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Poly[bis(μ_4-benzene-1,4-dicarboxylato)-(μ_4-succinato)diterbium(III)]

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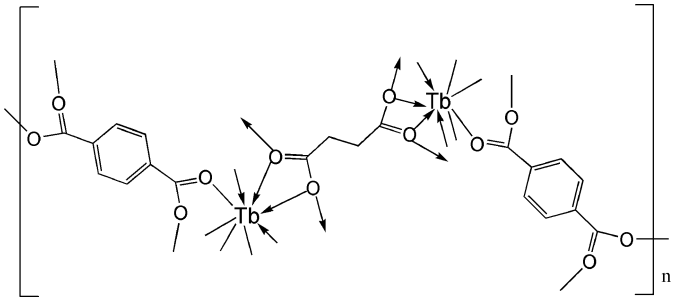
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.018; wR factor = 0.041; data-to-parameter ratio = 15.4.

In the title compound, $[Tb_2(C_4H_4O_4)(C_8H_4O_4)_2]_n$, the coordination around each Tb atom is distorted square-antiprismatic. The benzene-1,4-dicarboxylate and succinate anions bridge the antiprisms, forming a three-dimensional network. The succinate anion is located on a centre of inversion. The structure is isomorphous with the Dy, Gd, Er and Nd complexes.

Related literature

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



Experimental

Crystal data

$[Tb_2(C_4H_4O_4)(C_8H_4O_4)_2]$
M_r = 381.07
Orthorhombic, *Pbca*
a = 13.948 (3) Å
b = 6.8724 (14) Å
c = 21.844 (4) Å
V = 2093.9 (7) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 6.77 mm^{-1}
T = 293 (2) K
0.29 × 0.27 × 0.20 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.121, T_{max} = 0.257
18548 measured reflections
2376 independent reflections
2135 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.017
$wR(F^2)$ = 0.041
S = 1.07
2376 reflections
154 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.09 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL-Plus* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2699).

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supporting information

Acta Cryst. (2008). E**64**, m735 [doi:10.1107/S1600536808011355]

Poly[bis(μ_4-benzene-1,4-dicarboxylato)(μ_4-succinato)diterbium(III)]

Chun-Hui Yu

S1. Comment

Lanthanide complexes usually exhibit interesting framework structures and intense luminescence. In all types of rare-earth compounds, carboxylate anions with aromatic rings are widely used in the construction of high-dimensional lanthanide coordination polymers because these anions are able to act as bridging ligands in various ligating modes. However, rare-earth coordination polymers with mixed aromatic and fatty carboxylates are rarely studied (Wang & Li, 2005). In this paper, we present a new mixed carboxylate complex, namely $[Tb_2(1,4\text{-bdc})_2(suc)]_n$ (I), where 1,4-bdc=benzene-1,4-dicarboxylate and suc= succinate.

In (I), each Tb(III) center is coordinated by eight O atoms from 1,4-bdc and suc anions in a distorted square antiprism (Fig. 1). Each carboxylate moiety of the 1,4-bdc bridges two Tb(III) atoms, whereas each carboxylate group of suc links four Tb(III) atoms. In these modes, the central Tb(III) atoms are linked by 1,4-bdc and suc ligands, resulting in a rare three-dimensional framework structure (Fig. 2). The succinate anion is located on a centre of inversion. The structure of the title compound is isomorphous with the Dy (Li & Wang, 2005) Gd (Wang & Li, 2005), Er (He *et al.*, 2006) and the Nd (Li *et al.*, 2006) complex.

S2. Experimental

A mixture of 1,4-H_2bdc (0.5 mmol), H_2suc (0.5 mmol), NaOH (1 mmol) and $TbCl_3{\cdot}6H_2O$ (0.5 mmol) was suspended in 12 ml of deionized water and sealed in a 20-ml Teflon-lined autoclave. Upon heating at 185°C for ten days, the autoclave was slowly cooled to room temperature. The crystals were collected, washed with deionized water and dried.

S3. Refinement

H atoms bonded to C atom were positioned geometrically (C—H = 0.93 Å) and refined as riding, with U_{iso}(H)=1.2U_{eq}(carrier).

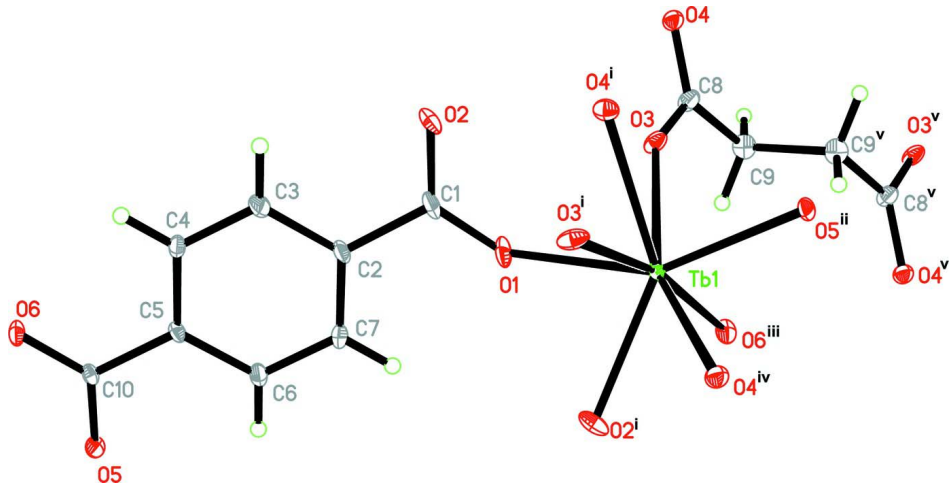

Figure 1

The structure of (I), showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Symmetry codes: (i) 0.5 - *x*, *y* - 1/2, *z*; (ii) 0.5 - *x*, -*y*, *z* + 1/2; (iii) *x* + 1/2, *y*, 0.5 - *z*; (iv) *x*, *y* - 1, *z*; (v) 1 - *x*, 1 - *y*, 1 - *z*.

Poly[bis(μ_4-benzene-1,4-dicarboxylato)(μ_4-succinato)diterbium(III)]

Crystal data

$[Tb_2(C_4H_4O_4)(C_8H_4O_4)_2]$
M_r = 381.07
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
a = 13.948 (3) Å
b = 6.8724 (14) Å
c = 21.844 (4) Å
V = 2093.9 (7) Å^3
Z = 8
F(000) = 1432
D_x = 2.418 Mg m^{-3}
Mo *Kα* radiation, λ = 0.71073 Å
Cell parameters from 15551 reflections
θ = 3.0–27.5°
μ = 6.77 mm^{-1}
T = 293 K
Block, colorless
0.29 × 0.27 × 0.20 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Radiation source: rotating anode
Graphite monochromator
Detector resolution: 10.0 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.121, T_{max} = 0.257
18548 measured reflections
2376 independent reflections
2135 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 27.5°, θ_{min} = 3.4°
h = −18→18
k = −8→8
l = −28→28

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.017
$wR(F^2)$ = 0.041
S = 1.07
2376 reflections
154 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

$w = 1/[\sigma^2(F_o^2) + (0.0163P)^2 + 4.6062P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 1.10$ e Å^{-3}
$\Delta\rho_{min} = -0.44$ e Å^{-3}

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}
C1	0.1795 (2)	0.2005 (4)	0.33571 (13)	0.0204 (6)
C2	0.1524 (2)	0.1513 (4)	0.27097 (13)	0.0187 (6)
C3	0.0612 (2)	0.1987 (5)	0.24969 (14)	0.0253 (7)
H3	0.0170	0.2563	0.2759	0.030*
C4	0.0363 (2)	0.1603 (5)	0.18965 (13)	0.0231 (7)
H4	−0.0247	0.1919	0.1756	0.028*
C5	0.1021 (2)	0.0744 (4)	0.15012 (12)	0.0148 (5)
C6	0.1935 (2)	0.0297 (5)	0.17129 (14)	0.0223 (6)
H6	0.2382	−0.0253	0.1449	0.027*
C7	0.2183 (2)	0.0667 (5)	0.23162 (14)	0.0242 (7)
H7	0.2792	0.0348	0.2457	0.029*
C8	0.3754 (2)	0.5305 (4)	0.46896 (15)	0.0202 (6)
C9	0.4829 (2)	0.5423 (5)	0.46975 (14)	0.0238 (7)
H9A	0.5034	0.6766	0.4660	0.029*
H9B	0.5095	0.4688	0.4358	0.029*
C10	0.0752 (2)	0.0328 (4)	0.08488 (12)	0.0126 (5)
O1	0.25854 (17)	0.1379 (4)	0.35567 (9)	0.0256 (5)
O2	0.12255 (18)	0.3032 (3)	0.36600 (10)	0.0274 (5)
O3	0.33421 (15)	0.3741 (3)	0.45414 (10)	0.0200 (4)
O4	0.32547 (15)	0.6772 (3)	0.48303 (9)	0.0178 (4)
O5	0.13755 (15)	−0.0398 (3)	0.05016 (9)	0.0173 (4)
O6	−0.00860 (15)	0.0752 (3)	0.06791 (9)	0.0184 (4)
Tb1	0.331426 (9)	0.019240 (18)	0.445275 (6)	0.01157 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0303 (17)	0.0194 (14)	0.0114 (13)	−0.0055 (12)	−0.0067 (12)	−0.0008 (12)
C2	0.0266 (16)	0.0182 (14)	0.0113 (13)	0.0008 (12)	−0.0074 (12)	−0.0024 (11)
C3	0.0226 (16)	0.0388 (19)	0.0146 (14)	0.0067 (13)	−0.0006 (12)	−0.0092 (14)
C4	0.0151 (14)	0.0381 (18)	0.0162 (14)	0.0072 (13)	−0.0058 (12)	−0.0084 (13)
C5	0.0169 (13)	0.0180 (13)	0.0094 (12)	−0.0011 (11)	−0.0012 (10)	−0.0023 (11)

C6	0.0173 (14)	0.0318 (17)	0.0179 (15)	0.0030 (12)	−0.0059 (11)	−0.0072 (13)
C7	0.0241 (16)	0.0305 (17)	0.0180 (14)	0.0078 (13)	−0.0104 (12)	−0.0039 (13)
C8	0.0167 (14)	0.0154 (14)	0.0285 (16)	0.0013 (11)	−0.0058 (12)	−0.0014 (12)
C9	0.0238 (16)	0.0236 (16)	0.0240 (16)	−0.0028 (12)	−0.0007 (13)	0.0018 (13)
C10	0.0161 (13)	0.0135 (13)	0.0082 (12)	−0.0042 (10)	−0.0014 (10)	0.0017 (10)
O1	0.0288 (12)	0.0363 (13)	0.0116 (9)	−0.0006 (10)	−0.0090 (9)	0.0023 (9)
O2	0.0365 (14)	0.0298 (12)	0.0159 (10)	0.0018 (10)	−0.0071 (10)	−0.0108 (10)
O3	0.0136 (10)	0.0126 (9)	0.0338 (12)	0.0003 (8)	−0.0069 (9)	−0.0015 (9)
O4	0.0175 (10)	0.0150 (9)	0.0209 (10)	0.0014 (8)	−0.0025 (8)	−0.0017 (8)
O5	0.0184 (10)	0.0253 (11)	0.0083 (9)	0.0039 (8)	0.0010 (7)	0.0000 (8)
O6	0.0134 (10)	0.0294 (11)	0.0123 (9)	−0.0010 (9)	−0.0036 (8)	−0.0009 (8)
Tb1	0.01146 (7)	0.01367 (7)	0.00960 (7)	−0.00056 (5)	−0.00011 (5)	−0.00135 (5)

Geometric parameters (Å, º)

C1—O2	1.252 (4)	C9—H9A	0.9700
C1—O1	1.261 (4)	C9—H9B	0.9700
C1—C2	1.503 (4)	C10—O5	1.257 (3)
C2—C7	1.386 (4)	C10—O6	1.260 (3)
C2—C3	1.393 (4)	O1—Tb1	2.352 (2)
C3—C4	1.382 (4)	O2—Tb1^{i}	2.370 (2)
C3—H3	0.9300	O3—Tb1	2.447 (2)
C4—C5	1.391 (4)	O3—Tb1^{i}	2.524 (2)
C4—H4	0.9300	O4—Tb1^{iii}	2.492 (2)
C5—C6	1.392 (4)	O4—Tb1^{i}	2.578 (2)
C5—C10	1.501 (4)	O5—Tb1^{iv}	2.3359 (19)
C6—C7	1.386 (4)	O6—Tb1^{v}	2.283 (2)
C6—H6	0.9300	Tb1—O6^{vi}	2.283 (2)
C7—H7	0.9300	Tb1—O5^{vii}	2.3359 (19)
C8—O3	1.261 (4)	Tb1—O2^{viii}	2.370 (2)
C8—O4	1.263 (4)	Tb1—O4^{ix}	2.492 (2)
C8—C9	1.501 (4)	Tb1—O3^{viii}	2.524 (2)
C8—Tb1^{i}	2.932 (3)	Tb1—O4^{viii}	2.578 (2)
C9—C9^{ii}	1.521 (6)	Tb1—C8^{viii}	2.932 (3)
O2—C1—O1	124.4 (3)	C8—O4—Tb1^{iii}	130.8 (2)
O2—C1—C2	117.7 (3)	C8—O4—Tb1^{i}	93.10 (17)
O1—C1—C2	117.9 (3)	Tb1^{iii}—O4—Tb1^{i}	108.64 (7)
C7—C2—C3	119.8 (3)	C10—O5—Tb1^{iv}	134.11 (18)
C7—C2—C1	120.7 (3)	C10—O6—Tb1^{v}	154.76 (19)
C3—C2—C1	119.4 (3)	O6^{vi}—Tb1—O5^{vii}	86.13 (7)
C4—C3—C2	120.1 (3)	O6^{vi}—Tb1—O1	105.02 (8)
C4—C3—H3	120.0	O5^{vii}—Tb1—O1	151.11 (8)
C2—C3—H3	120.0	O6^{vi}—Tb1—O2^{viii}	75.44 (8)
C3—C4—C5	120.3 (3)	O5^{vii}—Tb1—O2^{viii}	134.79 (8)
C3—C4—H4	119.8	O1—Tb1—O2^{viii}	74.10 (9)
C5—C4—H4	119.8	O6^{vi}—Tb1—O3	80.00 (7)
C4—C5—C6	119.5 (3)	O5^{vii}—Tb1—O3	81.91 (7)

C4—C5—C10	120.4 (3)	O1—Tb1—O3	74.17 (8)
C6—C5—C10	120.2 (3)	O2^{viii}—Tb1—O3	132.69 (8)
C7—C6—C5	120.3 (3)	O6^{vi}—Tb1—O4^{ix}	103.49 (7)
C7—C6—H6	119.9	O5^{vii}—Tb1—O4^{ix}	74.84 (7)
C5—C6—H6	119.9	O1—Tb1—O4^{ix}	126.02 (8)
C6—C7—C2	120.1 (3)	O2^{viii}—Tb1—O4^{ix}	70.12 (8)
C6—C7—H7	120.0	O3—Tb1—O4^{ix}	156.11 (7)
C2—C7—H7	120.0	O6^{vi}—Tb1—O3^{viii}	166.21 (7)
O3—C8—O4	119.4 (3)	O5^{vii}—Tb1—O3^{viii}	96.79 (7)
O3—C8—C9	120.2 (3)	O1—Tb1—O3^{viii}	78.76 (8)
O4—C8—C9	120.3 (3)	O2^{viii}—Tb1—O3^{viii}	93.23 (8)
O3—C8—Tb1^{i}	58.93 (15)	O3—Tb1—O3^{viii}	113.73 (5)
O4—C8—Tb1^{i}	61.42 (15)	O4^{ix}—Tb1—O3^{viii}	64.62 (7)
C9—C8—Tb1^{i}	170.4 (2)	O6^{vi}—Tb1—O4^{viii}	143.04 (7)
C8—C9—C9^{ii}	107.6 (3)	O5^{vii}—Tb1—O4^{viii}	79.52 (7)
C8—C9—H9A	110.2	O1—Tb1—O4^{viii}	75.72 (8)
C9^{ii}—C9—H9A	110.2	O2^{viii}—Tb1—O4^{viii}	136.68 (8)
C8—C9—H9B	110.2	O3—Tb1—O4^{viii}	64.43 (7)
C9^{ii}—C9—H9B	110.2	O4^{ix}—Tb1—O4^{viii}	105.25 (6)
H9A—C9—H9B	108.5	O3^{viii}—Tb1—O4^{viii}	50.58 (6)
O5—C10—O6	123.8 (2)	O6^{vi}—Tb1—C8^{viii}	168.43 (8)
O5—C10—C5	118.4 (2)	O5^{vii}—Tb1—C8^{viii}	90.44 (8)
O6—C10—C5	117.8 (2)	O1—Tb1—C8^{viii}	73.28 (9)
C1—O1—Tb1	141.6 (2)	O2^{viii}—Tb1—C8^{viii}	114.33 (9)
C1—O2—Tb1^{i}	124.6 (2)	O3—Tb1—C8^{viii}	88.58 (7)
C8—O3—Tb1	151.30 (19)	O4^{ix}—Tb1—C8^{viii}	86.20 (8)
C8—O3—Tb1^{i}	95.72 (17)	O3^{viii}—Tb1—C8^{viii}	25.35 (7)
Tb1—O3—Tb1^{i}	111.92 (8)	O4^{viii}—Tb1—C8^{viii}	25.48 (7)

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