Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Poly[di-μ_4-1,4-benzenedicarboxylato-μ_6-succinato-didysprosium(III)]

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Key indicators

Single-crystal X-ray study
T = 291 K
Mean σ(C–C) = 0.004 Å
R factor = 0.021
wR factor = 0.060
Data-to-parameter ratio = 15.8

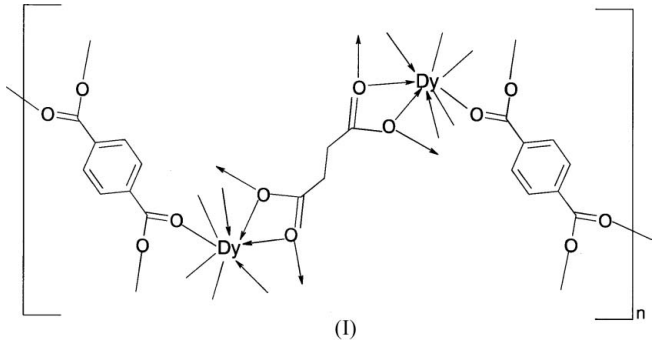
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

A new three-dimensional coordination polymer, $[Dy_2(C_4H_4O_4)(C_8H_4O_4)_2]_n$, has been synthesized under hydrothermal conditions. The coordination of the Dy atoms is distorted square antiprismatic. The antiprisms are bridged by the 1,4-benzenedicarboxylate and succinate ligands, forming a three-dimensional network. The succinate ion is located on an inversion center.

Received 7 November 2005
Accepted 18 November 2005
Online 26 November 2005

Comment

The title compound, (I), is isostructural with $[Gd_2(C_4H_4O_4)(C_8H_4O_4)_2]_n$ (Wang & Li, 2005). As depicted in Fig. 1, the Dy^{3+} ion is located at the center of a distorted square antiprism and is coordinated by four O atoms from four 1,4-benzenedicarboxylate (BDC) ligands and four O atoms from three succinate anions. The Dy—O distances range from 2.237 (2) to 2.5308 (19) Å. The Dy atoms are bridged by the succinate ligands, each of which lies on an inversion center, forming two-dimensional polymeric sheets parallel to the *ab* plane. These sheets are in turn bridged *via* BDC ligands, forming a three-dimensional framework.



(I)

Experimental

A mixture of $DyCl_3{\cdot}6H_2O$ (1.00 mmol, 0.38 g), 1,4-benzenedicarboxylic acid (0.50 mmol, 0.08 g), succinic acid (0.50 mmol, 0.06 g), NaOH (2.00 mmol, 0.08 g) and H_2O (10.0 ml) was heated in a 23 ml stainless steel reactor with a Teflon liner at 443 K for 48 h. On cooling, it was found that colorless column-like crystals had formed. These were filtered off and washed with water and acetone (yield 46%, based on Dy).

Crystal data

$[Dy_2(C_4H_4O_4)(C_8H_4O_4)_2]$
M_r = 769.30
Orthorhombic, *Pbca*
a = 13.8042 (9) Å
b = 6.7910 (4) Å
c = 21.7163 (13) Å
V = 2035.8 (2) Å^3
Z = 4
D_x = 2.510 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 147 reflections
θ = 3.3–26.7°
μ = 7.35 mm^{-1}
T = 291 (2) K
Column, colorless
0.32 × 0.11 × 0.08 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer	2453 independent reflections
φ and ω scans	2290 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$R_{int} = 0.028$
$T_{min} = 0.265$, $T_{max} = 0.563$	$\theta_{max} = 28.1^\circ$
10848 measured reflections	$h = -11 \rightarrow 18$
	$k = -8 \rightarrow 7$
	$l = -28 \rightarrow 28$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0378P)^2 + 2.3787P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.021$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.060$	$\Delta\rho_{max} = 0.85$ e Å^{-3}
$S = 1.01$	$\Delta\rho_{min} = -0.99$ e Å^{-3}
2453 reflections	Extinction correction: *SHELXL97*
155 parameters	Extinction coefficient: 0.00269 (12)
H-atom parameters constrained	

Table 1
Selected bond lengths (Å).

Dy—O2^{i}	2.237 (2)	Dy—O5^{iv}	2.408 (3)
Dy—O1	2.2931 (19)	Dy—O6^{v}	2.463 (2)
Dy—O3^{ii}	2.3093 (18)	Dy—O5	2.480 (2)
Dy—O4^{iii}	2.3305 (19)	Dy—O6	2.5308 (19)

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

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

Data collection: *SMART* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2004); software used to prepare material for publication: *SHELXTL*.

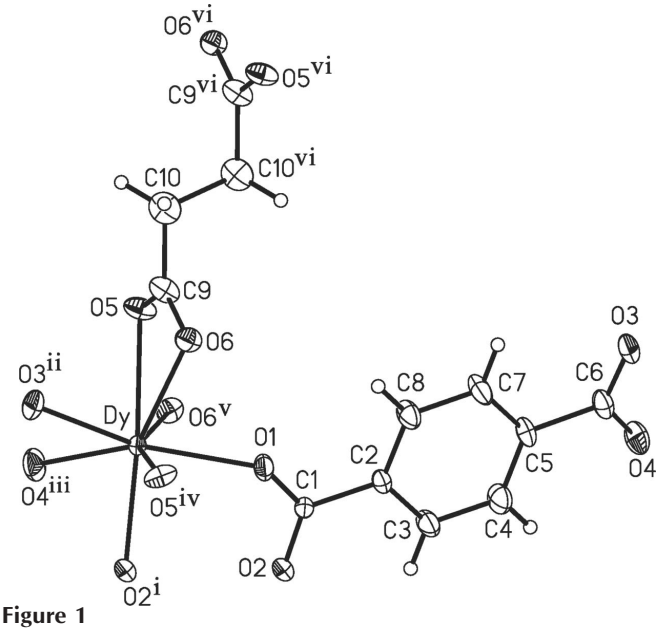


Figure 1
The coordination environment of the Dy atom with the atom-numbering scheme, showing displacement ellipsoids at the 45% probability level [symmetry codes: (i) $-x, -y, 1-z$; (ii) $\frac{1}{2}-x, -y, z-\frac{1}{2}$; (iii) $x, -\frac{1}{2}-y, z-\frac{1}{2}$; (iv) $\frac{1}{2}-x, \frac{1}{2}+y, z$; (v) $\frac{1}{2}-x, y-\frac{1}{2}, z$ (vi) $1-x, -y, 1-z$].

The project was supported by Jiangxi Provincial Educational Foundation (grant No. 2005–146) and Jiangxi University of Science and Technology Foundation (grand No. 2003–1).

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