Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

A new cobalt(II) complex with 5-(4-pyridyl)tetrazole ligands

Wei-Feng Zhu[a]* and Xing-Fen Zhou[b]

[a]Department of Chemistry, Nanjing Institute of Railway Technology, Suzhou 215137, People's Republic of China, and [b]Suzhou Institute of Trade & Commerce, Suzhou 215009, People's Republic of China
Correspondence e-mail: szhzhuweifeng@yahoo.cn

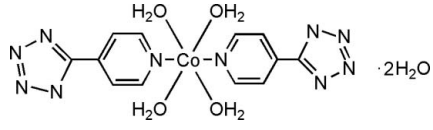
Received 28 September 2008; accepted 27 October 2008

Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.004 Å; R factor = 0.031; wR factor = 0.083; data-to-parameter ratio = 10.7.

A new mononuclear cobalt(II) complex, tetraaquabis[5-(4-pyridyl)tetrazolido-κN^5]cobalt(II) dihydrate, $[Co(C_6H_4N_5)_2(H_2O)_4]\cdot 2H_2O$, has been synthesized and structurally characterized. The Co^{II} atom is coordinated by two N atoms from 5-(4-pyridyl)tetrazole ligands (L), as well as four O atoms from coordinated water molecules. The molecule is centrosymmetric, with pairs of equivalent ligands lying *trans* to each other in a slightly distorted octahedral coordination geometry. A prominent feature of the complex is the formation of a three-dimensional supramolecular network *via* O—H···O and O—H···N hydrogen bonds.

Related literature

The corresponding complex with manganese(II) ion as the central metal atom (Lin *et al.*, 2005) has a similar structure to that of the title complex. For related literature, see: Detert & Schollmeier (1999).



Experimental

Crystal data

$[Co(C_6H_4N_5)_2(H_2O)_4]\cdot 2H_2O$
M_r = 459.31
Triclinic, $P\overline{1}$
a = 7.2087 (16) Å
b = 7.8002 (17) Å
c = 8.6702 (18) Å
α = 91.406 (3)°
β = 90.482 (3)°
γ = 100.953 (3)°
V = 478.45 (18) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.95 mm^{-1}
T = 294 (2) K
0.20 × 0.20 × 0.14 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick 1996)
T_{min} = 0.763, T_{max} = 0.890
2456 measured reflections
1684 independent reflections
1562 reflections with $I > 2\sigma(I)$
R_{int} = 0.013

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.083
S = 1.12
1684 reflections
157 parameters
9 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.49 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···N2^{i}	0.855 (10)	1.968 (10)	2.795 (3)	161.84 (3)
O1—H1B···O3^{ii}	0.857 (10)	1.93 (1)	2.753 (3)	161.83 (3)
O2—H2A···N3^{iii}	0.849 (10)	2.10 (1)	2.939 (3)	170.66 (3)
O2—H2B···O3^{iv}	0.851 (3)	1.90 (1)	2.745 (3)	172.44 (3)
O3—H3A···N5^{v}	0.853 (10)	1.99 (1)	2.840 (3)	177.52 (3)
O3—H3B···N4^{vi}	0.849 (10)	1.942 (10)	2.780 (3)	168.93 (3)

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

The authors thank the the Natural Science Foundation of Jiangsu for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BR2083).

References

Bruker (1998). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Detert, H. & Schollmeier, D. (1999). *Synthesis*, pp. 999–1004.
Lin, P., Clegg, W., Harrington, R. W. & Henderson, R. A. (2005). *Dalton. Trans.* pp. 2388-2394.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supplementary materials

Acta Cryst. (2008). E**64**, m1478 [**doi:10.1107/S1600536808034880**]

A new cobalt(II) complex with 5-(4-pyridyl)tetrazole ligands

W.-F. Zhu and X.-F. Zhou

Comment

A wide range of applications of tetrazoles have found in areas as diverse as coordination chemistry, medicinal chemistry and materials science. The study of complexes containing substituted tetrazole ligands is of interest to describe the ways in which tetrazoles bind to metal centres. However, in the title complex reported here, the substituted tetrazole ligands bind to metal centres by the N atoms from pyridyls. In this contribution, we chose 5-(4'-pyridyl)tetrazole (*L*) as organic ligands and synthesized a new mononuclear complex, namely $(CoL_2(H_2O)_4).H_2O$.

Single crystal X-ray diffraction analysis reveals that the vicinity of the cobalt(II) ion is constituted by two nitrogen atoms from the *L* ligands and four oxygen atoms from coordinated water moleculars. The molecule is centrosymmetric, so pairs of equivalent ligands lie *trans* to each other in a slightly distorted octahedral coordination geometry. Four oxygen atoms from coordinated water moleculars occupy the four equatorial positions while two nitrogen atoms, N(1) and N(1 A) from the *L* ligands are in the axial sites. A diagram of the molecule is shown in Fig. 1. The complex is further connected into a three dimensional supramolecular structure *via* O—H···O and O—H···N hydrogen bonds, which is shown in Fig. 2.

Experimental

The synthesis of the *L* ligand [*L* =5-(4'-pyridyl)tetrazole] was according to the previously published literature (Detert *et al.*, 1999). A solution of $CoCl_2.(H_2O)_6$ (0.0238 g, 0.1 mmol) in 10 ml water was added to the solution of *L* (0.0310 g, 0.2 mmol) in 5 ml water, the mixture was heated with stirring. After 3 h, the mixture was cooled to room temperature and filtered. The filtrate was allowed to stand in air at room temperature for several days. Red crystals suitable for X-ray diffraction were obtained. Calculated for $C_{12}H_{20}CoN_{10}O_6$: C 31.35, H 4.35, O 15.65, Co 12.83, N 30.48%; found: C 31.32, H 4.40%.

Refinement

To obtain a better refinement result, eight atoms, namely C(1), H(1), C(2), H(2), C(4), H(4), C(5) and H(5) have been restrained, and all the distance of C—H were fixed at 0.93 Å, with $U_{iso}(H) = 1.19U_{eq}(C)$. Other hydrogen atoms were positioned geometrically and refined using a riding model.

Figures

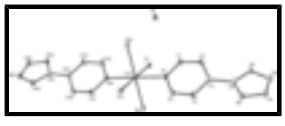


Fig. 1. An *ORTEP* view of the title complex with 30% thermal ellipsoids. The H atoms are omitted for clarity.

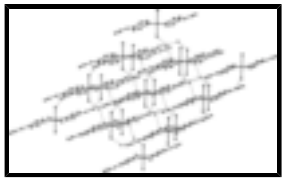


Fig. 2. The packing diagram of the title complex.

tetraaquabis[5-(4-pyridyl)tetrazolido-κN^5]cobalt(II) dihydrate

Crystal data

$[Co(C_6H_4N_5)_2(H_2O)_4]\cdot 2H_2O$	$Z = 1$
$M_r = 459.31$	$F_{000} = 237$
Triclinic, $P\overline{1}$	$D_x = 1.594$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 7.2087$ (16) Å	Cell parameters from 1859 reflections
$b = 7.8002$ (17) Å	$\theta = 2.7$–26.3°
$c = 8.6702$ (18) Å	$\mu = 0.95$ mm^{-1}
$\alpha = 91.406$ (3)°	$T = 294$ (2) K
$\beta = 90.482$ (3)°	Block, red
$\gamma = 100.953$ (3)°	0.20 × 0.20 × 0.14 mm
$V = 478.45$ (18) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	1684 independent reflections
Radiation source: fine-focus sealed tube	1562 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.013$
$T = 294(2)$ K	$\theta_{max} = 25.0^\circ$
phi and ω scans	$\theta_{min} = 2.4^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick 1996)	$h = -5\rightarrow 8$
$T_{min} = 0.763$, $T_{max} = 0.890$	$k = -8\rightarrow 9$
2456 measured reflections	$l = -10\rightarrow 7$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.031$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.083$	$w = 1/[\sigma^2(F_o^2) + (0.035P)^2 + 2.1646P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.12$	$(\Delta/\sigma)_{max} < 0.001$
1684 reflections	$\Delta\rho_{max} = 0.49$ e Å^{-3}

157 parameters	$\Delta\rho_{min} = -0.28$ e Å^{-3}
9 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Co1	0.5000	0.5000	0.0000	0.02432 (16)
O1	0.6737 (2)	0.6584 (2)	0.16137 (19)	0.0330 (4)
O2	0.7102 (3)	0.3451 (2)	−0.0278 (2)	0.0372 (4)
N1	0.3835 (3)	0.3267 (2)	0.1789 (2)	0.0285 (4)
N2	0.2607 (3)	0.0110 (3)	0.6942 (2)	0.0334 (5)
N3	0.2040 (3)	−0.1406 (3)	0.7653 (2)	0.0371 (5)
N4	0.1459 (3)	−0.2640 (3)	0.6620 (2)	0.0376 (5)
N5	0.1617 (3)	−0.1980 (3)	0.5206 (2)	0.0343 (5)
C1	0.3706 (4)	0.3835 (3)	0.3237 (3)	0.0353 (6)
H1	0.3975	0.5034	0.3441	0.042*
C2	0.3196 (4)	0.2748 (3)	0.4445 (3)	0.0372 (6)
H2	0.3120	0.3213	0.5435	0.045*
C3	0.2795 (3)	0.0948 (3)	0.4185 (3)	0.0265 (5)
C4	0.2848 (5)	0.0366 (3)	0.2677 (3)	0.0443 (7)
H4	0.2542	−0.0823	0.2433	0.053*
C5	0.3357 (5)	0.1551 (3)	0.1530 (3)	0.0445 (7)
H5	0.3366	0.1127	0.0519	0.053*
C6	0.2333 (3)	−0.0290 (3)	0.5441 (3)	0.0271 (5)
O3	0.0218 (2)	0.5988 (2)	0.25348 (19)	0.0332 (4)
H1A	0.670 (4)	0.7610 (19)	0.197 (3)	0.044 (8)*
H1B	0.782 (3)	0.629 (4)	0.170 (4)	0.073 (12)*
H2A	0.736 (4)	0.276 (3)	0.040 (2)	0.043 (8)*
H2B	0.794 (3)	0.372 (4)	−0.096 (3)	0.056 (10)*
H3A	0.066 (4)	0.662 (3)	0.332 (2)	0.040 (8)*
H3B	−0.018 (4)	0.4918 (15)	0.272 (3)	0.052 (9)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0335 (3)	0.0211 (2)	0.0174 (2)	0.00208 (17)	0.00210 (16)	0.00325 (16)
O1	0.0416 (10)	0.0277 (9)	0.0283 (9)	0.0039 (7)	−0.0052 (7)	−0.0036 (7)
O2	0.0474 (11)	0.0395 (10)	0.0289 (10)	0.0169 (8)	0.0099 (8)	0.0130 (8)
N1	0.0362 (10)	0.0248 (10)	0.0229 (10)	0.0014 (8)	0.0022 (8)	0.0034 (8)
N2	0.0459 (12)	0.0276 (11)	0.0247 (11)	0.0016 (9)	−0.0018 (9)	0.0068 (8)
N3	0.0489 (13)	0.0325 (11)	0.0279 (11)	0.0019 (9)	−0.0012 (9)	0.0104 (9)
N4	0.0499 (13)	0.0291 (11)	0.0313 (12)	−0.0004 (9)	−0.0018 (9)	0.0121 (9)
N5	0.0469 (12)	0.0264 (11)	0.0267 (11)	−0.0010 (9)	−0.0011 (9)	0.0078 (8)
C1	0.0497 (15)	0.0245 (12)	0.0282 (13)	−0.0019 (10)	0.0027 (11)	0.0028 (10)
C2	0.0527 (16)	0.0340 (14)	0.0217 (12)	−0.0001 (11)	0.0022 (11)	0.0016 (10)
C3	0.0282 (11)	0.0259 (12)	0.0245 (11)	0.0026 (9)	0.0013 (9)	0.0063 (9)

C4	0.077 (2)	0.0223 (13)	0.0296 (14)	−0.0022 (12)	0.0049 (13)	0.0022 (10)
C5	0.077 (2)	0.0301 (14)	0.0217 (12)	−0.0012 (13)	0.0043 (12)	0.0026 (10)
C6	0.0280 (11)	0.0275 (12)	0.0254 (11)	0.0040 (9)	0.0000 (9)	0.0057 (9)
O3	0.0422 (10)	0.0260 (9)	0.0292 (9)	0.0002 (8)	0.0012 (7)	0.0040 (7)

Geometric parameters (Å, °)

Co1—O1^{i}	2.0855 (16)	N3—N4	1.304 (3)
Co1—O1	2.0855 (16)	N4—N5	1.339 (3)
Co1—O2	2.1220 (17)	N5—C6	1.331 (3)
Co1—O2^{i}	2.1220 (17)	C1—C2	1.372 (3)
Co1—N1	2.1520 (19)	C1—H1	0.9300
Co1—N1^{i}	2.1521 (19)	C2—C3	1.391 (3)
O1—H1A	0.855 (10)	C2—H2	0.9300
O1—H1B	0.857 (10)	C3—C4	1.377 (3)
O2—H2A	0.849 (10)	C3—C6	1.471 (3)
O2—H2B	0.851 (10)	C4—C5	1.378 (4)
N1—C5	1.331 (3)	C4—H4	0.9300
N1—C1	1.331 (3)	C5—H5	0.9300
N2—C6	1.334 (3)	O3—H3A	0.853 (10)
N2—N3	1.342 (3)	O3—H3B	0.849 (10)
O1^{i}—Co1—O2	90.42 (7)	N4—N3—N2	109.21 (19)
O1—Co1—O2	89.58 (7)	N3—N4—N5	109.94 (19)
O1^{i}—Co1—O2^{i}	89.58 (7)	C6—N5—N4	104.62 (19)
O1—Co1—O2^{i}	90.42 (7)	N1—C1—C2	123.5 (2)
O1^{i}—Co1—N1	89.50 (7)	N1—C1—H1	118.2
O1—Co1—N1	90.50 (7)	C2—C1—H1	118.2
O2—Co1—N1	87.51 (7)	C1—C2—C3	119.9 (2)
O2^{i}—Co1—N1	92.49 (7)	C1—C2—H2	120.1
O1^{i}—Co1—N1^{i}	90.50 (7)	C3—C2—H2	120.1
O1—Co1—N1^{i}	89.50 (7)	C4—C3—C2	116.5 (2)
O2—Co1—N1^{i}	92.49 (7)	C4—C3—C6	121.0 (2)
O2^{i}—Co1—N1^{i}	87.51 (7)	C2—C3—C6	122.5 (2)
Co1—O1—H1A	130.6 (18)	C3—C4—C5	119.8 (2)
Co1—O1—H1B	112 (2)	C3—C4—H4	120.1
H1A—O1—H1B	114.2 (17)	C5—C4—H4	120.1
Co1—O2—H2A	123.1 (17)	N1—C5—C4	123.7 (2)
Co1—O2—H2B	118.7 (18)	N1—C5—H5	118.2
H2A—O2—H2B	115.9 (17)	C4—C5—H5	118.2
C5—N1—C1	116.5 (2)	N5—C6—N2	111.4 (2)
C5—N1—Co1	121.48 (16)	N5—C6—C3	123.4 (2)
C1—N1—Co1	121.77 (16)	N2—C6—C3	125.1 (2)
C6—N2—N3	104.82 (19)	H3A—O3—H3B	114.8 (16)

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1A···N2^{ii}	0.855 (10)	1.968 (10)	2.795 (3)	161.84 (3)
O1—H1B···O3^{iii}	0.857 (10)	1.93 (1)	2.753 (3)	161.83 (3)
O2—H2A···N3^{iv}	0.849 (10)	2.10 (1)	2.939 (3)	170.66 (3)
O2—H2B···O3^{i}	0.851 (3)	1.90 (1)	2.745 (3)	172.44 (3)
O3—H3A···N5^{v}	0.853 (10)	1.99 (1)	2.840 (3)	177.52 (3)
O3—H3B···N4^{vi}	0.849 (10)	1.942 (10)	2.780 (3)	168.93 (3)

Symmetry codes: (ii) −*x*+1, −*y*+1, −*z*+1; (iii) *x*+1, *y*, *z*; (iv) −*x*+1, −*y*, −*z*+1; (i) −*x*+1, −*y*+1, −*z*; (v) *x*, *y*+1, *z*; (vi) −*x*, −*y*, −*z*+1.

Fig. 1

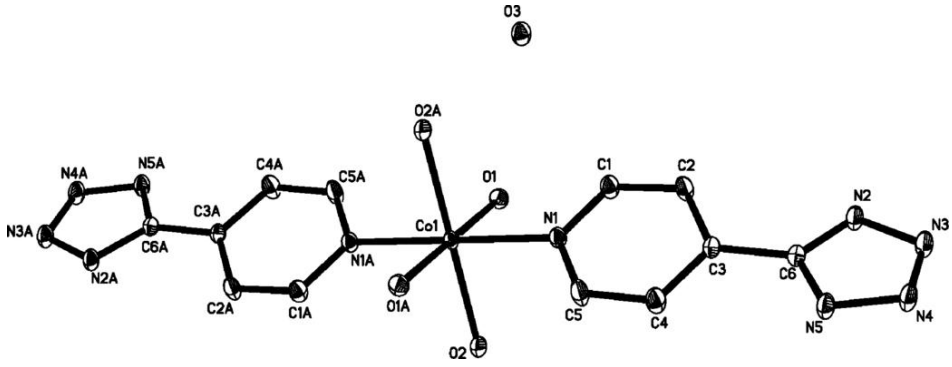

O3
O2A
N4A
N5A
C4A
C5A
O1
C1
C2
N2
N3A
C3A
Co1
N1
N3
C6A
N1A
C3
C6
N2A
C2A
C1A
O1A
C5
C4
N5
N4
O2

Fig. 2