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Poly[di-μ_4-benzene-1,4-dicarboxylato-μ_6-succinato-dieuropium(III)]

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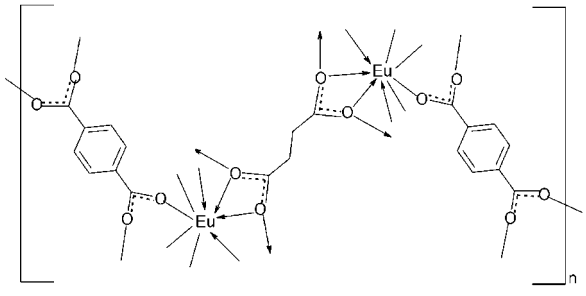
Key indicators: single-crystal X-ray study; T = 292 K; mean σ(C–C) = 0.004 Å; R factor = 0.016; wR factor = 0.040; data-to-parameter ratio = 15.9.

The title compound, $[Eu_2(C_4H_4O_4)(C_8H_4O_4)_2]_n$, has been synthesized by hydrothermal methods. The Eu atom is coordinated by four O atoms from four benzene-1,4-dicarboxylate (BDC) anions 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 anions into a three-dimensional coordination network. The succinate anions are located on centres of inversion.

Related literature

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



Experimental

Crystal data

$[Eu_2(C_4H_4O_4)(C_8H_4O_4)_2]$
M_r = 374.11
Orthorhombic, *Pbca*
a = 13.9501 (3) Å
b = 6.8696 (1) Å
c = 21.8409 (4) Å
V = 2093.05 (7) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 6.01 mm^{-1}
T = 292 (2) K
0.26 × 0.21 × 0.15 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.232, T_{max} = 0.415
11756 measured reflections
2458 independent reflections
2083 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.016
$wR(F^2)$ = 0.040
S = 1.10
2458 reflections
155 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.73 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}

Table 1
Selected bond lengths (Å).

Eu—O1	2.3355 (16)	Eu—O5^{iv}	2.4440 (18)
Eu—O2^{i}	2.2851 (17)	Eu—O5	2.5257 (17)
Eu—O3^{ii}	2.3486 (17)	Eu—O6^{v}	2.4958 (17)
Eu—O4^{iii}	2.3642 (17)	Eu—O6	2.5764 (16)

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*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NC2067).

References

Bruker (1998). *SMART* (Version 5.16), *SAINT* (Version 6.01) and *SHELXTL* (Version 6.14). Bruker AXS Inc., Madison, Wisconsin, USA.
He, Q., Zi, J.-F. & Zhang, F.-J. (2006). *Acta Cryst.* E**62**, m997–m998.
Li, Z.-F. & Wang, C.-X. (2005). *Acta Cryst.* E**61**, m2689–m2690.
Li, Z.-F., Wang, C.-X., Li, Y., Cai, D.-J. & Xiao, Y.-J. (2006). *Acta Cryst.* E**62**, m251–m252.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Wang, C.-X. & Li, Z.-F. (2005). *Acta Cryst.* E**61**, m2212–m2213.

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supplementary materials

Acta Cryst. (2007). E**63**, m2922 [**doi:10.1107/S1600536807054414**]

Poly[di-μ_4-benzene-1,4-dicarboxylato-μ_6-succinato-dieuropium(III)]

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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) and Er (He *et al.*, 2006)] analogues. The Eu^{3+} ion is located at the center of a distorted square antiprism and is coordinated by four oxygen atoms from four benzene-1,4-dicarboxylate anions and four oxygen atoms from three succinate anions (Fig. 1). The Eu—O bond distances ranging from 2.2851 (2) to 2.5764 (16) Å.

The succinate anions are located on centres of inversion and acts as a bis-chelating ligands for each two symmetry related Eu atoms. Each of the four oxygen atom are additionally connected by Eu atoms into layers which are parallel to the (001) plane. These layers are connected *via* the benzene-1,4-dicarboxylate anions into a three-dimensional coordination network.

Experimental

A mixture of $EuCl_3·6H_2O$ (2.00 mmol, 0.73 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_2O (20.0 ml) was heated in a 35 ml stainless steel autoclave with a teflon liner at 453 K for 48 h. After cooling to room temperature column-like crystals of the title compound has formed which were filtered off and washed with ethanol. Yield: 7% based on Eu.

Refinement

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

Figures

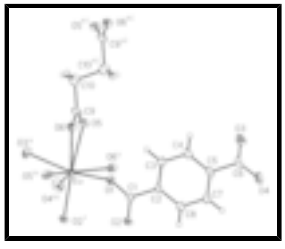


Fig. 1. The coordination environment of the Eu atom, with the atom-numbering scheme and displacement ellipsoids drawn at the 50% probability level. Symmetry codes: (i) 2 − *x*, 2 − *y*, 1 − *z*; (ii) 3/2 − *x*, 2 − *y*, *z* − 1/2; (iii) *x*, 3/2 − *y*, *z* − 1/2; (iv) 3/2 − *x*, *y* + 1/2, *z*; (v) 3/2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

Poly[di-μ$_4$-benzene-1,4-dicarboxylato-μ$_6$-succinato-dieuropium(III)]

Crystal data

$[Eu_2(C_4H_4O_4)(C_8H_4O_4)_2]$ $F_{000} = 1416$

M_r = 374.11	D_x = 2.374 Mg m^{-3}
Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 124 reflections
a = 13.9501 (3) Å	θ = 3.3–26.7º
b = 6.86960 (10) Å	μ = 6.01 mm^{-1}
c = 21.8409 (4) Å	*T* = 292 (2) K
V = 2093.05 (7) Å^3	Column, orange
Z = 8	0.26 × 0.21 × 0.15 mm

Data collection

Bruker SMART CCD area-detector diffractometer	2458 independent reflections
Radiation source: fine-focus sealed tube	2083 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.020
T = 292(2) K	θ_{max} = 28.0º
φ and ω scans	θ_{min} = 1.9º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −18→15
T_{min} = 0.232, T_{max} = 0.415	*k* = −7→9
11756 measured reflections	*l* = −28→28

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.016	$w = 1/[\sigma^2(F_o^2) + (0.0182P)^2 + 0.8889P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.040	$(\Delta/\sigma)_{max}$ = 0.014
S = 1.10	$\Delta\rho_{max}$ = 0.73 e Å^{-3}
2458 reflections	$\Delta\rho_{min}$ = −0.46 e Å^{-3}
155 parameters	Extinction correction: SHELXL, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.00043 (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}
Eu	0.831538 (8)	1.019333 (16)	0.445256 (5)	0.01307 (5)
O1	0.86262 (14)	1.0402 (3)	0.55012 (7)	0.0207 (4)
O2	1.00832 (12)	0.9242 (3)	0.56773 (7)	0.0218 (4)
C1	0.92483 (18)	0.9674 (3)	0.58479 (10)	0.0156 (5)
C2	0.89791 (18)	0.9259 (3)	0.65008 (10)	0.0175 (5)
C3	0.8072 (2)	0.9723 (4)	0.67128 (12)	0.0257 (6)
H3A	0.7629	1.0296	0.6450	0.031*
C4	0.7821 (2)	0.9335 (4)	0.73152 (11)	0.0278 (6)
H4A	0.7210	0.9645	0.7455	0.033*
C5	0.84800 (18)	0.8486 (4)	0.77108 (11)	0.0216 (5)
C6	0.82002 (19)	0.7999 (4)	0.83558 (11)	0.0231 (6)
C7	0.9384 (2)	0.8024 (4)	0.74985 (11)	0.0291 (6)
H7A	0.9828	0.7457	0.7762	0.035*
C8	0.96347 (19)	0.8400 (4)	0.68955 (11)	0.0280 (6)
H8A	1.0244	0.8076	0.6755	0.034*
O3	0.74136 (14)	0.8621 (3)	0.85578 (8)	0.0294 (4)
O4	0.87738 (14)	0.6966 (3)	0.86622 (8)	0.0312 (4)
O5	0.66579 (12)	0.8740 (3)	0.45395 (8)	0.0238 (4)
O6	0.67471 (12)	1.1767 (2)	0.48308 (8)	0.0202 (4)
C9	0.6250 (2)	1.0308 (4)	0.46890 (13)	0.0231 (6)
C10	0.5164 (2)	1.0421 (4)	0.46964 (14)	0.0297 (6)
H10A	0.4897	0.9678	0.4359	0.036*
H10B	0.4955	1.1762	0.4658	0.036*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Eu	0.01286 (8)	0.01546 (8)	0.01090 (7)	−0.00057 (4)	0.00000 (4)	−0.00124 (4)
O1	0.0211 (10)	0.0280 (10)	0.0130 (9)	0.0020 (7)	−0.0006 (7)	0.0010 (7)
O2	0.0158 (10)	0.0323 (10)	0.0173 (9)	−0.0014 (8)	0.0043 (7)	0.0021 (7)
C1	0.0182 (13)	0.0162 (12)	0.0124 (12)	−0.0030 (9)	0.0015 (10)	−0.0021 (9)
C2	0.0196 (14)	0.0214 (12)	0.0117 (11)	0.0003 (10)	0.0022 (10)	0.0024 (9)
C3	0.0244 (15)	0.0341 (15)	0.0185 (14)	0.0086 (11)	0.0028 (11)	0.0071 (11)
C4	0.0251 (16)	0.0375 (16)	0.0209 (14)	0.0081 (12)	0.0121 (12)	0.0045 (12)
C5	0.0276 (16)	0.0229 (13)	0.0142 (12)	0.0001 (10)	0.0062 (11)	0.0017 (10)
C6	0.0351 (17)	0.0198 (13)	0.0143 (12)	−0.0047 (11)	0.0056 (11)	0.0016 (10)
C7	0.0276 (17)	0.0413 (17)	0.0184 (13)	0.0056 (12)	0.0006 (12)	0.0100 (11)
C8	0.0221 (15)	0.0420 (17)	0.0200 (14)	0.0070 (12)	0.0062 (12)	0.0070 (11)
O3	0.0317 (12)	0.0397 (12)	0.0170 (9)	0.0004 (9)	0.0092 (8)	−0.0031 (8)
O4	0.0408 (12)	0.0309 (11)	0.0219 (10)	0.0037 (9)	0.0076 (9)	0.0101 (8)
O5	0.0181 (10)	0.0145 (9)	0.0388 (11)	0.0010 (7)	0.0061 (8)	−0.0017 (7)
O6	0.0201 (10)	0.0166 (9)	0.0241 (9)	−0.0026 (7)	0.0017 (7)	−0.0017 (7)

C9	0.0180 (14)	0.0218 (14)	0.0295 (14)	−0.0010 (10)	0.0096 (12)	0.0012 (11)
C10	0.0326 (18)	0.0235 (14)	0.0331 (16)	0.0028 (12)	0.0012 (13)	0.0018 (12)

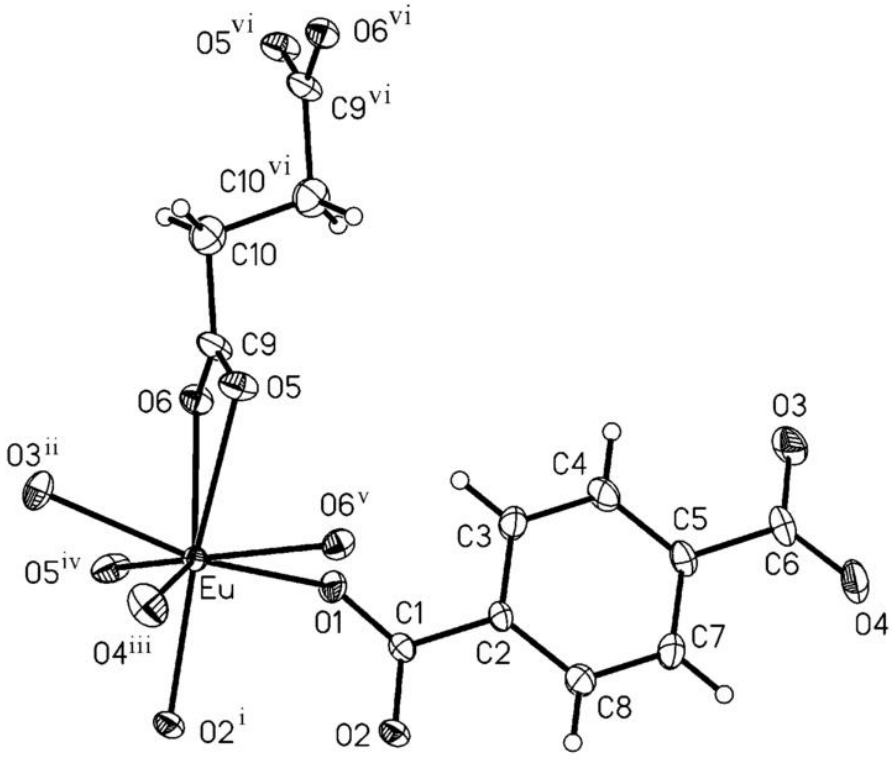
Geometric parameters (Å, °)

Eu—O1	2.3355 (16)	C4—C5	1.390 (3)
Eu—O2^{i}	2.2851 (17)	C4—H4A	0.9300
Eu—O3^{ii}	2.3486 (17)	C5—C7	1.381 (3)
Eu—O4^{iii}	2.3642 (17)	C5—C6	1.499 (3)
Eu—O5^{iv}	2.4440 (18)	C6—O3	1.258 (3)
Eu—O5	2.5257 (17)	C6—O4	1.261 (3)
Eu—O6^{v}	2.4958 (17)	C7—C8	1.387 (3)
Eu—O6	2.5764 (16)	C7—H7A	0.9300
Eu—Eu^{v}	4.11984 (14)	C8—H8A	0.9300
O1—C1	1.256 (3)	O5—C9	1.262 (3)
O2—C1	1.258 (3)	O6—C9	1.258 (3)
C1—C2	1.502 (3)	C9—C10	1.517 (4)
C2—C3	1.385 (4)	C10—C10^{vi}	1.517 (6)
C2—C8	1.388 (3)	C10—H10A	0.9700
C3—C4	1.387 (4)	C10—H10B	0.9700
C3—H3A	0.9300		
O2^{i}—Eu—O1	85.98 (6)	C4—C5—C6	120.4 (2)
O2^{i}—Eu—O3^{ii}	105.14 (6)	O3—C6—O4	124.0 (2)
O1—Eu—O3^{ii}	151.06 (6)	O3—C6—C5	118.7 (2)
O2^{i}—Eu—O4^{iii}	75.60 (6)	O4—C6—C5	117.3 (2)
O1—Eu—O4^{iii}	134.78 (6)	C5—C6—Eu^{vii}	146.06 (16)
O3^{ii}—Eu—O4^{iii}	74.16 (7)	C5—C7—C8	120.4 (2)
O2^{i}—Eu—O5^{iv}	79.96 (6)	C5—C7—H7A	119.8
O1—Eu—O5^{iv}	81.94 (6)	C8—C7—H7A	119.8
O4^{iii}—Eu—O5^{iv}	132.70 (6)	C7—C8—C2	120.2 (2)
O2^{i}—Eu—O6^{v}	103.61 (6)	C7—C8—H8A	119.9
O3^{ii}—Eu—O6^{v}	125.96 (6)	C2—C8—H8A	119.9
O4^{iii}—Eu—O6^{v}	70.09 (6)	C6—O3—Eu^{viii}	141.96 (17)
O3^{ii}—Eu—O5	78.65 (6)	C6—O4—Eu^{vii}	124.66 (17)
O5^{iv}—Eu—O5	113.72 (5)	C9—O5—Eu^{v}	151.43 (17)
O1—Eu—O6	79.48 (6)	C9—O5—Eu	95.47 (15)
O5^{iv}—Eu—O6	64.51 (5)	Eu^{v}—O5—Eu	111.98 (6)
O6^{v}—Eu—O6	105.07 (5)	C9—O6—Eu^{iv}	130.59 (17)
O1—C1—O2	123.7 (2)	C9—O6—Eu	93.16 (15)
O1—C1—C2	118.4 (2)	Eu^{iv}—O6—Eu	108.62 (6)
O2—C1—C2	117.9 (2)	O6—C9—O5	119.7 (2)
C3—C2—C8	119.5 (2)	O6—C9—C10	120.5 (2)
C3—C2—C1	120.1 (2)	O5—C9—C10	119.8 (2)
C8—C2—C1	120.4 (2)	O6—C9—Eu	61.44 (13)

C2—C3—C4	120.2 (2)	O5—C9—Eu	59.14 (13)
C2—C3—H3A	119.9	C10—C9—Eu	170.36 (19)
C4—C3—H3A	119.9	C9—C10—C10^{vi}	106.9 (3)
C3—C4—C5	120.3 (2)	C9—C10—H10A	110.3
C3—C4—H4A	119.9	C10^{vi}—C10—H10A	110.3
C5—C4—H4A	119.9	C9—C10—H10B	110.3
C7—C5—C4	119.5 (2)	C10^{vi}—C10—H10B	110.3
C7—C5—C6	120.1 (2)	H10A—C10—H10B	108.6

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*, −*y*+3/2, *z*+1/2; (viii) −*x*+3/2, −*y*+2, *z*+1/2.

Fig. 1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O6vi
C9vi
C10vi
C10
C9
O6
O5
O3ii
O6v
O5iv
Eu
O4iii
O1
C1
C2
C3
C4
C5
C6
O3
O4
C7
C8
O2i
O2