Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

Bis(aqua)bis(benzimidazole-κ*N*)-bis(5-fluorouracil-1-acetate-κ*O*)cobalt(II)

Mao-Lin Hu,[a]* Nan-Wen Zhu[b] and Hong-Ping Xiao[a]

[a]Department of Chemistry and Materials Science, Wenzhou Normal College, Wenzhou 325027, People's Republic of China, and [b]School of Environmental Science and Engineering, Shanghai Jiao Tong University, Shanghai 200240, People's Republic of China

Correspondence e-mail: maolin_hu@yahoo.com

Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
R factor = 0.054
wR factor = 0.142
Data-to-parameter ratio = 11.3

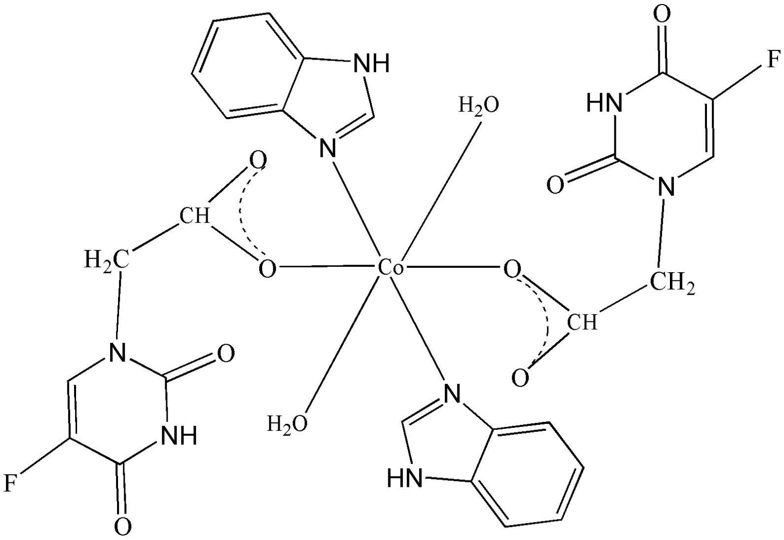
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 6 April 2005
Accepted 12 April 2005
Online 16 April 2005

In the centrosymmetric molecule of the title compound, $[Co(C_6H_4N_2O_4F)_2(C_7H_6N_2)_2(H_2O)_2]$, the Co^{II} ion is coordinated by two 5-fluorouracil-1-acetate anions *via* carboxylate O atoms, two water molecules and two benzimidazole ligands, forming a six-coordinate octahedral environment. N—H···O and O—H···O hydrogen-bond interactions are observed in the structure, leading to the formation of a three-dimensional network.

Comment

5-Fluorouracil-1-acetic acid is a derivative of 5-fluorouracil (5FU) from the pyrimidine family of bases. It is a cytotoxic analogue of the natural base thymine, which has proved useful in the chemotherapy of a number of cancers, particularly colorectal cancer (Markova Venelin Enchev & Timtcheva, 2005). Increasing attention has been paid to the anticancer activity of 5FU and its derivatives (Akgerman & Guney, 2000), but only a few of their transition metal complexes have been reported so far (Wang *et al.*, 1993). In an extension of this research, we report here the crystal structure of the title compound, (I).



(I)

The mononuclear molecule of (I) consists of a Co^{II} ion, two coordinated water molecules, two 5-fluorouracil-1-acetate anions coordinated through carboxylate O atoms, and two benzimidazole molecules. The Co^{II} cation lies on an inversion centre and the geometry around the Co^{II} ion is octahedral (Fig. 1 and Table 1). The equatorial square plane is formed by atoms O1, O1^{i}, N3 and N3^{i} atoms [symmetry code: (i) $-x$, $-y$,

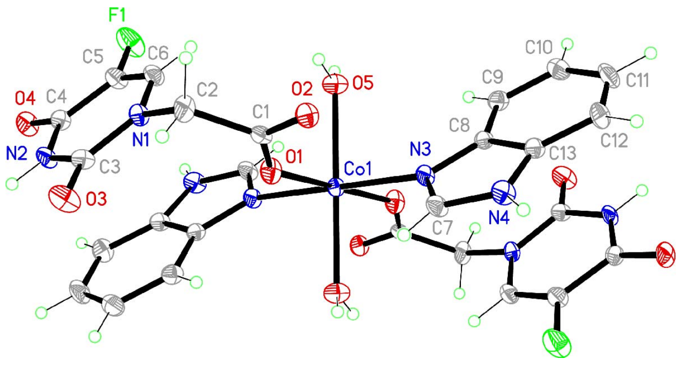


Figure 1

The coordination environment of the Co^{II} ion in (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii. Unlabelled atoms are related to labelled atoms by $-x, -y, 1-z$.

$1-z$], and is essentially planar (r.m.s. deviation 0.0011 Å). The two axial sites are occupied by atoms O5 and $O5^{i}$, with a Co—O bond distance of 2.173 (3) Å, longer than the average equatorial Co—O bond distance of 2.081 (3) Å.

Each molecule is linked to four adjacent molecules *via* N—H···O and O—H···O hydrogen-bond interactions, to form a three-dimensional network (Fig. 2 and Table 2).

Experimental

The title compound was synthesized in a hydrothermal process from a mixture of benzimidazole (2 mmol, 0.24 g), $CoCl_2·2H_2O$ (1 mmol, 0.16 g), 5-fluorouracil-1-acetic acid (2 mmol, 0.75 g) and water (20 ml) in a 30 ml Teflon-lined stainless steel reactor. The solution was heated to 421 K for 5 d. After the reaction, the system was slowly cooled to room temperature, and red crystals of (I) were collected and washed with distilled water.

Crystal data

$[Co(C_6H_4N_2O_4F)_2(C_7H_6N_2)_2(H_2O)_2]$
$M_r = 705.46$
Triclinic, $P\overline{1}$
$a = 7.368$ (13) Å
$b = 8.368$ (14) Å
$c = 12.07$ (2) Å
$\alpha = 88.59$ (3)°
$\beta = 88.38$ (3)°
$\gamma = 69.92$ (3)°
$V = 699$ (2) $Å^3$
$Z = 1$
$D_x = 1.677$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2778 reflections
$\theta = 2.6–24.9°$
$\mu = 0.70$ mm^{-1}
$T = 298$ (2) K
Block, red
0.43 × 0.33 × 0.23 mm

Data collection

Bruker APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{min} = 0.752$, $T_{max} = 0.855$
4448 measured reflections
2410 independent reflections
2064 reflections with $I > 2\sigma(I)$
$R_{int} = 0.035$
$\theta_{max} = 25.0°$
$h = -8 \rightarrow 8$
$k = -9 \rightarrow 9$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.142$
$S = 1.06$
2410 reflections
214 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0997P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.26$ e $Å^{-3}$
$\Delta\rho_{min} = -0.87$ e $Å^{-3}$

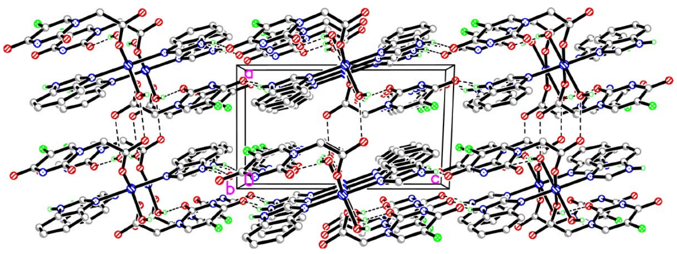


Figure 2

The three-dimensional network of (I), formed by hydrogen-bonding interactions, which are shown as dashed lines. H atoms not involved in these interactions have been omitted for clarity.

Table 1

Selected geometric parameters (Å, °).

Co1—O1	2.081 (3)	Co1—N3	2.125 (4)
Co1—$O1^{i}$	2.081 (3)	Co1—$O5^{i}$	2.173 (3)
Co1—$N3^{i}$	2.125 (4)	Co1—O5	2.173 (3)
O1—Co1—$O1^{i}$	180.00 (7)	$N3^{i}$—Co1—$O5^{i}$	90.65 (12)
O1—Co1—$N3^{i}$	86.88 (11)	N3—Co1—$O5^{i}$	89.35 (12)
$O1^{i}$—Co1—$N3^{i}$	93.12 (11)	O1—Co1—O5	90.38 (16)
O1—Co1—N3	93.12 (11)	$O1^{i}$—Co1—O5	89.62 (16)
$O1^{i}$—Co1—N3	86.88 (11)	$N3^{i}$—Co1—O5	89.35 (12)
$N3^{i}$—Co1—N3	180.00 (4)	N3—Co1—O5	90.65 (12)
O1—Co1—$O5^{i}$	89.62 (16)	$O5^{i}$—Co1—O5	180.000 (1)
$O1^{i}$—Co1—$O5^{i}$	90.38 (16)		

Symmetry code: (i) $-x, -y, 1-z$.

Table 2

Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4···$O4^{ii}$	0.86	2.12	2.905 (5)	152
O5—H5B···$O3^{iii}$	0.82	2.07	2.877 (4)	169

Symmetry codes: (ii) $x, y, z+1$; (iii) $x, y-1, z$.

H atoms were positioned geometrically and allowed to ride on their parent atoms at distances of Csp^2—H = 0.93 Å with $U_{iso}(H) = 1.2U_{eq}(C)$, Csp^3—H = 0.97 Å with $U_{iso}(H) = 1.5U_{eq}(C)$, N—H = 0.86 Å with $U_{iso}(H) = 1.2U_{eq}(N)$ and O—H = 0.82 Å with $U_{iso}(H) = 1.2U_{eq}(O)$. The highest peak is located 0.94 Å from atom Co1.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); 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, 2002); software used to prepare material for publication: *SHELXL97*.

This work was supported by the Wenzhou Technology Project Foundation of China (grant No. S2004A004), the Zhejiang Provincial Natural Science Foundation of China (grant No. Y404118) and the National Natural Science Foundation of China (grant No. 20471043).

References

Akgerman, A. & Guney, O. (2000). *J. Chem. Eng. Data*, **45**, 1049–1052.

Acta Cryst. (2005). E**61**, m898–m900   Hu *et al.* • $[Co(C_6H_4N_2O_4F)_2(C_7H_6N_2)_2(H_2O)_2]$ **m899**

Bruker (2002). *SADABS* (Version 2.03), *SAINT* (Version 6.02), *SMART* (Version 5.62) and *SHELXTL* (Version 6.10). Bruker AXS Inc., Madison, Wisconsin, USA.

Markova Venelin Enchev, N. & Timtcheva, I. (2005). *J. Phys. Chem. A*, **109**, 1981–1988.

Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

Wang, L. F., Yang, Z. Y., Peng, Z. R., Cheng, G. Q., Guo, H. Y., Sun, A. L., Wang, Q. & He, F. Y. (1993). *J. Coord. Chem.* **28**, 167–172.

m900 Hu *et al.* • $[Co(C_6H_4N_2O_4F)_2(C_7H_6N_2)_2(H_2O)_2]$ *Acta Cryst.* (2005). E**61**, m898–m900