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Poly[[[triaquaerbium(III)]-μ_3-succinato] chloride dihydrate]

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The title compound, $\{[\mathrm{Er}(\mathrm{C_4H_4O_4})(\mathrm{H_2O})_3]\mathrm{Cl}\cdot 2\mathrm{H_2O}\}_n$, crystallizes with an infinite polymeric structure, in which erbium(III) ions on twofold rotation axes are bridged by centrosymmetric succinate dianions. The carboxylate groups of the dicarboxylate coordinate in a tridentate-bridging manner to the otherwise water-coordinated $\mathrm{Er^{III}}$ ion. The structure is completed by $\mathrm{Cl^-}$ anions and uncoordinated water molecules.

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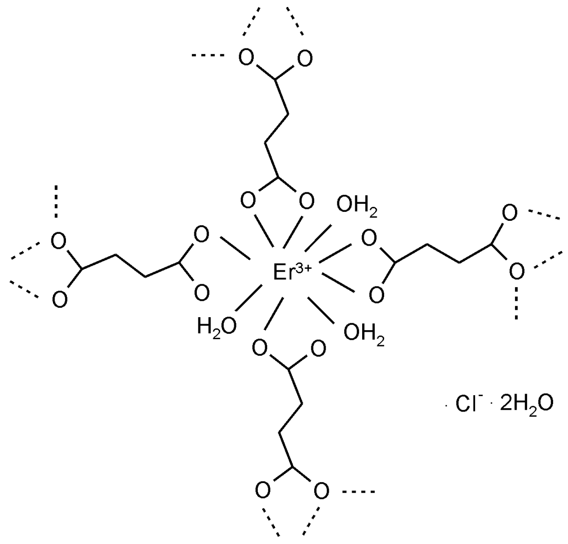
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.020
wR factor = 0.051
Data-to-parameter ratio = 14.7

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

Comment

The structural principles and design of coordination polymers for special applications have been the subject of numerous studies (Kitagawa *et al.*, 2004; Rao *et al.*, 2004). We have been especially interested in rare earth mono- and α,ω-dicarboxylates and those with mixed anions. In the course of this work, we have obtained the title compound, (I), $[\mathrm{Er(Succ)(H_2O)_3}]\mathrm{Cl}\cdot 2\mathrm{H_2O}$, where Succ is succinate (Nika, 2003).



(I)

Compound (I) forms a three-dimensional infinite network. The $\mathrm{Er^{III}}$ ion (on a twofold rotation axis) is coordinated by three water molecules, one of which also lies on this axis, and, in addition, by six O atoms of four different succinate anions (Fig. 1). These succinate anions themselves connect the $\mathrm{Er^{III}}$ ions, in a tridentate-bridging manner, to form infinite chains parallel to [001]. A crystallographic inversion centre is found midway between pairs of bridged Er atoms, and another at the centre of each succinate ligand.

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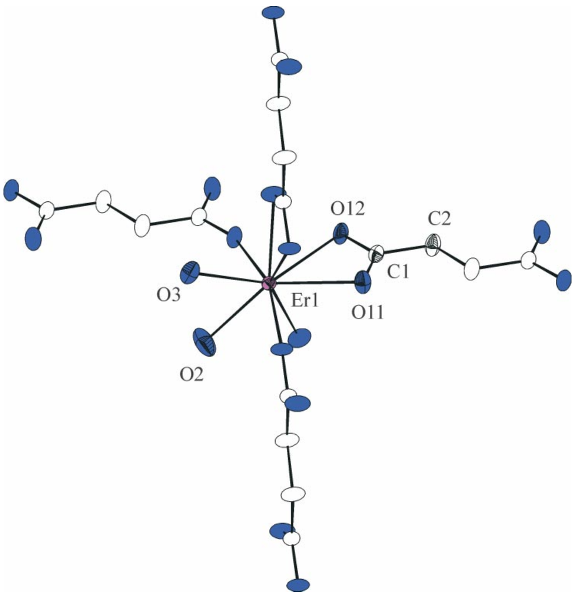

Figure 1
A perspective view of the local coordination environment of the Er atom in (I), with the atom-labelling scheme. Displacement ellipsoids are drawn at the 70% probability level. Symmetry-related atoms are drawn as empty ellipsoids. H atoms, solvent water molecules (O4) and Cl^- anions have been omitted for clarity.

The succinate ligands are planar and are oriented orthogonal to each other. In consequence, the Er-succinate chains are connected *via* succinate anions to give a three-dimensional network. The shortest distance between Er^{III} cations within a chain is 4.121 (2) Å. The Er—O distances range from 2.291 (2) to 2.652 (2) Å. The C—O and C—C distances and the O—C—O and O—C—C angles all lie in the expected ranges.

The connection of the Er—O chains through the succinate anions leads to the formation of channels running along [001], which are filled with uncoordinated water molecules [O4···Er1 4.554 (4) Å] and Cl^- anions [Cl1···Er1 5.063 (2) Å] (Fig. 2). The Cl^- anions are involved in hydrogen bonding (Table 2). Additional hydrogen bonds are observed between aqua ligands (O2 and O3) as donors, and uncoordinated water molecules (O4) and the carboxylic O atoms (O11) as acceptors.

Experimental

Compound (I) was prepared by dissolving $ErCl_3{\cdot}6H_2O$ (0.38 g, 1 mmol) and succinic acid (0.12 g, 1 mmol) in water (50 ml). Light pink crystals were obtained after a few days by slow evaporation of the solvent under ambient conditions.

Crystal data

$[Er(C_4H_4O_4)(H_2O)_3]Cl{\cdot}2H_2O$
$M_r = 408.86$
Monoclinic, $C2/c$
$a = 13.047$ (2) Å
$b = 11.6893$ (14) Å
$c = 7.8244$ (12) Å
$\beta = 109.954$ (17)°
$V = 1121.6$ (3) Å^3
$Z = 4$
$D_x = 2.421$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5000 reflections
$\theta = 2.4$–28.0°
$\mu = 7.75$ mm^{-1}
$T = 293$ (2) K
Block, light pink
0.2 × 0.15 × 0.1 mm

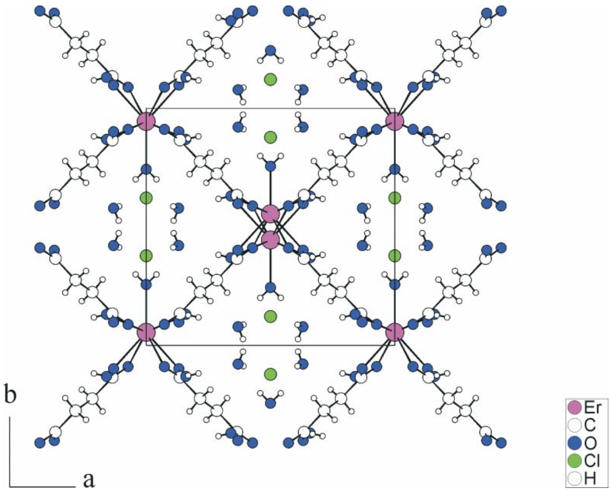

Figure 2
The unit-cell contents, in a view along the crystallographic c axis.

Data collection

Stoe IPDS-I diffractometer
φ scans
Absorption correction: numerical, [*X-RED* (Stoe & Cie, 2001); crystal shape optimized by *X-SHAPE* (Stoe & Cie, 1999)]
$T_{min} = 0.308$, $T_{max} = 0.370$
6684 measured reflections
1348 independent reflections
1234 reflections with $I > 2\sigma(I)$
$R_{int} = 0.039$
$\theta_{max} = 28.0°$
$h = -17 \rightarrow 17$
$k = -15 \rightarrow 15$
$l = -10 \rightarrow 10$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.020$
$wR(F^2) = 0.051$
$S = 1.12$
1348 reflections
92 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0329P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.08$ e Å^{-3}
$\Delta\rho_{min} = -0.77$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 1997)
Extinction coefficient: 0.0022 (2)

Table 1
Selected geometric parameters (Å, °).

Er1—O12^{i}	2.289 (3)	C1—O11	1.254 (5)
Er1—O2	2.344 (4)	C1—O12	1.280 (4)
Er1—O3	2.367 (3)	C1—C2	1.513 (5)
Er1—O11	2.423 (3)	C2—C2^{ii}	1.518 (7)
Er1—O12	2.654 (3)		
O11—C1—O12	119.1 (3)	C1—C2—C2^{ii}	114.8 (4)

Symmetry codes: (i) $x, -y, z-\frac{1}{2}$; (ii) $-x+\frac{5}{2}, -y-\frac{1}{2}, -z+2$.

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O2—H3···O4^{iii}	0.809 (19)	2.03 (2)	2.825 (5)	165 (5)
O4—H4···Cl1^{iv}	0.81 (2)	2.32 (3)	3.120 (4)	167 (8)
O4—H5···Cl1^{v}	0.81 (2)	2.31 (2)	3.118 (4)	171 (8)
O3—H6···O11^{vi}	0.82 (2)	1.97 (3)	2.742 (4)	157 (7)
O3—H7···O4	0.80 (2)	1.91 (2)	2.707 (5)	170 (5)

Symmetry codes: (iii) $x+\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$; (iv) $x-\frac{1}{2}, y+\frac{1}{2}, z$; (v) $-x+\frac{3}{2}, -y-\frac{1}{2}, -z+1$; (vi) $-x+2, -y, -z+1$.

The methylene H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H distances of 0.97 Å and U_{iso}(H) = 0.042 Å^2. The remaining H atoms were located in a difference Fourier map and refined, with O—H distances restrained to 0.82 (2) Å. The highest electron-density peak is located 1.22 Å from atom Er1.

Data collection: *IPDS* program system (Stoe & Cie, 1996); cell refinement: *IPDS* program system; data reduction: *IPDS* program system; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 1996); software used to prepare material for publication: *CIF-Editor* (Wieczorrek, 2004).

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