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Diaquabis[2,6-bis(1,2,4-triazol-2-yl)pyridine-κN^4]trinitratolathanum(III) monohydrate

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Key indicators

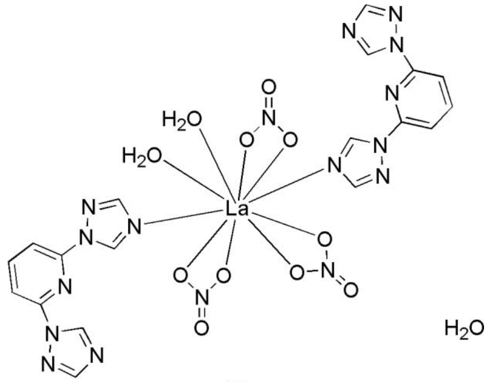
Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.005 Å
R factor = 0.032
wR factor = 0.069
Data-to-parameter ratio = 12.7

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

In the title complex, $[La(NO_3)_3(C_9H_7N_7)_2(H_2O)_2]\cdot H_2O$, the La^{III} atom is ten-coordinated by two N atoms of two monodentate 2,6-bis(1,2,4-triazolyl)pyridine ligands, six O atoms from three bidentate nitrate ligands, and two water molecules. In the crystal structure, a two-dimensional network is formed *via* O—H···O and O—H···N hydrogen bonds.

Comment

Interest has recently been focused on the self-assembly of coordination compounds because of their potential properties for ion exchange, gas storage, molecular sensing, and catalysis (Barnett & Champness, 2003; Hong *et al.*, 2004). Many topologically promising architectures have been constructed from new synthetic strategies using novel rigid or flexible spacer ligands (Wager *et al.*, 2002; Blake *et al.*, 1997). This group has investigated the design and control of the self-assembly of coordination polymers with rigid bridging btp ligands [btp = bis(2,6-bis(N'-1,2,4-triazolyl)pyridine] and have synthesized different dimensional structures from different metal salts with this ligand (Hong *et al.*, 2004; Ryu, Han *et al.*, 2005; Ryu, Lee *et al.*, 2005). We have concluded that the coordination environment of the metal is important for the construction of coordination polymers. In this study, we have used lanthanum nitrate to examine the structure generated in combination with the btp ligand and report here the crystal structure of the title compound, (I).



(I)

The asymmetric unit of (I) is shown in Fig. 1 and selected bond lengths and angles are given in Table 1. The La^{III} atom is ten-coordinated by two N atoms of two monodentate btp ligands, six O atoms from the bidentate nitrate ligands, and two water molecules. In the crystal structure, intermolecular O—H···O and O—H···N hydrogen bonds form a two-dimensional network (Table 2 and Fig. 2)

Experimental

Colorless rod-type crystals were obtained from a direct diffusion technique in which a methanol (4 ml) solution of $La(NO_3)_3$ (29.3 mg, 0.09 mmol) was carefully layered with a dichloromethane solution (4 ml) of a btp ligand (38.6 mg, 0.18 mmol). The btp ligand was prepared according to the literature (Hong *et al.*, 2004).

Crystal data

$[La(NO_3)_3(C_9H_7N_7)(H_2O)_2]\cdot H_2O$
$M_r = 805.42$
Monoclinic, $P2_1/c$
$a = 8.9000$ (5) Å
$b = 13.9649$ (8) Å
$c = 23.6361$ (13) Å
$\beta = 95.1110$ (10)°
$V = 2926.0$ (3) Å^3
$Z = 4$
$D_x = 1.828$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 1.55$ mm^{-1}
$T = 273$ (2) K
Rod, colorless
0.25 × 0.08 × 0.08 mm

Data collection

Bruker SMART CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
$T_{min} = 0.862$, $T_{max} = 0.883$
16236 measured reflections
5721 independent reflections
4382 reflections with $I > 2\sigma(I)$
$R_{int} = 0.041$
$\theta_{max} = 26.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.069$
$S = 1.03$
5721 reflections
451 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0235P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.48$ e Å^{-3}
$\Delta\rho_{min} = -0.42$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

La1—O11	2.497 (2)	La1—O52	2.633 (3)
La1—O12	2.516 (2)	La1—O42	2.662 (2)
La1—O31	2.600 (2)	La1—N21	2.664 (3)
La1—O41	2.620 (2)	La1—O32	2.683 (2)
La1—O51	2.629 (2)	La1—N11	2.723 (2)
O11—La1—O12	68.99 (8)	O31—La1—N21	117.70 (8)
O11—La1—O31	77.35 (8)	O41—La1—N21	118.18 (8)
O12—La1—O31	141.16 (8)	O51—La1—N21	114.55 (8)
O11—La1—O41	145.19 (8)	O52—La1—N21	68.13 (8)
O12—La1—O41	136.41 (8)	O42—La1—N21	73.29 (8)
O31—La1—O41	69.25 (8)	O11—La1—O32	66.25 (8)
O11—La1—O51	129.53 (8)	O12—La1—O32	126.64 (8)
O12—La1—O51	70.41 (8)	O31—La1—O32	48.11 (7)
O31—La1—O51	122.40 (8)	O41—La1—O32	96.81 (8)
O41—La1—O51	66.01 (8)	O51—La1—O32	162.60 (8)
O11—La1—O52	137.02 (8)	O52—La1—O32	128.13 (8)
O12—La1—O52	72.89 (8)	O42—La1—O32	65.25 (9)
O31—La1—O52	144.75 (8)	N21—La1—O32	70.07 (8)
O41—La1—O52	77.61 (9)	O11—La1—N11	75.68 (8)
O51—La1—O52	48.18 (8)	O12—La1—N11	77.56 (8)
O11—La1—O42	131.20 (8)	O31—La1—N11	75.80 (8)
O12—La1—O42	143.12 (9)	O41—La1—N11	86.67 (8)
O31—La1—O42	74.77 (8)	O51—La1—N11	67.35 (8)
O41—La1—O42	48.13 (7)	O52—La1—N11	114.67 (8)
O51—La1—O42	99.26 (8)	O42—La1—N11	132.49 (8)
O52—La1—O42	74.32 (9)	N21—La1—N11	154.21 (9)
O11—La1—N21	85.69 (8)	O32—La1—N11	116.42 (8)
O12—La1—N21	79.19 (8)		

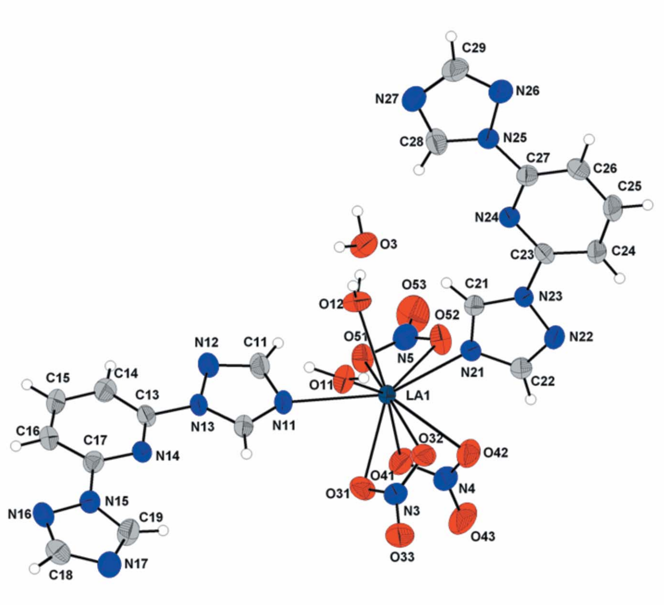


Figure 1
The asymmetric unit of (I) showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level.

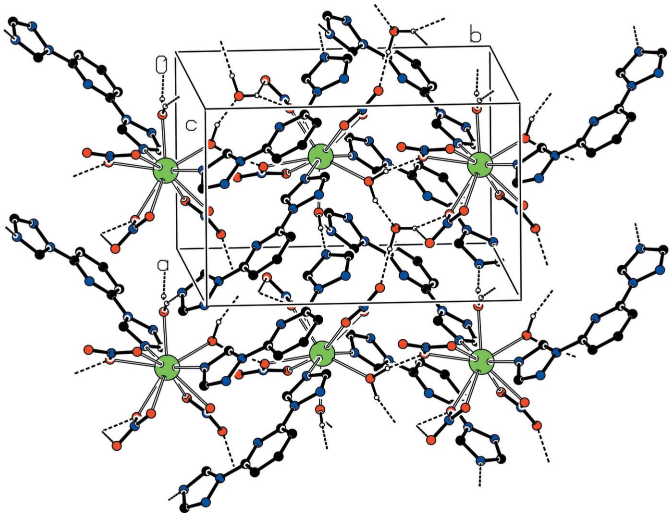


Figure 2
Part of the crystal structure of (I) showing hydrogen bonds as dahed lines. H atoms not involved in intermolecular interactions have been omitted for clarity.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H31···O53^{i}	0.96 (3)	1.86 (3)	2.801 (4)	168 (3)
O3—H32···O41^{ii}	0.94 (3)	1.87 (3)	2.777 (4)	160 (3)
O3—H32···O43^{ii}	0.94 (3)	2.52 (3)	3.206 (4)	130 (2)
O11—H111···N17^{iii}	0.95 (3)	1.89 (3)	2.820 (4)	164 (3)
O11—H112···N27^{iv}	0.95 (3)	1.84 (3)	2.787 (4)	173 (2)
O12—H121···O3	0.97 (3)	1.81 (3)	2.742 (4)	162 (3)
O12—H122···O31^{ii}	0.96 (3)	1.84 (3)	2.789 (3)	168 (3)

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

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Carbon-bound H atoms were placed in calculated positions with C—H distances of 0.93 Å. They were included in the refinement in the riding-model approximation with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C). The H atoms of the water molecules were located in a difference Fourier map and were refined with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C).

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); 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, 1998) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL*.

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