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Key indicators

Single-crystal X-ray study
 $T = 295$ K
Mean $\sigma(\text{C}-\text{C}) = 0.007$ Å
 R factor = 0.024
 wR factor = 0.061
Data-to-parameter ratio = 13.4For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.Poly[*diaquadi- μ_5 -succinato- μ_6 -succinato-*
didysprosium(III)]

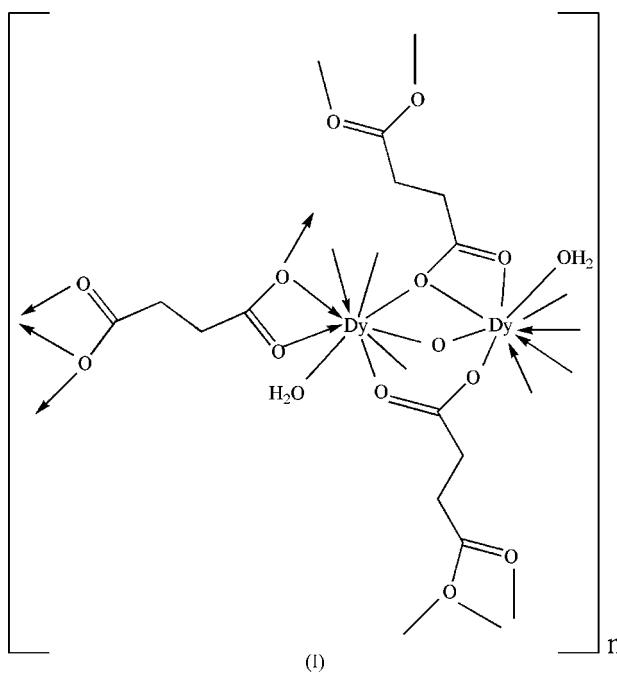
The title compound, $[\text{Dy}_2(\text{C}_4\text{H}_4\text{O}_4)_3(\text{H}_2\text{O})_2]$, has been synthesized under hydrothermal conditions. The asymmetric unit consists of two Dy^{3+} cations, three succinate anions and two aqua ligands. The succinate ligands exhibit *gauche* and *anti* conformations with different coordination modes. The Dy atoms are bridged into a three-dimensional network by succinate ligands.

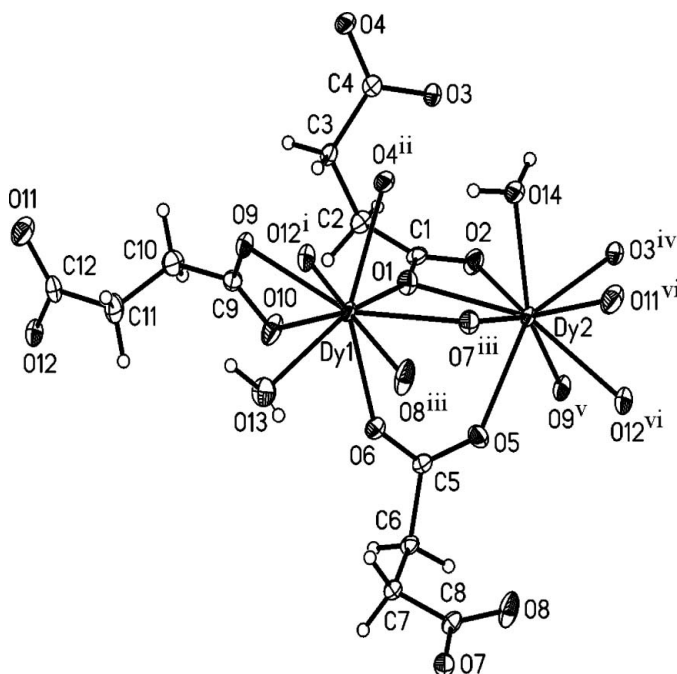
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Comment

The title compound, (I), is almost isostructural with the corresponding cerium complex (Seguatni *et al.*, 2004). The asymmetric unit consists of two Dy^{3+} cations (Dy1 and Dy2), three succinate anions (*L1*: O1–O4/C1–C4; *L2*: O5–O8/C5–C8; *L3*: O9–O12/C9–C12) and two aqua ligands (O13 and O14) (Fig. 1). Bond lengths and angles within the succinate anions exhibit normal values (Fleck, 2002; Serpaggi & Férey, 1999). The Dy atoms are each coordinated by nine O atoms of six succinate anions and one aqua ligand, forming a tricapped trigonal prism, with Dy–O bond lengths in the range 2.323 (3)–2.544 (3) Å (Table 1). The polyhedra are edge-shared, generating one-dimensional infinite chains along the [100] direction. The Dy1...Dy2 separation within the asymmetric unit is 4.028 (5) Å.




Figure 1

A part of the polymeric structure of the title compound, showing 45% probability displacement ellipsoids for non-H atoms. Symmetry codes: (i) $x, 1 + y, z$; (ii) $2 - x, 2 - y, 2 - z$; (iii) $1 - x, 2 - y, 1 - z$; (iv) $1 - x, 2 - y, 2 - z$; (v) $x - 1, y, z$; (vi) $x - 1, 1 + y, z$.

L1 and *L2*, with a *gauche* conformation [$C-C-C-C = 70.5(5)$ and $-89.6(5)^\circ$, respectively], function as chelating-bridging tridentate and bridging bidentate ligands, respectively; (ii) *L3*, with an *anti* conformation, functions as a chelating-bridging tetradentate ligand. Along the [001] direction, polyhedra are linked by the *gauche* dicarboxylate groups into layers parallel to (010) and they are pillared by the *anti* succinate anions, forming a three-dimensional framework.

The aqua ligands participate in extensive hydrogen-bonding interactions. Each water molecule forms hydrogen bonds to two carboxylate O atoms (Table 2), which make a significant contribution to the stability of the crystal structure.

Experimental

A mixture of $DyCl_3 \cdot 6H_2O$ (1.00 mmol, 0.38 g), succinic acid (1.00 mmol, 0.12 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. The colourless column-like crystals were filtered off and washed with water and acetone (yield 32%, based on Dy).

Crystal data

$[Dy_2(C_4H_4O_4)_3(H_2O)_2]$

$M_r = 709.25$

Triclinic, $P\bar{1}$

$a = 7.646(2) \text{ \AA}$

$b = 8.041(2) \text{ \AA}$

$c = 14.086(4) \text{ \AA}$

$\alpha = 96.915(4)^\circ$

$\beta = 97.004(4)^\circ$

$\gamma = 103.057(4)^\circ$

$V = 827.6(4) \text{ \AA}^3$

$Z = 2$

$D_x = 2.846 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation

Cell parameters from 256 reflections

$\theta = 3.3\text{--}26.7^\circ$

$\mu = 9.04 \text{ mm}^{-1}$

$T = 295(2) \text{ K}$

Needle, colourless

$0.18 \times 0.08 \times 0.06 \text{ mm}$

Data collection

Bruker SMART APEXII CCD

area-detector diffractometer

φ and ω scans

Absorption correction: multi-scan

(*SADABS*; Sheldrick, 1996)

$T_{\min} = 0.425, T_{\max} = 0.586$

4877 measured reflections

3413 independent reflections

2840 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.018$

$\theta_{\text{max}} = 26.9^\circ$

$h = -9 \rightarrow 10$

$k = -8 \rightarrow 10$

$l = -18 \rightarrow 17$

Refinement

Refinement on F^2

$R[F^2 > 2\sigma(F^2)] = 0.024$

$wR(F^2) = 0.061$

$S = 0.96$

3413 reflections

254 parameters

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.038P)^2]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} = 0.001$

$\Delta\rho_{\text{max}} = 1.19 \text{ e \AA}^{-3}$

$\Delta\rho_{\text{min}} = -1.49 \text{ e \AA}^{-3}$

Extinction correction: *SHELXL97*

Extinction coefficient: 0.0016 (2)

Table 1

Selected bond lengths (\AA).

Dy1—O1	2.361 (3)	Dy2—O1	2.544 (3)
Dy1—O4 ⁱ	2.439 (3)	Dy2—O2	2.430 (3)
Dy1—O6	2.332 (3)	Dy2—O3 ^{iv}	2.323 (3)
Dy1—O7 ⁱⁱ	2.488 (3)	Dy2—O5	2.377 (3)
Dy1—O8 ⁱⁱⁱ	2.440 (3)	Dy2—O7 ⁱⁱ	2.400 (3)
Dy1—O9	2.454 (3)	Dy2—O9 ^v	2.408 (3)
Dy1—O10	2.435 (4)	Dy2—O11 ^{vi}	2.453 (4)
Dy1—O12 ⁱⁱⁱ	2.436 (3)	Dy2—O12 ^{vi}	2.515 (3)
Dy1—O13	2.423 (3)	Dy2—O14	2.376 (3)

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

Table 2

Hydrogen-bond geometry ($\text{\AA}, ^\circ$).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O13—H13A \cdots O5 ^{vii}	0.85	1.97	2.816 (6)	173
O13—H13B \cdots O6	0.85	2.11	2.959 (6)	179
O14—H14A \cdots O4 ⁱ	0.85	2.01	2.843 (5)	166
O14—H14B \cdots O2 ^{iv}	0.85	1.89	2.733 (4)	173

Symmetry codes: (i) $-x + 2, -y + 2, -z + 2$; (iv) $-x + 1, -y + 2, -z + 2$; (vii) $x + 1, y, z$.

H atoms of methylene groups were included at calculated positions and treated as riding atoms, with C—H distances constrained to 0.97 \AA and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. The water H atoms were found in a difference map and refined with an O—H distance restraint of 0.85 (1) \AA and with $U_{\text{iso}}(\text{H}) = 0.05 \text{ \AA}^2$. The highest peak is located 0.87 \AA from atom Dy1 and the deepest hole 0.98 \AA from Dy2.

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*.

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