

# Poly[di-aqua-di- $\mu_6$ -succinato- $\mu_5$ -succinato-dierbium(III)]

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**Key indicators**

Single-crystal X-ray study  
 T = 298 K  
 Mean  $\sigma(\text{C}-\text{C}) = 0.010 \text{ \AA}$   
 R factor = 0.039  
 wR factor = 0.104  
 Data-to-parameter ratio = 13.2

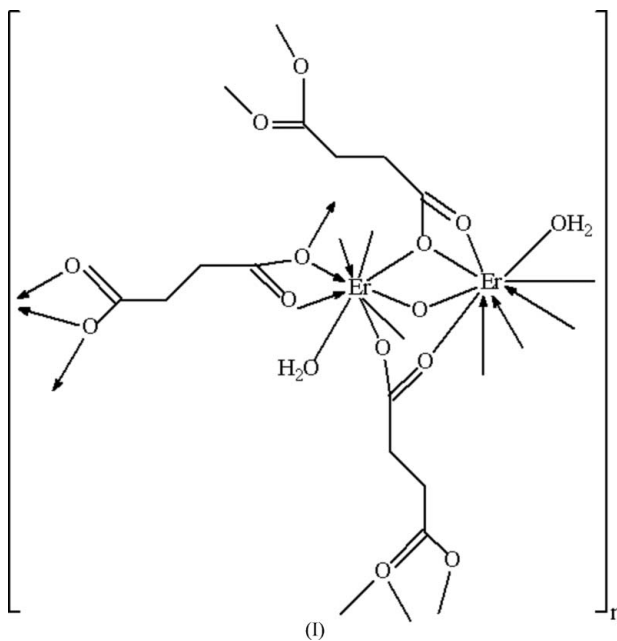
For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

In the title compound,  $[\text{Er}_2(\text{C}_4\text{H}_4\text{O}_4)_3(\text{H}_2\text{O})_2]_n$ , the asymmetric unit consists of two  $\text{Er}^{\text{III}}$  cations, three succinate anions and two coordinated water molecules. Both  $\text{Er}^{\text{III}}$  ions are in a tricapped trigonal-prismatic coordination environment. The Er atoms are bridged into a three-dimensional framework by succinate anions, which exhibit *anti* and *gauche* conformations with different coordination modes. The crystal structure is stabilized by  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bonds [ $\text{O}\cdots\text{O} = 2.715(8)-2.936(8) \text{ \AA}$ ].

Received 28 February 2006  
 Accepted 4 March 2006

**Comment**

The use of lanthanide metals with multifunctional carboxylic acids in assembling metal-organic frameworks has experienced an upsurge in recent years (Bünzli & Piguet, 2002), due to their variety of intriguing structural topologies and special magnetic, catalytic and luminescent properties. Some polymeric complexes, containing the lanthanide cations europium, gadolinium, dysprosium and cerium, in which the succinate acid ligand exhibits interesting behavior owing to its conformational flexibility and coordination diversity, have been synthesized and structurally investigated (Cui *et al.*, 2005; Fleck, 2002; Perles *et al.*, 2003, 2004; Seguatni *et al.*, 2004; Serpaggi *et al.*, 1999; Serpaggi & Férey, 1999; Zhou *et al.*, 2005; Wang *et al.*, 2006).



The asymmetric unit of the title compound, (I), contains two  $\text{Er}^{3+}$  cations, three succinate anions and two coordinated

water molecules. The Er atoms are each coordinated by nine O atoms of six succinate anions and one aqua ligand, forming a tricapped trigonal prism (Fig. 1). The bond lengths and angles compare well with those found in poly[[[triaquarerbium(III)]- $\mu_3$ -succinato] chloride dihydrate] (Nika *et al.*, 2005).

The three independent succinate anions may be divided into two groups according to their conformation and coordination mode: (i) the O1–O4/C1–C4 anion, with an *anti* conformation [C4–C3–C2–C1 = 179.0 (6)°], functions as a chelating–bridging ligand; (ii) the O5–O8/C5–C8 and O9–O12/C9–C12 anions, with *gauche* conformations [C8–C7–C6–C5 = –68.8 (8)° and C12–C11–C10–C9 = 75.9 (7)°], function as both chelating–bridging and bridging ligands. The polyhedra are linked by the *gauche* dicarboxylate groups into layers parallel to the *ac* plane, which are interconnected by the *anti* succinate anions, forming a three-dimensional framework.

The carboxylate groups of the bridging succinate ligands form O–H $\cdots$ O hydrogen bonds to coordinated water molecules (Table 2).

## Experimental

A mixture of Er(NO<sub>3</sub>)<sub>3</sub>·*n*H<sub>2</sub>O (1 mmol), succinic acid (118 mg, 1 mmol) and isonicotinic acid (124 mg, 1 mmol) in H<sub>2</sub>O–C<sub>2</sub>H<sub>5</sub>OH (12 ml, 5:1) was placed in a Teflon-lined stainless vessel and heated to 433 K for 72 h. The reaction system was then cooled to room temperature over a period of 24 h, giving red crystals, which were collected and washed with water (yield 0.0791 g, 29% based on Er). Analysis calculated for C<sub>12</sub>H<sub>16</sub>Er<sub>2</sub>O<sub>14</sub>: C 20.05, H 2.24%; found: C 19.86, H 2.13%.

### Crystal data

[Er <sub>2</sub> (C <sub>4</sub> H <sub>4</sub> O <sub>4</sub> ) <sub>3</sub> (H <sub>2</sub> O) <sub>2</sub> ]	Z = 2
<i>M<sub>r</sub></i> = 718.77	<i>D<sub>x</sub></i> = 2.816 Mg m <sup>–3</sup>
Triclinic, <i>P</i> 1	Mo <i>K</i> α radiation
<i>a</i> = 7.5576 (17) Å	Cell parameters from 1045 reflections
<i>b</i> = 8.4054 (18) Å	$\theta$ = 3.5–25.5°
<i>c</i> = 13.795 (3) Å	$\mu$ = 9.91 mm <sup>–1</sup>
$\alpha$ = 96.672 (3)°	<i>T</i> = 298 (2) K
$\beta$ = 98.394 (3)°	Block, red
$\gamma$ = 98.975 (3)°	0.25 × 0.18 × 0.10 mm
<i>V</i> = 847.6 (3) Å <sup>3</sup>	

### Data collection

Bruker SMART CCD area-detector diffractometer	3559 independent reflections
$\varphi$ and $\omega$ scans	3134 reflections with <i>I</i> > 2σ( <i>I</i> )
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	<i>R</i> <sub>int</sub> = 0.037
<i>T</i> <sub>min</sub> = 0.131, <i>T</i> <sub>max</sub> = 0.371	$\theta$ <sub>max</sub> = 27.1°
4914 measured reflections	<i>h</i> = –7 → 9
	<i>k</i> = –10 → 10
	<i>l</i> = –16 → 17

### Refinement

Refinement on <i>F</i> <sup>2</sup>	$w = 1/[\sigma^2(F_o^2) + (0.0489P)^2]$
$R[F^2 > 2\sigma(F^2)] = 0.039$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.104$	( $\Delta/\sigma$ ) <sub>max</sub> = 0.014
<i>S</i> = 1.02	$\Delta\rho$ <sub>max</sub> = 2.05 e Å <sup>–3</sup>
3559 reflections	$\Delta\rho$ <sub>min</sub> = –2.35 e Å <sup>–3</sup>
270 parameters	Extinction correction: SHELXTL
H atoms treated by a mixture of independent and constrained refinement	Extinction coefficient: 0.0027 (4)

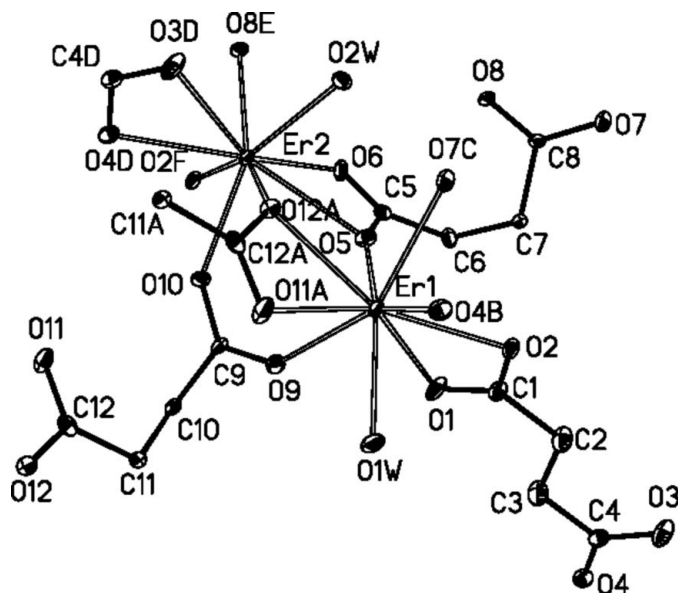


Figure 1

The local coordination environments of the Er<sup>III</sup> ions and succinate ligands in (I). Displacement ellipsoids are drawn at the 50% probability level. The atom-numbering scheme of the asymmetric unit is shown, together with symmetry-equivalent atoms [symmetry codes: (A) 1 – *x*, –*y*, 2 – *z*; (B) *x*, *y* – 1, *z*; (C) –*x*, –*y*, 1 – *z*; (D) *x* + 1, *y* – 1, *z*; (E) 1 – *x*, –*y*, 1 – *z*; (F) 1 + *x*, *y*, *z*]. H atoms have been omitted for clarity.

Table 1

Selected bond lengths (Å).

O2W–Er2	2.334 (5)	Er2–O2 <sup>vi</sup>	2.383 (5)
O12–Er2 <sup>i</sup>	2.366 (5)	Er2–O6	2.415 (5)
O12–Er1 <sup>i</sup>	2.457 (5)	Er2–O5	2.570 (5)
O11–Er1 <sup>i</sup>	2.428 (5)	Er1–O9	2.293 (5)
O3–Er2 <sup>ii</sup>	2.452 (5)	Er1–O5	2.306 (5)
O4–Er1 <sup>iii</sup>	2.437 (5)	Er1–O1W	2.385 (6)
O7–Er1 <sup>iv</sup>	2.459 (5)	Er1–O2	2.389 (5)
O8–Er2 <sup>v</sup>	2.291 (5)	Er1–O1	2.477 (5)
Er2–O10	2.337 (5)		

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

Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> –H $\cdots$ <i>A</i>	<i>D</i> –H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> –H $\cdots$ <i>A</i>
O1W–H1WB $\cdots$ O10 <sup>vii</sup>	0.84 (3)	2.10 (5)	2.853 (7)	149 (7)
O1W–H1WB $\cdots$ O11 <sup>vii</sup>	0.84 (3)	2.43 (7)	2.936 (8)	120 (7)
O2W–H2WA $\cdots$ O7 <sup>iv</sup>	0.83 (5)	1.98 (5)	2.784 (7)	163 (7)
O2W–H2WB $\cdots$ O6 <sup>v</sup>	0.84 (5)	1.87 (5)	2.715 (8)	178 (11)

Symmetry codes: (iv) –*x*, –*y*, –*z* + 1; (v) –*x* + 1, –*y*, –*z* + 1; (vii) *x* – 1, *y*, *z*.

Water H atoms were located in a difference Fourier map and refined isotropically, with O–H and H $\cdots$ H distance restraints of 0.84 (2) and 1.37 (2) Å, respectively. The methylene H atoms were placed in calculated positions and constrained to ride on their parent atoms, with C–H distances of 0.97 Å and *U*<sub>iso</sub>(H) = 1.2*U*<sub>eq</sub>(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:

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

The authors thank Hebei Polytechnic University and Hebei Normal University for supporting this work.

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