Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

Diaquabis(6-oxo-1,4,5,6-tetrahydropyridazine-3-carboxylato)cobalt(II) dihydrate

Qing Yu, Xiao-Ge Bao, Xiu-Qing Zhang, He-Dong Bian and Hong Liang*

College of Chemistry and Chemical Engineering, Guangxi Normal University, Guilin, Guangxi 541004, People's Republic of China

Correspondence e-mail:
yuqing@mailbox.gxnu.edu.cn

Received 8 October 2006
Accepted 18 November 2006

Key indicators

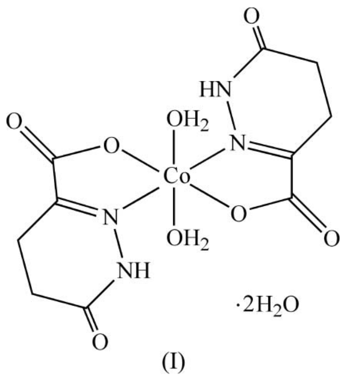
Single-crystal X-ray study
T = 294 K
Mean *σ*(C–C) = 0.011 Å
R factor = 0.083
wR factor = 0.201
Data-to-parameter ratio = 12.4

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

In the title complex, $[Co(C_5H_5N_2O_3)_2(H_2O)_2]\cdot 2H_2O$, the Co^{II} ion is octahedrally coordinated by two *O*,*N*-bidentate 6-oxo-1,4,5,6-tetrahydropyridazine-3-carboxylate ions and two water molecules. The complex molecule is centrosymmetric, with the Co^{II} ion located on an inversion center.

Comment

Pyridazine derivatives have attracted much attention because of their potential biological activities, such as adrenergic blocking properties, and antiarrhythmic and antifungal activities (Éliás *et al.*, 2003). We report here the structure of the title Co^{II} complex, (I), with a 6-oxo-1,4,5,6-tetrahydropyridazine-3-carboxylate (topca) ligand.



(I)

The molecular structure of (I) is shown in Fig. 1. The molecule of (I) is centrosymmetric; the Co^{II} ion is located on an inversion center and assumes a slightly distorted octahedral coordination geometry formed by two bidentate topca ions and two water molecules (Table 1). The topca acts as a *N*,*O*-chelating ligand and the five-membered chelate ring is planar.

N—H···O and O—H···O hydrogen bonding (Table 2) helps to stabilize the crystal structure of (I).

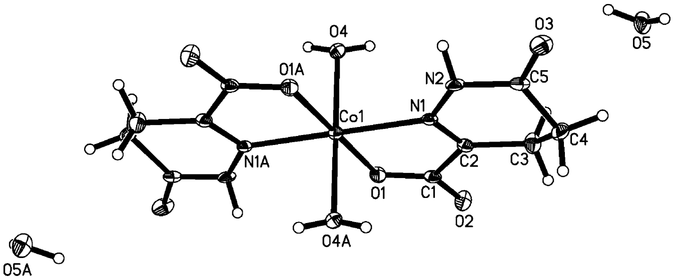


Figure 1
The molecular structure of (I), shown with 30% probability displacement ellipsoids (arbitrary spheres for the H atoms) [symmetry code: (A) $-x+2$, $-y$, $-z$].

doi:10.1107/S1600536806049427

Experimental

6-Oxo-1,4,5,6-tetrahydropyridazine-3-carboxylic acid (Htopca) was prepared according to Kline *et al.* (1961). Htopca (0.151 g, 1.0 mmol) was dissolved in water (5 ml), and a solution of $Co(ClO_4)_2 \cdot 6H_2O$ (0.183 g, 0.5 mmol) in methanol (10 ml) was added. The mixture was stirred at 338 K for 2 h and then cooled and filtered. The filtrate was allowed to evaporate slowly at room temperature. One month later, single crystals of (I) were obtained.

Crystal data

$[Co(C_5H_5N_2O_3)_2(H_2O)_2] \cdot 2H_2O$
$M_r = 413.21$
Monoclinic, $P2_1/c$
$a = 5.727$ (9) Å
$b = 18.48$ (3) Å
$c = 8.673$ (11) Å
$\beta = 114.07$ (8)°
$V = 838$ (2) Å^3

$Z = 2$
$D_x = 1.637$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 1.08$ mm^{-1}
$T = 294$ (2) K
Block, orange
0.20 × 0.12 × 0.08 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
$T_{min} = 0.812$, $T_{max} = 0.918$

3524 measured reflections
1429 independent reflections
1095 reflections with $I > 2\sigma(I)$
$R_{int} = 0.099$
$\theta_{max} = 25.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.083$
$wR(F^2) = 0.201$
$S = 1.06$
1429 reflections
115 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.085P)^2 + 4.3246P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.31$ e Å^{-3}
$\Delta\rho_{min} = -0.77$ e Å^{-3}

Table 1
Selected bond lengths (Å).

Co1—O1	2.096 (5)	Co1—O4	2.199 (5)
Co1—N1	2.169 (6)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2B···O1^{i}	0.88	2.41	3.256 (9)	160
N2—H2B···O4^{ii}	0.88	2.55	3.125 (8)	124
O4—H4A···O5^{iii}	0.85	1.92	2.769 (8)	176
O4—H4B···O3^{iv}	0.85	2.02	2.816 (8)	156
O5—H5A···O2^{i}	0.85	2.05	2.903 (8)	180
O5—H5B···O2^{v}	0.85	2.23	2.952 (8)	143

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

Water H atoms were located in a difference Fourier map and refined as riding, with O—H = 0.85 Å. The imino H atom was located in a difference Fourier map and refined as riding in its as-found relative position. Methylene H atoms were placed in calculated positions, with C—H = 0.97 Å, and refined in riding mode. For all H atoms, $U_{iso}(H) = 1.2U_{eq}$(carrier). The highest peak in the final difference map is located 1.10 Å from atom Co1.

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, 1997); software used to prepare material for publication: *SHELXTL*.

We gratefully acknowledge the Science Foundation of Guangxi, China, the Youth Science Foundation of Guangxi and the Teaching and Research Award Program for Outstanding Young Teachers in Higher Education Institutions of MOE, China.

References

Bruker (1997). *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (1998). *SMART* (Version 5.051), *SAINT* (Versions 5.01) and *SADABS* (Version 2.0). Bruker AXS Inc., Madison, Wisconsin, USA.
Éliás, O., Károlyházy, L., Horváth, G., Harmat, V. & Mátyus, P. (2003). *J. Mol. Struct. (THEOCHEM)*, **666–667**, 625–636.
Kline, G. B. & Cox, S. H. (1961). *J. Org. Chem.* **26**, 1854–1856.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.