

Poly[*diaqua*(μ_4 -3,5-dicarboxylatopyrazol-1-ido- $\kappa^6N^1,O^5:N^2,O^3:O^3':O^5,O^5'$)-lanthanum(III)]

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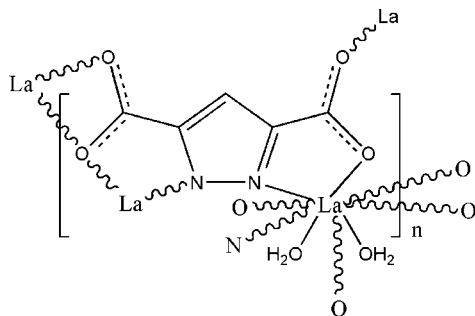
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 Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(C-C) = 0.004$ Å; R factor = 0.016; wR factor = 0.041; data-to-parameter ratio = 11.7.

In the title coordination polymer, $[La(C_5HN_2O_4)(H_2O)_2]_n$, the lanthanum(III) metal centre is nine-coordinated, with a distorted tricapped trigonal prismatic geometry, by the O atoms of two water molecules and by two N and five O atoms of two *N,O*-bidentate, one *O,O'*-bidentate and one *O*-monodentate 3,5-dicarboxylatopyrazol-1-ide ligands. The polymeric three-dimensional structure is stabilized by intermolecular O—H...O hydrogen bonds.

Related literature

For other coordination complexes with pyrazole-3,5-dicarboxylic acid ligands, see: Sakagami *et al.* (1996); Wang *et al.* (2007); Yang *et al.* (2004); King *et al.* (2003); Pan *et al.* (2000).



Experimental

Crystal data

 $[La(C_5HN_2O_4)(H_2O)_2]$
 $M_r = 328.02$

 Orthorhombic, *Pbca*
 $a = 12.5712$ (8) Å

 $b = 8.4350$ (6) Å

 $c = 16.0070$ (10) Å

 $V = 1697.35$ (19) Å³
 $Z = 8$

 Mo $K\alpha$ radiation

 $\mu = 5.04$ mm⁻¹
 $T = 293$ K

 $0.32 \times 0.24 \times 0.20$ mm

Data collection

Bruker APEXII CCD

diffractometer

Absorption correction: multi-scan

 (*SADABS*; Sheldrick, 1996)

 $T_{\min} = 0.239$, $T_{\max} = 0.365$

8554 measured reflections

1496 independent reflections

 1316 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.023$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.016$
 $wR(F^2) = 0.041$
 $S = 1.06$

1496 reflections

128 parameters

H-atom parameters constrained

 $\Delta\rho_{\text{max}} = 0.52$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.50$ e Å⁻³
Table 1

Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O5—H5A...O6	0.85	2.14	2.944 (3)	159
O5—H5B...O3 ⁱ	0.85	1.82	2.667 (3)	174
O6—H6A...O1 ⁱⁱ	0.85	2.20	2.999 (3)	155
O6—H6B...O1 ⁱⁱⁱ	0.85	2.12	2.908 (3)	153

Symmetry codes: (i) $-x + 2, -y + 1, -z + 1$; (ii) $-x + 2, y - \frac{1}{2}, -z + \frac{3}{2}$; (iii) $x + \frac{1}{2}, y, -z + \frac{3}{2}$.

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT-Plus* (Bruker, 2007); data reduction: *SAINT-Plus*; 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: RZ2328).

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supplementary materials

Acta Cryst. (2009). E65, m732 [doi:10.1107/S1600536809020479]

Poly[μ_4 -3,5-dicarboxylatopyrazol-1-ido- $\kappa^6 N^1, O^5: N^2, O^3: O^3', O^5, O^5'$]lanthanum(III)]

J. Xia and J.-F. Wei

Comment

In the past decade, the design and synthesis of metal–organic frameworks have drawn great attention. Pyrazole-3,5-dicarboxylic acid (H₃pdc) has been found to be a suitable ligand in this study for its various coordination modes and strong coordination ability. Some complexes of H₃pdc have been reported recently (Sakagami *et al.*, 1996; Wang *et al.*, 2007; Yang *et al.*, 2004; King *et al.*, 2003; Pan *et al.*, 2000). Herein, we report the synthesis and crystal structure of a new lanthanum complex with pdc³⁻ anions.

The coordination environment of the lanthanum(III) metal centre (Fig. 1) is provided by two N atoms and seven O atoms, of which the N atoms are from two pyrazole rings, five O atoms are from four carboxyl groups, and two O atoms are from water molecules. These atoms define a distorted tricapped trigonal prism, as commonly observed for nine-coordinate lanthanides. In the title complex, the La—O and La—N bond lengths are in the range 2.424 (2)–2.739 (2) and 2.621 (2)–2.665 (2) Å, respectively. The pdc³⁻ ligands link lanthanum(III) atoms to form a three-dimensional framework using a μ_4 coordination mode (Fig. 2). The crystal structure is stabilized by O—H...O hydrogen bonds (Table 1).

Experimental

All chemicals used (reagent grade) were commercially available. The compound was synthesized by heating a mixture of pyrazole-3,5-dicarboxylic acid (0.078 g, 0.5 mmol), lanthanum nitrate (0.129 g, 0.3 mmol) and water (10 ml) in a 20 ml acid digestion bomb at 180 °C for 3 d. Colourless single crystals suitable for X-ray analysis were obtained after cooling to room temperature.

Refinement

All H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.93, O—H = 0.85 Å and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $1.5U_{\text{eq}}(\text{O})$.

Figures

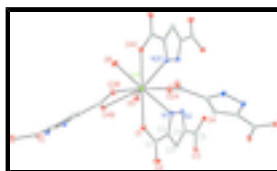


Fig. 1. The coordination environment of the lanthanum(III) atom, with the atom-numbering scheme, showing displacement ellipsoids drawn at the 30% probability level. H atoms are omitted for clarity. Symmetry codes: (A) $3/2-x, -1/2+y, z$; (B) $x, 1/2-y, 1/2+z$; (C) $2-x, -y, 1-z$.

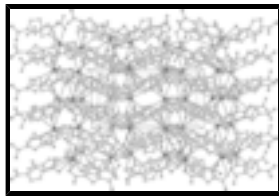


Fig. 2. Crystal packing of the title compound viewed along the a axis. H atoms are omitted for clarity.

Poly[diaqua(μ_4 -3,5-dicarboxylatopyrazol-1-ido- $\kappa^6N^1, O^5:N^2, O^3:O^3': O^5, O^5'$)lanthanum(III)]

Crystal data

[La(C₅HN₂O₄)(H₂O)₂]

$M_r = 328.02$

Orthorhombic, $Pbca$

Hall symbol: -P 2ac 2ab

$a = 12.5712$ (8) Å

$b = 8.4350$ (6) Å

$c = 16.0070$ (10) Å

$V = 1697.35$ (19) Å³

$Z = 8$

$F_{000} = 1232$

$D_x = 2.567$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 3962 reflections

$\theta = 2.5$ – 27.8°

$\mu = 5.04$ mm⁻¹

$T = 293$ K

Block, colourless

$0.32 \times 0.24 \times 0.20$ 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, 1996)

$T_{\min} = 0.239$, $T_{\max} = 0.365$

8554 measured reflections

1496 independent reflections

1316 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.023$

$\theta_{\text{max}} = 25.0^\circ$

$\theta_{\text{min}} = 3.0^\circ$

$h = -14 \rightarrow 13$

$k = -10 \rightarrow 10$

$l = -19 \rightarrow 15$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.016$

$wR(F^2) = 0.041$

$S = 1.06$

1496 reflections

128 parameters

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0185P)^2 + 2.3502P]$$

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

$(\Delta/\sigma)_{\text{max}} = 0.003$

$\Delta\rho_{\text{max}} = 0.52$ e Å⁻³

$\Delta\rho_{\text{min}} = -0.50$ e Å⁻³

Extinction correction: SHELXL97 (Sheldrick, 2008),

$$F_c^* = kFc[1 + 0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$$

Primary atom site location: structure-invariant direct methods Extinction coefficient: 0.00271 (13)

Secondary atom site location: difference Fourier map

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)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
La1	0.968426 (12)	0.009678 (17)	0.662201 (9)	0.01104 (9)
O1	0.80247 (17)	0.1816 (2)	0.67873 (12)	0.0212 (5)
O2	0.68279 (17)	0.3455 (3)	0.62560 (14)	0.0274 (5)
O3	0.9060 (2)	0.5049 (2)	0.31256 (13)	0.0222 (5)
O4	0.98606 (16)	0.2761 (2)	0.29004 (12)	0.0170 (4)
O5	1.0936 (2)	0.2221 (3)	0.60343 (15)	0.0325 (6)
H5A	1.0942	0.1442	0.6371	0.049*
H5B	1.0973	0.3066	0.6322	0.049*
O6	1.15184 (19)	-0.0151 (2)	0.73037 (16)	0.0338 (6)
H6A	1.1780	-0.1047	0.7434	0.051*
H6B	1.1851	0.0664	0.7475	0.051*
N1	0.89277 (19)	0.1436 (3)	0.52362 (14)	0.0162 (5)
N2	0.93750 (19)	0.1715 (3)	0.44839 (14)	0.0165 (5)
C1	0.7644 (2)	0.2632 (3)	0.61947 (19)	0.0153 (6)
C2	0.8238 (2)	0.2624 (3)	0.53938 (17)	0.0155 (6)
C3	0.8237 (2)	0.3719 (3)	0.47460 (18)	0.0190 (7)
H3	0.7841	0.4646	0.4698	0.023*
C4	0.8967 (2)	0.3099 (3)	0.41903 (17)	0.0160 (6)
C5	0.9322 (2)	0.3675 (3)	0.33671 (17)	0.0154 (6)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
La1	0.01164 (12)	0.01181 (12)	0.00967 (12)	0.00021 (6)	0.00036 (6)	-0.00053 (6)
O1	0.0230 (12)	0.0285 (11)	0.0122 (11)	0.0074 (9)	0.0021 (9)	0.0032 (9)
O2	0.0223 (12)	0.0311 (12)	0.0287 (13)	0.0141 (10)	0.0086 (10)	0.0075 (10)
O3	0.0358 (13)	0.0158 (11)	0.0150 (10)	0.0056 (9)	0.0055 (10)	0.0026 (8)
O4	0.0217 (11)	0.0158 (10)	0.0134 (11)	0.0024 (8)	0.0033 (8)	-0.0008 (8)
O5	0.0410 (15)	0.0214 (11)	0.0351 (13)	-0.0112 (11)	0.0097 (12)	-0.0019 (10)
O6	0.0253 (13)	0.0264 (12)	0.0496 (16)	-0.0030 (10)	-0.0187 (12)	0.0042 (10)

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N1	0.0190 (13)	0.0176 (12)	0.0120 (12)	0.0019 (10)	0.0034 (10)	0.0015 (9)
N2	0.0201 (13)	0.0186 (12)	0.0108 (12)	0.0022 (10)	0.0041 (10)	0.0027 (10)
C1	0.0151 (16)	0.0149 (14)	0.0159 (15)	-0.0019 (12)	0.0012 (11)	-0.0016 (11)
C2	0.0159 (15)	0.0169 (14)	0.0137 (15)	0.0016 (12)	0.0000 (12)	0.0006 (11)
C3	0.0235 (17)	0.0163 (14)	0.0173 (16)	0.0060 (12)	0.0011 (12)	0.0011 (12)
C4	0.0190 (16)	0.0153 (13)	0.0137 (15)	0.0014 (12)	0.0004 (12)	0.0016 (11)
C5	0.0159 (15)	0.0153 (14)	0.0149 (16)	-0.0021 (11)	-0.0020 (11)	0.0005 (12)

Geometric parameters (Å, °)

La1—O2 ⁱ	2.424 (2)	O4—La1 ⁱⁱⁱ	2.5929 (19)
La1—O3 ⁱⁱ	2.535 (2)	O4—La1 ^v	2.7388 (19)
La1—O1	2.554 (2)	O5—H5A	0.8500
La1—O6	2.559 (2)	O5—H5B	0.8500
La1—O5	2.564 (2)	O6—H6A	0.8500
La1—O4 ⁱⁱⁱ	2.5929 (19)	O6—H6B	0.8499
La1—N2 ⁱⁱⁱ	2.620 (2)	N1—C2	1.349 (4)
La1—N1	2.665 (2)	N1—N2	1.350 (3)
La1—O4 ⁱⁱ	2.7388 (19)	N2—C4	1.360 (4)
La1—C5 ⁱⁱ	3.014 (3)	N2—La1 ⁱⁱⁱ	2.620 (2)
La1—H5A	1.9874	C1—C2	1.483 (4)
O1—C1	1.266 (4)	C2—C3	1.389 (4)
O2—C1	1.242 (3)	C3—C4	1.380 (4)
O2—La1 ^{iv}	2.424 (2)	C3—H3	0.9300
O3—C5	1.266 (3)	C4—C5	1.474 (4)
O3—La1 ^v	2.535 (2)	C5—La1 ^v	3.014 (3)
O4—C5	1.269 (3)		
O2 ⁱ —La1—O3 ⁱⁱ	87.64 (7)	O2 ⁱ —La1—H5A	154.3
O2 ⁱ —La1—O1	73.08 (8)	O3 ⁱⁱ —La1—H5A	117.8
O3 ⁱⁱ —La1—O1	71.11 (7)	O1—La1—H5A	110.3
O2 ⁱ —La1—O6	139.71 (7)	O6—La1—H5A	54.3
O3 ⁱⁱ —La1—O6	82.55 (8)	O5—La1—H5A	15.9
O1—La1—O6	137.56 (7)	O4 ⁱⁱⁱ —La1—H5A	114.5
O2 ⁱ —La1—O5	142.39 (7)	N2 ⁱⁱⁱ —La1—H5A	80.6
O3 ⁱⁱ —La1—O5	124.93 (7)	N1—La1—H5A	82.7
O1—La1—O5	98.20 (7)	O4 ⁱⁱ —La1—H5A	73.1
O6—La1—O5	70.16 (8)	C5 ⁱⁱ —La1—H5A	96.4
O2 ⁱ —La1—O4 ⁱⁱⁱ	73.32 (7)	C1—O1—La1	122.68 (18)
O3 ⁱⁱ —La1—O4 ⁱⁱⁱ	75.12 (6)	C1—O2—La1 ^{iv}	170.3 (2)
O1—La1—O4 ⁱⁱⁱ	132.65 (6)	C5—O3—La1 ^v	99.48 (17)
O6—La1—O4 ⁱⁱⁱ	66.39 (6)	C5—O4—La1 ⁱⁱⁱ	120.58 (17)
O5—La1—O4 ⁱⁱⁱ	128.50 (7)	C5—O4—La1 ^v	89.78 (16)
O2 ⁱ —La1—N2 ⁱⁱⁱ	81.81 (8)	La1 ⁱⁱⁱ —O4—La1 ^v	148.37 (8)
O3 ⁱⁱ —La1—N2 ⁱⁱⁱ	138.85 (7)	La1—O5—H5B	114.9

O1—La1—N2 ⁱⁱⁱ	140.31 (7)	H5A—O5—H5B	107.7
O6—La1—N2 ⁱⁱⁱ	80.43 (8)	La1—O6—H6A	121.7
O5—La1—N2 ⁱⁱⁱ	83.25 (7)	La1—O6—H6B	120.9
O4 ⁱⁱⁱ —La1—N2 ⁱⁱⁱ	63.74 (7)	H6A—O6—H6B	116.7
O2 ⁱ —La1—N1	76.18 (7)	C2—N1—N2	107.8 (2)
O3 ⁱⁱ —La1—N1	134.47 (7)	C2—N1—La1	112.86 (17)
O1—La1—N1	63.52 (7)	N2—N1—La1	131.91 (17)
O6—La1—N1	135.32 (8)	N1—N2—C4	107.5 (2)
O5—La1—N1	67.51 (8)	N1—N2—La1 ⁱⁱⁱ	133.56 (17)
O4 ⁱⁱⁱ —La1—N1	135.91 (6)	C4—N2—La1 ⁱⁱⁱ	115.97 (17)
N2 ⁱⁱⁱ —La1—N1	81.13 (7)	O2—C1—O1	123.8 (3)
O2 ⁱ —La1—O4 ⁱⁱ	128.39 (7)	O2—C1—C2	119.1 (3)
O3 ⁱⁱ —La1—O4 ⁱⁱ	49.28 (6)	O1—C1—C2	117.0 (2)
O1—La1—O4 ⁱⁱ	67.31 (6)	N1—C2—C3	110.8 (3)
O6—La1—O4 ⁱⁱ	70.28 (7)	N1—C2—C1	119.2 (2)
O5—La1—O4 ⁱⁱ	76.32 (6)	C3—C2—C1	129.9 (3)
O4 ⁱⁱⁱ —La1—O4 ⁱⁱ	112.04 (2)	C4—C3—C2	103.2 (2)
N2 ⁱⁱⁱ —La1—O4 ⁱⁱ	148.53 (7)	C4—C3—H3	128.4
N1—La1—O4 ⁱⁱ	111.79 (6)	C2—C3—H3	128.4
O2 ⁱ —La1—C5 ⁱⁱ	107.57 (8)	N2—C4—C3	110.7 (2)
O3 ⁱⁱ —La1—C5 ⁱⁱ	24.47 (7)	N2—C4—C5	118.5 (2)
O1—La1—C5 ⁱⁱ	65.50 (7)	C3—C4—C5	130.8 (3)
O6—La1—C5 ⁱⁱ	76.66 (8)	O3—C5—O4	121.0 (3)
O5—La1—C5 ⁱⁱ	101.11 (7)	O3—C5—C4	119.7 (3)
O4 ⁱⁱⁱ —La1—C5 ⁱⁱ	94.58 (7)	O4—C5—C4	119.2 (2)
N2 ⁱⁱⁱ —La1—C5 ⁱⁱ	153.48 (8)	O3—C5—La1 ^v	56.04 (14)
N1—La1—C5 ⁱⁱ	124.88 (7)	O4—C5—La1 ^v	65.32 (14)
O4 ⁱⁱ —La1—C5 ⁱⁱ	24.90 (7)	C4—C5—La1 ^v	171.1 (2)
O2 ⁱ —La1—O1—C1	-89.3 (2)	La1—N1—N2—La1 ⁱⁱⁱ	55.4 (3)
O3 ⁱⁱ —La1—O1—C1	177.3 (2)	La1—O1—C1—O2	178.7 (2)
O6—La1—O1—C1	122.6 (2)	La1—O1—C1—C2	-3.1 (3)
O5—La1—O1—C1	53.1 (2)	N2—N1—C2—C3	-0.9 (3)
O4 ⁱⁱⁱ —La1—O1—C1	-135.8 (2)	La1—N1—C2—C3	152.7 (2)
N2 ⁱⁱⁱ —La1—O1—C1	-36.2 (3)	N2—N1—C2—C1	-178.8 (2)
N1—La1—O1—C1	-6.6 (2)	La1—N1—C2—C1	-25.2 (3)
O4 ⁱⁱ —La1—O1—C1	124.5 (2)	O2—C1—C2—N1	-161.5 (3)
C5 ⁱⁱ —La1—O1—C1	151.7 (2)	O1—C1—C2—N1	20.3 (4)
O2 ⁱ —La1—N1—C2	93.7 (2)	O2—C1—C2—C3	21.1 (5)
O3 ⁱⁱ —La1—N1—C2	21.3 (2)	O1—C1—C2—C3	-157.2 (3)
O1—La1—N1—C2	15.99 (18)	N1—C2—C3—C4	0.4 (3)
O6—La1—N1—C2	-115.99 (19)	C1—C2—C3—C4	178.0 (3)
O5—La1—N1—C2	-96.26 (19)	N1—N2—C4—C3	-0.9 (3)

supplementary materials

O4 ⁱⁱⁱ —La1—N1—C2	141.00 (17)	La1 ⁱⁱⁱ —N2—C4—C3	162.30 (19)
N2 ⁱⁱⁱ —La1—N1—C2	177.4 (2)	N1—N2—C4—C5	-179.6 (2)
O4 ⁱⁱ —La1—N1—C2	-32.5 (2)	La1 ⁱⁱⁱ —N2—C4—C5	-16.4 (3)
C5 ⁱⁱ —La1—N1—C2	-8.2 (2)	C2—C3—C4—N2	0.3 (3)
O2 ⁱ —La1—N1—N2	-120.8 (2)	C2—C3—C4—C5	178.8 (3)
O3 ⁱⁱ —La1—N1—N2	166.70 (19)	La1 ^v —O3—C5—O4	7.1 (3)
O1—La1—N1—N2	161.4 (2)	La1 ^v —O3—C5—C4	-170.7 (2)
O6—La1—N1—N2	29.5 (3)	La1 ⁱⁱⁱ —O4—C5—O3	-177.2 (2)
O5—La1—N1—N2	49.2 (2)	La1 ^v —O4—C5—O3	-6.5 (3)
O4 ⁱⁱⁱ —La1—N1—N2	-73.6 (2)	La1 ⁱⁱⁱ —O4—C5—C4	0.7 (3)
N2 ⁱⁱⁱ —La1—N1—N2	-37.1 (2)	La1 ^v —O4—C5—C4	171.4 (2)
O4 ⁱⁱ —La1—N1—N2	113.0 (2)	La1 ⁱⁱⁱ —O4—C5—La1 ^v	-170.65 (16)
C5 ⁱⁱ —La1—N1—N2	137.2 (2)	N2—C4—C5—O3	-171.1 (3)
C2—N1—N2—C4	1.1 (3)	C3—C4—C5—O3	10.5 (5)
La1—N1—N2—C4	-145.6 (2)	N2—C4—C5—O4	11.0 (4)
C2—N1—N2—La1 ⁱⁱⁱ	-157.9 (2)	C3—C4—C5—O4	-167.4 (3)

Symmetry codes: (i) $-x+3/2, y-1/2, z$; (ii) $x, -y+1/2, z+1/2$; (iii) $-x+2, -y, -z+1$; (iv) $-x+3/2, y+1/2, z$; (v) $x, -y+1/2, z-1/2$.

Hydrogen-bond geometry (Å, °)

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
O5—H5A···O6	0.85	2.14	2.944 (3)	159
O5—H5B···O3 ^{vi}	0.85	1.82	2.667 (3)	174
O6—H6A···O1 ^{vii}	0.85	2.20	2.999 (3)	155
O6—H6B···O1 ^{viii}	0.85	2.12	2.908 (3)	153

Symmetry codes: (vi) $-x+2, -y+1, -z+1$; (vii) $-x+2, y-1/2, -z+3/2$; (viii) $x+1/2, y, -z+3/2$.

Fig. 1

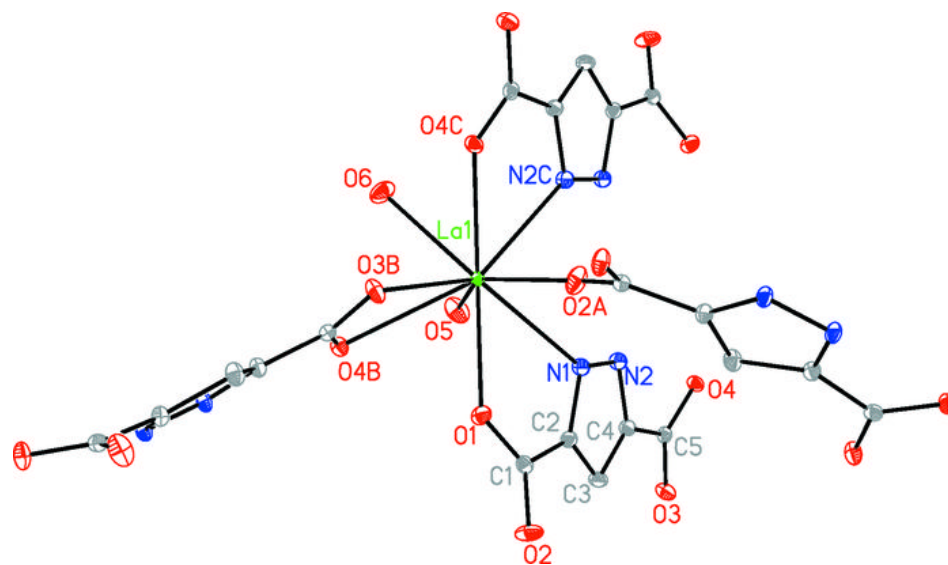


Fig. 2

