Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# Poly[[triaquatri-$\mu_5$-tartrato-dilanthanum(III)] dihydrate]

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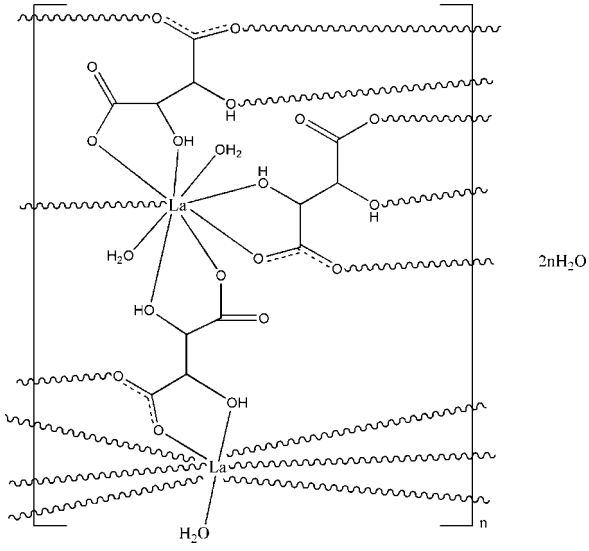
Received 18 April 2008; accepted 11 June 2008

Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.007 Å; disorder in solvent or counterion; $R$ factor = 0.026; $wR$ factor = 0.057; data-to-parameter ratio = 11.0.

In the title polymer, $\{[La_2(C_4H_4O_6)_3(H_2O)_3]\cdot 2H_2O\}_n$, two symmetry-independent $La^{III}$ ions are nine-coordinated and display a distorted monocapped square-antiprismatic geometry. One is coordinated by seven O atoms from four tartrate ligands and two water molecules, the other by eight O atoms from five tartrate ligands and one water molecule. The three tartrate ligands in the asymmetric unit act identically as $\mu_5$-ligands, which link lanthanum centres to form a three-dimensional coordination framework. An extensive network of hydrogen bonds is observed in the crystal structure, involving two uncoordinated water molecules, one of which is disordered over two positions, with occupancies of 0.550 (13) and 0.450 (13).

## Related literature

For related literature, see: Yaghi *et al.* (1998, 2003); Serre *et al.* (2004); James *et al.* (2003).




## Experimental

### Crystal data

$[La_2(C_4H_4O_6)_3(H_2O)_3]\cdot 2H_2O$
$M_r$ = 812.12
Monoclinic, $P2_1/c$
$a$ = 12.6271 (2) Å
$b$ = 12.9273 (2) Å
$c$ = 16.6556 (3) Å
$\beta$ = 127.801 (1)°
$V$ = 2148.22 (6) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 4.04 mm$^{-1}$
$T$ = 296 (2) K
0.25 × 0.21 × 0.18 mm

### Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.372, $T_{max}$ = 0.480
19115 measured reflections
3771 independent reflections
3226 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.047

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.057
$S$ = 1.05
3771 reflections
344 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.87 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.65 e Å$^{-3}$

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O3—H3$A$···O8$^{i}$ | 0.82 | 1.87 | 2.677 (4) | 169 |
| O4—H4···O18$^{ii}$ | 0.82 | 1.80 | 2.619 (4) | 174 |
| O9—H9···O16 | 0.82 | 2.46 | 3.177 (5) | 147 |
| O10—H10$A$···O8$^{iii}$ | 0.82 | 1.94 | 2.745 (4) | 167 |
| O15—H15···O2$^{i}$ | 0.82 | 1.82 | 2.632 (4) | 175 |
| O16—H16···O4$WA$ | 0.82 | 1.89 | 2.667 (9) | 158 |
| O16—H16···O4$WB$ | 0.82 | 1.94 | 2.708 (9) | 157 |

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

Data collection: *SMART* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *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*.

The author acknowledges South China Normal University for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BH2174).

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# supporting information

*Acta Cryst.* (2008). E**64**, m933 [doi:10.1107/S160053680801756X]

## Poly[[triaquatri-$\mu_5$-tartrato-dilanthanum(III)] dihydrate]

**Liu Shi-Zhu**

### S1. Comment

The use of multifunctional organic linker molecules to polymerize metal centers into open-framework materials has led to the development of a rich field of chemistry (Yaghi *et al.*, 1998, 2003; Serre *et al.*, 2004; James, 2003) owing to the potential applications of these materials in catalysis, separation, gas storage and molecular recognition. Among such novel open-framework materials, lanthanide oxalates are particularly noteworthy. The wide variety of coordination modes of the tartarate anion permits the use of metal-tartarate units as excellent building blocks to construct a great diversity of frameworks ranging from discrete oligomeric entities to one-, two- and three-dimensional networks. Recently, we obtained the title $La^{III}$ polymer, (I), and its crystal structure is reported here.

In the asymmetric unit of (I), two symmetry independent $La^{III}$ ions are nine-coordinated and display a distorted monocapped square antiprism geometry. One is coordinated by seven O atoms from four tartarate ligands and two coordinated water molecules, the other is defined by eight O atoms from five tartarate ligands and one coordinated water molecule (Fig. 1). All three unique tartarate ligands only act as one type of coordination mode, which link lanthanum centres to form a three-dimensional coordination framework (Fig. 2). The shortest La···La separations in the solid are 6.207 (2), 6.520 (3) and 6.535 (2) Å. The voids between the individual metal complex units are filled with classical hydrogen bonded (Table 1) interstitial disordered water molecules.

### S2. Experimental

A mixture of $La_2O_3$ (0.5 mmol), tartaric acid (1.5 mmol) and $H_2O$ (10 ml) in the presence of $HClO_4$ (0.385 mmol) was stirred vigorously for 20 min and then sealed in a Teflon-lined stainless-steel autoclave (20 ml, capacity). The autoclave was heated to 433 K and maintained at this temperature for 7 days, and then cooled to room temperature at 5 $K.h^{-1}$. The crystals were obtained in *ca.* 46% yield based on La.

### S3. Refinement

Lattice water molecule O4W is disordered over two sites, O4WA and O4WB, with refined occupancies of 0.450 (13) and 0.550 (13), respectively. Water H atoms were located in a difference map and refined isotropically with $U_{iso}$(H) = 1.5$U_{eq}$(O) and a regularized geometry: O—H bond lengths were restrained to 0.82 (2)/0.85 (1) Å and H···H separations were restrained to 1.35 (2) Å for coordinated and 1.39 Å for interstitial water molecules. In the final cycles, a riding model was applied for all water H atoms. All other H atoms were placed in calculated positions with a C—H distance of 0.98 Å and O—H distance of 0.82 Å, and refined using a riding model with $U_{iso}$(H) = 1.2$U_{eq}$(C) for CH groups and $U_{iso}$(H) = 1.5$U_{eq}$(O) for hydroxyl groups.

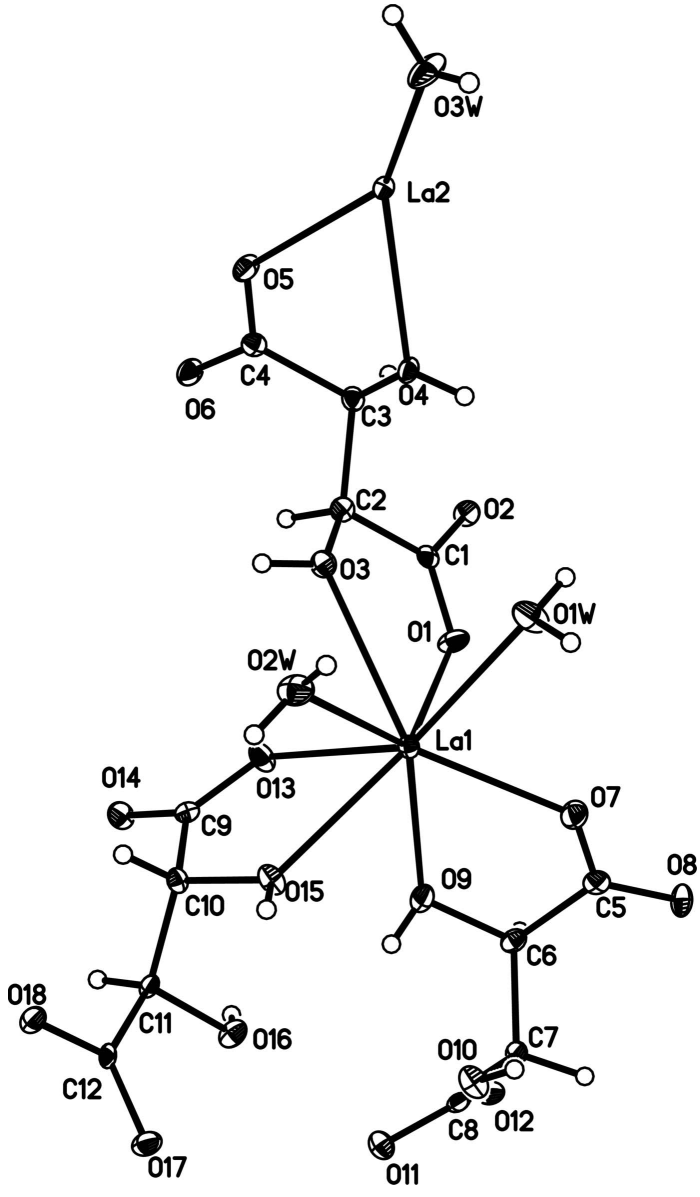


**Figure 1**

The structure of (I), showing the atomic numbering scheme. Non-H atoms are shown with 30% probability displacement ellipsoids.

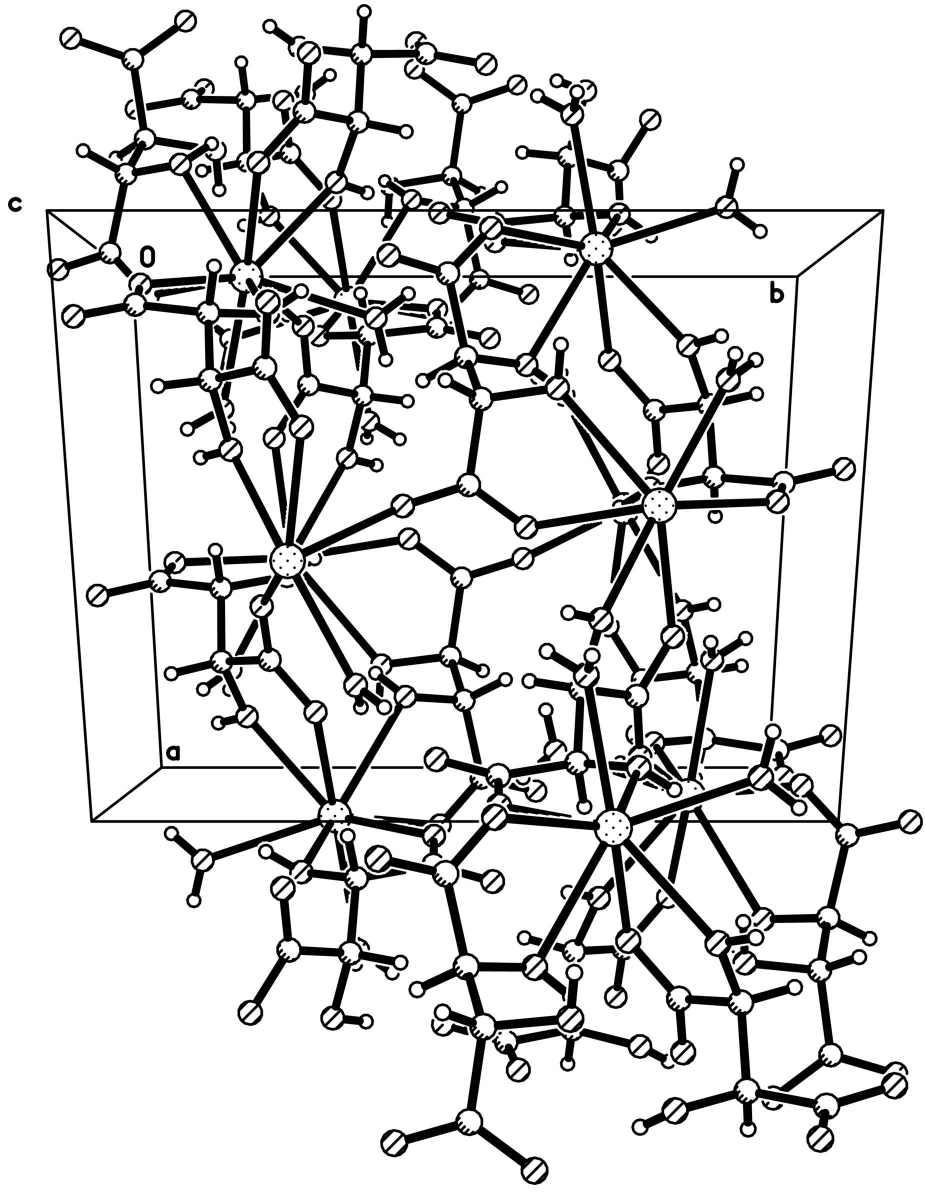


**Figure 2**

A packing view of (I), showing the inter and intramolecular hydrogen bonds.

**Poly[[triaquatri-$\mu_5$-tartrato-dilanthanum(III)] dihydrate]**

*Crystal data*

$[La_2(C_4H_4O_6)_3(H_2O)_3]\cdot 2H_2O$
$M_r = 812.12$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 12.6271\ (2)$ Å
$b = 12.9273\ (2)$ Å
$c = 16.6556\ (3)$ Å
$\beta = 127.801\ (1)°$
$V = 2148.22\ (6)$ Å$^3$
$Z = 4$
$F(000) = 1568$
$D_x = 2.511$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 15678 reflections
$\theta = 1.4$–$28.0°$
$\mu = 4.04$ mm$^{-1}$
$T = 296$ K
Block, colourless
0.25 × 0.21 × 0.18 mm

*Data collection*

Bruker APEXII area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.372, $T_{max}$ = 0.480
19115 measured reflections
3771 independent reflections
3226 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.047
$\theta_{max}$ = 25.2°, $\theta_{min}$ = 2.0°
$h$ = −15→15
$k$ = −15→14
$l$ = −19→19

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.057
$S$ = 1.05
3771 reflections
344 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0203P)^2 + 3.8165P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.87 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.65 e Å$^{-3}$

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| C1 | −0.0900 (4) | 0.9566 (4) | 0.5698 (3) | 0.0155 (10) | |
| C2 | −0.1083 (4) | 0.8523 (4) | 0.5199 (3) | 0.0177 (10) | |
| H2 | −0.0295 | 0.8416 | 0.5224 | 0.021* | |
| C3 | −0.2308 (4) | 0.8455 (4) | 0.4086 (3) | 0.0176 (10) | |
| H3 | −0.2432 | 0.9136 | 0.3782 | 0.021* | |
| C4 | −0.2140 (4) | 0.7672 (4) | 0.3482 (3) | 0.0174 (10) | |
| C5 | 0.0357 (5) | 1.0235 (4) | 0.9197 (3) | 0.0183 (10) | |
| C6 | 0.1840 (4) | 0.9984 (4) | 0.9767 (3) | 0.0184 (10) | |
| H6 | 0.2249 | 1.0587 | 0.9697 | 0.022* | |
| C7 | 0.2635 (4) | 0.9782 (3) | 1.0918 (3) | 0.0165 (10) | |
| H7 | 0.2333 | 1.0265 | 1.1193 | 0.020* | |
| C8 | 0.4144 (4) | 0.9950 (4) | 1.1463 (3) | 0.0172 (10) | |
| C9 | 0.2706 (4) | 0.7265 (4) | 0.8239 (3) | 0.0171 (10) | |
| C10 | 0.2636 (4) | 0.6536 (4) | 0.8918 (3) | 0.0152 (10) | |
| H10 | 0.2424 | 0.5841 | 0.8623 | 0.018* | |
| C11 | 0.3977 (4) | 0.6497 (3) | 0.9974 (3) | 0.0150 (10) | |
| H11 | 0.4687 | 0.6446 | 0.9899 | 0.018* | |
| C12 | 0.4096 (4) | 0.5570 (3) | 1.0589 (3) | 0.0137 (10) | |
| La1 | −0.02226 (2) | 0.81431 (2) | 0.77118 (2) | 0.01422 (8) | |
| La2 | −0.54797 (2) | 0.73846 (2) | 0.22545 (2) | 0.01381 (8) | |
| O1 | −0.0471 (3) | 0.9566 (3) | 0.6612 (2) | 0.0248 (8) | |
| O2 | −0.1144 (3) | 1.0376 (2) | 0.5208 (2) | 0.0207 (7) | |
| O3 | −0.1053 (3) | 0.7743 (2) | 0.5816 (2) | 0.0221 (7) | |
| H3A | −0.0661 | 0.7267 | 0.5776 | 0.033* | |
| O4 | −0.3519 (3) | 0.8206 (2) | 0.3936 (2) | 0.0184 (7) | |

| | | | | | |
|---|---|---|---|---|---|
| H4 | −0.3650 | 0.8645 | 0.4222 | 0.028* | |
| O5 | −0.3178 (3) | 0.7172 (2) | 0.2791 (2) | 0.0221 (8) | |
| O6 | −0.1040 (3) | 0.7609 (3) | 0.3649 (2) | 0.0232 (8) | |
| O7 | −0.0495 (3) | 0.9637 (3) | 0.8484 (2) | 0.0255 (8) | |
| O8 | 0.0074 (3) | 1.1045 (2) | 0.9438 (3) | 0.0226 (8) | |
| O9 | 0.1947 (3) | 0.9140 (3) | 0.9266 (3) | 0.0294 (8) | |
| H9 | 0.2372 | 0.8703 | 0.9710 | 0.044* | |
| O10 | 0.2457 (3) | 0.8752 (2) | 1.1112 (2) | 0.0237 (8) | |
| H10A | 0.1714 | 0.8711 | 1.0973 | 0.036* | |
| O11 | 0.4892 (3) | 0.9167 (2) | 1.1844 (2) | 0.0214 (7) | |
| O12 | 0.4517 (3) | 1.0853 (2) | 1.1460 (2) | 0.0213 (7) | |
| O13 | 0.1759 (3) | 0.7910 (3) | 0.7713 (3) | 0.0256 (8) | |
| O14 | 0.3687 (3) | 0.7181 (3) | 0.8235 (2) | 0.0235 (8) | |
| O15 | 0.1587 (3) | 0.6864 (2) | 0.8953 (2) | 0.0197 (7) | |
| H15 | 0.1438 | 0.6427 | 0.9228 | 0.030* | |
| O16 | 0.4191 (3) | 0.7419 (2) | 1.0529 (2) | 0.0212 (7) | |
| H16 | 0.4526 | 0.7832 | 1.0370 | 0.032* | |
| O17 | 0.4440 (3) | 0.5724 (2) | 1.1455 (2) | 0.0238 (8) | |
| O18 | 0.3836 (3) | 0.4696 (2) | 1.0164 (2) | 0.0194 (7) | |
| O1W | −0.2694 (3) | 0.8479 (3) | 0.6519 (3) | 0.0322 (9) | |
| H1W | −0.3029 | 0.8425 | 0.6809 | 0.048* | |
| H2W | −0.3074 | 0.8967 | 0.6129 | 0.048* | |
| O2W | −0.1015 (3) | 0.6276 (3) | 0.7134 (2) | 0.0307 (8) | |
| H4W | −0.1775 | 0.6138 | 0.6932 | 0.046* | |
| H3W | −0.0543 | 0.5815 | 0.7543 | 0.046* | |
| O3W | −0.7660 (3) | 0.6479 (3) | 0.1489 (3) | 0.0363 (10) | |
| H6W | −0.8076 | 0.6421 | 0.1715 | 0.054* | |
| H5W | −0.8025 | 0.6085 | 0.1004 | 0.054* | |
| O5W | 0.6940 (6) | 0.5141 (5) | 0.6746 (7) | 0.139 (3) | |
| H10W | 0.6504 | 0.5618 | 0.6312 | 0.208* | |
| H9W | 0.6446 | 0.4937 | 0.6900 | 0.208* | |
| O4WA | 0.4665 (13) | 0.9039 (8) | 0.9799 (8) | 0.056 (5) | 0.450 (13) |
| H4WA | 0.4304 | 0.8494 | 0.9818 | 0.084* | 0.450 (13) |
| H4WB | 0.4877 | 0.8889 | 0.9417 | 0.084* | 0.450 (13) |
| O4WB | 0.5902 (11) | 0.8436 (8) | 1.0338 (7) | 0.072 (4) | 0.550 (13) |
| H4WC | 0.5854 | 0.8295 | 0.9818 | 0.108* | 0.550 (13) |
| H4WD | 0.5400 | 0.8961 | 1.0169 | 0.108* | 0.550 (13) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.008 (2) | 0.020 (3) | 0.017 (3) | −0.0002 (18) | 0.008 (2) | 0.000 (2) |
| C2 | 0.018 (2) | 0.019 (3) | 0.019 (2) | −0.0007 (19) | 0.013 (2) | 0.001 (2) |
| C3 | 0.014 (2) | 0.018 (3) | 0.019 (3) | −0.0001 (18) | 0.010 (2) | −0.001 (2) |
| C4 | 0.018 (3) | 0.020 (3) | 0.016 (2) | −0.0001 (19) | 0.011 (2) | 0.002 (2) |
| C5 | 0.026 (3) | 0.015 (3) | 0.017 (2) | 0.000 (2) | 0.015 (2) | 0.005 (2) |
| C6 | 0.023 (2) | 0.016 (3) | 0.018 (2) | −0.0038 (19) | 0.013 (2) | −0.003 (2) |
| C7 | 0.025 (3) | 0.010 (2) | 0.019 (2) | 0.0028 (19) | 0.015 (2) | 0.003 (2) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C8 | 0.025 (3) | 0.015 (3) | 0.013 (2) | 0.000 (2) | 0.012 (2) | −0.002 (2) |
| C9 | 0.019 (3) | 0.020 (3) | 0.013 (2) | −0.0007 (19) | 0.010 (2) | −0.001 (2) |
| C10 | 0.015 (2) | 0.015 (3) | 0.020 (2) | 0.0020 (18) | 0.013 (2) | 0.0033 (19) |
| C11 | 0.020 (2) | 0.014 (2) | 0.016 (2) | 0.0004 (18) | 0.013 (2) | −0.0021 (19) |
| C12 | 0.010 (2) | 0.016 (3) | 0.018 (2) | 0.0019 (18) | 0.0102 (19) | −0.002 (2) |
| La1 | 0.01520 (14) | 0.01340 (16) | 0.01582 (14) | 0.00137 (10) | 0.01041 (12) | 0.00210 (11) |
| La2 | 0.01507 (14) | 0.01329 (15) | 0.01485 (14) | −0.00060 (10) | 0.01008 (12) | −0.00145 (11) |
| O1 | 0.035 (2) | 0.024 (2) | 0.0153 (18) | −0.0022 (15) | 0.0153 (16) | −0.0006 (15) |
| O2 | 0.0321 (19) | 0.0115 (18) | 0.0204 (18) | 0.0018 (14) | 0.0170 (16) | 0.0048 (14) |
| O3 | 0.0296 (19) | 0.0142 (18) | 0.0211 (18) | 0.0049 (14) | 0.0148 (16) | 0.0042 (14) |
| O4 | 0.0148 (16) | 0.0217 (19) | 0.0211 (18) | −0.0020 (13) | 0.0123 (14) | −0.0078 (14) |
| O5 | 0.0188 (18) | 0.027 (2) | 0.0230 (18) | −0.0058 (14) | 0.0140 (15) | −0.0108 (15) |
| O6 | 0.0202 (18) | 0.031 (2) | 0.0234 (19) | −0.0026 (14) | 0.0158 (15) | −0.0061 (15) |
| O7 | 0.0218 (18) | 0.025 (2) | 0.0244 (19) | −0.0017 (14) | 0.0116 (16) | −0.0084 (16) |
| O8 | 0.0267 (18) | 0.0119 (18) | 0.034 (2) | −0.0001 (14) | 0.0208 (16) | −0.0045 (15) |
| O9 | 0.0268 (19) | 0.033 (2) | 0.0237 (19) | 0.0059 (15) | 0.0129 (16) | −0.0087 (16) |
| O10 | 0.0199 (17) | 0.0202 (19) | 0.033 (2) | 0.0000 (14) | 0.0170 (16) | 0.0073 (16) |
| O11 | 0.0196 (17) | 0.0160 (18) | 0.0259 (18) | −0.0002 (14) | 0.0126 (15) | 0.0017 (15) |
| O12 | 0.0273 (18) | 0.0150 (19) | 0.0174 (17) | −0.0051 (14) | 0.0115 (15) | −0.0027 (14) |
| O13 | 0.0247 (19) | 0.031 (2) | 0.028 (2) | 0.0126 (15) | 0.0197 (16) | 0.0147 (16) |
| O14 | 0.0207 (18) | 0.033 (2) | 0.0245 (19) | 0.0064 (15) | 0.0181 (16) | 0.0072 (16) |
| O15 | 0.0174 (17) | 0.0201 (19) | 0.0271 (19) | 0.0030 (13) | 0.0164 (15) | 0.0106 (15) |
| O16 | 0.0309 (19) | 0.0135 (18) | 0.0235 (18) | −0.0071 (14) | 0.0189 (16) | −0.0049 (14) |
| O17 | 0.037 (2) | 0.0175 (19) | 0.0171 (18) | 0.0001 (15) | 0.0166 (16) | 0.0003 (15) |
| O18 | 0.0267 (18) | 0.0165 (19) | 0.0195 (17) | −0.0007 (14) | 0.0164 (15) | −0.0011 (14) |
| O1W | 0.0219 (19) | 0.051 (2) | 0.028 (2) | 0.0068 (16) | 0.0173 (16) | 0.0164 (18) |
| O2W | 0.035 (2) | 0.022 (2) | 0.0256 (19) | −0.0047 (16) | 0.0143 (17) | −0.0026 (16) |
| O3W | 0.027 (2) | 0.052 (3) | 0.039 (2) | −0.0224 (17) | 0.0246 (18) | −0.0308 (19) |
| O5W | 0.117 (5) | 0.100 (5) | 0.255 (10) | 0.012 (4) | 0.142 (6) | 0.041 (6) |
| O4WA | 0.103 (11) | 0.045 (7) | 0.053 (7) | −0.036 (7) | 0.064 (8) | −0.019 (5) |
| O4WB | 0.090 (9) | 0.075 (8) | 0.056 (6) | −0.033 (7) | 0.047 (6) | 0.005 (5) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—O2 | 1.245 (5) | La1—O2W | 2.563 (3) |
| C1—O1 | 1.266 (5) | La1—O9 | 2.679 (3) |
| C1—C2 | 1.525 (6) | La1—O3 | 2.698 (3) |
| C2—O3 | 1.424 (5) | La2—O5 | 2.478 (3) |
| C2—C3 | 1.524 (6) | La2—O14$^{ii}$ | 2.488 (3) |
| C2—H2 | 0.9800 | La2—O17$^{iii}$ | 2.496 (3) |
| C3—O4 | 1.427 (5) | La2—O3W | 2.505 (3) |
| C3—C4 | 1.531 (6) | La2—O11$^{iii}$ | 2.529 (3) |
| C3—H3 | 0.9800 | La2—O4 | 2.569 (3) |
| C4—O6 | 1.241 (5) | La2—O12$^{iv}$ | 2.606 (3) |
| C4—O5 | 1.269 (5) | La2—O16$^{iii}$ | 2.641 (3) |
| C5—O8 | 1.249 (5) | La2—O10$^{iii}$ | 2.730 (3) |
| C5—O7 | 1.265 (5) | O3—H3A | 0.8187 |
| C5—C6 | 1.527 (6) | O4—H4 | 0.8211 |

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| C6—O9 | 1.430 (5) | O6—La1$^{v}$ | 2.534 (3) |
| C6—C7 | 1.547 (6) | O9—H9 | 0.8167 |
| C6—H6 | 0.9800 | O10—La2$^{vi}$ | 2.730 (3) |
| C7—O10 | 1.420 (5) | O10—H10A | 0.8180 |
| C7—C8 | 1.543 (6) | O11—La2$^{vi}$ | 2.529 (3) |
| C7—H7 | 0.9800 | O12—La2$^{vii}$ | 2.606 (3) |
| C8—O11 | 1.258 (5) | O14—La2$^{viii}$ | 2.488 (3) |
| C8—O12 | 1.260 (5) | O15—H15 | 0.8188 |
| C9—O14 | 1.249 (5) | O16—La2$^{vi}$ | 2.641 (3) |
| C9—O13 | 1.268 (5) | O16—H16 | 0.8184 |
| C9—C10 | 1.516 (6) | O17—La2$^{vi}$ | 2.496 (3) |
| C10—O15 | 1.426 (5) | O1W—H1W | 0.8167 |
| C10—C11 | 1.520 (6) | O1W—H2W | 0.8174 |
| C10—H10 | 0.9800 | O2W—H4W | 0.8180 |
| C11—O16 | 1.429 (5) | O2W—H3W | 0.8220 |
| C11—C12 | 1.523 (6) | O3W—H6W | 0.8155 |
| C11—H11 | 0.9800 | O3W—H5W | 0.8177 |
| C12—O17 | 1.241 (5) | O5W—H10W | 0.8468 |
| C12—O18 | 1.265 (5) | O5W—H9W | 0.8478 |
| La1—O7 | 2.458 (3) | O4WA—H4WA | 0.8498 |
| La1—O1 | 2.476 (3) | O4WA—H4WB | 0.8499 |
| La1—O1W | 2.505 (3) | O4WA—H4WD | 0.7409 |
| La1—O13 | 2.519 (3) | O4WB—H4WC | 0.8505 |
| La1—O6$^{i}$ | 2.534 (3) | O4WB—H4WD | 0.8503 |
| La1—O15 | 2.537 (3) | | |

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| O2—C1—O1 | 122.7 (4) | O1—La1—O3 | 59.64 (10) |
| O2—C1—C2 | 119.5 (4) | O1W—La1—O3 | 72.73 (10) |
| O1—C1—C2 | 117.8 (4) | O13—La1—O3 | 69.61 (10) |
| O3—C2—C3 | 113.3 (4) | O6$^{i}$—La1—O3 | 129.38 (10) |
| O3—C2—C1 | 107.7 (4) | O15—La1—O3 | 109.80 (10) |
| C3—C2—C1 | 114.6 (4) | O2W—La1—O3 | 66.30 (10) |
| O3—C2—H2 | 106.9 | O9—La1—O3 | 131.08 (10) |
| C3—C2—H2 | 106.9 | O5—La2—O14$^{ii}$ | 131.51 (10) |
| C1—C2—H2 | 106.9 | O5—La2—O17$^{iii}$ | 75.65 (10) |
| O4—C3—C2 | 113.9 (4) | O14$^{ii}$—La2—O17$^{iii}$ | 130.47 (10) |
| O4—C3—C4 | 107.5 (4) | O5—La2—O3W | 144.32 (11) |
| C2—C3—C4 | 113.1 (4) | O14$^{ii}$—La2—O3W | 70.40 (10) |
| O4—C3—H3 | 107.3 | O17$^{iii}$—La2—O3W | 69.74 (11) |
| C2—C3—H3 | 107.3 | O5—La2—O11$^{iii}$ | 80.05 (10) |
| C4—C3—H3 | 107.3 | O14$^{ii}$—La2—O11$^{iii}$ | 101.25 (11) |
| O6—C4—O5 | 124.2 (4) | O17$^{iii}$—La2—O11$^{iii}$ | 126.38 (10) |
| O6—C4—C3 | 118.9 (4) | O3W—La2—O11$^{iii}$ | 128.09 (11) |
| O5—C4—C3 | 116.8 (4) | O5—La2—O4 | 61.24 (9) |
| O8—C5—O7 | 124.6 (4) | O14$^{ii}$—La2—O4 | 72.79 (10) |
| O8—C5—C6 | 117.5 (4) | O17$^{iii}$—La2—O4 | 129.34 (10) |
| O7—C5—C6 | 117.8 (4) | O3W—La2—O4 | 140.56 (10) |
| O9—C6—C5 | 108.5 (4) | O11$^{iii}$—La2—O4 | 72.77 (10) |

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| O9—C6—C7 | 111.8 (4) | O5—La2—O12$^{iv}$ | 76.47 (10) |
| C5—C6—C7 | 115.0 (4) | O14$^{ii}$—La2—O12$^{iv}$ | 78.72 (10) |
| O9—C6—H6 | 107.0 | O17$^{iii}$—La2—O12$^{iv}$ | 68.33 (10) |
| C5—C6—H6 | 107.0 | O3W—La2—O12$^{iv}$ | 82.92 (11) |
| C7—C6—H6 | 107.0 | O11$^{iii}$—La2—O12$^{iv}$ | 147.59 (10) |
| O10—C7—C8 | 108.0 (3) | O4—La2—O12$^{iv}$ | 76.44 (10) |
| O10—C7—C6 | 111.6 (4) | O5—La2—O16$^{iii}$ | 76.20 (10) |
| C8—C7—C6 | 109.6 (3) | O14$^{ii}$—La2—O16$^{iii}$ | 149.60 (10) |
| O10—C7—H7 | 109.2 | O17$^{iii}$—La2—O16$^{iii}$ | 60.38 (10) |
| C8—C7—H7 | 109.2 | O3W—La2—O16$^{iii}$ | 93.63 (10) |
| C6—C7—H7 | 109.2 | O11$^{iii}$—La2—O16$^{iii}$ | 67.75 (10) |
| O11—C8—O12 | 125.4 (4) | O4—La2—O16$^{iii}$ | 125.67 (9) |
| O11—C8—C7 | 117.3 (4) | O12$^{iv}$—La2—O16$^{iii}$ | 126.16 (9) |
| O12—C8—C7 | 117.2 (4) | O5—La2—O10$^{iii}$ | 136.93 (10) |
| O14—C9—O13 | 124.9 (4) | O14$^{ii}$—La2—O10$^{iii}$ | 72.81 (10) |
| O14—C9—C10 | 117.5 (4) | O17$^{iii}$—La2—O10$^{iii}$ | 118.40 (10) |
| O13—C9—C10 | 117.6 (4) | O3W—La2—O10$^{iii}$ | 70.51 (11) |
| O15—C10—C9 | 109.0 (3) | O11$^{iii}$—La2—O10$^{iii}$ | 58.50 (9) |
| O15—C10—C11 | 111.5 (4) | O4—La2—O10$^{iii}$ | 111.26 (10) |
| C9—C10—C11 | 110.6 (4) | O12$^{iv}$—La2—O10$^{iii}$ | 146.07 (9) |
| O15—C10—H10 | 108.6 | O16$^{iii}$—La2—O10$^{iii}$ | 77.54 (10) |
| C9—C10—H10 | 108.6 | C1—O1—La1 | 131.0 (3) |
| C11—C10—H10 | 108.6 | C2—O3—La1 | 121.9 (3) |
| O16—C11—C10 | 110.8 (4) | C2—O3—H3A | 103.0 |
| O16—C11—C12 | 108.7 (3) | La1—O3—H3A | 114.7 |
| C10—C11—C12 | 112.6 (4) | C3—O4—La2 | 119.8 (2) |
| O16—C11—H11 | 108.2 | C3—O4—H4 | 108.6 |
| C10—C11—H11 | 108.2 | La2—O4—H4 | 121.1 |
| C12—C11—H11 | 108.2 | C4—O5—La2 | 127.0 (3) |
| O17—C12—O18 | 125.4 (4) | C4—O6—La1$^{v}$ | 135.2 (3) |
| O17—C12—C11 | 118.4 (4) | C5—O7—La1 | 131.3 (3) |
| O18—C12—C11 | 116.2 (4) | C6—O9—La1 | 121.6 (2) |
| O7—La1—O1 | 78.94 (11) | C6—O9—H9 | 104.2 |
| O7—La1—O1W | 76.88 (11) | La1—O9—H9 | 104.9 |
| O1—La1—O1W | 75.70 (11) | C7—O10—La2$^{vi}$ | 123.3 (2) |
| O7—La1—O13 | 123.42 (11) | C7—O10—H10A | 108.1 |
| O1—La1—O13 | 76.42 (10) | La2$^{vi}$—O10—H10A | 126.4 |
| O1W—La1—O13 | 140.85 (11) | C8—O11—La2$^{vi}$ | 131.4 (3) |
| O7—La1—O6$^{i}$ | 74.88 (11) | C8—O12—La2$^{vii}$ | 133.4 (3) |
| O1—La1—O6$^{i}$ | 145.67 (10) | C9—O13—La1 | 126.5 (3) |
| O1W—La1—O6$^{i}$ | 77.03 (10) | C9—O14—La2$^{viii}$ | 143.6 (3) |
| O13—La1—O6$^{i}$ | 137.11 (10) | C10—O15—La1 | 123.8 (2) |
| O7—La1—O15 | 115.51 (10) | C10—O15—H15 | 110.8 |
| O1—La1—O15 | 136.82 (10) | La1—O15—H15 | 120.3 |
| O1W—La1—O15 | 145.22 (10) | C11—O16—La2$^{vi}$ | 122.1 (2) |
| O13—La1—O15 | 61.51 (10) | C11—O16—H16 | 105.4 |
| O6$^{i}$—La1—O15 | 75.61 (10) | La2$^{vi}$—O16—H16 | 126.4 |
| O7—La1—O2W | 142.04 (11) | C12—O17—La2$^{vi}$ | 128.9 (3) |

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| O1—La1—O2W | 125.34 (11) | La1—O1W—H1W | 111.2 |
| O1W—La1—O2W | 81.70 (12) | La1—O1W—H2W | 127.1 |
| O13—La1—O2W | 92.68 (11) | H1W—O1W—H2W | 105.8 |
| O6$^{i}$—La1—O2W | 69.95 (11) | La1—O2W—H4W | 116.7 |
| O15—La1—O2W | 69.01 (10) | La1—O2W—H3W | 117.0 |
| O7—La1—O9 | 60.31 (10) | H4W—O2W—H3W | 104.7 |
| O1—La1—O9 | 87.05 (11) | La2—O3W—H6W | 128.7 |
| O1W—La1—O9 | 136.24 (11) | La2—O3W—H5W | 124.9 |
| O13—La1—O9 | 68.26 (11) | H6W—O3W—H5W | 105.5 |
| O6$^{i}$—La1—O9 | 98.66 (11) | H10W—O5W—H9W | 105.7 |
| O15—La1—O9 | 69.45 (10) | H4WA—O4WA—H4WB | 105.2 |
| O2W—La1—O9 | 138.45 (11) | H4WA—O4WA—H4WD | 106.4 |
| O7—La1—O3 | 133.15 (10) | H4WC—O4WB—H4WD | 105.1 |

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

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O3—H3*A*···O8$^{iv}$ | 0.82 | 1.87 | 2.677 (4) | 169 |
| O4—H4···O18$^{vii}$ | 0.82 | 1.80 | 2.619 (4) | 174 |
| O9—H9···O16 | 0.82 | 2.46 | 3.177 (5) | 147 |
| O10—H10*A*···O8$^{ix}$ | 0.82 | 1.94 | 2.745 (4) | 167 |
| O15—H15···O2$^{iv}$ | 0.82 | 1.82 | 2.632 (4) | 175 |
| O16—H16···O4*WA* | 0.82 | 1.89 | 2.667 (9) | 158 |
| O16—H16···O4*WB* | 0.82 | 1.94 | 2.708 (9) | 157 |

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