

Yu-Hong Ma,* Pi-Zhuang Ma,
Huan-Qin Zhu and Chang-Cheng
LiuDepartment of Materials and Oil, PLA Xu Zhou
Air Force College, Xuzhou 221000, Jiangsu
Province, People's Republic of ChinaCorrespondence e-mail:
mayuhong2010@yahoo.com.cn

Key indicators

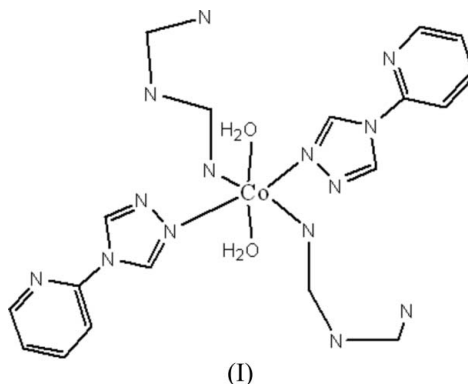
Single-crystal X-ray study
 $T = 300\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.003\text{ \AA}$
 R factor = 0.028
 wR factor = 0.070
Data-to-parameter ratio = 11.4For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.Diaquabis(dicyanamido)bis[4-(2-pyridyl)-
4*H*-1,2,4-triazole- κN^1]cobalt(II)

The title complex, $[\text{Co}(\text{C}_2\text{N}_3)_2(\text{C}_7\text{H}_6\text{N}_4)_2(\text{H}_2\text{O})_2]$ or $[\text{Co}(\text{dca})_2(\text{pytrz})_2(\text{H}_2\text{O})_2]$, where pytrz is 4-(2-pyridyl)-4*H*-1,2,4-triazole and dca is the dicyanamido monoanion, was prepared using pytrz, Na(dca) and $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$. The Co^{II} atom lies on a center of inversion and is coordinated in a slightly distorted octahedral geometry by two pytrz ligands, two dca ligands and two *trans*-oriented water molecules. In the crystal structure, complex molecules are linked by $\text{O}-\text{H} \cdots \text{N}$ hydrogen bonds into a two-dimensional network and further into a three-dimensional network *via* weak $\text{C}-\text{H} \cdots \text{N}$ hydrogen bonds.

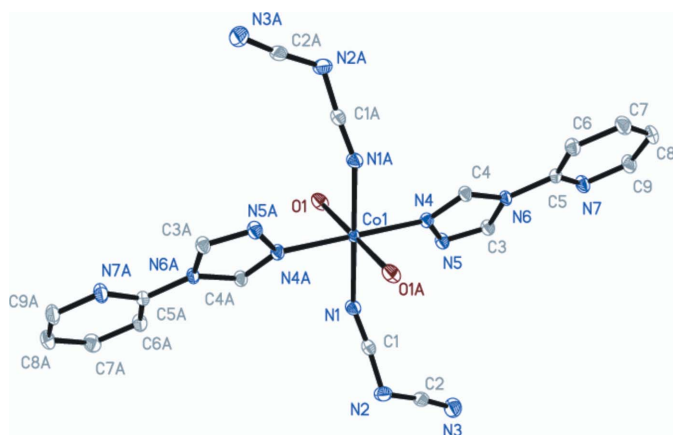
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Comment

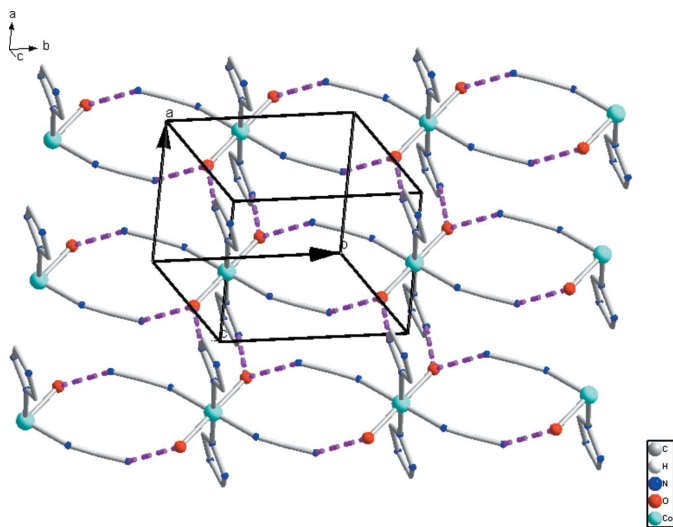
Transition metal complexes using 1,2,4-triazole derivatives as ligands are of great interest as many compounds based on these ligands have shown intriguing structures with interesting properties (Kahn & Martinez, 1998). In addition, supramolecular polymer chemistry is a branch of modern science that is developing rapidly (Lehn, 1995, 1999; Ouahab, 1997). In our current research, relating to these topics, we have synthesized the title compound, (I), and determined its crystal structure.



The molecular structure of (I) is shown in Fig. 1 and selected geometric parameters are listed in Table 1. The Co^{II} atom lies on a center of inversion and is coordinated in a slightly distorted octahedral environment through two N atoms from two pytrz ligands and two N atoms from two dca ligands in the equatorial plane, and two aqua ligands [pytrz is 4-(2-pyridyl)-4*H*-1,2,4-triazole and dca is the dicyanamido monoanion]. The dihedral angle between the pyridine and triazole rings is $4.77(4)^\circ$. In the crystal structure, the coordinated water molecules act as hydrogen-bond donors to N atoms of both the dca ligands and the triazole groups of pytrz ligands to give intermolecular $\text{O}-\text{H} \cdots \text{N}$ hydrogen bonds,


Figure 1

The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level. Atoms labeled with the suffix A are related by the symmetry operator $(1 - x, 2 - y, -z)$. H atoms have been omitted.


Figure 2

A two-dimensional hydrogen-bonded layer of (I). Dashed lines indicate the non-bonded contacts between N and O atoms involved in hydrogen bonds. H atoms have been omitted.

which assemble the title complex into two-dimensional layers (Fig. 2). Furthermore, weak intermolecular $C-H \cdots N$ hydrogen bonds link these layers into a three-dimensional network (Table 2).

Experimental

To a solution of $CoCl_2 \cdot 6H_2O$ (0.5 mmol) in EtOH (10 ml) was added a solution of pytrz (0.5 mmol) in water (15 ml). The mixture was stirred for 30 min and then Na(dca) (0.4 mmol) was added to the solution. The mixture was then refluxed for 3 h and stirred for 5 h at room temperature. After filtration, the filtrate was allowed to stand at room temperature. After a few weeks, red crystals of the title compound were obtained. Analysis calculated for $C_{18}H_{16}CoN_{14}O_2$: C 41.62, H 3.10, N 37.75%; found: C 41.50, H 3.12, N 37.57%.

Crystal data

$[Co(C_2N_3)_2(C_7H_6N_4)_2(H_2O)_2]$
 $M_r = 519.38$
 Triclinic, $P\bar{1}$
 $a = 5.8684$ (17) Å
 $b = 7.661$ (2) Å
 $c = 11.716$ (4) Å
 $\alpha = 89.794$ (5)°
 $\beta = 88.512$ (5)°
 $\gamma = 85.991$ (5)°

$V = 525.3$ (3) Å³
 $Z = 1$
 $D_x = 1.642$ Mg m⁻³
 Mo $K\alpha$ radiation
 $\mu = 0.87$ mm⁻¹
 $T = 300$ (2) K
 Block, red
 $0.30 \times 0.20 \times 0.16$ mm

Data collection

Bruker SMART CCD
 diffractometer
 φ and ω scans
 Absorption correction: multi-scan
 (SADABS; Sheldrick, 1996)
 $T_{min} = 0.812$, $T_{max} = 0.870$

2180 measured reflections
 1830 independent reflections
 1693 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.016$
 $\theta_{max} = 25.0^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.028$
 $wR(F^2) = 0.070$
 $S = 1.06$
 1830 reflections
 160 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0298P)^2 + 0.2298P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{max} < 0.001$
 $\Delta\rho_{max} = 0.23$ e Å⁻³
 $\Delta\rho_{min} = -0.47$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Co1—N1	2.0800 (17)	Co1—O1	2.1391 (14)
Co1—N4	2.1245 (16)		
N1 ⁱ —Co1—N1	180	N4—Co1—O1 ⁱ	90.64 (6)
N1—Co1—N4	90.88 (6)	N1—Co1—O1	92.45 (7)
N1—Co1—N4 ⁱ	89.12 (6)	N4—Co1—O1	89.36 (6)
N4—Co1—N4 ⁱ	180	O1 ⁱ —Co1—O1	180
N1—Co1—O1 ⁱ	87.55 (7)		

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

Table 2

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O1—H1A ⁱⁱ ···N2 ⁱⁱ	0.85	2.16	2.991 (2)	166
O1—H1B ⁱⁱⁱ ···N5 ⁱⁱⁱ	0.98	2.06	3.006 (2)	161
C3—H3···N7 ^{iv}	0.93	2.51	3.374 (3)	154
C4—H4···N3 ^v	0.93	2.44	3.352 (3)	167
C6—H6···N3 ^v	0.93	2.48	3.374 (3)	162

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

H atoms bonded to C atoms were placed in calculated positions ($C-H = 0.93$ Å) and were included in a riding-model approximation. The aqua H atoms were located in a difference Fourier map and were refined as riding in their as-found positions. For all H atoms, $U_{iso}(H) = 1.2U_{eq}(C, O)$.

Data collection: SMART-NT (Bruker, 1998); cell refinement: SAINT-NT (Bruker, 1998); data reduction: SAINT-NT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1990); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL-NT (Bruker, 1998); software used to prepare material for publication: SHELXTL-NT.

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