

Poly[diaqua(μ -oxalato)(μ -2-oxidopyridinium-3-carboxylato)lanthanum(III)]

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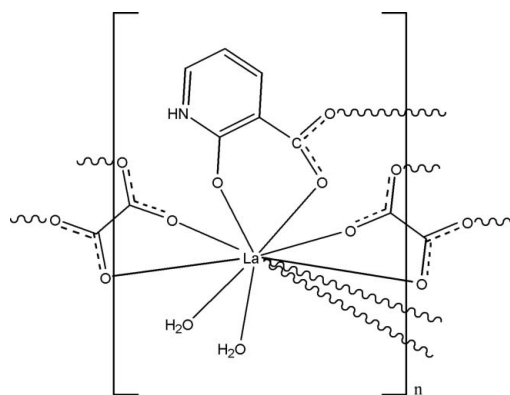
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.007$ Å; R factor = 0.025; wR factor = 0.069; data-to-parameter ratio = 11.3.

In the title complex, $[\text{La}(\text{C}_6\text{H}_4\text{NO}_3)(\text{C}_2\text{O}_4)(\text{H}_2\text{O})_2]_n$, the La^{III} ion is coordinated by eight O atoms from two 2-oxidopyridinium-3-carboxylate ligands, two oxalate ligands and two water molecules in a distorted bicapped square-antiprismatic geometry. The carboxylate groups link adjacent La^{III} ions, forming two-dimensional layers that are further linked by $\text{N}-\text{H}\cdots\text{O}$ and $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds.

Related literature

 For related structures, see: Huang *et al.* (2009); Xu *et al.* (2009).


Experimental

Crystal data

$[\text{La}(\text{C}_6\text{H}_4\text{NO}_3)(\text{C}_2\text{O}_4)(\text{H}_2\text{O})_2]$
 $M_r = 401.06$
 Triclinic, $P\bar{1}$
 $a = 8.0856$ (18) Å
 $b = 8.5493$ (19) Å
 $c = 9.388$ (3) Å
 $\alpha = 109.281$ (3)°
 $\beta = 104.702$ (3)°
 $\gamma = 104.940$ (2)°
 $V = 549.5$ (2) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 3.93$ mm⁻¹
 $T = 293$ K
 $0.20 \times 0.18 \times 0.17$ mm

Data collection

Bruker APEXII CCD diffractometer
 Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
 $T_{\text{min}} = 0.460$, $T_{\text{max}} = 0.512$
 2843 measured reflections
 1946 independent reflections
 1870 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.020$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.025$
 $wR(F^2) = 0.069$
 $S = 1.10$
 1946 reflections
 172 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.92$ e Å⁻³
 $\Delta\rho_{\text{min}} = -1.37$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N1}-\text{H1A}\cdots\text{O4}^i$	0.86	1.96	2.789 (5)	162
$\text{O1W}-\text{H1W}\cdots\text{O6}^i$	0.85	2.01	2.805 (5)	155
$\text{O2W}-\text{H4W}\cdots\text{O2W}^{ii}$	0.85	2.00	2.853 (7)	180
$\text{O2W}-\text{H3W}\cdots\text{O7}^{iii}$	0.85	1.97	2.753 (5)	152

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *S SAINT* (Bruker, 2004); data reduction: *S SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BI2356).

References

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supplementary materials

Acta Cryst. (2009). E65, m682 [doi:10.1107/S1600536809018194]

Poly[diaqua(μ -oxalato)(μ -2-oxidopyridinium-3-carboxylato)lanthanum(III)]

Z. Hu and Z.-B. Zhu

Comment

Whereas a large number of metal derivatives of oxalic acid have been reported, there are few examples of metal derivatives of 2-oxynicotinic acid and oxalic acid: the crystal structures of praseodymium (Xu *et al.*, 2009) and dysprosium (Huang *et al.*, 2009) derivatives have been reported only. We report here a lanthanum(III) complex formed by reaction of lanthanum nitrate, 2-oxynicotinic acid and oxalic acid under hydrothermal conditions.

As illustrated in Fig. 1, each La^{III} centre adopts a distorted bicapped square-antiprismatic geometry, defined by eight O atoms from two 2-oxynicotinate ligands, two oxalate ligands, and two water molecules. The 2-oxynicotinate ligands and oxalate ligands link the La^{III} ions to form layers in the *bc* plane in which the shortest La \cdots La separation is 4.429 (3) Å. These layers are connected through O—H \cdots O and N—H \cdots O hydrogen bonding (Table 1) involving 2-oxynicotinate ligands, oxalate ligands and the coordinating water molecules, forming a three-dimensional supramolecular network motif (Fig. 2).

Experimental

A mixture of La₂O₃ (0.245 g, 0.75 mmol), 2-oxynicotinic acid (0.127 g, 1 mmol), oxalic acid (0.09 g, 1 mmol), water (10 ml) and HNO₃ (0.024 g, 0.385 mmol) was stirred vigorously for 20 min then sealed in a Teflon-lined stainless-steel autoclave (20 ml capacity). The autoclave was heated and maintained at 433 K for 4 days, then cooled to room temperature at 5 K h⁻¹ to yield colourless block crystals.

Refinement

H atoms bound to C and N atoms were placed at calculated positions and refined as riding with N—H = 0.86 Å, C—H = 0.93 Å and with $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C/N})$. H atoms of the water molecules were tentatively located in difference Fourier maps and refined with distance restraints of O—H = 0.850 (1) Å and H \cdots H = 1.350 (1) Å. In the final cycles of refinement, the O—H distances were normalized to 0.85 Å and the H atoms were refined as riding with $U_{\text{iso}}(\text{H}) = 1.5 U_{\text{eq}}(\text{O})$. Atom H4W forms a symmetrical H-bond about a centre of inversion and therefore is included with site occupancy factor 0.5. The alternative position H4W' points towards the centroid of an adjacent pyridyl ring.

Figures

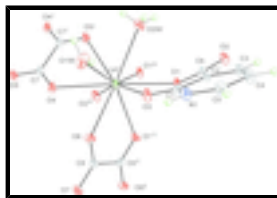


Fig. 1. The molecular structure showing displacement ellipsoids at 30% probability for non-H atoms. Symmetry codes: (i) $-x, -y, -z$; (ii) $-x, 1 - y, 1 - z$; (iii) $-x, -y, 1 - z$. The H atoms on O2W are disordered.

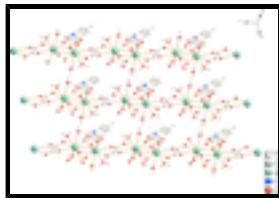


Fig. 2. Packing diagram showing part of the 2-D layers (horizontal).

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Crystal data

[La(C₆H₄NO₃)(C₂O₄)(H₂O)₂]

$M_r = 401.06$

Triclinic, *PT*

Hall symbol: -P 1

$a = 8.0856$ (18) Å

$b = 8.5493$ (19) Å

$c = 9.388$ (3) Å

$\alpha = 109.281$ (3)°

$\beta = 104.702$ (3)°

$\gamma = 104.940$ (2)°

$V = 549.5$ (2) Å³

$Z = 2$

$F_{000} = 384$

$D_x = 2.424$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 2827 reflections

$\theta = 2.5$ – 28.3 °

$\mu = 3.93$ mm⁻¹

$T = 293$ K

Block, colourless

$0.20 \times 0.18 \times 0.17$ mm

Data collection

Bruker APEXII CCD
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 293$ K

φ and ω scans

Absorption correction: multi-scan
(SADABS; Sheldrick, 2003)

$T_{\min} = 0.460$, $T_{\max} = 0.512$

2843 measured reflections

1946 independent reflections

1870 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.020$

$\theta_{\max} = 25.2$ °

$\theta_{\min} = 2.5$ °

$h = -7 \rightarrow 9$

$k = -10 \rightarrow 10$

$l = -11 \rightarrow 11$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.025$

$wR(F^2) = 0.069$

$S = 1.10$

1946 reflections

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0415P)^2 + 0.4664P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.92$ e Å⁻³

172 parameters

$$\Delta\rho_{\min} = -1.37 \text{ e } \text{\AA}^{-3}$$

Primary atom site location: structure-invariant direct methods

Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness 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 threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *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)
C1	0.5156 (6)	0.3528 (6)	0.7873 (5)	0.0193 (9)	
C2	0.4448 (6)	0.2225 (6)	0.8439 (5)	0.0190 (9)	
C3	0.5510 (7)	0.2276 (6)	0.9869 (5)	0.0278 (10)	
H3A	0.5043	0.1411	1.0209	0.033*	
C4	0.7265 (7)	0.3590 (7)	1.0820 (6)	0.0340 (12)	
H4A	0.7963	0.3617	1.1788	0.041*	
C5	0.7924 (6)	0.4829 (7)	1.0291 (6)	0.0310 (11)	
H5A	0.9085	0.5728	1.0910	0.037*	
C6	0.2549 (6)	0.0837 (6)	0.7555 (5)	0.0195 (9)	
C7	0.0124 (6)	0.0944 (6)	0.0035 (5)	0.0209 (9)	
C8	0.0714 (6)	0.5526 (5)	0.4754 (5)	0.0180 (8)	
La1	0.14649 (3)	0.16626 (3)	0.39929 (2)	0.01432 (11)	
N1	0.6911 (5)	0.4769 (5)	0.8873 (5)	0.0253 (8)	
H1A	0.7393	0.5561	0.8570	0.030*	
O1	0.1395 (4)	0.0964 (4)	0.6424 (3)	0.0215 (7)	
O2	0.2093 (4)	-0.0404 (4)	0.7976 (4)	0.0285 (7)	
O3	0.4372 (4)	0.3643 (4)	0.6604 (4)	0.0276 (7)	
O4	0.1045 (5)	0.2240 (4)	0.1390 (4)	0.0258 (7)	
O5	-0.0601 (5)	0.1020 (4)	-0.1273 (4)	0.0275 (7)	
O6	0.1897 (4)	0.4906 (4)	0.4461 (4)	0.0238 (7)	
O7	0.0581 (4)	0.6932 (4)	0.4686 (4)	0.0263 (7)	
O1W	0.4501 (5)	0.2684 (5)	0.3496 (4)	0.0400 (9)	
H1W	0.5512	0.3270	0.4309	0.060*	
H2W	0.4721	0.1911	0.2808	0.060*	
O2W	0.3055 (5)	-0.0633 (5)	0.4169 (4)	0.0329 (8)	
H3W	0.2604	-0.1491	0.4396	0.049*	
H4W	0.4214	-0.0254	0.4667	0.049*	0.50
H4W'	0.2871	-0.1202	0.3175	0.049*	0.50

supplementary materials

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.018 (2)	0.016 (2)	0.018 (2)	0.0023 (17)	0.0060 (17)	0.0040 (17)
C2	0.017 (2)	0.017 (2)	0.0160 (19)	0.0019 (17)	0.0018 (17)	0.0062 (17)
C3	0.027 (2)	0.023 (2)	0.024 (2)	0.002 (2)	0.000 (2)	0.012 (2)
C4	0.024 (3)	0.034 (3)	0.024 (2)	0.001 (2)	-0.011 (2)	0.012 (2)
C5	0.017 (2)	0.029 (3)	0.029 (2)	0.001 (2)	-0.0042 (19)	0.006 (2)
C6	0.016 (2)	0.020 (2)	0.016 (2)	-0.0004 (17)	0.0025 (17)	0.0074 (17)
C7	0.021 (2)	0.024 (2)	0.017 (2)	0.0035 (18)	0.0066 (18)	0.0103 (18)
C8	0.014 (2)	0.014 (2)	0.017 (2)	0.0005 (17)	-0.0001 (16)	0.0029 (17)
La1	0.01183 (15)	0.01383 (16)	0.01434 (15)	0.00163 (11)	0.00223 (11)	0.00694 (11)
N1	0.0186 (19)	0.022 (2)	0.027 (2)	-0.0013 (16)	0.0045 (16)	0.0110 (17)
O1	0.0154 (15)	0.0253 (17)	0.0172 (15)	0.0003 (13)	-0.0005 (12)	0.0118 (13)
O2	0.0215 (17)	0.0269 (18)	0.0325 (18)	0.0002 (14)	0.0028 (14)	0.0192 (15)
O3	0.0211 (17)	0.0312 (18)	0.0235 (16)	-0.0002 (14)	0.0014 (14)	0.0163 (14)
O4	0.0326 (19)	0.0190 (16)	0.0157 (15)	-0.0002 (14)	0.0040 (14)	0.0068 (13)
O5	0.0369 (19)	0.0238 (16)	0.0163 (15)	0.0085 (15)	0.0030 (14)	0.0093 (13)
O6	0.0193 (16)	0.0192 (16)	0.0336 (17)	0.0070 (13)	0.0107 (14)	0.0116 (14)
O7	0.0294 (18)	0.0209 (16)	0.0373 (18)	0.0110 (14)	0.0169 (15)	0.0177 (14)
O1W	0.0197 (18)	0.057 (2)	0.0307 (19)	0.0001 (17)	0.0090 (15)	0.0158 (18)
O2W	0.0285 (18)	0.040 (2)	0.043 (2)	0.0178 (16)	0.0155 (16)	0.0276 (17)

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

C1—O3	1.248 (5)	La1—O6	2.574 (3)
C1—N1	1.382 (6)	La1—O5 ⁱ	2.582 (3)
C1—C2	1.437 (6)	La1—O3	2.585 (3)
C2—C3	1.377 (6)	La1—O1W	2.598 (3)
C2—C6	1.489 (6)	La1—O4	2.606 (3)
C3—C4	1.395 (7)	La1—O7 ⁱⁱ	2.608 (3)
C3—H3A	0.930	La1—O1 ⁱⁱⁱ	2.612 (3)
C4—C5	1.357 (7)	La1—O2W	2.634 (3)
C4—H4A	0.930	La1—O2 ⁱⁱⁱ	2.691 (3)
C5—N1	1.351 (6)	N1—H1A	0.860
C5—H5A	0.930	O1—La1 ⁱⁱⁱ	2.612 (3)
C6—O2	1.252 (5)	O2—La1 ⁱⁱⁱ	2.691 (3)
C6—O1	1.279 (5)	O5—La1 ⁱ	2.582 (3)
C7—O4	1.250 (5)	O7—La1 ⁱⁱ	2.608 (3)
C7—O5	1.251 (5)	O1W—H1W	0.850
C7—C7 ⁱ	1.550 (9)	O1W—H2W	0.850
C8—O6	1.253 (5)	O2W—H3W	0.850
C8—O7	1.255 (5)	O2W—H4W	0.850
C8—C8 ⁱⁱ	1.537 (8)	O2W—H4W'	0.850
La1—O1	2.553 (3)		

O3—C1—N1	118.0 (4)	O1—La1—O1 ⁱⁱⁱ	61.92 (11)
O3—C1—C2	127.4 (4)	O6—La1—O1 ⁱⁱⁱ	130.59 (10)
N1—C1—C2	114.6 (4)	O5 ⁱ —La1—O1 ⁱⁱⁱ	70.65 (10)
C3—C2—C1	120.0 (4)	O3—La1—O1 ⁱⁱⁱ	127.57 (9)
C3—C2—C6	118.0 (4)	O1W—La1—O1 ⁱⁱⁱ	148.31 (12)
C1—C2—C6	121.9 (4)	O4—La1—O1 ⁱⁱⁱ	111.41 (10)
C2—C3—C4	121.8 (4)	O7 ⁱⁱ —La1—O1 ⁱⁱⁱ	72.58 (10)
C2—C3—H3A	119.1	O1—La1—O2W	68.95 (10)
C4—C3—H3A	119.1	O6—La1—O2W	147.03 (10)
C5—C4—C3	118.1 (4)	O5 ⁱ —La1—O2W	64.56 (10)
C5—C4—H4A	121.0	O3—La1—O2W	78.73 (11)
C3—C4—H4A	121.0	O1W—La1—O2W	72.87 (12)
N1—C5—C4	120.6 (4)	O4—La1—O2W	115.38 (10)
N1—C5—H5A	119.7	O7 ⁱⁱ —La1—O2W	138.08 (10)
C4—C5—H5A	119.7	O1 ⁱⁱⁱ —La1—O2W	81.33 (10)
O2—C6—O1	121.1 (4)	O1—La1—O2 ⁱⁱⁱ	105.06 (9)
O2—C6—C2	119.0 (4)	O6—La1—O2 ⁱⁱⁱ	92.61 (10)
O1—C6—C2	119.8 (4)	O5 ⁱ —La1—O2 ⁱⁱⁱ	66.21 (10)
O4—C7—O5	126.4 (4)	O3—La1—O2 ⁱⁱⁱ	157.15 (11)
O4—C7—C7 ⁱ	116.9 (4)	O1W—La1—O2 ⁱⁱⁱ	131.48 (11)
O5—C7—C7 ⁱ	116.7 (5)	O4—La1—O2 ⁱⁱⁱ	67.14 (10)
O6—C8—O7	126.1 (4)	O7 ⁱⁱ —La1—O2 ⁱⁱⁱ	65.52 (10)
O6—C8—C8 ⁱⁱ	117.3 (4)	O1 ⁱⁱⁱ —La1—O2 ⁱⁱⁱ	49.08 (9)
O7—C8—C8 ⁱⁱ	116.6 (4)	O2W—La1—O2 ⁱⁱⁱ	118.71 (11)
O1—La1—O6	115.01 (10)	C5—N1—C1	124.9 (4)
O1—La1—O5 ⁱ	116.73 (10)	C5—N1—H1A	117.6
O6—La1—O5 ⁱ	127.50 (10)	C1—N1—H1A	117.6
O1—La1—O3	65.68 (10)	C6—O1—La1	135.9 (3)
O6—La1—O3	74.38 (10)	C6—O1—La1 ⁱⁱⁱ	96.3 (3)
O5 ⁱ —La1—O3	136.55 (11)	La1—O1—La1 ⁱⁱⁱ	118.08 (11)
O1—La1—O1W	121.99 (10)	C6—O2—La1 ⁱⁱⁱ	93.3 (2)
O6—La1—O1W	78.71 (11)	C1—O3—La1	136.4 (3)
O5 ⁱ —La1—O1W	81.66 (11)	C7—O4—La1	118.5 (3)
O3—La1—O1W	65.28 (11)	C7—O5—La1 ⁱ	119.4 (3)
O1—La1—O4	172.10 (10)	C8—O6—La1	120.7 (3)
O6—La1—O4	65.38 (10)	C8—O7—La1 ⁱⁱ	119.8 (3)
O5 ⁱ —La1—O4	62.14 (10)	La1—O1W—H1W	118.9
O3—La1—O4	120.98 (10)	La1—O1W—H2W	118.3
O1W—La1—O4	65.90 (11)	H1W—O1W—H2W	105.2
O1—La1—O7 ⁱⁱ	69.92 (10)	La1—O2W—H3W	122.1
O6—La1—O7 ⁱⁱ	62.13 (9)	La1—O2W—H4W	119.6
O5 ⁱ —La1—O7 ⁱⁱ	131.12 (11)	H3W—O2W—H4W	105.2

supplementary materials

O3—La1—O7 ⁱⁱ	91.67 (11)	La1—O2W—H4W'	101.0
O1W—La1—O7 ⁱⁱ	139.07 (11)	H3W—O2W—H4W'	100.6
O4—La1—O7 ⁱⁱ	104.60 (10)	H4W—O2W—H4W'	105.2
O3—C1—C2—C3	179.2 (4)	N1—C1—O3—La1	168.2 (3)
N1—C1—C2—C3	-0.4 (6)	C2—C1—O3—La1	-11.5 (7)
O3—C1—C2—C6	-3.1 (7)	O1—La1—O3—C1	22.7 (4)
N1—C1—C2—C6	177.2 (4)	O6—La1—O3—C1	150.2 (4)
C1—C2—C3—C4	1.3 (7)	O5 ⁱ —La1—O3—C1	-81.2 (4)
C6—C2—C3—C4	-176.5 (4)	O1W—La1—O3—C1	-125.3 (4)
C2—C3—C4—C5	-0.6 (8)	O4—La1—O3—C1	-162.1 (4)
C3—C4—C5—N1	-0.8 (8)	O7 ⁱⁱ —La1—O3—C1	89.7 (4)
C3—C2—C6—O2	-11.8 (6)	O1 ⁱⁱⁱ —La1—O3—C1	20.6 (5)
C1—C2—C6—O2	170.5 (4)	O2W—La1—O3—C1	-49.1 (4)
C3—C2—C6—O1	165.6 (4)	O2 ⁱⁱⁱ —La1—O3—C1	92.9 (5)
C1—C2—C6—O1	-12.0 (6)	O5—C7—O4—La1	160.6 (4)
C4—C5—N1—C1	1.7 (7)	C7 ⁱ —C7—O4—La1	-20.2 (6)
O3—C1—N1—C5	179.3 (4)	O6—La1—O4—C7	-157.7 (3)
C2—C1—N1—C5	-1.0 (6)	O5 ⁱ —La1—O4—C7	20.9 (3)
O2—C6—O1—La1	-137.1 (4)	O3—La1—O4—C7	150.7 (3)
C2—C6—O1—La1	45.4 (6)	O1W—La1—O4—C7	114.1 (3)
O2—C6—O1—La1 ⁱⁱⁱ	5.4 (4)	O7 ⁱⁱ —La1—O4—C7	-108.3 (3)
C2—C6—O1—La1 ⁱⁱⁱ	-172.0 (3)	O1 ⁱⁱⁱ —La1—O4—C7	-31.6 (4)
O6—La1—O1—C6	-98.9 (4)	O2W—La1—O4—C7	58.8 (3)
O5 ⁱ —La1—O1—C6	90.3 (4)	O2 ⁱⁱⁱ —La1—O4—C7	-53.3 (3)
O3—La1—O1—C6	-41.3 (4)	O4—C7—O5—La1 ⁱ	159.7 (4)
O1W—La1—O1—C6	-6.8 (4)	C7 ⁱ —C7—O5—La1 ⁱ	-19.6 (6)
O7 ⁱⁱ —La1—O1—C6	-142.8 (4)	O7—C8—O6—La1	-165.0 (3)
O1 ⁱⁱⁱ —La1—O1—C6	136.7 (5)	C8 ⁱⁱ —C8—O6—La1	15.1 (6)
O2W—La1—O1—C6	45.5 (4)	O1—La1—O6—C8	-63.1 (3)
O2 ⁱⁱⁱ —La1—O1—C6	160.9 (4)	O5 ⁱ —La1—O6—C8	106.6 (3)
O6—La1—O1—La1 ⁱⁱⁱ	124.39 (13)	O3—La1—O6—C8	-116.0 (3)
O5 ⁱ —La1—O1—La1 ⁱⁱⁱ	-46.43 (16)	O1W—La1—O6—C8	176.7 (3)
O3—La1—O1—La1 ⁱⁱⁱ	-178.07 (17)	O4—La1—O6—C8	108.2 (3)
O1W—La1—O1—La1 ⁱⁱⁱ	-143.50 (14)	O7 ⁱⁱ —La1—O6—C8	-15.6 (3)
O7 ⁱⁱ —La1—O1—La1 ⁱⁱⁱ	80.43 (14)	O1 ⁱⁱⁱ —La1—O6—C8	10.4 (4)
O1 ⁱⁱⁱ —La1—O1—La1 ⁱⁱⁱ	0.0	O2W—La1—O6—C8	-152.6 (3)
O2W—La1—O1—La1 ⁱⁱⁱ	-91.27 (15)	O2 ⁱⁱⁱ —La1—O6—C8	44.9 (3)
O2 ⁱⁱⁱ —La1—O1—La1 ⁱⁱⁱ	24.16 (15)	O6—C8—O7—La1 ⁱⁱ	-165.3 (3)
O1—C6—O2—La1 ⁱⁱⁱ	-5.2 (4)	C8 ⁱⁱ —C8—O7—La1 ⁱⁱ	14.7 (6)
C2—C6—O2—La1 ⁱⁱⁱ	172.2 (3)		

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

Hydrogen-bond geometry (Å, °)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N1-H1A\cdots O4^{iv}$	0.86	1.96	2.789 (5)	162
$O1W-H1W\cdots O6^{iv}$	0.85	2.01	2.805 (5)	155
$O2W-H4W\cdots O2W^v$	0.85	2.00	2.853 (7)	180
$O2W-H3W\cdots O7^{vi}$	0.85	1.97	2.753 (5)	152

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

Fig. 1

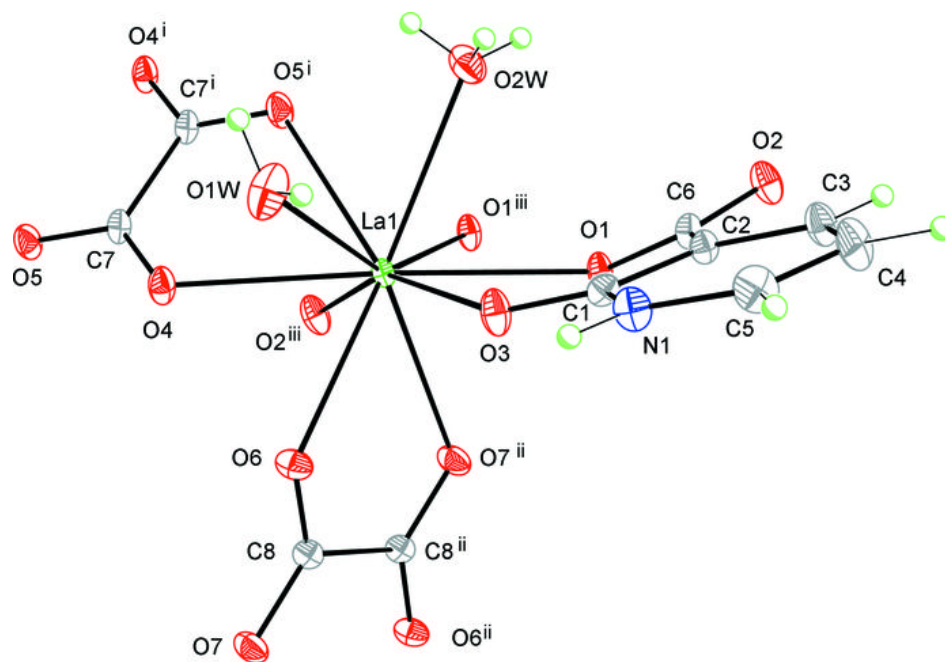


Fig. 2

