

***catena*-Poly[[diaqua(isonicotinato-*O,O'*)europium(III)]-di- μ -isonicotinato-*O:O'*]**

Xi-Rui Zeng *et al.*

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catena-Poly[[diaqua(isonicotinato-*O,O'*)europium(III)]-di- μ -isonicotinato-*O:O'*]Xi-Rui Zeng,^{a*} Yan Xu,^b Ren-Geng Xiong,^b Li-Juan Zhang^b
and Xiao-Zeng You^b^aDepartment of Chemistry, JingGangShan Normal College, 343009 Jian, Jiangxi, People's Republic of China, and ^bCoordination Chemistry Institute and, State Key Laboratory of Coordination Chemistry, Nanjing University, 210093 Nanjing, Jiangsu, People's Republic of China

Correspondence e-mail: zengrj@public1.jappt.jx.cn

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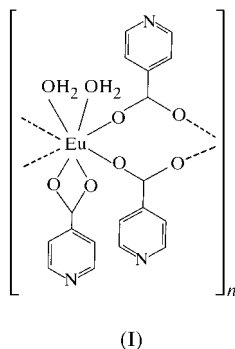
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The title complex, $[\text{Eu}(\text{C}_6\text{H}_4\text{O}_2)_3(\text{H}_2\text{O})_2]$, has a double carboxylate-bridged infinite-chain structure, with one chelating carboxylate group on each Eu ion centre, which also binds to two water molecules to yield an eight-coordinate square-antiprismatic geometry, with Eu—O bond lengths in the range 2.338 (3)–2.594 (3) Å. The pyridine N atoms of the isonicotinate groups do not coordinate to the Eu ions; instead, they direct the formation of Eu^{III} coordination polymers *via* hydrogen bonding with coordinated water molecules.

Comment

There has been considerable interest in rare earth isonicotinates (Moore *et al.*, 1972; Chupakhina *et al.*, 1963; Xu *et al.*, 1997; Ye & Qin, 1991). In this paper, we report that *catena*-poly[[[diaqua(isonicotinato-*O,O'*)europium(III)]-di- μ -isonicotinato-*O:O'*] dihydrate], (I), has a one-dimensional chain structure instead of the dimers reported for the Sm^{III} and La^{III} isonicotinates (Moore *et al.*, 1972).



In the title compound, the isonicotinates are coordinated to the Eu^{III} ions solely through the carboxylate O atoms, leaving

the pyridine N atoms uncoordinated, and two isonicotinates act as bridging ligands between all adjacent Eu ions, thus forming a one-dimensional structure. In other words, the complex has a double carboxylate-bridged infinite chain, with one chelating carboxylate group on each Eu ion centre. The chelating carboxyl groups of isonicotinate have two Eu—O distances of 2.594 (3) and 2.445 (3) Å. A prominent feature is that the distances of the bridging isonicotinates have two shorter Eu—O distances: O1ⁱⁱ is 2.403 (3) Å from Eu1 and O2 is 2.338 (3) Å from Eu1, which represents a weak interaction between the metal ion and the C atom of the carboxylate group (see Table 1 for symmetry code).

The coordination sphere of each Eu ion is completed by two water molecules to yield an eight-coordinate square-antiprismatic geometry. The Eu1—OW1 and Eu1—OW2 bond lengths are 2.449 (3) and 2.444 (3) Å, respectively. The presence of water molecules permits hydrogen bonding to the N and O atoms of adjacent chain units, whose relevant geometric parameters are quoted in Table 2. This hydrogen bonding occurs between different chain units, so that the bulk structure is bound together by these hydrogen bonds into a three-dimensional network.

Experimental

Isonicotinic acid (0.1 g) and $\text{Eu}(\text{CF}_3\text{COO})_3$ (0.1 g) were mixed with ethanol (1 ml) and water (0.1 ml) in a heavy-walled Pyrex tube. The Pyrex tube was sealed under vacuum (while frozen with liquid nitrogen). The tube was kept in oven at the temperature 350 K for 24 h, after which time, colourless prismatic crystals were obtained.

Crystal data

$[\text{Eu}(\text{C}_6\text{H}_4\text{O}_2)_3(\text{H}_2\text{O})_2]$
 $M_r = 554.30$
 Monoclinic, $P2_1/c$
 $a = 9.4860$ (19) Å
 $b = 18.974$ (4) Å
 $c = 10.759$ (2) Å
 $\beta = 92.48$ (3)°
 $V = 1934.7$ (7) Å³
 $Z = 4$

$D_x = 1.903$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 25 reflections
 $\theta = 2.63$ – 6.87°
 $\mu = 3.295$ mm⁻¹
 $T = 293$ (2) K
 Prism, colourless
 $0.32 \times 0.26 \times 0.24$ mm

Data collection

CAD-4 diffractometer
 ω - 2θ scans
 Absorption correction: empirical
 from ψ scan (North *et al.*, 1968)
 $T_{\min} = 0.348$, $T_{\max} = 0.452$
 3615 measured reflections
 3402 independent reflections
 3060 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.017$
 $\theta_{\text{max}} = 24.97^\circ$
 $h = 0 \rightarrow 11$
 $k = 0 \rightarrow 22$
 $l = -12 \rightarrow 12$
 3 standard reflections
 every 97 reflections
 intensity decay: none

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.025$
 $wR(F^2) = 0.070$
 $S = 1.091$
 3402 reflections
 271 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0460P)^2 + 1.4090P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.002$
 $\Delta\rho_{\text{max}} = 0.729$ e Å⁻³
 $\Delta\rho_{\text{min}} = -2.005$ e Å⁻³

Table 1

Selected geometric parameters (Å).

Eu1—O2	2.338 (3)	Eu1—O2W	2.445 (3)
Eu1—O6 ⁱ	2.359 (3)	Eu1—O1W	2.450 (3)
Eu1—O5	2.370 (3)	Eu1—O4	2.453 (2)
Eu1—O1 ⁱⁱ	2.403 (3)	Eu1—O3	2.594 (3)

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

Table 2

Hydrogen-bonding geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O1W—H1 \cdots O3 ⁱ	0.95 (7)	1.84 (7)	2.784 (4)	165 (8)
O1W—H2 \cdots N3 ⁱⁱ	0.97 (1)	1.84 (7)	2.799 (5)	166 (6)
O2W—H3 \cdots O4 ⁱⁱⁱ	0.88 (6)	1.88 (5)	2.752 (4)	165 (3)
O2W—H4 \cdots N1 ^{iv}	0.86 (3)	1.96 (7)	2.800 (4)	161 (9)

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

The deepest difference electron-density hole was 1.07 Å from the Eu1 atom.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; program(s) used to solve structure:

SHELXS97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXTL* (Sheldrick, 1997); software used to prepare material for publication: *SHELXTL*.

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