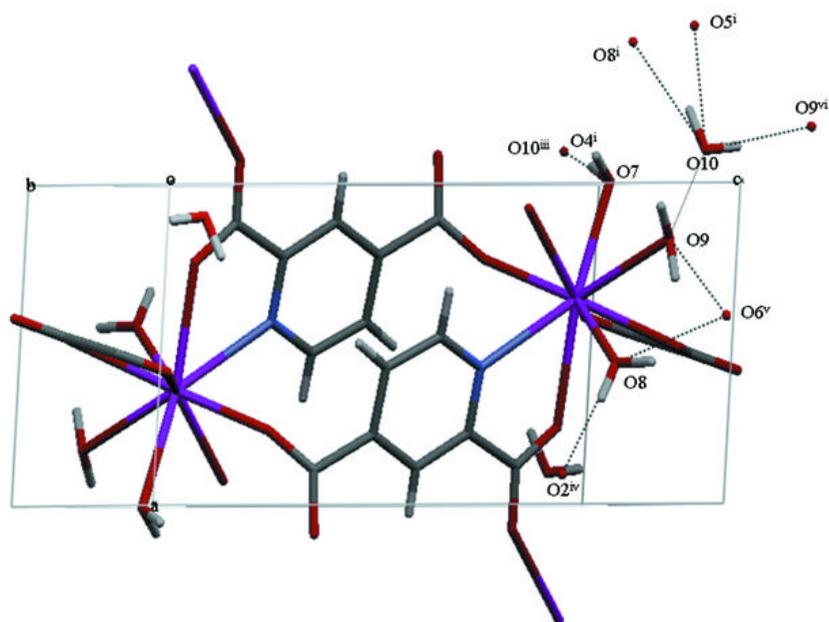


Fig. 3

