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Diaquabis(2-methylpyrazine-5-carboxylato)-cobalt(II)

Fu-Ying Liu,[a] Rui-Ling Shang,[b] Lin Du,[a] Qi-Hua Zhao[a]* and Rui-Bing Fang[a]

[a]Department of Chemistry, Key Laboratory of Medicinal Chemistry for Natural Resource, Ministry of Education, Yunnan University, Kunming 650091, People's Republic of China, and [b]Department of Chemistry and Chemical Engineering, Southeast University, Nanjing 210096, People's Republic of China

Correspondence e-mail: qhzhao@ynu.edu.cn

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Key indicators

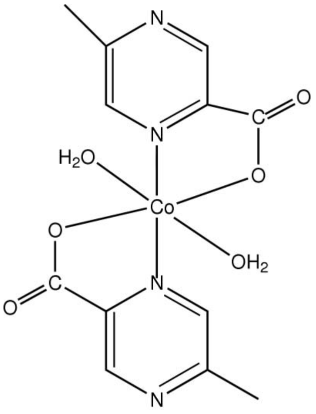
Single-crystal X-ray study
T = 298 K
Mean *σ*(C–C) = 0.003 Å
R factor = 0.030
wR factor = 0.084
Data-to-parameter ratio = 14.1

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

The title compound, $[Co(C_6H_6N_2O_2)_2(H_2O)_2]$, was obtained from $Co(CH_3COO)_2\cdot 6H_2O$ and 2-methylpyrazine-5-carboxylic acid. The crystal structure reveals that the Co atom is located on a crystallographic inversion center and is six-coordinated in a distorted octahedral geometry by 2-methylpyrazine-5-carboxylate anions and water molecules. The structure is stabilized both by hydrogen bonds forming a two-dimensional network parallel to the *ab* plane and by *π*–*π* stacking interactions between the 2-methylpyrazine-5-carboxylate ligands.

Comment

We have employed the ligand 2-methylpyrazine-5-carboxylate ($MePycza^-$) in reactions with different transition metals to design novel frameworks. A series of complexes based on this ligand presents various structural motifs and dimensionalities (Ciurtin *et al.*, 2001, 2003) because of the strong binding capabilities of the MePyzca ligand with two N atoms and two carboxylate O atoms. In the literature, there are some reports on the compounds obtained from the reaction of the MePyzca ligand with transition metals, such as $[Cu(MePyzca)_2(H_2O)]\cdot 3H_2O$ (Dong *et al.*, 2000), $\{[Cu(MePyzca)_2Cu_2Br_2]_2\}_n$ (Ciurtin *et al.*, 2001) and $\{[CdI(MePyzca)(H_2O)_21.5]_2\}_n$ (Ciurtin *et al.*, 2003). Here, we present the synthesis and crystal structure of a Co^{II} complex of MePyzca, (I).


(I)

The molecular structure of (I) (Fig. 1) shows Co on a crystallographic inversion center. The coordination environment of the Co^{II} center consists of two oxygen donors and two nitrogen donors from two 2-methylpyrazine-5-carboxylate chelating ligands and two water oxygen donors. The distorted octahedral coordination geometry (Table 1) may be described as an equatorial plane defined by N and O atoms from two 2-methylpyrazine-5-carboxylate ligands and axial positions

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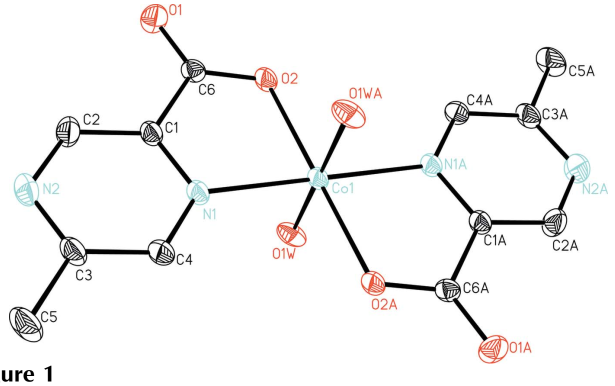

Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted. [Symmetry code: (A) $-x+1$, $-y$, $-z+1$.]

occupied by the two water oxygen donors. The carboxylate group, defined by C6, O1 and O2, is essentially coplanar with the pyrazine ring [O2—C6—C1—N1 = 0.5 (2)°]. The Co1/O2/N1 plane makes a dihedral angle of 3.39 (15)° with the pyrazine ring. The Co—O(water) and Co—N bond lengths are slightly smaller and the Co—O(acid) bond lengths are slightly larger then the corresponding values for other reported cobalt(II) complexes (Liang *et al.*, 2002; Ciurtin *et al.*, 2002).

The crystal structure is stabilized by O—H···O hydrogen-bonding interactions between O atoms of the carboxylate groups of the MePyzca ligands and O atoms of the water molecules (geometric details in Table 2). The hydrogen bonds link the molecules into layers parallel to the *ab* plane. Furthermore, there are π–π stacking interactions between the pyrazine rings and C═O groups of the ligand at position ($1+x$, y, z) with a distance of 3.4562 (5) Å between the centroids, which also stabilize the crystal packing (Fig. 2).

Experimental

A solution of MePyzcaH (27.63 mg, 0.2 mmol) in EtOH/H_2O (1:1 *v*/*v*, 5 ml) was added to a solution of $Co(CH_3COO)_2\cdot 6H_2O$ (24.91 mg, 0.1 mmol) in EtOH/H_2O (1:1 *v*/*v*, 15 ml). The mixture was stirred for 30 min. The resulting solution was filtered and allowed to stand undisturbed at room temperature. After several days, red block-shaped crystals of (I) were obtained from the mother liquor.

Crystal data

$[Co(C_6H_6N_2O_2)_2(H_2O)_2]$
$M_r = 369.20$
Triclinic, $P\overline{1}$
$a = 5.1051$ (10) Å
$b = 6.3653$ (13) Å
$c = 12.281$ (3) Å
$\alpha = 103.53$ (3)°
$\beta = 91.06$ (3)°
$\gamma = 108.28$ (3)°
$V = 366.59$ (16) Å^3
$Z = 1$
$D_x = 1.672$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 1.21$ mm^{-1}
$T = 298$ (2) K
Block, red
0.29 × 0.19 × 0.15 mm

Data collection

Bruker APEX-II CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
$T_{min} = 0.761$, $T_{max} = 0.836$
2378 measured reflections
1627 independent reflections
1569 reflections with $I > 2\sigma(I)$
$R_{int} = 0.011$
$\theta_{max} = 28.1°$

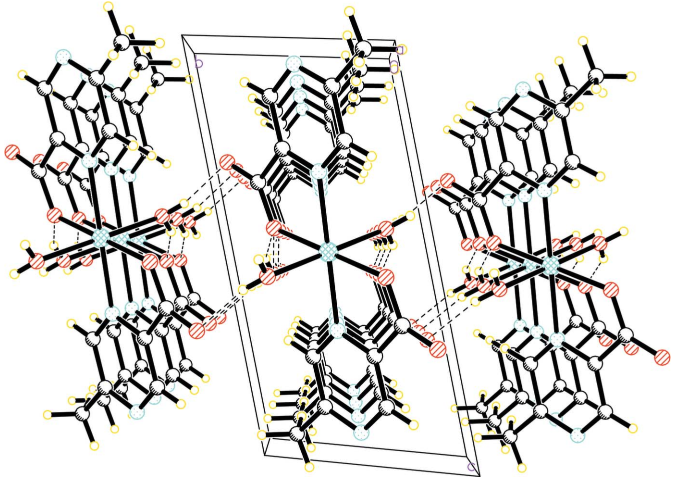

Figure 2
The crystal packing of complex (I), viewed down *a*, showing the hydrogen bonds as dashed lines and the π–π stacking interaction.

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.084$
$S = 1.05$
1627 reflections
115 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0519P)^2 + 0.1476P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.024$
$\Delta\rho_{max} = 0.38$ e Å^{-3}
$\Delta\rho_{min} = -0.28$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.023 (6)

Table 1
Selected geometric parameters (Å, °).

Co1—O2	2.0763 (14)	Co1—N1	2.1176 (16)
Co1—O1W	2.0854 (19)		
O2—Co1—O1W	90.19 (6)	O2^{i}—Co1—N1	101.03 (6)
O2^{i}—Co1—O1W	89.81 (6)	O1W—Co1—N1	91.70 (8)
O2—Co1—N1	78.97 (6)	O1W^{i}—Co1—N1	88.30 (8)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1WA···O2^{ii}	0.79 (3)	1.98 (3)	2.727 (2)	156.45
O1W—H1WB···O1^{iii}	0.76 (3)	1.94 (3)	2.675 (3)	164.62

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

The C-bound H atoms were included in the riding model approximation with C—H distances of 0.93 and 0.96 Å [$U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}(C)$]. The H atoms of the water molecule were located in a difference Fourier map and refined freely.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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