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

# *catena*-Poly[[aqua(4-ethylbenzoic acid-*κO*)lanthanum(III)]-tri-*μ*-4-ethylbenzoato]

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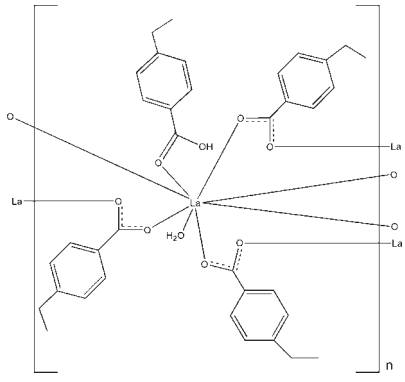
Received 1 January 2010; accepted 15 January 2010

Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.006 Å; disorder in main residue; $R$ factor = 0.038; $wR$ factor = 0.077; data-to-parameter ratio = 18.1.

The reaction of lanthanum nitrate and 4-ethylbenzoic acid (EBAH) in aqueous solution yielded the title polymer, $[La(C_9H_9O_2)_3(C_9H_{10}O_2)(H_2O)]_n$. The asymmetric unit contains one $La^{III}$ atom, three 4-ethylbenzoate (EBA) ligands, one neutral EBAH ligand and one coordinated water molecule. Each $La^{III}$ ion is eight-coordinated by six O atoms from six bridging-bidentate EBA ligands, one O atom from a monodentate EBAH ligand and one water O atom in a distorted bicapped trigonal-prismatic geometry. The adjacent $La^{III}$ ions are linked by the carboxylate groups of EBA ligands in a bridging-bidetate coordination mode, resulting in an infinite chain structure along the $c$ axis. O—H···O hydrogen-bonding interactions involving the water molecules, carboxylate groups and carboxyl H atoms are formed within the one-dimensional polymer. One of the ethyl groups is disordered over two positions with occupancies of 0.717 (7) and 0.283 (7).

## Related literature

For information on lanthanum complexes, see: Ishii *et al.* (2002); Kim *et al.* (2001); Luneau & Rey (2005); Wang *et al.* (2006); Yu *et al.* (2003).




## Experimental

### *Crystal data*

$[La(C_9H_9O_2)_3(C_9H_{10}O_2)(H_2O)]$
$M_r$ = 754.58
Triclinic, $P\overline{1}$
$a$ = 9.5319 (3) Å
$b$ = 14.0378 (5) Å
$c$ = 14.9847 (5) Å
$\alpha$ = 65.024 (2)°
$\beta$ = 74.942 (2)°
$\gamma$ = 74.734 (2)°
$V$ = 1727.91 (10) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 1.29 mm$^{-1}$
$T$ = 296 K
0.35 × 0.32 × 0.23 mm

### *Data collection*

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
$T_{min}$ = 0.643, $T_{max}$ = 0.744
22559 measured reflections
7733 independent reflections
6206 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.050

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.077
$S$ = 1.01
7733 reflections
427 parameters
14 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.63 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.73 e Å$^{-3}$

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| La1—O7$^{i}$ | 2.446 (2) | La1—O8 | 2.479 (2) |
| La1—O1 | 2.451 (2) | La1—O5 | 2.581 (2) |
| La1—O2$^{ii}$ | 2.457 (2) | La1—O9 | 2.624 (2) |
| La1—O6$^{i}$ | 2.466 (2) | La1—O3 | 2.672 (2) |

Symmetry codes: (i) $-x+1, -y, -z+1$; (ii) $-x+2, -y, -z+1$.

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O4—H4$A$···O5 | 0.82 | 1.84 | 2.652 (3) | 171 |
| O9—H9$B$···O2 | 0.82 | 2.04 | 2.829 (3) | 161 |

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); 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 authors acknowledge support from the Doctoral Foundation of Henan Polytechnic University (B2008–58 648265).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GK2253).

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# supplementary materials

*Acta Cryst.* (2010). E**66**, m183-m184 [ **doi:10.1107/S160053681000190X** ]

# *catena*-Poly[[aqua(4-ethylbenzoic acid-*κO*)lanthanum(III)]-tri-$\mu$-4-ethylbenzoato]

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## Comment

Recently, the use of lanthanide salts for the synthesis of coordination polymer has attracted more and more attentions due to their high coordination numbers along with distinguished magnetic and luminescent properties (Ishii *et al.*, 2002; Luneau & Rey, 2005; Yu *et al.*, 2003). As an important family of multidentate O-donor ligands, aromatic carboxylate ligands have been extensively employed in the preparation of metal-organic complexes because of their potential properties and intriguing structural topologies (Kim *et al.*, 2001; Wang *et al.*, 2006). Herein, we report the structure of the title $La^{III}$ coordibation polymer.

The asymmetric unit of the title compound, $[La(C_9H_9O_2)_3(C_9H_{10}O_2)(H_2O)]_n$ contains one $La^{III}$ cation, three anionic EBA ligands, one neutral ligand EBAH and one water molecule, as illustrated in Fig. 1. The $La^{III}$ atom is coordinated by eight O atoms from six bridging-bidentate EBA ligands, one monodentate EBAH ligand and one water molecule. The $La^{III}$ center adopts a distorted bicapped trigonal prism geometry. The carboxylate groups of EBA ligands link the adjacent $La^{III}$ ions in bridging-bidetate coordination modeto form an infinite chain structure running along the c axis. The shortest intermetallic distance La···La is 4.2601 (4) Å, indicating a weak metal-metal interaction. The coordinating water, carboxylate O atoms of EBA ligands and carboxylic H atom of EBAH ligand are involved in O—H···O hydrogen-bonding interactions. These hydrogen bonds are all intramolecular, *i.e.* stabilize the one-dimensional chain structure of the title polymer (Table 2).

## Experimental

A mixture of $La(NO_3)_3.6H_2O$ (0.225 g, 0.52 mmol), EBAH (0.126 g, 0.84 mmol), melamine (0.026 g, 0.20 mmol) and distilled water (10 ml) was sealed in a 25 ml Teflon-lined stainless autoclave. The mixture was heated at 423 K for 7 days to give the colorless prism crystals suitable for X-ray diffraction analysis.

## Refinement

All H atoms bounded to C atoms were positioned geometrically and allowed to ride on their parent atoms, with C (phenyl)—H = 0.93 Å, C (methyl)—H = 0.96 Å, and C (methylene)—H = 0.97 Å, respectively with $U_{iso}$ (H) = 1.2 $U_{eq}$(C). The ethyl group C8—C9 was treated as disordered over two sites, with refined ccupancies 0.717 (7) and 0.283 (7). Positions of the water H atoms and the carboxylic H atom were found from a difference Fourier map and O—H distances constrained to 0.82 Å. Among 14 restraints used in the refinement are those used to restrain geometry of the disordered ethyl group and SHELXL-97 ISOR restraint imposed on the displacement ellipsoids of C27 and C9A.

**Figures**

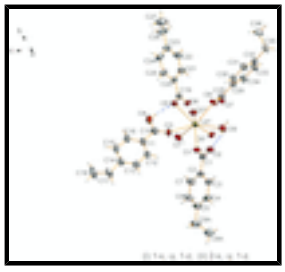


Fig. 1. The coordination environment of $La^{III}$ in the title complex with the atom-labeling scheme[symmetry codes: (i) -*x* + 1, -*y*, -*z* + 1; (ii) -*x* + 2, -*y*, -*z* + 1] Displacement ellipsoids for non-hydrogen atoms are drawn at the 30% probability level. Hydrogen bonds are shown as dashed lines.

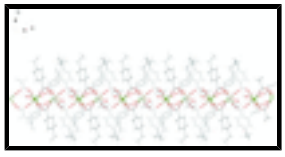


Fig. 2. The one-dimensional chain structure of the title compound.

**_catena_-Poly[[aqua(4-ethylbenzoic acid-κ*O*)lanthanum(III)]-tri-μ-4-ethylbenzoato]**

*Crystal data*

| | |
|---|---|
| $[La(C_9H_9O_2)_3(C_9H_{10}O_2)(H_2O)]$ | $Z = 2$ |
| $M_r = 754.58$ | $F(000) = 768$ |
| Triclinic, $P\overline{1}$ | $D_x = 1.450$ Mg m$^{-3}$ |
| Hall symbol: -P 1 | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| $a = 9.5319$ (3) Å | Cell parameters from 4271 reflections |
| $b = 14.0378$ (5) Å | $\theta = 1.6$–$27.4°$ |
| $c = 14.9847$ (5) Å | $\mu = 1.29$ mm$^{-1}$ |
| $\alpha = 65.024$ (2)° | $T = 296$ K |
| $\beta = 74.942$ (2)° | Prism, colorless |
| $\gamma = 74.734$ (2)° | 0.35 × 0.32 × 0.23 mm |
| $V = 1727.91$ (10) Å$^3$ | |

*Data collection*

| | |
|---|---|
| Bruker APEXII CCD diffractometer | 7733 independent reflections |
| Radiation source: fine-focus sealed tube | 6206 reflections with $I > 2\sigma(I)$ |
| graphite | $R_{int} = 0.050$ |
| φ and ω scans | $\theta_{max} = 27.4°$, $\theta_{min} = 1.6°$ |
| Absorption correction: multi-scan (SADABS; Bruker, 2007) | $h = -12 \rightarrow 12$ |
| $T_{min} = 0.643$, $T_{max} = 0.744$ | $k = -17 \rightarrow 18$ |
| 22559 measured reflections | $l = -19 \rightarrow 19$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |

| | |
|---|---|
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.038$ | H-atom parameters constrained |
| $wR(F^2) = 0.077$ | $w = 1/[\sigma^2(F_o^2) + (0.028P)^2 + 0.4P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.01$ | $(\Delta/\sigma)_{max} = 0.001$ |
| 7733 reflections | $\Delta\rho_{max} = 0.63$ e Å$^{-3}$ |
| 427 parameters | $\Delta\rho_{min} = -0.73$ e Å$^{-3}$ |
| 14 restraints | Extinction correction: SHELXL97 (Sheldrick, 2008) |
| Primary atom site location: structure-invariant direct methods | Extinction coefficient: none |

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| La1 | 0.70393 (2) | 0.005772 (14) | 0.529430 (14) | 0.03202 (7) | |
| O1 | 0.8939 (2) | −0.14429 (17) | 0.60351 (17) | 0.0452 (6) | |
| O2 | 1.1201 (2) | −0.12633 (17) | 0.51839 (17) | 0.0425 (6) | |
| O3 | 0.7662 (3) | 0.01235 (19) | 0.69039 (17) | 0.0476 (6) | |
| O4 | 0.5733 (3) | 0.1064 (2) | 0.7549 (2) | 0.0716 (9) | |
| H4A | 0.5546 | 0.1300 | 0.6982 | 0.086* | |
| O5 | 0.5373 (2) | 0.16617 (17) | 0.56793 (17) | 0.0438 (6) | |
| O6 | 0.3932 (3) | 0.11669 (17) | 0.50875 (17) | 0.0451 (6) | |
| O7 | 0.4662 (3) | 0.08426 (18) | 0.32269 (17) | 0.0480 (6) | |
| O8 | 0.6584 (3) | 0.11814 (19) | 0.35678 (17) | 0.0483 (6) | |
| O9 | 0.9081 (3) | −0.0388 (2) | 0.39017 (18) | 0.0582 (7) | |
| H9A | 0.9185 | 0.0072 | 0.3337 | 0.087* | |
| H9B | 0.9818 | −0.0684 | 0.4164 | 0.087* | |
| C1 | 1.0302 (4) | −0.1780 (2) | 0.5892 (2) | 0.0369 (8) | |
| C2 | 1.0876 (4) | −0.2861 (2) | 0.6599 (2) | 0.0382 (8) | |
| C3 | 1.2323 (4) | −0.3347 (3) | 0.6403 (3) | 0.0510 (10) | |
| H3 | 1.2948 | −0.2994 | 0.5832 | 0.061* | |
| C4 | 1.2843 (5) | −0.4349 (3) | 0.7050 (3) | 0.0686 (12) | |
| H4 | 1.3809 | −0.4675 | 0.6900 | 0.082* | |
| C5 | 1.1953 (6) | −0.4879 (3) | 0.7917 (3) | 0.0717 (13) | |
| C6 | 1.0516 (5) | −0.4374 (3) | 0.8123 (3) | 0.0695 (13) | |
| H6 | 0.9906 | −0.4712 | 0.8711 | 0.083* | |
| C7 | 0.9980 (4) | −0.3380 (3) | 0.7470 (3) | 0.0545 (10) | |
| H7 | 0.9011 | −0.3058 | 0.7615 | 0.065* | |
| C8A | 1.243 (2) | −0.6017 (18) | 0.8639 (16) | 0.110 (7) | 0.717 (7) |
| H8A | 1.2931 | −0.5979 | 0.9108 | 0.131* | 0.717 (7) |
| H8B | 1.1553 | −0.6318 | 0.9019 | 0.131* | 0.717 (7) |
| C9A | 1.3372 (10) | −0.6726 (6) | 0.8198 (6) | 0.119 (3) | 0.717 (7) |
| H9C | 1.3514 | −0.7432 | 0.8701 | 0.178* | 0.717 (7) |
| H9D | 1.4307 | −0.6496 | 0.7902 | 0.178* | 0.717 (7) |
| H9E | 1.2930 | −0.6729 | 0.7693 | 0.178* | 0.717 (7) |
| C8B | 1.271 (7) | −0.592 (5) | 0.863 (4) | 0.110 (7) | 0.283 (7) |
| H8C | 1.2841 | −0.6473 | 0.8382 | 0.131* | 0.283 (7) |

| | | | | | |
|---|---|---|---|---|---|
| H8D | 1.3690 | −0.5825 | 0.8627 | 0.131* | 0.283 (7) |
| C9B | 1.199 (3) | −0.6280 (15) | 0.9635 (18) | 0.119 (3) | 0.283 (7) |
| H9F | 1.2268 | −0.7040 | 0.9943 | 0.178* | 0.283 (7) |
| H9G | 1.0938 | −0.6101 | 0.9652 | 0.178* | 0.283 (7) |
| H9H | 1.2256 | −0.5945 | 0.9993 | 0.178* | 0.283 (7) |
| C10 | 0.6986 (4) | 0.0379 (3) | 0.7597 (3) | 0.0446 (8) | |
| C11 | 0.7491 (4) | −0.0046 (3) | 0.8568 (3) | 0.0461 (9) | |
| C12 | 0.8705 (5) | −0.0842 (3) | 0.8747 (3) | 0.0613 (11) | |
| H12 | 0.9191 | −0.1116 | 0.8259 | 0.074* | |
| C13 | 0.9214 (5) | −0.1240 (3) | 0.9641 (3) | 0.0703 (13) | |
| H13 | 1.0038 | −0.1779 | 0.9743 | 0.084* | |
| C14 | 0.8540 (5) | −0.0862 (3) | 1.0379 (3) | 0.0637 (11) | |
| C15 | 0.7330 (5) | −0.0069 (4) | 1.0200 (3) | 0.0802 (15) | |
| H15 | 0.6844 | 0.0199 | 1.0691 | 0.096* | |
| C16 | 0.6812 (5) | 0.0343 (4) | 0.9305 (3) | 0.0711 (13) | |
| H16 | 0.5995 | 0.0888 | 0.9202 | 0.085* | |
| C17 | 0.9168 (6) | −0.1315 (4) | 1.1346 (3) | 0.0830 (15) | |
| H17A | 0.9530 | −0.2072 | 1.1509 | 0.100* | |
| H17B | 1.0009 | −0.0983 | 1.1223 | 0.100* | |
| C18 | 0.8160 (7) | −0.1179 (5) | 1.2215 (4) | 0.124 (2) | |
| H18A | 0.7852 | −0.0431 | 1.2089 | 0.186* | |
| H18B | 0.8651 | −0.1520 | 1.2785 | 0.186* | |
| H18C | 0.7312 | −0.1494 | 1.2344 | 0.186* | |
| C19 | 0.4269 (3) | 0.1873 (2) | 0.5257 (2) | 0.0353 (7) | |
| C20 | 0.3432 (3) | 0.2980 (2) | 0.4932 (2) | 0.0368 (8) | |
| C21 | 0.2418 (4) | 0.3307 (3) | 0.4299 (3) | 0.0502 (9) | |
| H21 | 0.2218 | 0.2815 | 0.4105 | 0.060* | |
| C22 | 0.1699 (5) | 0.4353 (3) | 0.3953 (3) | 0.0617 (11) | |
| H22 | 0.1025 | 0.4553 | 0.3527 | 0.074* | |
| C23 | 0.1952 (5) | 0.5096 (3) | 0.4220 (3) | 0.0616 (11) | |
| C24 | 0.2970 (5) | 0.4781 (3) | 0.4853 (4) | 0.0733 (14) | |
| H24 | 0.3158 | 0.5278 | 0.5045 | 0.088* | |
| C25 | 0.3715 (5) | 0.3726 (3) | 0.5205 (3) | 0.0603 (11) | |
| H25 | 0.4399 | 0.3528 | 0.5623 | 0.072* | |
| C26 | 0.1122 (6) | 0.6239 (3) | 0.3830 (4) | 0.0977 (18) | |
| H26A | 0.0694 | 0.6333 | 0.3271 | 0.117* | |
| H26B | 0.0312 | 0.6329 | 0.4351 | 0.117* | |
| C27 | 0.1952 (8) | 0.7071 (4) | 0.3512 (5) | 0.133 (2) | |
| H27A | 0.1389 | 0.7739 | 0.3146 | 0.199* | |
| H27B | 0.2859 | 0.6923 | 0.3090 | 0.199* | |
| H27C | 0.2168 | 0.7111 | 0.4085 | 0.199* | |
| C28 | 0.5754 (4) | 0.1295 (2) | 0.2983 (2) | 0.0381 (8) | |
| C29 | 0.6127 (3) | 0.2007 (2) | 0.1914 (2) | 0.0367 (8) | |
| C30 | 0.7214 (4) | 0.2619 (3) | 0.1596 (3) | 0.0476 (9) | |
| H30 | 0.7741 | 0.2584 | 0.2055 | 0.057* | |
| C31 | 0.7529 (4) | 0.3279 (3) | 0.0608 (3) | 0.0527 (10) | |
| H31 | 0.8253 | 0.3694 | 0.0415 | 0.063* | |
| C32 | 0.6798 (4) | 0.3339 (3) | −0.0099 (3) | 0.0513 (10) | |
| C33 | 0.5723 (5) | 0.2719 (3) | 0.0215 (3) | 0.0579 (11) | |

| | | | | |
|---|---|---|---|---|
| H33 | 0.5222 | 0.2739 | −0.0251 | 0.069* |
| C34 | 0.5373 (4) | 0.2069 (3) | 0.1209 (3) | 0.0520 (10) |
| H34 | 0.4628 | 0.1670 | 0.1405 | 0.062* |
| C35 | 0.7126 (5) | 0.4099 (3) | −0.1179 (3) | 0.0732 (13) |
| H35A | 0.8179 | 0.4101 | −0.1368 | 0.088* |
| H35B | 0.6846 | 0.3844 | −0.1606 | 0.088* |
| C36 | 0.6326 (7) | 0.5210 (4) | −0.1346 (4) | 0.117 (2) |
| H36A | 0.5286 | 0.5209 | −0.1135 | 0.176* |
| H36B | 0.6519 | 0.5650 | −0.2043 | 0.176* |
| H36C | 0.6659 | 0.5488 | −0.0967 | 0.176* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| La1 | 0.02659 (10) | 0.03400 (11) | 0.03639 (11) | −0.00694 (7) | −0.01086 (7) | −0.01010 (8) |
| O1 | 0.0330 (13) | 0.0440 (13) | 0.0504 (15) | −0.0023 (11) | −0.0126 (11) | −0.0096 (11) |
| O2 | 0.0350 (13) | 0.0397 (12) | 0.0501 (14) | −0.0112 (10) | −0.0132 (11) | −0.0082 (11) |
| O3 | 0.0458 (14) | 0.0621 (16) | 0.0420 (14) | −0.0068 (12) | −0.0105 (12) | −0.0263 (12) |
| O4 | 0.0567 (18) | 0.100 (2) | 0.0626 (18) | 0.0178 (16) | −0.0241 (15) | −0.0452 (17) |
| O5 | 0.0373 (13) | 0.0446 (13) | 0.0541 (15) | −0.0007 (11) | −0.0208 (11) | −0.0193 (12) |
| O6 | 0.0475 (14) | 0.0380 (13) | 0.0555 (15) | −0.0107 (11) | −0.0110 (12) | −0.0201 (11) |
| O7 | 0.0421 (14) | 0.0552 (15) | 0.0432 (14) | −0.0194 (12) | −0.0068 (11) | −0.0092 (12) |
| O8 | 0.0434 (14) | 0.0552 (15) | 0.0399 (14) | −0.0118 (12) | −0.0186 (11) | −0.0033 (12) |
| O9 | 0.0387 (14) | 0.0818 (19) | 0.0522 (16) | −0.0015 (13) | −0.0134 (12) | −0.0255 (14) |
| C1 | 0.0369 (19) | 0.0352 (17) | 0.044 (2) | −0.0107 (15) | −0.0145 (16) | −0.0136 (15) |
| C2 | 0.0368 (19) | 0.0337 (17) | 0.046 (2) | −0.0073 (14) | −0.0195 (16) | −0.0090 (15) |
| C3 | 0.048 (2) | 0.044 (2) | 0.056 (2) | −0.0015 (17) | −0.0182 (19) | −0.0126 (18) |
| C4 | 0.063 (3) | 0.052 (2) | 0.079 (3) | 0.010 (2) | −0.026 (2) | −0.018 (2) |
| C5 | 0.084 (3) | 0.045 (2) | 0.073 (3) | −0.002 (2) | −0.037 (3) | −0.002 (2) |
| C6 | 0.072 (3) | 0.055 (2) | 0.062 (3) | −0.023 (2) | −0.019 (2) | 0.008 (2) |
| C7 | 0.046 (2) | 0.052 (2) | 0.060 (3) | −0.0148 (18) | −0.0183 (19) | −0.0066 (19) |
| C8A | 0.118 (10) | 0.072 (6) | 0.097 (5) | 0.014 (8) | −0.043 (7) | 0.003 (4) |
| C9A | 0.141 (6) | 0.069 (4) | 0.135 (6) | 0.008 (4) | −0.062 (5) | −0.022 (4) |
| C8B | 0.118 (10) | 0.072 (6) | 0.097 (5) | 0.014 (8) | −0.043 (7) | 0.003 (4) |
| C9B | 0.141 (6) | 0.069 (4) | 0.135 (6) | 0.008 (4) | −0.062 (5) | −0.022 (4) |
| C10 | 0.039 (2) | 0.052 (2) | 0.049 (2) | −0.0111 (17) | −0.0124 (17) | −0.0205 (18) |
| C11 | 0.041 (2) | 0.058 (2) | 0.043 (2) | −0.0056 (17) | −0.0096 (17) | −0.0236 (18) |
| C12 | 0.066 (3) | 0.067 (3) | 0.047 (2) | 0.003 (2) | −0.012 (2) | −0.026 (2) |
| C13 | 0.071 (3) | 0.074 (3) | 0.057 (3) | 0.011 (2) | −0.021 (2) | −0.024 (2) |
| C14 | 0.063 (3) | 0.077 (3) | 0.049 (2) | −0.005 (2) | −0.016 (2) | −0.022 (2) |
| C15 | 0.081 (3) | 0.109 (4) | 0.052 (3) | 0.017 (3) | −0.019 (2) | −0.048 (3) |
| C16 | 0.064 (3) | 0.088 (3) | 0.058 (3) | 0.020 (2) | −0.021 (2) | −0.038 (2) |
| C17 | 0.089 (4) | 0.104 (4) | 0.052 (3) | −0.010 (3) | −0.031 (3) | −0.019 (3) |
| C18 | 0.109 (5) | 0.202 (7) | 0.064 (4) | −0.002 (5) | −0.031 (3) | −0.058 (4) |
| C19 | 0.0304 (17) | 0.0358 (17) | 0.0388 (19) | −0.0061 (14) | −0.0045 (14) | −0.0139 (15) |
| C20 | 0.0323 (17) | 0.0371 (17) | 0.0411 (19) | −0.0046 (14) | −0.0063 (15) | −0.0159 (15) |
| C21 | 0.051 (2) | 0.044 (2) | 0.055 (2) | −0.0051 (17) | −0.0187 (19) | −0.0139 (18) |
| C22 | 0.058 (3) | 0.050 (2) | 0.066 (3) | −0.002 (2) | −0.024 (2) | −0.008 (2) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C23 | 0.054 (3) | 0.044 (2) | 0.069 (3) | 0.0001 (19) | −0.004 (2) | −0.014 (2) |
| C24 | 0.087 (3) | 0.049 (3) | 0.100 (4) | −0.007 (2) | −0.020 (3) | −0.043 (3) |
| C25 | 0.066 (3) | 0.049 (2) | 0.081 (3) | 0.001 (2) | −0.028 (2) | −0.037 (2) |
| C26 | 0.083 (4) | 0.046 (3) | 0.128 (5) | 0.002 (2) | −0.004 (3) | −0.015 (3) |
| C27 | 0.157 (5) | 0.058 (3) | 0.184 (6) | −0.007 (3) | −0.073 (5) | −0.028 (4) |
| C28 | 0.0319 (18) | 0.0368 (17) | 0.0400 (19) | −0.0034 (15) | −0.0093 (15) | −0.0091 (15) |
| C29 | 0.0316 (17) | 0.0368 (17) | 0.0379 (18) | −0.0031 (14) | −0.0080 (14) | −0.0111 (15) |
| C30 | 0.045 (2) | 0.056 (2) | 0.042 (2) | −0.0144 (18) | −0.0121 (17) | −0.0128 (17) |
| C31 | 0.045 (2) | 0.058 (2) | 0.050 (2) | −0.0221 (18) | 0.0001 (18) | −0.0124 (19) |
| C32 | 0.058 (2) | 0.047 (2) | 0.041 (2) | −0.0027 (19) | −0.0059 (19) | −0.0143 (17) |
| C33 | 0.077 (3) | 0.059 (2) | 0.041 (2) | −0.011 (2) | −0.027 (2) | −0.0126 (19) |
| C34 | 0.058 (2) | 0.051 (2) | 0.051 (2) | −0.0212 (19) | −0.0182 (19) | −0.0104 (18) |
| C35 | 0.083 (3) | 0.076 (3) | 0.037 (2) | −0.011 (3) | 0.004 (2) | −0.009 (2) |
| C36 | 0.133 (5) | 0.071 (3) | 0.064 (3) | 0.011 (3) | 0.019 (3) | 0.015 (3) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| La1—O7$^{i}$ | 2.446 (2) | C12—C13 | 1.380 (5) |
| La1—O1 | 2.451 (2) | C12—H12 | 0.9300 |
| La1—O2$^{ii}$ | 2.457 (2) | C13—C14 | 1.365 (5) |
| La1—O6$^{i}$ | 2.466 (2) | C13—H13 | 0.9300 |
| La1—O8 | 2.479 (2) | C14—C15 | 1.369 (5) |
| La1—O5 | 2.581 (2) | C14—C17 | 1.528 (6) |
| La1—O9 | 2.624 (2) | C15—C16 | 1.383 (5) |
| La1—O3 | 2.672 (2) | C15—H15 | 0.9300 |
| La1—O6 | 2.989 (2) | C16—H16 | 0.9300 |
| O1—C1 | 1.255 (4) | C17—C18 | 1.455 (6) |
| O2—C1 | 1.262 (4) | C17—H17A | 0.9700 |
| O2—La1$^{ii}$ | 2.457 (2) | C17—H17B | 0.9700 |
| O3—C10 | 1.212 (4) | C18—H18A | 0.9600 |
| O4—C10 | 1.318 (4) | C18—H18B | 0.9600 |
| O4—H4A | 0.8200 | C18—H18C | 0.9600 |
| O5—C19 | 1.272 (4) | C19—C20 | 1.482 (4) |
| O6—C19 | 1.255 (4) | C20—C25 | 1.381 (5) |
| O6—La1$^{i}$ | 2.466 (2) | C20—C21 | 1.385 (5) |
| O7—C28 | 1.255 (4) | C21—C22 | 1.381 (5) |
| O7—La1$^{i}$ | 2.446 (2) | C21—H21 | 0.9300 |
| O8—C28 | 1.263 (4) | C22—C23 | 1.358 (6) |
| O9—H9A | 0.8199 | C22—H22 | 0.9300 |
| O9—H9B | 0.8200 | C23—C24 | 1.390 (6) |
| C1—C2 | 1.494 (4) | C23—C26 | 1.524 (5) |
| C2—C7 | 1.382 (5) | C24—C25 | 1.399 (5) |
| C2—C3 | 1.385 (5) | C24—H24 | 0.9300 |
| C3—C4 | 1.377 (5) | C25—H25 | 0.9300 |
| C3—H3 | 0.9300 | C26—C27 | 1.428 (7) |
| C4—C5 | 1.380 (6) | C26—H26A | 0.9700 |
| C4—H4 | 0.9300 | C26—H26B | 0.9700 |
| C5—C6 | 1.389 (6) | C27—H27A | 0.9600 |

| | | | |
|---|---|---|---|
| C5—C8B | 1.527 (12) | C27—H27B | 0.9600 |
| C5—C8A | 1.530 (9) | C27—H27C | 0.9600 |
| C6—C7 | 1.377 (5) | C28—C29 | 1.494 (4) |
| C6—H6 | 0.9300 | C29—C30 | 1.380 (5) |
| C7—H7 | 0.9300 | C29—C34 | 1.388 (5) |
| C8A—C9A | 1.42 (3) | C30—C31 | 1.378 (5) |
| C8A—H8A | 0.9700 | C30—H30 | 0.9300 |
| C8A—H8B | 0.9700 | C31—C32 | 1.376 (5) |
| C9A—H9C | 0.9600 | C31—H31 | 0.9300 |
| C9A—H9D | 0.9600 | C32—C33 | 1.379 (5) |
| C9A—H9E | 0.9600 | C32—C35 | 1.520 (5) |
| C8B—C9B | 1.41 (3) | C33—C34 | 1.385 (5) |
| C8B—H8C | 0.9700 | C33—H33 | 0.9300 |
| C8B—H8D | 0.9700 | C34—H34 | 0.9300 |
| C9B—H9F | 0.9600 | C35—C36 | 1.491 (6) |
| C9B—H9G | 0.9600 | C35—H35A | 0.9700 |
| C9B—H9H | 0.9600 | C35—H35B | 0.9700 |
| C10—C11 | 1.478 (5) | C36—H36A | 0.9600 |
| C11—C16 | 1.374 (5) | C36—H36B | 0.9600 |
| C11—C12 | 1.374 (5) | C36—H36C | 0.9600 |
| $O7^{i}$—La1—O1 | 85.28 (8) | C12—C11—C10 | 119.7 (3) |
| $O7^{i}$—La1—$O2^{ii}$ | 138.39 (8) | C11—C12—C13 | 120.8 (4) |
| O1—La1—$O2^{ii}$ | 88.76 (7) | C11—C12—H12 | 119.6 |
| $O7^{i}$—La1—$O6^{i}$ | 72.11 (8) | C13—C12—H12 | 119.6 |
| O1—La1—$O6^{i}$ | 88.38 (8) | C14—C13—C12 | 121.7 (4) |
| $O2^{ii}$—La1—$O6^{i}$ | 148.91 (8) | C14—C13—H13 | 119.1 |
| $O7^{i}$—La1—O8 | 129.46 (8) | C12—C13—H13 | 119.1 |
| O1—La1—O8 | 134.90 (8) | C13—C14—C15 | 117.3 (4) |
| $O2^{ii}$—La1—O8 | 81.26 (8) | C13—C14—C17 | 119.6 (4) |
| $O6^{i}$—La1—O8 | 79.01 (8) | C15—C14—C17 | 123.1 (4) |
| $O7^{i}$—La1—O5 | 78.89 (8) | C14—C15—C16 | 121.6 (4) |
| O1—La1—O5 | 137.55 (8) | C14—C15—H15 | 119.2 |
| $O2^{ii}$—La1—O5 | 78.19 (7) | C16—C15—H15 | 119.2 |
| $O6^{i}$—La1—O5 | 122.55 (7) | C11—C16—C15 | 120.7 (4) |
| O8—La1—O5 | 83.19 (8) | C11—C16—H16 | 119.7 |
| $O7^{i}$—La1—O9 | 138.96 (8) | C15—C16—H16 | 119.7 |
| O1—La1—O9 | 69.14 (8) | C18—C17—C14 | 116.4 (4) |
| $O2^{ii}$—La1—O9 | 74.56 (8) | C18—C17—H17A | 108.2 |
| $O6^{i}$—La1—O9 | 75.51 (8) | C14—C17—H17A | 108.2 |
| O8—La1—O9 | 65.79 (8) | C18—C17—H17B | 108.2 |
| O5—La1—O9 | 141.12 (8) | C14—C17—H17B | 108.2 |
| $O7^{i}$—La1—O3 | 70.76 (8) | H17A—C17—H17B | 107.3 |
| O1—La1—O3 | 67.79 (7) | C17—C18—H18A | 109.5 |
| $O2^{ii}$—La1—O3 | 68.89 (8) | C17—C18—H18B | 109.5 |
| $O6^{i}$—La1—O3 | 137.01 (8) | H18A—C18—H18B | 109.5 |

| | | | |
|---|---|---|---|
| O8—La1—O3 | 142.87 (8) | C17—C18—H18C | 109.5 |
| O5—La1—O3 | 69.82 (7) | H18A—C18—H18C | 109.5 |
| O9—La1—O3 | 122.91 (7) | H18B—C18—H18C | 109.5 |
| O7$^{i}$—La1—O6 | 69.86 (7) | O6—C19—O5 | 120.5 (3) |
| O1—La1—O6 | 154.19 (7) | O6—C19—C20 | 120.8 (3) |
| O2$^{ii}$—La1—O6 | 114.27 (7) | O5—C19—C20 | 118.7 (3) |
| O6$^{i}$—La1—O6 | 77.73 (7) | C25—C20—C21 | 118.4 (3) |
| O8—La1—O6 | 63.95 (7) | C25—C20—C19 | 120.4 (3) |
| O5—La1—O6 | 45.66 (7) | C21—C20—C19 | 121.0 (3) |
| O9—La1—O6 | 126.33 (7) | C22—C21—C20 | 120.9 (4) |
| O3—La1—O6 | 108.39 (7) | C22—C21—H21 | 119.5 |
| C1—O1—La1 | 141.5 (2) | C20—C21—H21 | 119.5 |
| C1—O2—La1$^{ii}$ | 144.6 (2) | C23—C22—C21 | 121.5 (4) |
| C10—O3—La1 | 136.8 (2) | C23—C22—H22 | 119.2 |
| C10—O4—H4A | 109.2 | C21—C22—H22 | 119.2 |
| C19—O5—La1 | 104.12 (19) | C22—C23—C24 | 118.3 (4) |
| C19—O6—La1$^{i}$ | 172.4 (2) | C22—C23—C26 | 119.8 (5) |
| C19—O6—La1 | 85.22 (18) | C24—C23—C26 | 122.0 (4) |
| La1$^{i}$—O6—La1 | 102.27 (7) | C23—C24—C25 | 120.9 (4) |
| C28—O7—La1$^{i}$ | 140.7 (2) | C23—C24—H24 | 119.5 |
| C28—O8—La1 | 139.7 (2) | C25—C24—H24 | 119.5 |
| La1—O9—H9A | 119.0 | C20—C25—C24 | 119.9 (4) |
| La1—O9—H9B | 105.1 | C20—C25—H25 | 120.0 |
| H9A—O9—H9B | 117.6 | C24—C25—H25 | 120.0 |
| O1—C1—O2 | 123.7 (3) | C27—C26—C23 | 116.9 (5) |
| O1—C1—C2 | 117.6 (3) | C27—C26—H26A | 108.1 |
| O2—C1—C2 | 118.7 (3) | C23—C26—H26A | 108.1 |
| C7—C2—C3 | 119.0 (3) | C27—C26—H26B | 108.1 |
| C7—C2—C1 | 120.4 (3) | C23—C26—H26B | 108.1 |
| C3—C2—C1 | 120.5 (3) | H26A—C26—H26B | 107.3 |
| C4—C3—C2 | 120.3 (4) | C26—C27—H27A | 109.5 |
| C4—C3—H3 | 119.8 | C26—C27—H27B | 109.5 |
| C2—C3—H3 | 119.8 | H27A—C27—H27B | 109.5 |
| C3—C4—C5 | 121.1 (4) | C26—C27—H27C | 109.5 |
| C3—C4—H4 | 119.5 | H27A—C27—H27C | 109.5 |
| C5—C4—H4 | 119.5 | H27B—C27—H27C | 109.5 |
| C4—C5—C6 | 118.2 (4) | O7—C28—O8 | 125.1 (3) |
| C4—C5—C8B | 115.9 (19) | O7—C28—C29 | 117.8 (3) |
| C6—C5—C8B | 125.3 (17) | O8—C28—C29 | 117.1 (3) |
| C4—C5—C8A | 123.8 (8) | C30—C29—C34 | 118.1 (3) |
| C6—C5—C8A | 117.9 (8) | C30—C29—C28 | 121.8 (3) |
| C7—C6—C5 | 121.0 (4) | C34—C29—C28 | 120.1 (3) |
| C7—C6—H6 | 119.5 | C31—C30—C29 | 120.8 (3) |
| C5—C6—H6 | 119.5 | C31—C30—H30 | 119.6 |
| C6—C7—C2 | 120.3 (4) | C29—C30—H30 | 119.6 |
| C6—C7—H7 | 119.9 | C32—C31—C30 | 121.6 (4) |
| C2—C7—H7 | 119.9 | C32—C31—H31 | 119.2 |

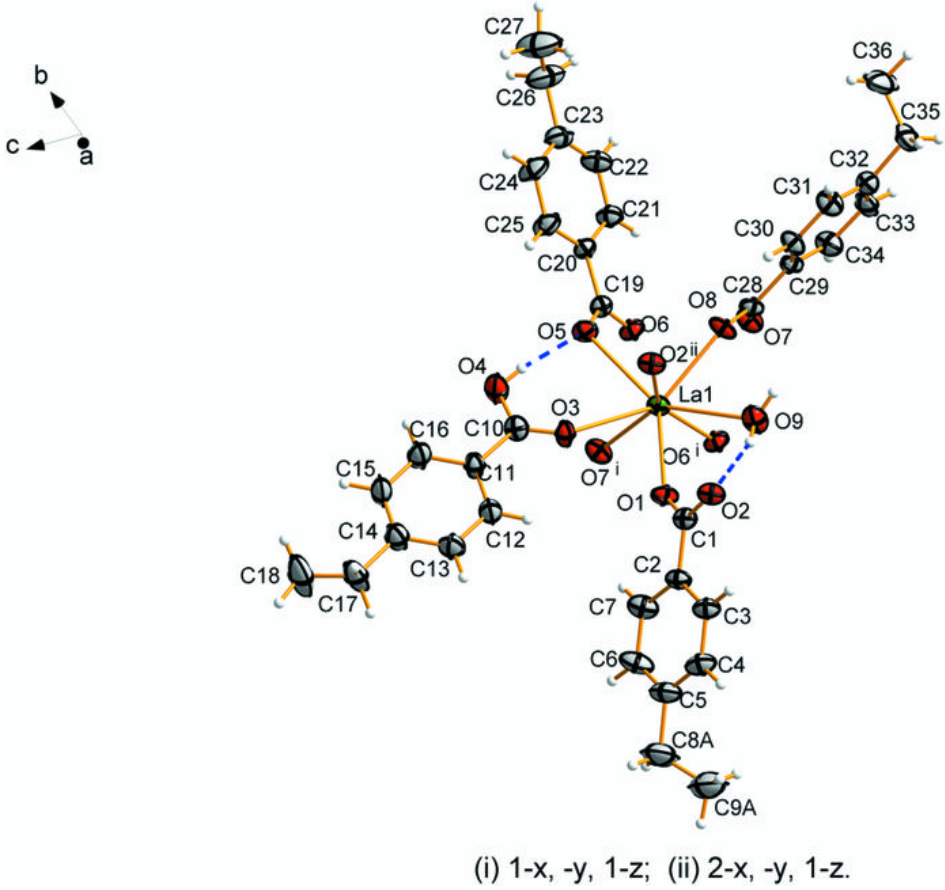
| | | | |
|---|---|---|---|
| C9A—C8A—C5 | 116.0 (15) | C30—C31—H31 | 119.2 |
| C9A—C8A—H8A | 108.3 | C31—C32—C33 | 117.7 (3) |
| C5—C8A—H8A | 108.3 | C31—C32—C35 | 120.8 (4) |
| C9A—C8A—H8B | 108.3 | C33—C32—C35 | 121.5 (4) |
| C5—C8A—H8B | 108.3 | C32—C33—C34 | 121.4 (4) |
| H8A—C8A—H8B | 107.4 | C32—C33—H33 | 119.3 |
| C9B—C8B—C5 | 116 (3) | C34—C33—H33 | 119.3 |
| C9B—C8B—H8C | 108.2 | C33—C34—C29 | 120.4 (4) |
| C5—C8B—H8C | 108.2 | C33—C34—H34 | 119.8 |
| C5—C8B—H8D | 108.2 | C29—C34—H34 | 119.8 |
| H8C—C8B—H8D | 107.4 | C36—C35—C32 | 112.5 (3) |
| C8B—C9B—H9F | 109.5 | C36—C35—H35A | 109.1 |
| C8B—C9B—H9G | 109.5 | C32—C35—H35A | 109.1 |
| H9F—C9B—H9G | 109.5 | C36—C35—H35B | 109.1 |
| C8B—C9B—H9H | 109.5 | C32—C35—H35B | 109.1 |
| H9F—C9B—H9H | 109.5 | H35A—C35—H35B | 107.8 |
| H9G—C9B—H9H | 109.5 | C35—C36—H36A | 109.5 |
| O3—C10—O4 | 122.7 (3) | C35—C36—H36B | 109.5 |
| O3—C10—C11 | 123.2 (3) | H36A—C36—H36B | 109.5 |
| O4—C10—C11 | 114.1 (3) | C35—C36—H36C | 109.5 |
| C16—C11—C12 | 117.8 (4) | H36A—C36—H36C | 109.5 |
| C16—C11—C10 | 122.5 (3) | H36B—C36—H36C | 109.5 |

Symmetry codes: (i) −*x*+1, −*y*, −*z*+1; (ii) −*x*+2, −*y*, −*z*+1.

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O4—H4A···O5 | 0.82 | 1.84 | 2.652 (3) | 171 |
| O9—H9B···O2 | 0.82 | 2.04 | 2.829 (3) | 161 |

**Fig. 1**




(i) 1-x, -y, 1-z; (ii) 2-x, -y, 1-z.

**Fig. 2**