metal-organic papers

Poly[[bis[μ-1-ethyl-6-fluoro-4-oxo-7-(1-piperazinyl)-1,4-dihydro-1,8-naphthyridine-3-carboxylato]-cobalt(II)] dihydrate]

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In the title compound, $\{[Co(C_{15}H_{16}FN_4O_3)_2]\cdot2H_2O\}_n$, the Co^{II} atom (site symmetry $\bar{1}$) exists in a distorted *trans*-CoN_2O_4 octahedral geometry that is defined by two monodentate *N*-bonded and two bidentate *O,O*-bonded 1-ethyl-6-fluoro-4-oxo-7-(1-piperazine)-1,4-dihydro-1,8-naphthyridine-3-carboxylate (enox) monoanions. The extended two-dimensional structure is a square grid.

Comment

Enoxacin (H-Enox, 1-ethyl-6-fluoro-4-oxo-7-piperazine-1,4-dihydro-1,8-naphthyridine-3-carboxylic acid) is a member of the class of quinolones that is used to treat infections (Mizuki *et al.*, 1996). Manganese(II) and cadmium(II) derivatives of enox have been reported (Yu *et al.*, 2005; Zhang *et al.*, 2006). The title cobalt(II) derivative, (I), a two-dimensional coordination polymer in which the anion acts in a bridging mode, is reported here (Fig. 1).

(I)
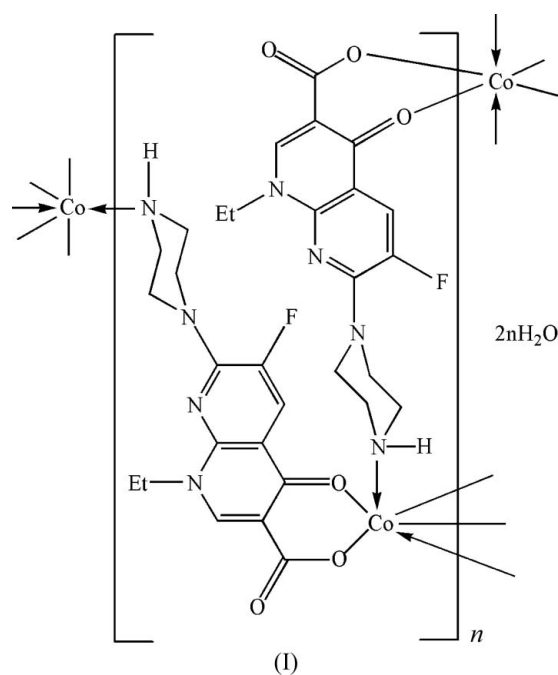
The Co^{II} atom (site symmetry $\bar{1}$) in (I) is coordinated (Table 1) by four O atoms and two N atoms from four enoxacin ligands (two *N*-monodentate and two *O,O*-bidentate), forming an approximate square grid (Fig. 2) propagating in $(10\bar{2})$. The disordered uncoordinated water molecules occupy cavities within the grid. An N—H···O hydrogen bond (Table 2) to carboxylate atom O2 (not bonded to Co) completes the structure.

Experimental

A mixture of Co(CH₃COO)₂·4H₂O (0.062 g, 0.25 mmol), Henox (0.13 g, 0.5 mmol) and water (12 ml) was stirred for 30 min in air. The mixture was then transferred to a 23 ml Teflon-lined hydrothermal bomb. The bomb was kept at 423 K for 72 h under autogenous pressure. Pink single crystals of (I) suitable for X-ray analysis were obtained from the reaction mixture after cooling.

Crystal data

$[Co(C_{15}H_{16}FN_4O_3)_2]\cdot 2H_2O$	$Z = 2$
$M_r = 729.57$	$D_x = 1.470$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 5.9422$ (4) Å	$\mu = 0.59$ mm^{-1}
$b = 21.4433$ (16) Å	$T = 273$ (2) K
$c = 13.147$ (1) Å	Prism, pink
$\beta = 100.290$ (2)°	$0.32 \times 0.26 \times 0.18$ mm
$V = 1648.3$ (2) Å^3	

Data collection

Bruker SMART CCD diffractometer	8212 measured reflections
ω scans	2921 independent reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	2204 reflections with $I > 2\sigma(I)$
$T_{min} = 0.833$, $T_{max} = 0.901$	$R_{int} = 0.049$
	$\theta_{max} = 25.1°$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0722P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.049$	$+ 0.8753P]$
$wR(F^2) = 0.140$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} < 0.001$
2921 reflections	$\Delta\rho_{max} = 0.58$ e Å^{-3}
231 parameters	$\Delta\rho_{min} = -0.28$ e Å^{-3}
H atoms treated by a mixture of independent and constrained refinement	

Table 1
Selected bond lengths (Å).

Co1—O1	2.047 (2)	Co1—N4^i	2.254 (2)
Co1—O3	2.0718 (19)		

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

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

| D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
N4—H4⋯O2^{ii}	0.86 (3)	2.29 (3)	3.124 (4)	163 (2)

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

The carbon-bound H atoms were positioned geometrically (C—H = 0.93–0.97 Å) and refined as riding, with $U_{iso}(H) = 1.2U_{eq}(C)$. The N-bound H atom was located in a difference map and refined with a distance restraint of 0.86 (1) Å and with $U_{iso}(H) = 1.2U_{eq}(N)$. The uncoordinated water molecule is disordered over two adjacent [O⋯O = 2.138 (6) Å] positions; the fractional site occupancies refined to 0.557 (5):0.443 (5) (sum constrained to unity). The water H atoms could not be placed due to this disorder.
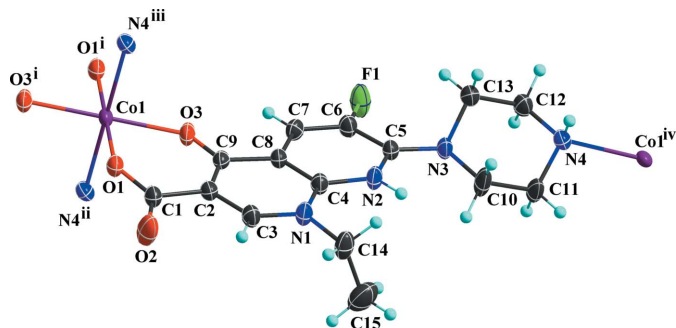
Figure 1
The asymmetric unit of (I), extended to show the Co coordination, showing 50% displacement ellipsoids (H atoms and water molecule O atoms have been omitted for clarity). [Symmetry codes: (i) $1 - x, 1 - y, 1 - z$; (ii) $-x, y + \frac{1}{2}, -z + \frac{1}{2}$; (iii) $x + 1, -y + \frac{1}{2}, z + \frac{1}{2}$.]
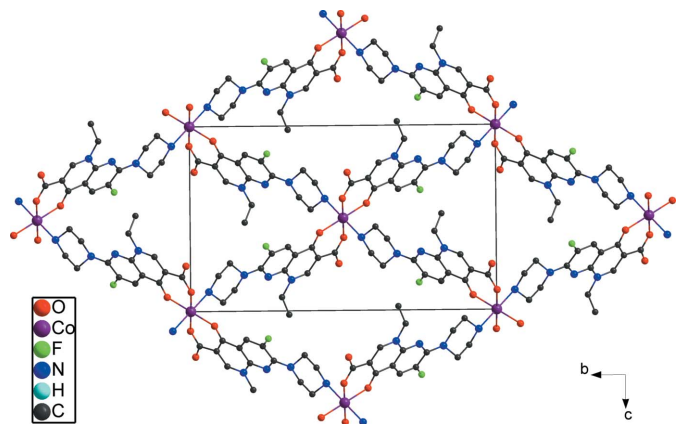
Figure 2
A view of part of a two-dimensional polymeric sheet in (I) showing the square-grid connectivity (H atoms and water molecule O atoms have been omitted for clarity).

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*.

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