Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Poly[[tetraaquabis(5-carboxypyridine-2-carboxylato-κ^2N,O)bis(μ_4-pyridine-2,5-dicarboxylato-$\kappa^5N,O:O:O':O''$)-dilanthanum(III)] dihydrate]

Fan Zhang, Bin Yu, Xiao-Qing Wang, Guang-Qiu Shen and De-Zhong Shen*

Department of Chemistry, Tsinghua University, Beijing 100084, People's Republic of China
Correspondence e-mail: xqwang@mail.tsinghua.edu.cn

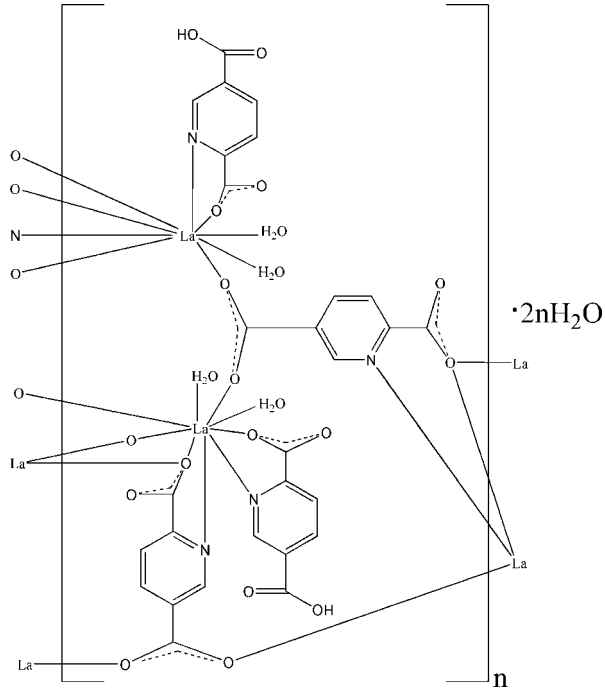
Received 26 June 2007; accepted 1 July 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.020 Å; R factor = 0.064; wR factor = 0.174; data-to-parameter ratio = 11.4.

The title compound, $\{[La_2(C_7H_4NO_4)_2(C_7H_3NO_4)_2(H_2O)_4]\cdot 2H_2O\}_n$, was prepared by a hydrothermal reaction at 433 K. The asymmetric unit contains two La^{III} ions. Each La^{III} ion is nine-coordinated in a slightly distorted tricapped trigonal–prismatic coordination geometry, formed by two N atoms from 5-carboxypyridine-2-carboxylate (Hpydc) and pyridine-2,5-dicarboxylate (pydc) ligands, five O atoms from carboxylate groups of one Hpydc and four pydc ligands, and two water molecules. Adjacent La^{III} ions are linked together through single bridging carboxylate O atoms and carboxylate groups in a *syn–anti* mode, forming a two-dimensional layered polymeric structure. Extensive O—H···O hydrogen bonding connects adjacent layers into an infinite three-dimensional supramolecular network structure. The crystal studied was an inversion twin.

Related literature

For general background, see: Chae *et al.* (2004); Seo *et al.* (2000); Bradshaw *et al.* (2004); Lu *et al.* (2006); Liang *et al.* (2000, 2001); Min *et al.* (2001); Xu *et al.* (2001); Gao *et al.* (2005). For related structures, see: Song *et al.* (2005); Qin *et al.* (2005).



Experimental

Crystal data

$[La_2(C_7H_4NO_4)_2(C_7H_3NO_4)_2(H_2O)_4]\cdot 2H_2O$
M_r = 1048.35
Monoclinic, $P2_1$
a = 9.2203 (18) Å
b = 19.744 (4) Å
c = 9.3552 (19) Å
β = 101.72 (3)°
V = 1667.5 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.63 mm^{-1}
T = 293 (2) K
0.35 × 0.34 × 0.27 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.428, T_{max} = 0.490
12319 measured reflections
5778 independent reflections
5491 reflections with $I > 2\sigma(I)$
R_{int} = 0.093

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.174
S = 1.06
5778 reflections
505 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.82 e Å^{-3}
$\Delta\rho_{min}$ = −3.93 e Å^{-3}
Absolute structure: Flack (1983), with 2752 Friedel pairs
Flack parameter: 0.50 (4)

Table 1
Selected bond lengths (Å).

La1—O1	2.520 (10)	La2—O6	2.522 (9)
La1—O5	2.531 (10)	La2—O8^{iii}	2.599 (9)
La1—O8^{i}	2.658 (9)	La2—O10	2.498 (10)
La1—O13^{ii}	2.584 (10)	La2—O13	2.626 (10)
La1—O15^{i}	2.531 (9)	La2—O16^{i}	2.551 (10)
La1—O19	2.570 (11)	La2—O17	2.613 (10)
La1—O20	2.543 (10)	La2—O18	2.505 (10)
La1—N1	2.778 (13)	La2—N3	2.681 (12)
La1—N2^{i}	2.703 (12)	La2—N4	2.786 (12)

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

 doi:10.1107/S1600536807032059

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

D—H···A	D—H	H···A	D···A	D—H···A
O22—H22B···O21^{iv}	0.85	2.03	2.88 (2)	176
O22—H22A···O2^{v}	0.85	1.85	2.702 (17)	177
O21—H21C···O17^{vi}	0.85	1.99	2.833 (15)	171
O21—H21B···O9^{ii}	0.85	1.77	2.612 (15)	171
O20—H20B···O11^{i}	0.85	2.09	2.759 (14)	136
O20—H20A···O8^{i}	0.85	2.47	3.020 (14)	123
O20—H20A···O10^{ii}	0.85	2.06	2.687 (14)	130
O19—H19B···O16^{i}	0.85	1.98	2.787 (15)	158
O19—H19A···O14^{ii}	0.85	1.80	2.605 (15)	157
O18—H18C···O3^{vii}	0.85	1.91	2.728 (15)	162
O18—H18A···O1^{viii}	0.85	1.89	2.706 (14)	161
O17—H17C···O16^{i}	0.85	2.49	2.955 (14)	115
O17—H17C···O5	0.85	2.12	2.791 (14)	135
O17—H17A···O7^{iii}	0.85	1.76	2.608 (14)	174
O12—H12A···O21^{vii}	0.82	1.76	2.564 (15)	166
O4—H4B···O22^{ix}	0.82	1.82	2.534 (14)	145

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

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, 1997); software used to prepare material for publication: *SHELXTL*.

The authors acknowledge financial support by the National Natural Science Foundation of China (grant No. 50590402).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2283).

References

Bradshaw, D., Prior, T. J., Cussen, E. J., Claridge, J. B. & Rosseinsky, M. J. (2004). *J. Am. Chem. Soc.* **126**, 6106–6114.

Bruker (1997). *SMART*, *SAINT* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.

Chae, H. K., Siberio-Pérez, D. Y., Kim, J., Go, Y. B., Eddaoudi, M., Matzger, A. J., O'Keeffe, M. & Yaghi, O. M. (2004). *Nature* (*London*), **427**, 523–527.

Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.

Gao, H.-L., Cheng, C., Ding, B., Shi, W., Song, H.-B., Cheng, P., Liao, D.-Z., Yan, S.-P. & Jiang, Z.-H. (2005). *J. Mol. Struct.* **738**, 105–111.

Liang, Y.-C., Cao, R., Su, W.-P., Hong, M.-C. & Zhang, W.-J. (2000). *Angew. Chem. Int. Ed.* **39**, 3304–3307.

Liang, Y.-C., Hong, M.-C., Su, W.-P., Cao, R. & Zhang, W.-J. (2001). *Inorg. Chem.* **40**, 4574–4582.

Lu, W.-G., Su, C.-Y., Lu, T.-B., Jiang, L. & Chen, J.-M. (2006). *J. Am. Chem. Soc.* **128**, 34–35.

Min, D., Yoon, S. S., Lee, C. Y., Han, W. S. & Lee, S. W. (2001). *Bull. Korean Chem. Soc.* **22**, 1041–1044.

Qin, C., Wang, X.-L., Wang, E.-B. & Su, Z.-M. (2005). *Inorg. Chem.* **44**, 7122–7129.

Seo, J. S., Whang, D., Lee, H., Jun, S. I., Oh, J., Jeon, Y. J. & Kim, K. (2000). *Nature* (*London*), **404**, 982–986.

Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.

Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

Song, Y.-S., Yan, B. & Chen, Z.-X. (2005). *J. Mol. Struct.* **750**, 101–108.

Xu, H.-T., Zheng, N.-W., Xu, H.-H., Wu, Y.-G., Yang, R.-Y., Ye, E.-Y. & Jin, X.-L. (2001). *J. Mol. Struct.* **597**, 1–5.

supplementary materials

Acta Cryst. (2007). E**63**, m2069-m2070 [**doi:10.1107/S1600536807032059**]

Poly[[tetraaquabis(5-carboxypyridine-2-carboxylato-κ^2N,O)bis(μ_4-pyridine-2,5-dicarboxylato-$\kappa^5N,O:O:O':O''$)dilanthanum(III)] dihydrate]

F. Zhang, B. Yu, X.-Q. Wang, G.-Q. Shen and D.-Z. Shen

Comment

In recent years, studies on the syntheses, structures and properties of coordination complexes containing lanthanum and aromatic carboxylate have intensely attracted much attention, because they possess potential application on catalysis, separation, gas deposition and luminescence (Chae *et al.*, 2004; Seo *et al.*, 2000; Bradshaw *et al.*, 2004; Lu *et al.*, 2006). As a multi-functional ligand, pyridine-2,5-dicarboxylic acid has been widely used in the preparation of 3 d-4f heterometallic coordination polymers (Liang *et al.*, 2000; Liang *et al.*, 2001) and transition metallic supra-molecular compounds (Min *et al.*, 2001; Xu *et al.*, 2001; Gao *et al.*, 2005). However the investigation on the lanthanum complexes is relative limited (Song *et al.*, 2005). We report here the crystal structure of the title La^{III} polymeric compound.

A segment of the polymeric structure of the title compound is illustrated in Fig. 1. Each La^{III} ion is nine-coordinated by two nitrogen atoms from Hpydc and pydc ligands, five oxygen atoms from carboxylate groups of one Hpydc and four pydc ligands and two water molecules. The $pydc^{2-}$ anion acts as chelating-bridging pentadentate ligand towards four La^{III} ions. The pyridine nitrogen atom and the *ortho*-carboxylic oxygen atom chelate one La ion, and this oxygen atom and other two carboxylic oxygen atoms of the pydc ligand bridge another three different La ions. The $Hpydc^{-}$ anion acts as chelating bidentate ligand towards the La ion with a pyridine nitrogen atom and the *ortho* carboxylic oxygen atom, which is similar to the coordination mode of Hpydc in $[Dy(Hpydc)(pydc)(phen)(H_2O)\cdot H_2O]_n$ [phen=1,10-phenanthroline] (Song *et al.*, 2005) and [Ln(Hpydc)(pydc)] [Ln = Sm, Eu, Gd] (Qin *et al.*, 2005). The La···La separations in the same unit and between adjacent units are 4.339 (9) and 5.619 (9) Å, respectively. The La center is in a slightly distorted tricapped trigonal prism coordination geometry. Adjacent La ions are linked together through single-atom carboxylate oxygen atom and carboxylate group in the *syn*-anti mode, forming a two-dimensional polymeric layer structure as represented in Fig. 2. Selected geometric parameters are listed in Table 1. The La—O bond lengths fall in range from 2.498 (10) to 2.658 (9) Å.

Extensive N—H···O and O—H···O hydrogen bonding occur in the crystal structure of the title compound, and connect adjacent layers into the infinite three-dimensional supramolecular network structure (Table 2 and Fig. 3).

Experimental

A mixture of $La(NO_3)_3\cdot 6H_2O$ (0.060 g, 0.25 mmol), pyridine-2,5-dicarboxylic acid (0.084 g, 0.50 mmol) and H_2O (15 ml) was sealed in a 25 ml stainless steel reactor with a Teflon liner and heated at 433 K for 72 h. The mixture was cooled slowly to room temperature at a rate of 10 $K.h^{-1}$. Straw yellow prism crystals of the title complex were collected by filtration and were obtained in 21% yield. Analysis calculated for $C_{14}H_{13}LaN_2O_{11}$ (%): C 32.08, H 2.50, N 5.34; found: C 32.11, H 2.53, N 5.36

Refinement

Aromatic H atoms were placed in geometrically idealized positions with C—H = 0.93 Å and refined in the riding-model approximation with U_{iso}(H) = 1.2U_{eq}(C). Carboxyl H atoms were placed in calculated position with O—H = 0.82 Å and refined in riding mode with U_{iso}(H) = 1.5U_{eq}(O). Water H atoms were placed in calculated positions with O—H = 0.85 Å and refined in riding mode with U_{iso}(H) = 1.2U_{eq}(O). The highest peak and deepest hole appear at 1.22 Å from H14 and 0.83 Å from H21A, respectively.

Figures

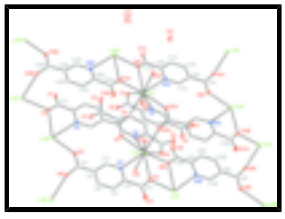


Fig. 1. The structure of the title compound with displacement ellipsoids drawn at the 50% probability level. H atoms have been omitted for clarity.

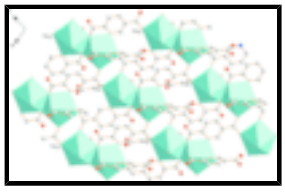


Fig. 2. View of the two-dimensional network in the crystal structure of the title compound. H atoms and uncoordinated water molecules have been omitted.

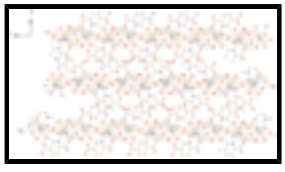


Fig. 3. View of the packing of the three-dimensional network of the title compound along the *b* axis (H atoms and uncoordinated water molecules have been omitted for clarity).

Poly[[tetraaquabis(5-carboxypyridine-2-carboxylato-κ^2N,O)bis(μ_4– pyridine-2,5-dicarboxylato-$\kappa^5N,O:O:O':O''$)dilanthanum(III)] dihydrate]

Crystal data

$[La_2(C_7H_4NO_4)_2(C_7H_3NO_4)_2(H_2O)_4]\cdot 2H_2O$	F_{000} = 1024
M_r = 1048.35	D_x = 2.088 Mg m^{-3}
Monoclinic, $P2_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2yb	Cell parameters from 3211 reflections
a = 9.2203 (18) Å	θ = 2.2–20.5°
b = 19.744 (4) Å	μ = 2.63 mm^{-1}
c = 9.3552 (19) Å	T = 293 (2) K
β = 101.72 (3)°	Prism, yellow
V = 1667.5 (6) Å^3	0.35 × 0.34 × 0.27 mm
Z = 2	

Data collection

Bruker SMART CCD area-detector diffractometer	5778 independent reflections
Radiation source: fine-focus sealed tube	5491 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.093$
$T = 293(2)$ K	$\theta_{max} = 25.0^{o}$
φ and ω scans	$\theta_{min} = 3.0^{o}$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -10 \rightarrow 10$
$T_{min} = 0.428$, $T_{max} = 0.490$	$k = -23 \rightarrow 23$
12319 measured reflections	$l = -11 \rightarrow 11$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.064$	$w = 1/[\sigma^2(F_o^2) + (0.0958P)^2 + 9.9455P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.174$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.06$	$\Delta\rho_{max} = 1.82$ e Å^{-3}
5778 reflections	$\Delta\rho_{min} = -3.93$ e Å^{-3}
505 parameters	Extinction correction: none
1 restraint	Absolute structure: Flack (1983), 2752 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.50 (4)
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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
La1	0.46937 (8)	0.05700 (3)	0.39796 (8)	0.0112 (2)
La2	0.28724 (8)	0.07667 (3)	0.93428 (8)	0.0107 (2)
N1	0.5695 (13)	−0.0629 (6)	0.5397 (14)	0.016 (3)

N2	−0.2524 (13)	0.0334 (6)	0.3592 (13)	0.014 (3)
N3	0.0116 (13)	0.1009 (6)	0.9728 (13)	0.015 (3)
N4	0.1862 (13)	0.1969 (6)	0.7924 (13)	0.014 (3)
O1	0.3674 (11)	−0.0545 (5)	0.2910 (11)	0.015 (2)
O2	0.2676 (12)	−0.1539 (5)	0.3372 (12)	0.024 (2)
O3	0.9397 (13)	−0.0864 (6)	0.8710 (13)	0.024 (3)
O4	0.8767 (12)	−0.1922 (5)	0.9100 (13)	0.026 (3)
H4B	0.9385	−0.1884	0.9860	0.038*
O5	0.2708 (11)	0.0173 (5)	0.5298 (11)	0.014 (2)
O6	0.1288 (10)	0.0513 (5)	0.6871 (10)	0.0148 (19)
O7	−0.3646 (11)	−0.0298 (6)	0.0010 (12)	0.021 (2)
O8	−0.4868 (10)	0.0364 (5)	0.1292 (10)	0.011 (2)
O9	0.4727 (13)	0.2909 (5)	1.0127 (13)	0.029 (3)
O10	0.3905 (11)	0.1868 (5)	1.0408 (11)	0.016 (2)
O11	−0.1719 (12)	0.2227 (5)	0.4463 (12)	0.020 (2)
O12	−0.0761 (13)	0.3223 (5)	0.3902 (13)	0.026 (3)
H12A	−0.1476	0.3221	0.3218	0.040*
O13	0.2497 (11)	0.0993 (5)	1.2010 (11)	0.015 (2)
O14	0.1265 (12)	0.1662 (6)	1.3299 (12)	0.023 (2)
O15	−0.3697 (10)	0.0818 (5)	0.6455 (10)	0.0145 (19)
O16	−0.5110 (11)	0.1124 (5)	0.7993 (11)	0.017 (2)
O17	0.3846 (11)	−0.0285 (5)	0.8125 (11)	0.016 (2)
H17A	0.4683	−0.0311	0.8705	0.019*
H17C	0.3985	−0.0053	0.7400	0.019*
O18	0.1967 (11)	−0.0318 (5)	1.0239 (11)	0.016 (2)
H18A	0.2358	−0.0457	1.1090	0.019*
H18C	0.1178	−0.0542	0.9929	0.019*
O19	0.3764 (12)	0.1608 (5)	0.5188 (12)	0.018 (2)
H19A	0.2862	0.1573	0.4756	0.022*
H19B	0.3869	0.1431	0.6031	0.022*
O20	0.5648 (11)	0.1658 (5)	0.3042 (12)	0.019 (2)
H20A	0.5504	0.1549	0.2145	0.022*
H20B	0.6562	0.1606	0.3414	0.022*
O21	0.7230 (12)	0.3388 (5)	0.1594 (13)	0.027 (3)
H21B	0.6464	0.3190	0.1118	0.033*
H21C	0.7003	0.3796	0.1734	0.033*
O22	0.1319 (14)	0.7993 (6)	0.0723 (16)	0.040 (3)
H22A	0.1775	0.8147	0.1540	0.048*
H22B	0.1779	0.8119	0.0068	0.048*
C1	0.3653 (16)	−0.1095 (7)	0.3636 (16)	0.016 (3)
C2	0.4906 (16)	−0.1192 (7)	0.4931 (16)	0.015 (3)
C3	0.5209 (16)	−0.1821 (8)	0.5549 (17)	0.017 (3)
H3A	0.4613	−0.2191	0.5205	0.021*
C4	0.6448 (16)	−0.1899 (7)	0.6723 (17)	0.018 (3)
H4A	0.6699	−0.2318	0.7156	0.021*
C5	0.7253 (16)	−0.1331 (7)	0.7187 (17)	0.016 (3)
C6	0.8590 (16)	−0.1344 (7)	0.8433 (17)	0.017 (3)
C7	0.6853 (16)	−0.0696 (8)	0.6544 (16)	0.016 (3)
H7A	0.7393	−0.0315	0.6913	0.019*

C8	0.1461 (15)	0.0313 (7)	0.5627 (16)	0.014 (3)
C9	0.0120 (16)	0.0184 (7)	0.4480 (16)	0.013 (3)
C10	0.0192 (16)	−0.0138 (7)	0.3160 (16)	0.015 (3)
H10A	0.1094	−0.0302	0.3007	0.018*
C11	−0.1064 (15)	−0.0214 (7)	0.2089 (17)	0.014 (3)
H11A	−0.1001	−0.0431	0.1221	0.017*
C12	−0.2384 (16)	0.0021 (7)	0.2280 (16)	0.014 (3)
C13	−0.3733 (15)	0.0021 (7)	0.1096 (16)	0.014 (3)
C14	−0.1313 (15)	0.0397 (7)	0.4643 (16)	0.014 (3)
H14	−0.1410	0.0590	0.5526	0.017*
C15	0.1360 (16)	0.1339 (7)	1.2190 (16)	0.014 (3)
C16	−0.0017 (16)	0.1304 (7)	1.0937 (16)	0.013 (3)
C17	−0.1335 (16)	0.1583 (7)	1.1211 (17)	0.016 (3)
H17B	−0.1360	0.1813	1.2073	0.019*
C18	−0.2594 (16)	0.1499 (7)	1.0130 (16)	0.014 (3)
H18B	−0.3503	0.1665	1.0259	0.017*
C19	−0.2479 (16)	0.1164 (7)	0.8852 (16)	0.014 (3)
C20	−0.3863 (15)	0.1042 (7)	0.7739 (16)	0.013 (3)
C21	−0.1135 (15)	0.0917 (7)	0.8690 (15)	0.014 (3)
H21A	−0.1075	0.0679	0.7846	0.017*
C22	0.3880 (16)	0.2428 (7)	0.9726 (16)	0.017 (3)
C23	0.2723 (16)	0.2512 (7)	0.8339 (16)	0.016 (3)
C24	0.2569 (17)	0.3121 (7)	0.7608 (17)	0.018 (3)
H24A	0.3219	0.3478	0.7911	0.022*
C25	0.1432 (17)	0.3188 (7)	0.6423 (17)	0.017 (3)
H25A	0.1294	0.3596	0.5917	0.021*
C26	0.0477 (16)	0.2643 (7)	0.5970 (16)	0.015 (3)
C27	−0.0788 (16)	0.2672 (7)	0.4702 (16)	0.015 (3)
C28	0.0747 (16)	0.2054 (7)	0.6777 (16)	0.015 (3)
H28A	0.0109	0.1691	0.6503	0.018*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
La1	0.0075 (4)	0.0194 (4)	0.0072 (4)	0.0004 (3)	0.0030 (3)	−0.0004 (3)
La2	0.0075 (4)	0.0192 (4)	0.0057 (4)	0.0007 (3)	0.0022 (3)	−0.0004 (3)
N1	0.013 (6)	0.022 (6)	0.012 (7)	0.001 (5)	0.002 (5)	0.000 (5)
N2	0.010 (6)	0.024 (6)	0.008 (6)	0.002 (5)	0.003 (5)	−0.003 (5)
N3	0.012 (6)	0.024 (6)	0.008 (6)	0.000 (5)	0.002 (5)	−0.001 (5)
N4	0.012 (6)	0.023 (6)	0.008 (6)	0.000 (5)	0.003 (5)	0.001 (5)
O1	0.013 (5)	0.024 (5)	0.008 (5)	0.001 (4)	0.003 (4)	0.001 (4)
O2	0.018 (6)	0.032 (6)	0.019 (6)	−0.008 (5)	−0.005 (5)	0.002 (5)
O3	0.023 (6)	0.026 (6)	0.020 (6)	−0.004 (5)	−0.004 (5)	−0.001 (5)
O4	0.022 (6)	0.032 (6)	0.018 (6)	−0.003 (5)	−0.005 (5)	0.003 (4)
O5	0.011 (5)	0.025 (5)	0.009 (5)	0.002 (4)	0.005 (4)	−0.001 (4)
O6	0.011 (4)	0.024 (5)	0.010 (5)	0.001 (4)	0.004 (4)	−0.001 (4)
O7	0.012 (5)	0.037 (6)	0.011 (6)	0.004 (5)	−0.003 (4)	−0.009 (5)
O8	0.003 (4)	0.023 (5)	0.007 (5)	0.002 (3)	−0.001 (4)	−0.004 (4)

O9	0.023 (6)	0.031 (6)	0.028 (7)	−0.007 (5)	−0.006 (5)	0.002 (5)
O10	0.014 (5)	0.023 (5)	0.010 (5)	0.001 (4)	0.001 (4)	0.001 (4)
O11	0.013 (5)	0.029 (6)	0.015 (6)	−0.001 (5)	−0.002 (4)	−0.002 (4)
O12	0.021 (6)	0.035 (6)	0.017 (6)	−0.003 (5)	−0.011 (5)	0.009 (4)
O13	0.016 (5)	0.023 (5)	0.010 (5)	−0.002 (4)	0.008 (4)	0.000 (4)
O14	0.017 (6)	0.035 (6)	0.016 (6)	0.005 (5)	0.001 (5)	−0.012 (5)
O15	0.011 (5)	0.024 (5)	0.008 (5)	0.002 (4)	0.001 (4)	−0.002 (4)
O16	0.011 (5)	0.027 (5)	0.012 (5)	0.000 (4)	0.002 (4)	0.001 (4)
O17	0.014 (5)	0.025 (5)	0.009 (5)	0.004 (4)	0.004 (4)	0.003 (4)
O18	0.012 (5)	0.028 (5)	0.010 (5)	−0.005 (4)	0.006 (4)	0.003 (4)
O19	0.014 (5)	0.028 (6)	0.012 (6)	0.003 (4)	0.000 (4)	0.002 (5)
O20	0.013 (5)	0.030 (6)	0.013 (6)	−0.002 (4)	0.001 (4)	0.001 (4)
O21	0.022 (6)	0.024 (5)	0.030 (7)	−0.005 (4)	−0.009 (5)	0.006 (5)
O22	0.034 (8)	0.045 (7)	0.036 (8)	0.000 (6)	−0.003 (6)	−0.002 (6)
C1	0.012 (7)	0.023 (7)	0.011 (8)	0.001 (6)	0.003 (6)	−0.001 (6)
C2	0.011 (7)	0.023 (7)	0.011 (8)	0.000 (6)	0.003 (6)	0.001 (6)
C3	0.014 (8)	0.024 (7)	0.014 (8)	0.000 (6)	0.002 (6)	0.001 (6)
C4	0.013 (8)	0.026 (7)	0.014 (8)	0.001 (6)	0.001 (6)	0.001 (6)
C5	0.012 (7)	0.024 (7)	0.011 (7)	0.001 (6)	0.003 (6)	0.001 (6)
C6	0.014 (8)	0.025 (7)	0.012 (8)	0.003 (6)	0.003 (6)	0.001 (6)
C7	0.012 (7)	0.024 (7)	0.012 (8)	0.001 (6)	0.003 (6)	0.000 (6)
C8	0.011 (7)	0.023 (7)	0.009 (7)	0.001 (6)	0.003 (6)	0.000 (6)
C9	0.008 (7)	0.024 (7)	0.008 (7)	0.000 (6)	0.002 (6)	0.000 (6)
C10	0.011 (7)	0.024 (7)	0.010 (7)	0.000 (6)	0.004 (6)	−0.001 (6)
C11	0.010 (7)	0.024 (7)	0.008 (8)	0.001 (5)	0.003 (6)	−0.002 (6)
C12	0.012 (7)	0.023 (7)	0.008 (7)	−0.001 (6)	0.000 (6)	−0.005 (6)
C13	0.008 (7)	0.023 (7)	0.009 (8)	−0.001 (5)	0.002 (6)	−0.001 (6)
C14	0.010 (7)	0.024 (8)	0.008 (7)	−0.001 (5)	0.003 (5)	−0.002 (5)
C15	0.011 (7)	0.022 (7)	0.010 (8)	−0.001 (5)	0.002 (6)	0.000 (6)
C16	0.010 (7)	0.023 (7)	0.007 (7)	0.001 (6)	0.005 (6)	0.001 (5)
C17	0.013 (7)	0.025 (7)	0.011 (7)	0.001 (6)	0.003 (6)	−0.001 (6)
C18	0.011 (7)	0.024 (7)	0.008 (7)	−0.001 (6)	0.004 (6)	−0.001 (6)
C19	0.012 (7)	0.023 (7)	0.008 (7)	−0.001 (6)	0.004 (6)	0.000 (6)
C20	0.010 (7)	0.022 (6)	0.008 (7)	−0.001 (6)	0.002 (6)	0.003 (6)
C21	0.011 (7)	0.024 (8)	0.009 (7)	0.001 (5)	0.004 (5)	−0.001 (5)
C22	0.013 (7)	0.024 (7)	0.013 (8)	0.001 (6)	0.002 (6)	−0.002 (6)
C23	0.012 (7)	0.024 (7)	0.012 (8)	0.001 (6)	0.003 (6)	−0.001 (6)
C24	0.015 (8)	0.025 (7)	0.013 (8)	−0.002 (6)	−0.001 (6)	0.000 (6)
C25	0.015 (7)	0.023 (7)	0.012 (8)	−0.001 (6)	0.000 (6)	0.002 (6)
C26	0.011 (7)	0.024 (7)	0.010 (7)	0.000 (5)	0.003 (6)	−0.001 (6)
C27	0.012 (7)	0.024 (7)	0.010 (7)	0.000 (6)	0.003 (6)	0.000 (5)
C28	0.012 (7)	0.024 (7)	0.010 (8)	0.000 (6)	0.003 (6)	−0.001 (6)

Geometric parameters (Å, °)

La1—O1	2.520 (10)	O16—La2^{iv}	2.551 (10)
La1—O5	2.531 (10)	O17—H17A	0.8500
La1—O8^{i}	2.658 (9)	O17—H17C	0.8500

La1—O13^{ii}	2.584 (10)	O18—H18A	0.8500
La1—O15^{i}	2.531 (9)	O18—H18C	0.8500
La1—O19	2.570 (11)	O19—H19A	0.8500
La1—O20	2.543 (10)	O19—H19B	0.8501
La1—N1	2.778 (13)	O20—H20A	0.8500
La1—N2^{i}	2.703 (12)	O20—H20B	0.8500
La2—O6	2.522 (9)	O21—H21B	0.8500
La2—O8^{iii}	2.599 (9)	O21—H21C	0.8500
La2—O10	2.498 (10)	O22—H22A	0.8500
La2—O13	2.626 (10)	O22—H22B	0.8500
La2—O16^{i}	2.551 (10)	C1—C2	1.51 (2)
La2—O17	2.613 (10)	C2—C3	1.38 (2)
La2—O18	2.505 (10)	C3—C4	1.42 (2)
La2—N3	2.681 (12)	C3—H3A	0.9300
La2—N4	2.786 (12)	C4—C5	1.37 (2)
N1—C2	1.351 (19)	C4—H4A	0.9300
N1—C7	1.357 (19)	C5—C7	1.41 (2)
N2—C14	1.335 (18)	C5—C6	1.51 (2)
N2—C12	1.403 (19)	C7—H7A	0.9300
N2—La1^{iv}	2.703 (12)	C8—C9	1.49 (2)
N3—C16	1.300 (19)	C9—C10	1.40 (2)
N3—C21	1.361 (18)	C9—C14	1.42 (2)
N4—C28	1.337 (19)	C10—C11	1.38 (2)
N4—C23	1.344 (19)	C10—H10A	0.9300
O1—C1	1.282 (17)	C11—C12	1.35 (2)
O2—C1	1.246 (18)	C11—H11A	0.9300
O3—C6	1.201 (18)	C12—C13	1.488 (19)
O4—C6	1.296 (18)	C14—H14	0.9300
O4—H4B	0.8200	C15—C16	1.545 (19)
O5—C8	1.279 (17)	C16—C17	1.40 (2)
O6—C8	1.270 (17)	C17—C18	1.39 (2)
O7—C13	1.211 (18)	C17—H17B	0.9300
O8—C13	1.290 (17)	C18—C19	1.39 (2)
O8—La2^{v}	2.599 (9)	C18—H18B	0.9300
O8—La1^{iv}	2.658 (9)	C19—C21	1.37 (2)
O9—C22	1.237 (18)	C19—C20	1.494 (19)
O10—C22	1.276 (18)	C21—H21A	0.9300
O11—C27	1.216 (18)	C22—C23	1.512 (19)
O12—C27	1.323 (18)	C23—C24	1.38 (2)
O12—H12A	0.8200	C24—C25	1.37 (2)
O13—C15	1.291 (17)	C24—H24A	0.9300
O13—La1^{vi}	2.584 (10)	C25—C26	1.40 (2)
O14—C15	1.237 (18)	C25—H25A	0.9300
O15—C20	1.317 (18)	C26—C28	1.38 (2)
O15—La1^{iv}	2.531 (9)	C26—C27	1.486 (19)
O16—C20	1.232 (18)	C28—H28A	0.9300
O1—La1—O5	71.0 (3)	C15—O13—La2	118.8 (9)

O1—La1—O15^{i}	129.4 (3)	La1^{vi}—O13—La2	112.8 (4)
O5—La1—O15^{i}	87.8 (3)	C20—O15—La1^{iv}	138.1 (8)
O1—La1—O20	136.7 (3)	C20—O16—La2^{iv}	149.6 (10)
O5—La1—O20	139.9 (3)	La2—O17—H17A	96.8
O15^{i}—La1—O20	88.4 (3)	La2—O17—H17C	92.3
O1—La1—O19	137.8 (3)	H17A—O17—H17C	106.2
O5—La1—O19	72.1 (3)	La2—O18—H18A	118.8
O15^{i}—La1—O19	68.2 (3)	La2—O18—H18C	130.6
O20—La1—O19	69.4 (4)	H18A—O18—H18C	108.8
O1—La1—O13^{ii}	79.9 (3)	La1—O19—H19A	96.2
O5—La1—O13^{ii}	84.7 (3)	La1—O19—H19B	95.5
O15^{i}—La1—O13^{ii}	145.0 (3)	H19A—O19—H19B	108.9
O20—La1—O13^{ii}	76.0 (3)	La1—O20—H20A	97.6
O19—La1—O13^{ii}	76.9 (3)	La1—O20—H20B	98.1
O1—La1—O8^{i}	66.8 (3)	H20A—O20—H20B	108.5
O5—La1—O8^{i}	132.7 (3)	H21B—O21—H21C	108.2
O15^{i}—La1—O8^{i}	136.2 (3)	H22A—O22—H22B	108.5
O20—La1—O8^{i}	70.9 (3)	O2—C1—O1	125.4 (13)
O19—La1—O8^{i}	131.8 (3)	O2—C1—C2	118.4 (13)
O13^{ii}—La1—O8^{i}	67.8 (3)	O1—C1—C2	116.2 (12)
O1—La1—N2^{i}	94.8 (3)	N1—C2—C3	123.9 (13)
O5—La1—N2^{i}	144.3 (3)	N1—C2—C1	115.4 (12)
O15^{i}—La1—N2^{i}	76.1 (3)	C3—C2—C1	120.7 (13)
O20—La1—N2^{i}	72.3 (3)	C2—C3—C4	118.9 (13)
O19—La1—N2^{i}	127.4 (3)	C2—C3—H3A	120.5
O13^{ii}—La1—N2^{i}	126.0 (3)	C4—C3—H3A	120.5
O8^{i}—La1—N2^{i}	61.0 (3)	C5—C4—C3	117.2 (14)
O1—La1—N1	60.4 (4)	C5—C4—H4A	121.4
O5—La1—N1	73.0 (3)	C3—C4—H4A	121.4
O15^{i}—La1—N1	69.6 (3)	C4—C5—C7	121.1 (14)
O20—La1—N1	141.2 (3)	C4—C5—C6	122.4 (13)
O19—La1—N1	125.3 (4)	C7—C5—C6	116.5 (13)
O13^{ii}—La1—N1	138.8 (3)	O3—C6—O4	125.5 (14)
O8^{i}—La1—N1	102.8 (3)	O3—C6—C5	121.6 (13)
N2^{i}—La1—N1	71.6 (4)	O4—C6—C5	112.8 (12)
O10—La2—O18	137.5 (3)	N1—C7—C5	121.4 (14)
O10—La2—O6	129.9 (3)	N1—C7—H7A	119.3
O18—La2—O6	88.1 (3)	C5—C7—H7A	119.3
O10—La2—O16^{i}	72.5 (3)	O6—C8—O5	125.1 (13)
O18—La2—O16^{i}	136.8 (3)	O6—C8—C9	118.3 (12)
O6—La2—O16^{i}	86.9 (3)	O5—C8—C9	116.5 (13)
O10—La2—O16^{i}	72.5 (3)	C10—C9—C14	116.1 (13)

O18—La2—O16^{i}	136.8 (3)	C10—C9—C8	122.1 (13)
O6—La2—O16^{i}	86.9 (3)	C14—C9—C8	121.8 (13)
O16^{i}—La2—O16^{i}	0.0 (4)	C11—C10—C9	120.4 (14)
O10—La2—O8^{iii}	78.5 (3)	C11—C10—H10A	119.8
O18—La2—O8^{iii}	77.1 (3)	C9—C10—H10A	119.8
O6—La2—O8^{iii}	144.6 (3)	C12—C11—C10	121.0 (14)
O16^{i}—La2—O8^{iii}	82.6 (3)	C12—C11—H11A	119.5
O16^{i}—La2—O8^{iii}	82.6 (3)	C10—C11—H11A	119.5
O10—La2—O17	136.8 (3)	C11—C12—N2	120.9 (13)
O18—La2—O17	68.5 (4)	C11—C12—C13	122.8 (14)
O6—La2—O17	68.2 (3)	N2—C12—C13	116.1 (12)
O16^{i}—La2—O17	69.8 (3)	O7—C13—O8	125.8 (13)
O16^{i}—La2—O17	69.8 (3)	O7—C13—C12	115.9 (13)
O8^{iii}—La2—O17	76.4 (3)	O8—C13—C12	118.2 (12)
O10—La2—O13	65.6 (3)	N2—C14—C9	123.3 (13)
O18—La2—O13	73.1 (3)	N2—C14—H14	118.4
O6—La2—O13	137.9 (3)	C9—C14—H14	118.4
O16^{i}—La2—O13	132.3 (3)	O14—C15—O13	125.5 (13)
O16^{i}—La2—O13	132.3 (3)	O14—C15—C16	118.2 (13)
O8^{iii}—La2—O13	68.1 (3)	O13—C15—C16	116.2 (12)
O17—La2—O13	132.3 (3)	N3—C16—C17	125.0 (14)
O10—La2—N3	94.9 (3)	N3—C16—C15	118.1 (13)
O18—La2—N3	73.6 (3)	C17—C16—C15	116.9 (13)
O6—La2—N3	76.7 (3)	C18—C17—C16	116.6 (14)
O16^{i}—La2—N3	145.4 (3)	C18—C17—H17B	121.7
O16^{i}—La2—N3	145.4 (3)	C16—C17—H17B	121.7
O8^{iii}—La2—N3	127.4 (3)	C17—C18—C19	119.0 (14)
O17—La2—N3	128.3 (3)	C17—C18—H18B	120.5
O13—La2—N3	62.0 (3)	C19—C18—H18B	120.5
O10—La2—N4	60.8 (4)	C21—C19—C18	119.6 (14)
O18—La2—N4	141.8 (3)	C21—C19—C20	122.0 (13)
O6—La2—N4	69.9 (3)	C18—C19—C20	118.2 (13)
O16^{i}—La2—N4	74.7 (3)	O16—C20—O15	120.4 (13)
O16^{i}—La2—N4	74.7 (3)	O16—C20—C19	122.9 (13)
O8^{iii}—La2—N4	137.6 (3)	O15—C20—C19	116.7 (12)
O17—La2—N4	125.5 (4)	N3—C21—C19	121.9 (13)
O13—La2—N4	102.2 (3)	N3—C21—H21A	119.0
N3—La2—N4	71.2 (4)	C19—C21—H21A	119.0
C2—N1—C7	117.4 (13)	O9—C22—O10	124.5 (14)
C2—N1—La1	116.2 (9)	O9—C22—C23	117.9 (13)
C7—N1—La1	126.4 (10)	O10—C22—C23	117.5 (12)
C14—N2—C12	118.3 (12)	N4—C23—C24	124.0 (14)
C14—N2—La1^{iv}	124.0 (9)	N4—C23—C22	115.7 (13)
C12—N2—La1^{iv}	116.8 (8)	C24—C23—C22	120.4 (13)

C16—N3—C21	117.7 (12)	C25—C24—C23	118.1 (14)
C16—N3—La2	117.2 (9)	C25—C24—H24A	120.9
C21—N3—La2	124.7 (9)	C23—C24—H24A	120.9
C28—N4—C23	116.4 (13)	C24—C25—C26	120.2 (14)
C28—N4—La2	128.1 (10)	C24—C25—H25A	119.9
C23—N4—La2	114.9 (9)	C26—C25—H25A	119.9
C1—O1—La1	125.0 (9)	C28—C26—C25	116.7 (13)
C6—O4—H4B	109.5	C28—C26—C27	119.5 (13)
C8—O5—La1	145.6 (9)	C25—C26—C27	123.7 (13)
C8—O6—La2	138.2 (8)	O11—C27—O12	125.6 (13)
C13—O8—La2^{v}	128.2 (8)	O11—C27—C26	122.0 (13)
C13—O8—La1^{iv}	119.9 (8)	O12—C27—C26	112.4 (12)
La2^{v}—O8—La1^{iv}	111.2 (3)	N4—C28—C26	124.6 (14)
C22—O10—La2	126.1 (9)	N4—C28—H28A	117.7
C27—O12—H12A	109.5	C26—C28—H28A	117.7
C15—O13—La1^{vi}	128.2 (9)		
O1—La1—N1—C2	−12.5 (9)	La1—O1—C1—O2	146.7 (12)
O5—La1—N1—C2	64.9 (10)	La1—O1—C1—C2	−31.7 (17)
O15^{i}—La1—N1—C2	159.0 (11)	C7—N1—C2—C3	0(2)
O20—La1—N1—C2	−141.6 (10)	La1—N1—C2—C3	−177.3 (12)
O19—La1—N1—C2	117.4 (10)	C7—N1—C2—C1	−178.7 (13)
O13^{ii}—La1—N1—C2	4.7 (13)	La1—N1—C2—C1	4.0 (16)
O8^{i}—La1—N1—C2	−66.2 (11)	O2—C1—C2—N1	−162.9 (14)
N2^{i}—La1—N1—C2	−119.4 (11)	O1—C1—C2—N1	15.6 (19)
O1—La1—N1—C7	170.5 (13)	O2—C1—C2—C3	18 (2)
O5—La1—N1—C7	−112.0 (12)	O1—C1—C2—C3	−163.1 (14)
O15^{i}—La1—N1—C7	−18.0 (11)	N1—C2—C3—C4	−2(2)
O20—La1—N1—C7	41.5 (14)	C1—C2—C3—C4	176.8 (13)
O19—La1—N1—C7	−59.6 (13)	C2—C3—C4—C5	1(2)
O13^{ii}—La1—N1—C7	−172.3 (10)	C3—C4—C5—C7	1(2)
O8^{i}—La1—N1—C7	116.9 (12)	C3—C4—C5—C6	179.6 (13)
N2^{i}—La1—N1—C7	63.6 (11)	C4—C5—C6—O3	170.4 (15)
O10—La2—N3—C16	−39.9 (11)	C7—C5—C6—O3	−11 (2)
O18—La2—N3—C16	98.3 (11)	C4—C5—C6—O4	−8(2)
O6—La2—N3—C16	−169.8 (11)	C7—C5—C6—O4	170.9 (14)
O16^{i}—La2—N3—C16	−105.9 (11)	C2—N1—C7—C5	2(2)
O16^{i}—La2—N3—C16	−105.9 (11)	La1—N1—C7—C5	179.4 (11)
O8^{iii}—La2—N3—C16	39.4 (12)	C4—C5—C7—N1	−3(2)
O17—La2—N3—C16	142.4 (10)	C6—C5—C7—N1	178.4 (13)
O13—La2—N3—C16	19.0 (10)	La2—O6—C8—O5	0(2)
N4—La2—N3—C16	−96.7 (11)	La2—O6—C8—C9	175.4 (9)
O10—La2—N3—C21	132.3 (10)	La1—O5—C8—O6	−104.4 (18)
O18—La2—N3—C21	−89.5 (10)	La1—O5—C8—C9	79.9 (19)
O6—La2—N3—C21	2.4 (10)	O6—C8—C9—C10	−169.6 (13)
O16^{i}—La2—N3—C21	66.3 (12)	O5—C8—C9—C10	6(2)

O16^{i}—La2—N3—C21	66.3 (12)	O6—C8—C9—C14	12 (2)
O8^{iii}—La2—N3—C21	−148.4 (9)	O5—C8—C9—C14	−172.0 (13)
O17—La2—N3—C21	−45.4 (12)	C14—C9—C10—C11	2(2)
O13—La2—N3—C21	−168.8 (11)	C8—C9—C10—C11	−176.3 (13)
N4—La2—N3—C21	75.5 (10)	C9—C10—C11—C12	0(2)
O10—La2—N4—C28	−172.5 (13)	C10—C11—C12—N2	−2(2)
O18—La2—N4—C28	−41.6 (15)	C10—C11—C12—C13	172.9 (14)
O6—La2—N4—C28	16.9 (11)	C14—N2—C12—C11	1(2)
O16^{i}—La2—N4—C28	109.2 (12)	La1^{iv}—N2—C12—C11	−169.3 (11)
O16^{i}—La2—N4—C28	109.2 (12)	C14—N2—C12—C13	−174.5 (12)
O8^{iii}—La2—N4—C28	169.3 (10)	La1^{iv}—N2—C12—C13	15.7 (15)
O17—La2—N4—C28	58.7 (13)	La2^{v}—O8—C13—O7	−16 (2)
O13—La2—N4—C28	−119.8 (12)	La1^{iv}—O8—C13—O7	153.7 (12)
N3—La2—N4—C28	−65.4 (12)	La2^{v}—O8—C13—C12	162.2 (9)
O10—La2—N4—C23	16.5 (10)	La1^{iv}—O8—C13—C12	−27.8 (16)
O18—La2—N4—C23	147.4 (9)	C11—C12—C13—O7	11 (2)
O6—La2—N4—C23	−154.0 (11)	N2—C12—C13—O7	−174.1 (13)
O16^{i}—La2—N4—C23	−61.7 (10)	C11—C12—C13—O8	−167.7 (14)
O16^{i}—La2—N4—C23	−61.7 (10)	N2—C12—C13—O8	7.3 (19)
O8^{iii}—La2—N4—C23	−1.6 (13)	C12—N2—C14—C9	2(2)
O17—La2—N4—C23	−112.3 (10)	La1^{iv}—N2—C14—C9	171.2 (10)
O13—La2—N4—C23	69.2 (11)	C10—C9—C14—N2	−4(2)
N3—La2—N4—C23	123.7 (11)	C8—C9—C14—N2	175.0 (13)
O5—La1—O1—C1	−56.9 (11)	La1^{vi}—O13—C15—O14	17 (2)
O15^{i}—La1—O1—C1	13.5 (12)	La2—O13—C15—O14	−155.8 (12)
O20—La1—O1—C1	158.6 (10)	La1^{vi}—O13—C15—C16	−158.9 (9)
O19—La1—O1—C1	−87.4 (11)	La2—O13—C15—C16	28.0 (15)
O13^{ii}—La1—O1—C1	−144.7 (11)	C21—N3—C16—C17	−5(2)
O8^{i}—La1—O1—C1	145.2 (11)	La2—N3—C16—C17	167.4 (12)
N2^{i}—La1—O1—C1	89.5 (11)	C21—N3—C16—C15	173.2 (12)
N1—La1—O1—C1	23.8 (10)	La2—N3—C16—C15	−14.0 (16)
O1—La1—O5—C8	−120.5 (16)	O14—C15—C16—N3	174.7 (14)
O15^{i}—La1—O5—C8	106.3 (16)	O13—C15—C16—N3	−8.8 (19)
O20—La1—O5—C8	21.3 (18)	O14—C15—C16—C17	−7(2)
O19—La1—O5—C8	38.4 (16)	O13—C15—C16—C17	169.9 (13)
O13^{ii}—La1—O5—C8	−39.5 (16)	N3—C16—C17—C18	4(2)
O8^{i}—La1—O5—C8	−92.5 (16)	C15—C16—C17—C18	−174.7 (13)
N2^{i}—La1—O5—C8	168.6 (15)	C16—C17—C18—C19	−1(2)
N1—La1—O5—C8	175.6 (17)	C17—C18—C19—C21	1(2)
O10—La2—O6—C8	95.6 (14)	C17—C18—C19—C20	176.4 (13)
O18—La2—O6—C8	−105.5 (13)	La2^{iv}—O16—C20—O15	110.5 (19)
O16^{i}—La2—O6—C8	31.6 (13)	La2^{iv}—O16—C20—C19	−67 (2)
O16^{i}—La2—O6—C8	31.6 (13)	La1^{iv}—O15—C20—O16	8(2)

O8^{iii}—La2—O6—C8	−41.0 (16)	La1^{iv}—O15—C20—C19	−174.1 (9)
O17—La2—O6—C8	−37.9 (13)	C21—C19—C20—O16	163.5 (14)
O13—La2—O6—C8	−167.5 (12)	C18—C19—C20—O16	−12 (2)
N3—La2—O6—C8	−179.1 (14)	C21—C19—C20—O15	−15 (2)
N4—La2—O6—C8	106.4 (14)	C18—C19—C20—O15	170.0 (13)
O18—La2—O10—C22	−156.8 (11)	C16—N3—C21—C19	4(2)
O6—La2—O10—C22	−9.0 (13)	La2—N3—C21—C19	−167.7 (10)
O16^{i}—La2—O10—C22	61.3 (11)	C18—C19—C21—N3	−2(2)
O16^{i}—La2—O10—C22	61.3 (11)	C20—C19—C21—N3	−177.7 (12)
O8^{iii}—La2—O10—C22	147.1 (12)	La2—O10—C22—O9	−158.6 (12)
O17—La2—O10—C22	91.6 (12)	La2—O10—C22—C23	22.0 (18)
O13—La2—O10—C22	−141.9 (12)	C28—N4—C23—C24	−4(2)
N3—La2—O10—C22	−85.8 (12)	La2—N4—C23—C24	168.3 (12)
N4—La2—O10—C22	−20.6 (11)	C28—N4—C23—C22	174.1 (12)
O10—La2—O13—C15	85.7 (10)	La2—N4—C23—C22	−13.8 (16)
O18—La2—O13—C15	−104.7 (9)	O9—C22—C23—N4	178.0 (14)
O6—La2—O13—C15	−37.5 (11)	O10—C22—C23—N4	−3(2)
O16^{i}—La2—O13—C15	116.3 (9)	O9—C22—C23—C24	−4(2)
O16^{i}—La2—O13—C15	116.3 (9)	O10—C22—C23—C24	175.3 (14)
O8^{iii}—La2—O13—C15	172.6 (10)	N4—C23—C24—C25	3(2)
O17—La2—O13—C15	−142.4 (9)	C22—C23—C24—C25	−175.0 (14)
N3—La2—O13—C15	−24.7 (9)	C23—C24—C25—C26	−1(2)
N4—La2—O13—C15	36.0 (10)	C24—C25—C26—C28	0(2)
O10—La2—O13—La1^{vi}	−88.4 (4)	C24—C25—C26—C27	179.6 (14)
O18—La2—O13—La1^{vi}	81.1 (4)	C28—C26—C27—O11	10 (2)
O6—La2—O13—La1^{vi}	148.4 (4)	C25—C26—C27—O11	−169.3 (15)
O16^{i}—La2—O13—La1^{vi}	−57.8 (5)	C28—C26—C27—O12	−169.6 (13)
O16^{i}—La2—O13—La1^{vi}	−57.8 (5)	C25—C26—C27—O12	11 (2)
O8^{iii}—La2—O13—La1^{vi}	−1.5 (4)	C23—N4—C28—C26	3(2)
O17—La2—O13—La1^{vi}	43.5 (6)	La2—N4—C28—C26	−167.7 (11)
N3—La2—O13—La1^{vi}	161.2 (5)	C25—C26—C28—N4	−1(2)
N4—La2—O13—La1^{vi}	−138.1 (4)	C27—C26—C28—N4	179.2 (13)

Symmetry codes: (i) *x*+1, *y*, *z*; (ii) *x*, *y*, *z*−1; (iii) *x*+1, *y*, *z*+1; (iv) *x*−1, *y*, *z*; (v) *x*−1, *y*, *z*−1; (vi) *x*, *y*, *z*+1.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O22—H22B···O21^{vii}	0.85	2.03	2.88 (2)	176
O22—H22A···O2^{viii}	0.85	1.85	2.702 (17)	177
O21—H21C···O17^{ix}	0.85	1.99	2.833 (15)	171
O21—H21B···O9^{ii}	0.85	1.77	2.612 (15)	171
O20—H20B···O11^{i}	0.85	2.09	2.759 (14)	136
O20—H20A···O8^{i}	0.85	2.47	3.020 (14)	123
O20—H20A···O10^{ii}	0.85	2.06	2.687 (14)	130

O19—H19B···O16^{i}	0.85	1.98	2.787 (15)	158
O19—H19A···O14^{ii}	0.85	1.80	2.605 (15)	157
O18—H18C···O3^{iv}	0.85	1.91	2.728 (15)	162
O18—H18A···O1^{vi}	0.85	1.89	2.706 (14)	161
O17—H17C···O16^{i}	0.85	2.49	2.955 (14)	115
O17—H17C···O5	0.85	2.12	2.791 (14)	135
O17—H17A···O7^{iii}	0.85	1.76	2.608 (14)	174
O12—H12A···O21^{iv}	0.82	1.76	2.564 (15)	166
O4—H4B···O22^{x}	0.82	1.82	2.534 (14)	145

Symmetry codes: (vii) −*x*+1, *y*+1/2, −*z*; (viii) *x*, *y*+1, *z*; (ix) −*x*+1, *y*+1/2, −*z*+1; (ii) *x*, *y*, *z*−1; (i) *x*+1, *y*, *z*; (iv) *x*−1, *y*, *z*; (vi) *x*, *y*, *z*+1; (iii) *x*+1, *y*, *z*+1; (x) *x*+1, *y*−1, *z*+1.

Fig. 1

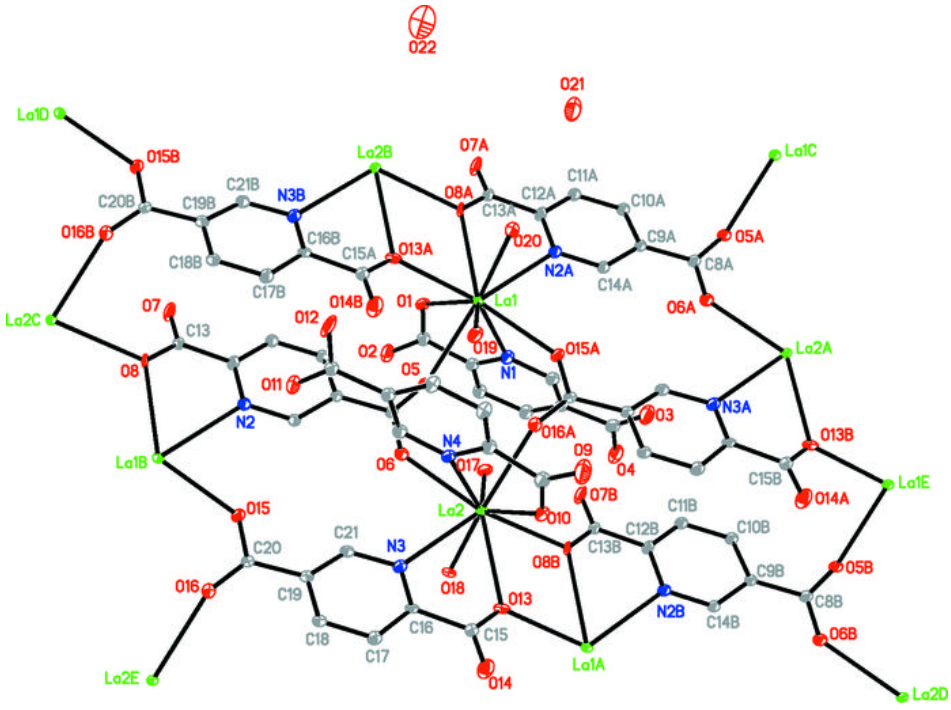

O22
O21
La1D
O15B
La2B
O7A
La1C
C20B
C19B
C21B
N3B
O8A
C12A
C11A
C10A
O16B
C16B
C13A
O20
C9A
O5A
C18B
C15A
O13A
N2A
C14A
C8A
C17B
O14B
O1
La1
O6A
La2C
O7
C13
O12
O2
O19
O15A
La2A
O8
O5
N1
O11
N2
O3
N3A
O16A
N4
O9
O13B
La1B
O6
O17
O4
C15B
La1E
O7B
O14A
O15
La2
C11B
C21
C20
N3
C12B
C10B
O10
C13B
O8B
C9B
O5B
O16
O18
C19
O13
N2B
C8B
C18
C16
C15
C14B
O6B
C17
La1A
La2E
O14
La2D

Fig. 2

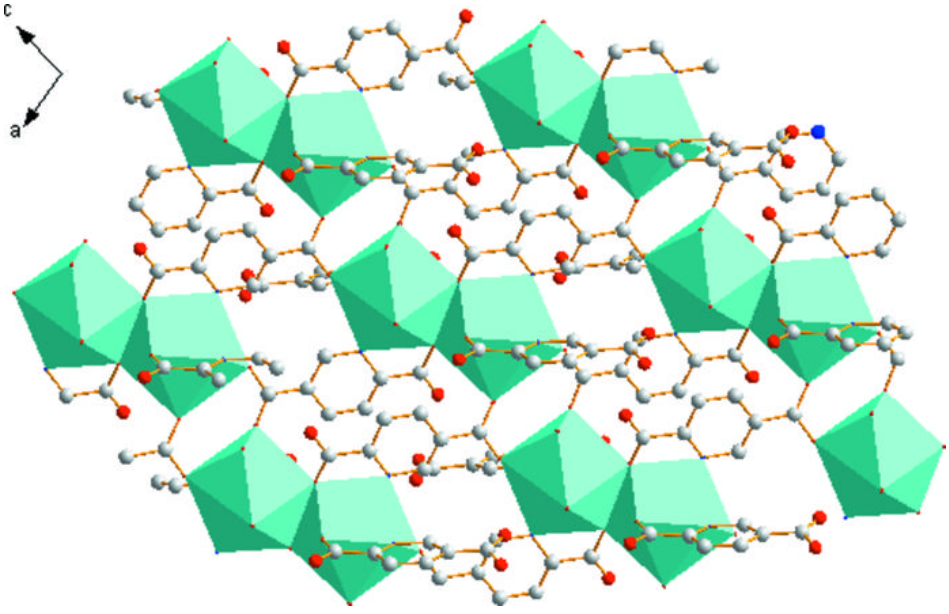


Fig. 3