Poly[di-μ4-1,4-benzenedicarboxylato-μ6-succinato-dierbium(III)]

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A three-dimensional coordination polymer, $[Er_2(C_4H_4O_4)(C_8H_4O_4)_2]_n$, has been synthesized under hydrothermal conditions. The coordination polyhedron around the Er atom is a distorted square antiprism; antiprisms are linked into a three-dimensional network by the 1,4-benzenedicarboxylate ligands and succinate anions. The succinate anion is located on a centre of inversion.

Comment

The title compound, (I), is isostructural with its $[M_2(C_4H_4O_4)(C_8H_4O_4)_2]_n$ [M = Gd (Wang & Li, 2005), Dy (Li & Wang, 2005), Nd (Li *et al.*, 2006)] analogues. As depicted in Fig. 1, the Er^{3+} ion is located at the centre of a distorted square antiprismatic geometry and is coordinated by four O atoms from four 1,4-benzenedicarboxylate (BDC) ligands and four O atoms from three succinate anions. The Er—O bond distances range from 2.2203 (18) to 2.5127 (18)Å, with an average of 2.364Å, similar to those found in the previously reported isostructural complexes.

(I)
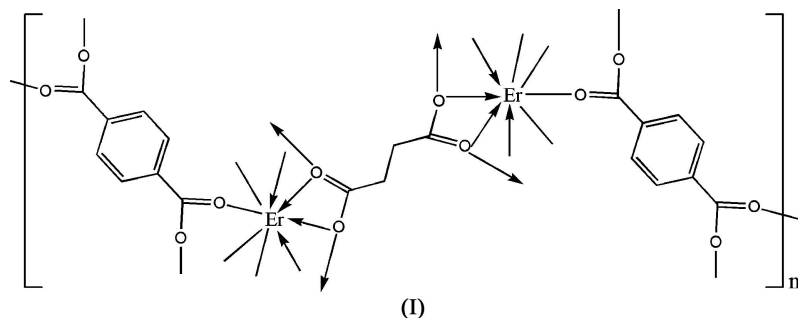
In (I), the succinate ligand is located on an inversion centre and functions as an octadentate ligand, bis-chelating two Er atoms with each O atom bridging to another Er atom; the BDC ligand functions as a tetradentate ligand, bis-bridging four Er atoms. In this mode, the Er^{3+} ions are linked into a two-dimensional polymeric sheet parallel to the (001) plane by the succinate ligands, and a three-dimensional framework is formed *via* bridging BDC ligands.

Experimental

A mixture of $ErCl_3 \cdot 6H_2O$ (1.0 mmol, 0.38 g), 1,4-benzenedicarboxylic acid (1.0 mmol, 0.17 g), succinic acid (0.5 mmol, 0.06 g), NaOH (3.0 ml, 1 M) and H_2O (10.0 ml) was heated in a 23 ml stainless steel reactor with a Teflon liner at 453 K for 48 h. Orange columnar crystals were filtered off and washed with ethanol (yield: 52%, based on Er).

Crystal data

[Er$_2$(C$_4$H$_4$O$_4$)(C$_8$H$_4$O$_4$)$_2$]
$M_r = 778.83$
Orthorhombic, $Pbca$
$a = 13.7859$ (2) Å
$b = 6.7632$ (1) Å
$c = 21.6642$ (3) Å
$V = 2019.90$ (5) Å^3

$Z = 4$
$D_x = 2.561$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 8.32$ mm^{-1}
$T = 295$ (2) K
Column, orange
$0.21 \times 0.14 \times 0.08$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.244$, $T_{max} = 0.518$

11606 measured reflections
2419 independent reflections
2127 reflections with $I > 2\sigma(I)$
$R_{int} = 0.021$
$\theta_{max} = 28.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.016$
$wR(F^2) = 0.045$
$S = 1.04$
2419 reflections
155 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0253P)^2 + 1.5821P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.45$ e Å^{-3}
$\Delta\rho_{min} = -0.68$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.00119 (6)

Table 1
Selected bond lengths (Å).

Er—O1	2.2724 (18)	Er—O5	2.4622 (18)
Er—O2^i	2.2203 (18)	Er—O5^{iv}	2.393 (2)
Er—O3^{ii}	2.2888 (17)	Er—O6	2.5127 (18)
Er—O4^{iii}	2.3077 (18)	Er—O6^v	2.4541 (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) $-x+\frac{3}{2}, y-\frac{1}{2}, z$.

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

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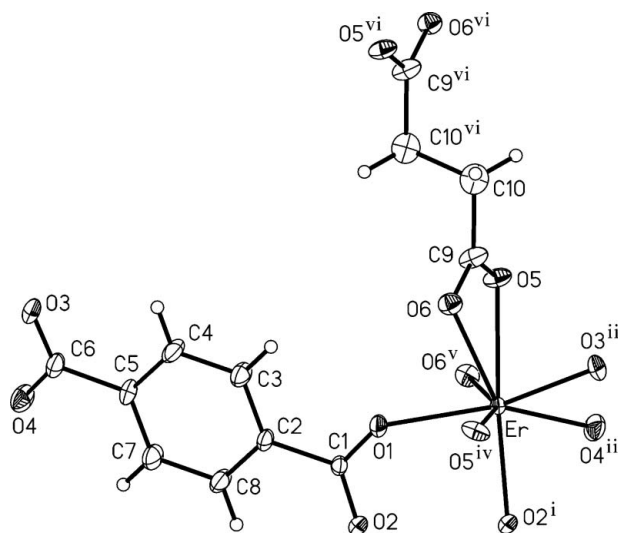

Figure 1
The coordination environment of the Er atom in (I), showing the atom-numbering scheme and displacement ellipsoids drawn at the 50% probability level. [Symmetry codes: (i) $2-x, 2-y, 1-z$; (ii) $\frac{3}{2}-x, 2-y, z-\frac{1}{2}$; (iii) $x, \frac{3}{2}-y, z-\frac{1}{2}$; (iv) $\frac{3}{2}-x, \frac{1}{2}+y, z$; (v) $\frac{3}{2}-x, y-\frac{1}{2}, z$; (vi) $1-x, 2-y, 1-z$.]

SHELXTL (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

References

Bruker (1998). *SMART* (Version 5.16), *SAINT* (Version 6.01) and *SHELXTL* (Version 6.14). Bruker AXS Inc., Madison, Wisconsin, USA.
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.