# metal-organic compounds

# Poly[bis(μ4-benzene-1,4-dicarboxylato)-μ6-succinato-dilanthanum(III)]

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The title compound, $[La_2(C_4H_4O_4)(C_8H_4O_4)_2]_n$, was synthesized by hydrothermal methods. The La atom is coordinated by four O atoms from four benzene-1,4-dicarboxylate (BDC) ligands and four O atoms from three succinate anions, in a distorted square antiprismatic coordination geometry. The antiprisms are bridged by the benzene-1,4-dicarboxylate and succinate ligands, forming a three-dimensional network. The succinate ion is located on a centre of inversion.

## Related literature

For related literature, see: Li & Wang (2005); Li *et al.* (2006); Wang & Li (2005); He *et al.* (2006).
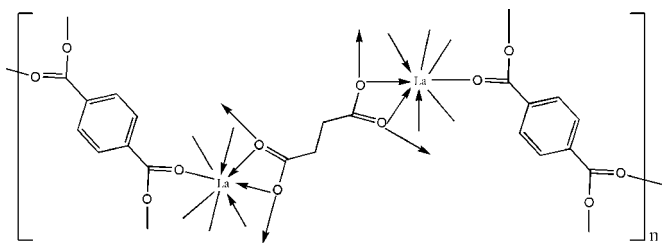


## Experimental

### Crystal data

| | |
|---|---|
| $[La_2(C_4H_4O_4)(C_8H_4O_4)_2]$ | $V$ = 2214.06 (9) Å$^3$ |
| $M_r$ = 361.06 | $Z$ = 8 |
| Orthorhombic, $Pbca$ | Mo $K\alpha$ radiation |
| $a$ = 14.2014 (4) Å | $\mu$ = 3.87 mm$^{-1}$ |
| $b$ = 7.0513 (1) Å | $T$ = 291 (2) K |
| $c$ = 22.1100 (5) Å | $0.33 \times 0.27 \times 0.18$ mm |

### Data collection

| | |
|---|---|
| Bruker SMART CCD area-detector diffractometer | 11927 measured reflections |
| Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996) | 2505 independent reflections |
| | 1974 reflections with $I > 2\sigma(I)$ |
| $T_{min}$ = 0.293, $T_{max}$ = 0.492 | $R_{int}$ = 0.029 |

### Refinement

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)]$ = 0.021 | 155 parameters |
| $wR(F^2)$ = 0.051 | H-atom parameters constrained |
| $S$ = 1.02 | $\Delta\rho_{max}$ = 0.31 e Å$^{-3}$ |
| 2505 reflections | $\Delta\rho_{min}$ = −0.53 e Å$^{-3}$ |

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

| | | | |
|---|---|---|---|
| La—O1 | 2.4380 (18) | La—O5 | 2.6244 (19) |
| La—O2$^i$ | 2.390 (2) | La—O5$^{iv}$ | 2.532 (2) |
| La—O3$^{ii}$ | 2.446 (2) | La—O6$^v$ | 2.573 (2) |
| La—O4$^{iii}$ | 2.450 (2) | La—O6 | 2.6884 (19) |

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1998); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*

## References

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**supplementary materials**

# Poly[bis($\mu_4$-benzene-1,4-dicarboxylato)-$\mu_6$-succinato-dilanthanum(III)]

## Q. He and B.-J. Huang

## Comment

The title compound, (I), is isostructural with its $[M_2(C_8H_4O_4)_2(C_4H_4O_4)]_n$ [$M$ = Gd (Wang & Li, 2005), Dy ((Li & Wang, 2005), Nd (Li *et al.*, 2006), Er (He *et al.*, 2006)] analogues. As depicted in Fig.1, The La$^{3+}$ ion is located at the center of a distorted square antiprism geometry and is coordinated by four oxygen atoms from four BDC and four from three succinate anions. The La—O bond distances ranging from 2.390 (2) to 2.6884 (19) Å.

In (I), the succinate ligand is located on an inversion centre and functions as an octadentate ligand, bis-chelating two La atoms with each O atom bridging to another La atom. In this mode, the La atoms are linked into a two-dimensional polymeric sheet parallel to the (001) plane. These sheets are in turn bridged *via* benzene-1,4-dicarboxylate ligands, forming a three-dimensional framework.

## Experimental

A mixture of LaCl$_3$·6H$_2$O (2.00 mmol, 0.70 g), benzene-1,4-dicarboxylic acid (1.0 mmol, 0.16 g), succinic acid (1.0 mmol, 0.10 g), NaOH (6.0 ml, 1 mol/*L*) and H$_2$O (20.0 ml) was heated in a 35 ml stainless steel reactor with a Teflon liner at 453 K for 48 h. The column-like crystals were filtered and washed with ethanol. Yield: 14% based on Nd.

## Refinement

H atoms were included at calculated positions and treated as riding atoms, with C—H distances of 0.93–0.97 Å and $U_{iso}$(H) = 1.2$U_{eq}$(C)].
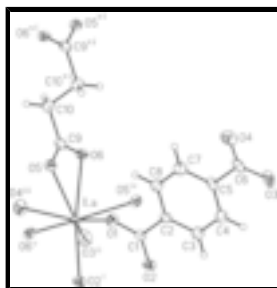
## Figures



Fig. 1. The coordination environment of the La atom, with the atom-numbering scheme, showing displacement ellipsoids drawn at the 50% probability level. Symmetry codes: (i) 2 − $x$, 2 − $y$, 1 − $z$; (ii) 3/2 − $x$, 2 − $y$, $z$ + 1/2; (iii) $x$, 3/2 − $y$, $z$ + 1/2; (iv) 3/2 − $x$, $y$ + 1/2, $z$; (v) 3/2 − $x$, $y$ − 1/2, $z$; (vi) 1 − $x$, 2 − $y$, 1 − $z$.

**Poly[bis(μ₄-benzene-1,4-dicarboxylato)-μ₆-succinato-dilanthanum(III)]**

*Crystal data*

| | |
|---|---|
| $[La_2(C_4H_4O_4)(C_8H_4O_4)_2]$ | $F_{000} = 1368$ |
| $M_r = 361.06$ | $D_x = 2.166$ Mg m$^{-3}$ |
| Orthorhombic, *Pbca* | Mo *Kα* radiation<br>$λ = 0.71073$ Å |
| Hall symbol: -P 2ac 2ab | Cell parameters from 168 reflections |
| $a = 14.2014$ (4) Å | $θ = 3.3–26.7º$ |
| $b = 7.0513$ (1) Å | $μ = 3.87$ mm$^{-1}$ |
| $c = 22.1100$ (5) Å | $T = 291$ (2) K |
| $V = 2214.06$ (9) Å$^3$ | Column, colorless |
| $Z = 8$ | $0.33 × 0.27 × 0.18$ mm |

*Data collection*

| | |
|---|---|
| Bruker SMART CCD area-detector diffractometer | 2505 independent reflections |
| Radiation source: fine-focus sealed tube | 1974 reflections with $I > 2σ(I)$ |
| Monochromator: graphite | $R_{int} = 0.029$ |
| $T = 291(2)$ K | $θ_{max} = 27.5º$ |
| φ and ω scans | $θ_{min} = 1.8º$ |
| Absorption correction: multi-scan (SADABS; Sheldrick, 1996) | $h = −18→18$ |
| $T_{min} = 0.293$, $T_{max} = 0.492$ | $k = −9→5$ |
| 11927 measured reflections | $l = −28→29$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Hydrogen site location: inferred from neighbouring sites |
| Least-squares matrix: full | H-atom parameters constrained |
| $R[F^2 > 2σ(F^2)] = 0.021$ | $w = 1/[σ^2(F_o^2) + (0.0243P)^2 + 1.3924P]$<br>where $P = (F_o^2 + 2F_c^2)/3$ |
| $wR(F^2) = 0.051$ | $(Δ/σ)_{max} = 0.030$ |
| $S = 1.02$ | $Δρ_{max} = 0.31$ e Å$^{-3}$ |
| 2505 reflections | $Δρ_{min} = −0.53$ e Å$^{-3}$ |
| 155 parameters | Extinction correction: SHELXTL (Bruker, 1998), $Fc^* = kFc[1+0.001xFc^2λ^3/\sin(2θ)]^{-1/4}$ |
| Primary atom site location: structure-invariant direct methods | Extinction coefficient: 0.00116 (9) |
| 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 ($Å^2$)*

|       | $x$ | $y$ | $z$ | $U_{iso}*/U_{eq}$ |
|-------|------|------|------|------|
| La   | 0.833810 (10) | 1.02208 (2) | 0.554317 (6) | 0.01592 (7) |
| O1   | 0.86146 (16) | 1.0440 (3) | 0.44571 (8) | 0.0277 (5) |
| O2   | 1.00219 (14) | 0.9173 (3) | 0.43107 (8) | 0.0279 (5) |
| C1   | 0.92144 (19) | 0.9655 (4) | 0.41250 (12) | 0.0198 (6) |
| C2   | 0.89650 (19) | 0.9240 (4) | 0.34781 (12) | 0.0225 (6) |
| C3   | 0.8095 (2) | 0.9761 (5) | 0.32544 (14) | 0.0326 (8) |
| H3A  | 0.7667 | 1.0383 | 0.3503 | 0.039* |
| C4   | 0.7857 (2) | 0.9356 (5) | 0.26579 (14) | 0.0359 (8) |
| H4A  | 0.7269 | 0.9697 | 0.2509 | 0.043* |
| C5   | 0.8497 (2) | 0.8446 (5) | 0.22869 (13) | 0.0289 (7) |
| C6   | 0.8238 (2) | 0.7940 (5) | 0.16472 (14) | 0.0341 (8) |
| C7   | 0.9370 (2) | 0.7938 (5) | 0.25116 (13) | 0.0361 (8) |
| H7A  | 0.9803 | 0.7333 | 0.2262 | 0.043* |
| C8   | 0.9603 (2) | 0.8325 (5) | 0.31042 (13) | 0.0337 (8) |
| H8A  | 1.0189 | 0.7971 | 0.3253 | 0.040* |
| O3   | 0.74602 (16) | 0.8515 (4) | 0.14369 (9) | 0.0424 (6) |
| O4   | 0.88149 (19) | 0.6945 (4) | 0.13534 (10) | 0.0486 (7) |
| O5   | 0.66405 (13) | 0.8794 (3) | 0.54300 (10) | 0.0285 (5) |
| O6   | 0.67149 (13) | 1.1776 (3) | 0.51616 (9) | 0.0247 (4) |
| C9   | 0.6242 (2) | 1.0327 (5) | 0.52874 (16) | 0.0293 (7) |
| C10  | 0.5157 (2) | 1.0426 (5) | 0.52970 (16) | 0.0376 (8) |
| H10A | 0.4907 | 0.9706 | 0.5635 | 0.045* |
| H10B | 0.4946 | 1.1729 | 0.5331 | 0.045* |

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

|     | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|-----|------|------|------|------|------|------|
| La | 0.01657 (9) | 0.01669 (11) | 0.01450 (9) | −0.00152 (6) | −0.00020 (6) | 0.00152 (6) |
| O1 | 0.0323 (11) | 0.0345 (15) | 0.0162 (10) | 0.0050 (9) | 0.0015 (8) | −0.0020 (9) |
| O2 | 0.0243 (10) | 0.0378 (14) | 0.0217 (10) | −0.0031 (10) | −0.0081 (8) | −0.0016 (9) |
| C1 | 0.0228 (14) | 0.0197 (17) | 0.0169 (13) | −0.0048 (11) | −0.0036 (11) | −0.0002 (11) |
| C2 | 0.0240 (14) | 0.0248 (18) | 0.0186 (14) | −0.0005 (12) | −0.0043 (11) | −0.0025 (12) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C3 | 0.0340 (16) | 0.039 (2) | 0.0246 (16) | 0.0136 (14) | −0.0038 (13) | −0.0070 (14) |
| C4 | 0.0333 (18) | 0.042 (2) | 0.0320 (17) | 0.0112 (15) | −0.0141 (14) | −0.0037 (16) |
| C5 | 0.0432 (19) | 0.0241 (19) | 0.0195 (14) | −0.0012 (13) | −0.0091 (13) | −0.0032 (13) |
| C6 | 0.055 (2) | 0.0244 (19) | 0.0225 (15) | −0.0097 (15) | −0.0123 (15) | −0.0019 (14) |
| C7 | 0.0396 (18) | 0.044 (2) | 0.0243 (15) | 0.0122 (15) | −0.0044 (14) | −0.0143 (15) |
| C8 | 0.0294 (16) | 0.048 (2) | 0.0234 (15) | 0.0107 (15) | −0.0088 (13) | −0.0119 (15) |
| O3 | 0.0468 (15) | 0.0549 (19) | 0.0256 (11) | −0.0100 (12) | −0.0167 (10) | 0.0095 (11) |
| O4 | 0.0760 (18) | 0.0420 (18) | 0.0279 (12) | 0.0110 (14) | −0.0163 (12) | −0.0156 (12) |
| O5 | 0.0216 (10) | 0.0155 (13) | 0.0483 (13) | 0.0007 (8) | −0.0087 (9) | 0.0021 (10) |
| O6 | 0.0236 (10) | 0.0165 (12) | 0.0339 (11) | −0.0013 (8) | −0.0039 (8) | 0.0024 (9) |
| C9 | 0.0193 (15) | 0.022 (2) | 0.0463 (19) | −0.0011 (12) | −0.0118 (14) | 0.0020 (15) |
| C10 | 0.042 (2) | 0.026 (2) | 0.045 (2) | 0.0062 (15) | −0.0048 (16) | −0.0042 (17) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| La—O1 | 2.4380 (18) | C4—C5 | 1.382 (4) |
| La—O2$^i$ | 2.390 (2) | C4—H4A | 0.9300 |
| La—O3$^{ii}$ | 2.446 (2) | C5—C7 | 1.383 (4) |
| La—O4$^{iii}$ | 2.450 (2) | C5—C6 | 1.504 (4) |
| La—O5 | 2.6244 (19) | C6—O4 | 1.259 (4) |
| La—O5$^{iv}$ | 2.532 (2) | C6—O3 | 1.265 (4) |
| La—O6$^v$ | 2.573 (2) | C7—C8 | 1.378 (4) |
| La—O6 | 2.6884 (19) | C7—H7A | 0.9300 |
| O1—C1 | 1.253 (3) | C8—H8A | 0.9300 |
| O2—C1 | 1.265 (3) | O5—C9 | 1.260 (4) |
| C1—C2 | 1.502 (3) | O6—C9 | 1.254 (4) |
| C2—C3 | 1.380 (4) | C9—C10 | 1.542 (4) |
| C2—C8 | 1.386 (4) | C10—C10$^{vi}$ | 1.512 (7) |
| C3—C4 | 1.391 (4) | C10—H10A | 0.9700 |
| C3—H3A | 0.9300 | C10—H10B | 0.9700 |
| O2$^i$—La—O1 | 87.98 (7) | C3—C2—C8 | 119.7 (3) |
| O2$^i$—La—O3$^{ii}$ | 106.10 (7) | C3—C2—C1 | 120.0 (2) |
| O1—La—O3$^{ii}$ | 147.90 (8) | C8—C2—C1 | 120.3 (2) |
| O2$^i$—La—O4$^{iii}$ | 75.13 (8) | C2—C3—C4 | 120.1 (3) |
| O1—La—O4$^{iii}$ | 135.66 (8) | C2—C3—H3A | 119.9 |
| O3$^{ii}$—La—O4$^{iii}$ | 76.39 (9) | C4—C3—H3A | 119.9 |
| O2$^i$—La—O5$^{iv}$ | 79.84 (7) | C5—C4—C3 | 119.9 (3) |
| O1—La—O5$^{iv}$ | 80.66 (7) | C5—C4—H4A | 120.1 |
| O3$^{ii}$—La—O5$^{iv}$ | 73.90 (8) | C3—C4—H4A | 120.1 |
| O4$^{iii}$—La—O5$^{iv}$ | 133.58 (8) | C7—C5—C4 | 119.8 (3) |
| O2$^i$—La—O6$^v$ | 103.99 (7) | C7—C5—C6 | 119.7 (3) |
| O1—La—O6$^v$ | 75.02 (7) | C4—C5—C6 | 120.5 (3) |
| O3$^{ii}$—La—O6$^v$ | 126.55 (7) | O4—C6—O3 | 123.8 (3) |
| O4$^{iii}$—La—O6$^v$ | 70.07 (7) | O4—C6—C5 | 117.3 (3) |
| O5$^{iv}$—La—O6$^v$ | 155.16 (7) | O3—C6—C5 | 118.9 (3) |

| | | | |
|---|---|---|---|
| O2<sup>i</sup>—La—O5 | 167.61 (7) | C8—C7—C5 | 120.3 (3) |
| O1—La—O5 | 94.49 (7) | C8—C7—H7A | 119.8 |
| O3<sup>ii</sup>—La—O5 | 77.94 (7) | C5—C7—H7A | 119.8 |
| O4<sup>iii</sup>—La—O5 | 94.85 (8) | C7—C8—C2 | 120.1 (3) |
| O5<sup>iv</sup>—La—O5 | 112.53 (6) | C7—C8—H8A | 119.9 |
| O6<sup>v</sup>—La—O5 | 65.15 (6) | C2—C8—H8A | 119.9 |
| O2<sup>i</sup>—La—O6 | 143.61 (7) | C6—O3—La<sup>vii</sup> | 144.9 (2) |
| O1—La—O6 | 78.65 (7) | C6—O4—La<sup>viii</sup> | 123.0 (2) |
| O3<sup>ii</sup>—La—O6 | 72.99 (7) | C9—O5—La<sup>v</sup> | 152.08 (19) |
| O4<sup>iii</sup>—La—O6 | 136.12 (8) | C9—O5—La | 96.17 (18) |
| O5<sup>iv</sup>—La—O6 | 64.75 (6) | La<sup>v</sup>—O5—La | 111.17 (7) |
| O6<sup>v</sup>—La—O6 | 104.90 (6) | C9—O6—La<sup>iv</sup> | 132.9 (2) |
| O5—La—O6 | 48.61 (7) | C9—O6—La | 93.29 (17) |
| O2<sup>i</sup>—La—C9 | 167.94 (8) | La<sup>iv</sup>—O6—La | 107.90 (7) |
| O1—La—C9 | 88.44 (9) | O6—C9—O5 | 120.9 (3) |
| O3<sup>ii</sup>—La—C9 | 71.73 (9) | O6—C9—C10 | 120.1 (3) |
| O4<sup>iii</sup>—La—C9 | 115.04 (9) | O5—C9—C10 | 118.9 (3) |
| O5<sup>iv</sup>—La—C9 | 88.21 (7) | O6—C9—La | 62.32 (15) |
| O6<sup>v</sup>—La—C9 | 86.18 (7) | O5—C9—La | 59.41 (15) |
| O5—La—C9 | 24.42 (8) | C10—C9—La | 168.4 (2) |
| O6—La—C9 | 24.40 (7) | C10<sup>vi</sup>—C10—C9 | 105.4 (3) |
| C1—O1—La | 131.18 (18) | C10<sup>vi</sup>—C10—H10A | 110.7 |
| C1—O2—La<sup>i</sup> | 151.6 (2) | C9—C10—H10A | 110.7 |
| O1—C1—O2 | 123.0 (2) | C10<sup>vi</sup>—C10—H10B | 110.7 |
| O1—C1—C2 | 118.9 (2) | C9—C10—H10B | 110.7 |
| O2—C1—C2 | 118.1 (2) | H10A—C10—H10B | 108.8 |

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

**Fig. 1**