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Poly[[bis[μ-1-ethyl-6-fluoro-1,4-dihydro-4-oxo-7-(1-piperazinyl)quinoline-3-carboxylato-$\kappa^3O^3,O^4:N^7$]cobalt(II)] dihydrate]

Zhe An,[a,b] Wen Xu[c] and Rong-Shun Wang[a]*

[a]Institute of Functional Materials Chemistry, Faculty of Chemistry, Northeast Normal University, Changchun, 130024, People's Republic of China, [b]School of Pharmaceutical Science, Harbin Medical University, Harbin, 150086, People's Republic of China, and [c]Department of Hematology, Second Hospital, Jilin University, Changchun, Jilin,130041, People's Republic of China

Correspondence e-mail: wangrs@nenu.edu.cn

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Key indicators

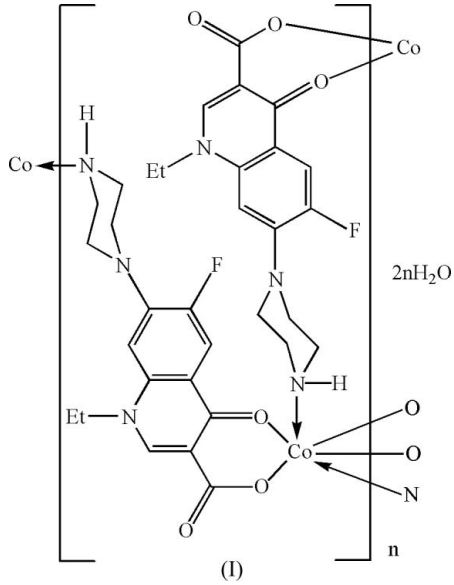
Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.003 Å
H-atom completeness 90%
Disorder in solvent or counterion
R factor = 0.043
wR factor = 0.142
Data-to-parameter ratio = 15.9

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

In the title compound, $\{[Co(C_{16}H_{17}FN_3O_3)_2]\cdot 2H_2O\}_n$, the Co atom 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-1,4-dihydro-4-oxo-7-(1-piperazinyl)-3-quinoline carboxylate ligands. The extended two-dimensional structure exhibits a 13.33 × 16.19 Å square grid. The Co atom lies on a center of inversion.

Comment

Norfloxacin (Norf, 1-ethyl-6-fluoro-1,4-dihydro-4-oxo-7-(1-piperazinyl)-3-quinolinecarboxylic acid) is a member of the class of quinolones, which is used to treat infections (Mizuki *et al.*, 1996). Cadmium(II) and zinc(II) complexes with norf have been reported (Chen *et al.*, 2001; Wang *et al.*, 2004). The cobalt(II) complex with norf, (I), a two-dimensional coordination polymer in which the ligand acts in a bridging mode, is reported here (Fig. 1).



(I)

In the complex (I), the Co atom, lying on a crystallographic center of inversion, is coordinated by four O atoms from two bidentate *O*,*O*′-bonded ligands and two N atoms from two monodentate *N*-bonded ligands, forming a square-grid structure (Fig. 2). The disordered water molecules occupy the cavities.

Experimental

A mixture of $Co(CH_3COO)_2\cdot 4H_2O$ (0.062 g, 0.25 mmol), Hnorf (0.16 g, 0.5 mmol) and water (12 ml) was stirred for 20 min in air. The

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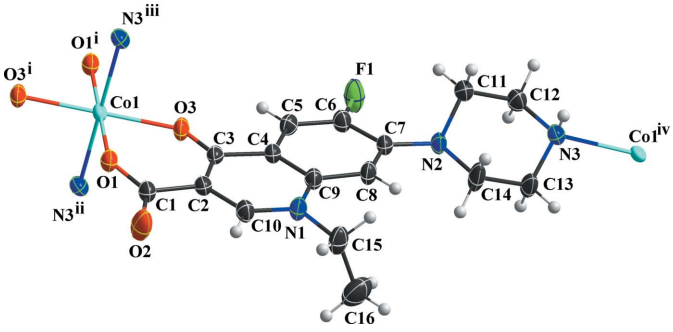

Figure 1
The asymmetric unit of (I), extended to show the Co coordination. Displacement ellipsoids are drawn at the 50% probability level. Water molecules have been omitted. [Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $-x, y-\frac{1}{2}, -z+\frac{1}{2}$; (iii) $x+1, -y+\frac{3}{2}, z+\frac{1}{2}$; (iv) $-x, y+\frac{1}{2}, -z+\frac{1}{2}$.]

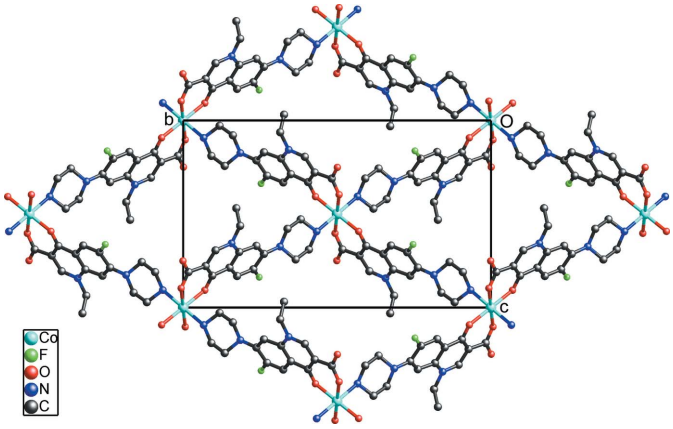

Figure 2
Part of a two-dimensional polymeric sheet in (I), showing the square-grid connectivity. H atoms and water molecules have been omitted for clarity.

mixture was then transferred to a 23 ml Teflon-lined hydrothermal bomb. The bomb was kept at 433 K for 72 h under autogenous pressure. Pink crystals of (I) suitable for X-ray analysis were obtained from the reaction mixture.

Crystal data

$[Co(C_{16}H_{17}FN_3O_3)_2]\cdot 2H_2O$
$M_r = 731.61$
Monoclinic, $P2_1/c$
$a = 5.8530\ (12)$ Å
$b = 21.587\ (4)$ Å
$c = 13.278\ (3)$ Å
$\beta = 99.48\ (3)^\circ$
$V = 1654.8\ (6)$ Å^3
$Z = 2$
$D_x = 1.468$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.59$ mm^{-1}
$T = 295\ (2)$ K
Prism, pink
0.35 × 0.28 × 0.19 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.790$, $T_{max} = 0.854$
15910 measured reflections
3779 independent reflections
2889 reflections with $I > 2\sigma(I)$
$R_{int} = 0.038$
$\theta_{max} = 27.5^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.142$
$S = 1.07$
3779 reflections
237 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0884P)^2 + 0.3041P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.72$ e Å^{-3}
$\Delta\rho_{min} = -0.34$ e Å^{-3}

The C-bound H atoms were positioned geometrically and refined as riding, with C—H = 0.93 (aromatic H), 0.97 (CH_2) and 0.96 Å (CH_3) and $U_{iso}(H) = 1.2U_{eq}(C)$. The N-bound H atom was located in a difference map and refined with a distance restraint of 0.86 (1) Å and $U_{iso}(H) = 1.5U_{eq}(N)$. The water molecules O1*W* and O2*W* are disordered with the sites assigned half-occupancy. The H atoms of the water molecules were not located because of the disorder.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 2001); software used to prepare material for publication: *SHELXL97*.

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