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# Poly[($\mu_3$-isonicotinato-$\kappa^3N$:$O$:$O'$)($\mu_4$-tetraoxidochromato-$\kappa^5O$:$O'$:$O'$,$O''$:$O''$)erbium(III)]

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**Key indicators**

Single-crystal X-ray study
$T$ = 298 K
Mean $\sigma$(C–C) = 0.011 Å
$R$ factor = 0.023
$wR$ factor = 0.075
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.

The title compound, $[Er\{CrO_4\}(C_6H_4NO_2)]_n$ or $[CrEr(C_6H_4NO_2)O_4]_n$, obtained by a hydrothermal reaction, is a three-dimentional polymer consisting of inorganic layers of Er$^{III}$ ions and $[CrO_4]^{2-}$ anions pillared by organic isonicotinate (IN) ligands. Each Er$^{III}$ ion is eight-coordinated by one N atom from one IN ligand, two carboxylate O atoms from two IN ligands and five O atoms from four $[CrO_4]^{2-}$ anions. The inorganic layer consists of $[Er(CrO_4)]_n$ chains running along the $b$ direction, linked together in the $a$ direction. Each $[CrO_4]^{2-}$ anion in the structure binds four Er$^{III}$ ions in a $\mu_4$-pentadentate coordination mode.

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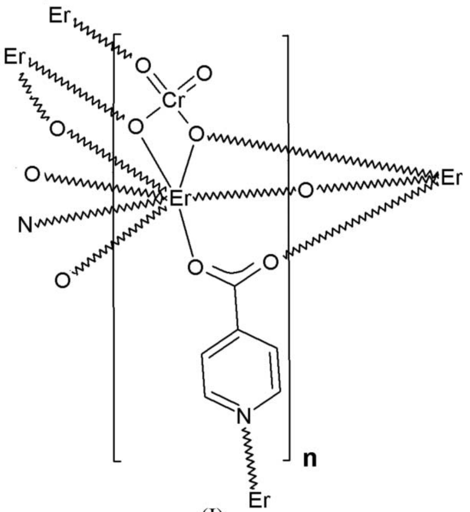
## Comment

The design of coordination polymers has become an active research area (Hill, 1998; Serre *et al.*, 2002) because of their potential application as functional solid materials (Rowsell & Yaghi, 2006; Piguet *et al.*, 1997; Wu *et al.*, 2003). Among the large number of reported structures, the rational synthesis of organic–inorganic hybrid compounds containing chiral or double helical arrays is of particular interest (Lu *et al.*, 2002; Evans *et al.*, 2001). Here, we report the synthesis and crystal structure of the title compound, $[Er(IN)CrO_4]_n$, (I) (IN is isonicotinate).



(I)

Fig. 1 shows an ellipsoid plot of the erbium coordination environment. Each Er$^{III}$ ion is eight-coordinated by one N atom from one IN ligand, two carboxylate O atoms from two IN ligands and five O atoms from four $[CrO_4]^{2-}$ anions (Fig. 1). Therefore, the coordination environment around the Er$^{III}$ ion contains three IN and four chromate ions.

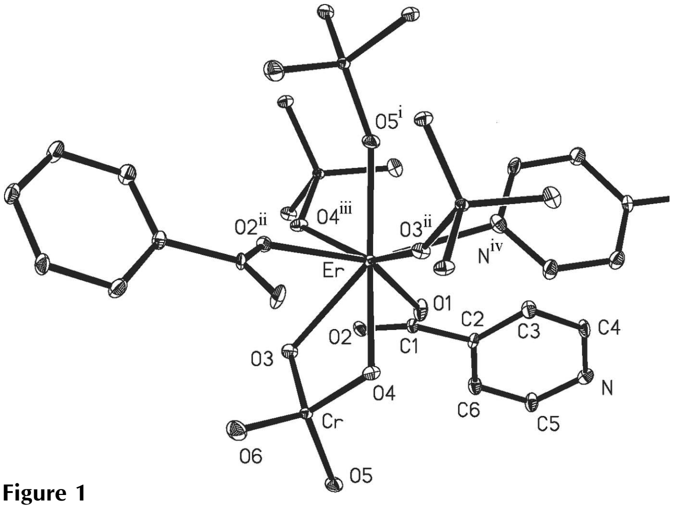


**Figure 1**
The asymmetric unit of (I), expanded to show the complete environment of Er, with 30% probability displacement ellipsoids. H atoms have been omitted for clarity. [Symmetry codes: (i) $x, y, z$; (ii) $-x + \frac{1}{2}, -y, z + \frac{1}{2}$; (iii) $-x, y + \frac{1}{2}, -z + \frac{1}{2}$; (iv) $x + \frac{1}{2}, -y + \frac{1}{2}, -z$.]

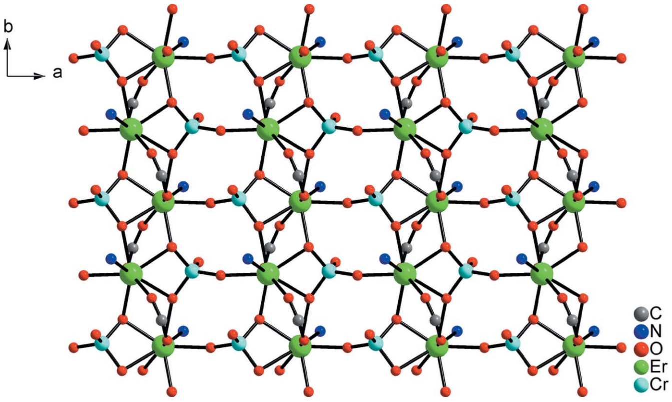


**Figure 2**
[001] view of the inorganic layered structure of (I).

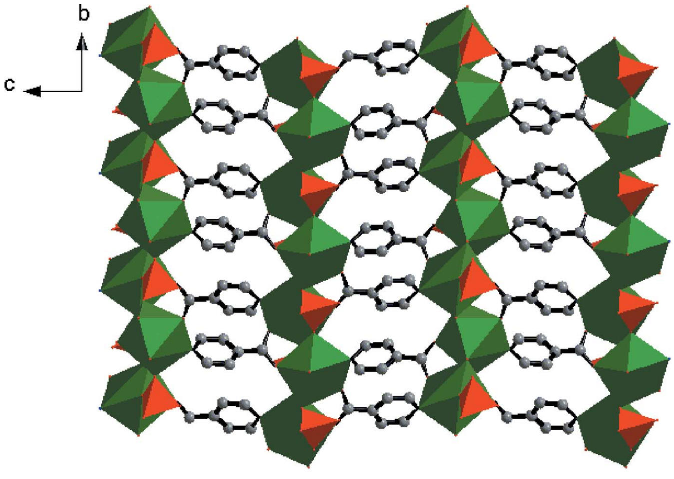


**Figure 3**
A polyhedral representation of the three-dimensional structure of (I), at right angles to that in Fig. 2, showing the inorganic layers in projection (as vertical columns), horizontally linked by the organic ligands. Colour code: red, [$CrO_4$] unit; green, [$ErNO_7$] unit.

The Er—O distances are in the range 2.277 (5)–2.532 (5)Å [average 2.343 (5) Å], shorter than those in similar structures such as $[Ln(INO)(H_2O)(SO_4)]_n$ (Ln = La, Ce, Pr; INO is isonicotinate-*N*-oxide; He *et al.*, 2005), where the Ln—O distances span 2.449 (3)–2.691 (3), 2.423 (2)–2.671 (2) and 2.408 (4)–2.648 (4) Å, respectively. The O—Er—O bond angles range from 76.7 (2) to 152.45 (19)°.

The three-dimensional crystal structure of (I) comprises $[Er(CrO_4)]_n$ chains running along *b*, then linked together in the *a* direction, to form the inorganic layers shown in Fig. 2. These layers, in turn, are pillared by the organic IN ligand into a tightly bound three-dimensional structure (Fig. 3).

Within each chain, both the Er$^{III}$ cations and the $[CrO_4]^{2-}$ anions are disposed in a zigzag-like arrangement, where each pair of Er ions is bridged by two $\mu$-O bridges of two $[CrO_4]^{2-}$ anions to form an $[Er_2O_2]$ rhombic unit. These units form a chain by sharing their two Er$^{III}$ vertices. There is an Er$\cdots$Er separation of 3.935 (2) Å and an Er$\cdots$Cr separation of 3.140 (2) Å for neighboring cations along each $[Er(CrO_4)]_n$ chain. Each $[CrO_4]^{2-}$ anion provides two $\mu$-O atoms (O3 and O4) to bridge three Er$^{III}$ ions of a triangle in the chain. The fourth O atom of the $[CrO_4]^{2-}$ anion is non-coordinated. As a result, each $[CrO_4]^{2-}$ anion in the structure binds four Er$^{III}$ ions in a $\mu_4$-pentadentate coordination mode. The Cr—O bond distances are in the range 1.589 (6)–1.705 (5) Å, similar to those found in the related $[\{Cu(bpy)_2\}_3(\mu\text{-}CrO_4)](ClO_4)_4\cdot H_2O$ (bpy is 2,2′-bipyridine; Yin *et al.*, 2002).

## Experimental

The pH of a mixture of $K_2Cr_2O_7$ (0.34 mmol), HIN (0.50 mmol), $Er_2O_3$ (0.25 mmol) and deionized water (13 ml) was adjusted to 2.0 by the addition of HCl solution (4 *M*) whilst stirring and the resulting mixture was then heated at 423 K for 3 d under autogenous pressure in a sealed 25 ml Teflon-lined stainless steel vessel. Yellow crystals were isolated after the reaction solution was cooled (yield 51%).

*Crystal data*

$[CrEr(C_6H_4NO_2)O_4]$
$M_r = 405.36$
Orthorhombic, $P2_12_12_1$
$a = 6.636$ (3) Å
$b = 6.980$ (3) Å
$c = 18.980$ (8) Å
$V = 879.1$ (7) Å$^3$
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 10.72$ mm$^{-1}$
$T = 298$ (2) K
$0.12 \times 0.05 \times 0.03$ mm

*Data collection*

Siemens SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996) $T_{min} = 0.52$, $T_{max} = 0.73$
6991 measured reflections
2010 independent reflections
1879 reflections with $I > 2\sigma(I)$
$R_{int} = 0.036$

*Refinement*

$R[F^2 > 2\sigma(F^2)] = 0.023$
$wR(F^2) = 0.075$
$S = 1.01$
2010 reflections
137 parameters
H-atom parameters constrained
$\Delta\rho_{max} = 1.99$ e Å$^{-3}$
$\Delta\rho_{min} = -2.34$ e Å$^{-3}$
Absolute structure: Flack (1983), 811 Friedel pairs
Flack parameter: 0.001 (19)

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**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| Er—O1 | 2.277 (5) | Er—O4$^{iii}$ | 2.336 (6) |
| Er—O5$^{i}$ | 2.282 (5) | Er—O4 | 2.362 (6) |
| Er—O2$^{ii}$ | 2.297 (5) | Er—O3 | 2.532 (5) |
| Er—O3$^{ii}$ | 2.315 (5) | Er—N$^{iv}$ | 2.571 (6) |

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

All H atoms were positioned geometrically and allowed to ride with C—H distances of 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$. The highest residual density peak and deepest hole are located 0.66 Å from C3 and 1.26 Å from O3, respectively.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1994); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1994); software used to prepare material for publication: *SHELXL97*.

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