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catena-Poly[[[diaqua(6-carboxypyridine-2-carboxylato-κ^3O,N,O')erbium(III)]-μ-pyridine-2,6-dicarboxylato-$\kappa^4O,N,O':O$] tetrahydrate]

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In the title structure, $\{[Er(C_7H_3NO_4)(C_7H_4NO_4)(H_2O)_2]\cdot 4H_2O\}_n$, the Er^{III} atom is nine-coordinated by a tridendate pyridine-2,6-dicarboxylate (pdc) ligand, a tridentate 6-carboxypyridine-2-carboxylate ligand (Hpdc), two water molecules and a bridging carboxylate O atom from a symmetry-related ligand, forming a one-dimensional chain structure propagating along the *c* axis. In the crystal structure, intermolecular O—H···O hydrogen bonds link these chains into a three-dimensional network.

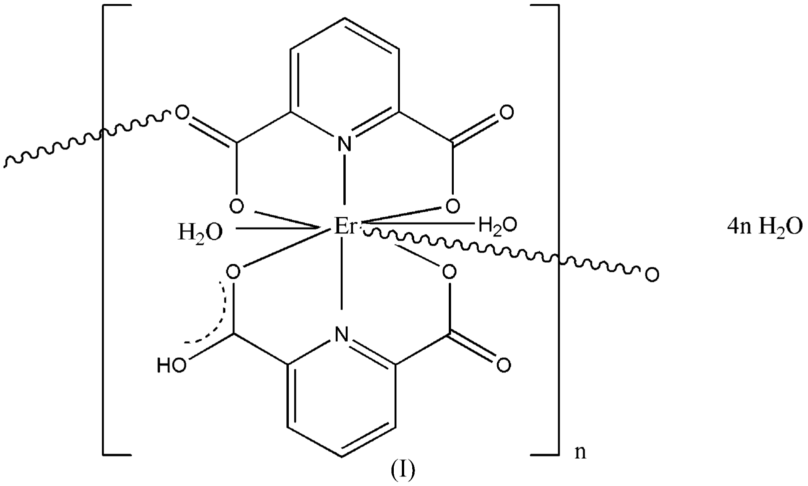
Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.006 Å
R factor = 0.031
wR factor = 0.086
Data-to-parameter ratio = 15.3

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

Comment

Research into inorganic coordination polymeric complexes has developed rapidly in recent years, owning to the potential applications of these compounds as functional materials. Much of the work has so far been focused on coordination polymers containing transition metals (Li *et al.*, 2004; Zhu *et al.*, 2003). However, recent years have seen an upsurge in the use of lanthanide metals for constructing metal-organic framework (MOF) structures (Bunzli *et al.*, 2002; Wu *et al.*, 2002). We have used pyridine-2,6-dicarboxylic acid and $Er(NO_3)_3\cdot 6H_2O$ to form the title polymeric linear coordination compound, (I), under hydrothermal conditions and we report its crystal structure here.



(I)

Part of the linear structure of (I) is shown in Fig. 1 and selected bond lengths are given in Table 1. Each Er^{III} atom is coordinated by a tridendate pyridine-2,6-dicarboxylate ligand, a tridentate 6-carboxypyridine-2-carboxylate ligand, two water molecules and one O atom from a symmetry-related carboxylate group. In the crystal structure, a three-dimensional network is formed *via* intermolecular O—H···O

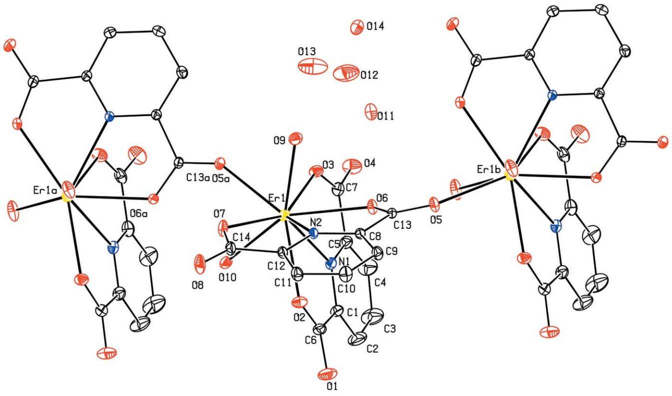


Figure 1
Part of the linear chain structure of (I), propagating along the crystallographic *c* axis, showing 30% probability ellipsoids. H atoms are not shown; atoms labelled with the suffix a are related by the symmetry operation $(x, -y + \frac{3}{2}, z - \frac{1}{2})$.

hydrogen bonds (Table 2 and Fig. 2). Compound (I) is isostructural with its Pr and Ce analogues (Ghosh & Bharadwaj, 2003).

Experimental

A mixture of erbium(III) nitrate hexahydrate (1 mmol, 0.463 g) and pyridine-2,6-dicarboxylic acid (2 mmol, 0.334 g) in dimethylformamide (10 ml) and pyridine (2 ml) was placed in a Teflon-lined autoclave and heated under autogenous pressure to 453 K for 72 h. This was then left to cool to room temperature (RT) and on allowing the filtrate from the reaction to evaporate at RT, a crystalline solid formed after several days.

Crystal data

$[Er(C_7H_3NO_4)(C_7H_4NO_4)(H_2O)_2]\cdot 4H_2O$
$M_r = 606.57$
Monoclinic, $P2_1/c$
$a = 13.9915$ (15) Å
$b = 11.2079$ (12) Å
$c = 12.8282$ (14) Å
$\beta = 102.439$ (2)°
$V = 1964.4$ (4) Å^3
$Z = 4$
$D_x = 2.051$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 4.35$ mm^{-1}
$T = 292$ (2) K
Block, colourless
0.20 × 0.10 × 0.10 mm

Data collection

Bruker SMART CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{\min} = 0.462$, $T_{\max} = 0.650$
16162 measured reflections
4276 independent reflections
3976 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.047$
$\theta_{\max} = 27.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.031$
$wR(F^2) = 0.086$
$S = 1.05$
4276 reflections
280 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0536P)^2 + 3.616P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 1.04$ e Å^{-3}
$\Delta\rho_{\min} = -0.81$ e Å^{-3}

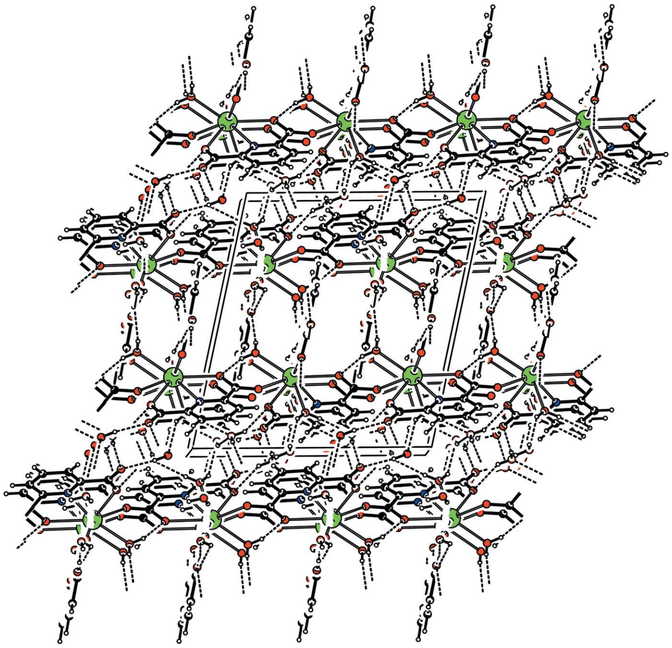


Figure 2
Part of the crystal structure, viewed approximately along the *b* axis, showing hydrogen bonds as dashed lines.

Table 1
Selected bond lengths (Å).

Er1—O9	2.382 (3)	Er1—O6	2.507 (3)
Er1—O10	2.427 (3)	Er1—O2	2.508 (3)
Er1—O3	2.436 (3)	Er1—N3	2.559 (3)
Er1—O5$^{\rm i}$	2.437 (3)	Er1—N4	2.560 (3)
Er1—O7	2.461 (3)		

Symmetry code: (i) $x, -y + \frac{3}{2}, z - \frac{1}{2}$.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*O*···O12$^{\rm ii}$	0.88	1.69	2.476 (6)	147
O9—H9*A*···O11	0.82	1.92	2.738 (4)	176
O9—H9*B*···O14$^{\rm iii}$	0.82	2.04	2.734 (4)	142
O10—H10*A*···O4$^{\rm iv}$	0.81	1.96	2.735 (4)	161
O10—H10*B*···O6$^{\rm i}$	0.81	1.99	2.714 (4)	148
O11—H11*A*···O8$^{\rm v}$	0.82	2.11	2.894 (4)	161
O11—H11*B*···O7$^{\rm vi}$	0.81	2.17	2.917 (4)	154
O12—H12*A*···O4	0.82	1.83	2.640 (5)	170
O12—H12*B*···O13	0.94	2.17	2.790 (7)	123
O13—H13*A*···O14	1.09	2.58	3.012 (6)	103
O13—H13*B*···O3	0.82	2.24	2.953 (5)	146
O14—H14*A*···O11	0.82	2.18	2.902 (4)	148
O14—H14*B*···O8$^{\rm vi}$	0.82	1.89	2.686 (4)	167

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

All C-bound H atoms were placed in calculated positions, with C—H distances of 0.93 Å. H atoms bonded to O atoms were included in their as-found positions (0.81–1.09 Å). All H atoms were refined in the riding-model approximation, with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$ or $1.5U_{\rm eq}({\rm O})$. In the final difference Fourier, two significant residual

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density peaks of 1.04 and 1.03 Å^3 are located 0.86 and 0.83 Å, respectively, from atom Er1.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); 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, 2000); software used to prepare material for publication: *SHELXTL*.

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