metal-organic compounds

Poly[bis(μ4-benzene-1,4-dicarboxylato)-(μ4-succinato)diterbium(III)]

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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).
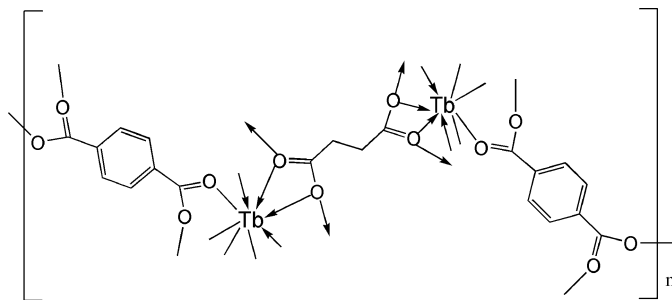
Experimental

Crystal data

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

Data collection

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

Refinement

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

References

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supplementary materials

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

C.-H. Yu

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-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.

Experimental

A mixture of 1,4-H$_2$bdc (0.5 mmol), H$_2$suc (0.5 mmol), NaOH (1 mmol) and TbCl$_3$·6H$_2$O (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.

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).
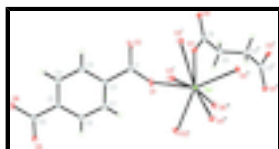
Figures

Fig. 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*.

supplementary materials

Poly[bis(μ$_4$-benzene-1,4-dicarboxylato)(μ$_4$-succinato)diterbium(III)]

Crystal data

[Tb$_2$(C$_4$H$_4$O$_4$)(C$_8$H$_4$O$_4$)$_2$]	$F(000) = 1432$
$M_r = 381.07$	$D_x = 2.418$ Mg m^{-3}
Orthorhombic, *Pbca*	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ac 2ab	Cell parameters from 15551 reflections
$a = 13.948$ (3) Å	$\theta = 3.0–27.5°$
$b = 6.8724$ (14) Å	$\mu = 6.77$ mm^{-1}
$c = 21.844$ (4) Å	$T = 293$ K
$V = 2093.9$ (7) Å^3	Block, colorless
$Z = 8$	$0.29 \times 0.27 \times 0.20$ mm

Data collection

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

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.017$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.041$	H-atom parameters constrained
$S = 1.07$	$w = 1/[\sigma^2(F_o^2) + (0.0163P)^2 + 4.6062P]$ where $P = (F_o^2 + 2F_c^2)/3$
2376 reflections	$(\Delta/\sigma)_{max} = 0.001$
154 parameters	$\Delta\rho_{max} = 1.10$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.44$ 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, °)

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.

Fig. 1