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Diaquabis[5-(pyrazin-2-yl)tetrazolato]-cobalt(II)

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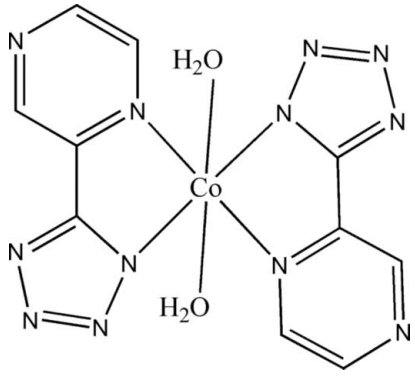
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.034; wR factor = 0.083; data-to-parameter ratio = 14.0.

In the title complex, $[Co(C_5H_3N_3)_2(H_2O)_2]$, prepared in a one-pot synthesis, the Co^{II} atom (site symmetry $\overline{1}$), is coordinated by four N atoms from two 5-(2-pyrazinyl)tetrazolate ligands and by two water molecules in a distorted *trans*-CoO_2N_4 octahedral geometry. A supramolecular network is formed *via* intermolecular O—H···N hydrogen bonds.

Related literature

For related literature, see: Demko & Sharpless (2001*a*, 2001*b*); Deng *et al.* (2007); Eddaoudi *et al.* (2001); Rizk *et al.* (2005).



Experimental

Crystal data

$[Co(C_5H_3N_3)_2(H_2O)_2]$
M_r = 389.23
Monoclinic, $P2_1/n$
a = 6.0676 (1) Å
b = 11.4221 (2) Å
c = 10.7096 (2) Å
β = 105.652 (1)°
V = 714.70 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.24 mm^{-1}
T = 293 (2) K
0.18 × 0.16 × 0.15 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.808, T_{max} = 0.836
6011 measured reflections
1693 independent reflections
1325 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.083
S = 1.06
1693 reflections
121 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

Table 1
Selected bond lengths (Å).

Co1—O1W	2.0638 (18)	Co1—N1	2.1856 (16)
Co1—N6	2.1076 (17)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1W···N5^{i}	0.777 (15)	2.067 (15)	2.832 (2)	168 (2)
O1W—H2W···N3^{ii}	0.819 (15)	1.928 (15)	2.740 (2)	171 (2)

Symmetry codes: (i) $x-1, y, z$; (ii) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); 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, 2004); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2381).

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supplementary materials

Acta Cryst. (2007). E**63**, m1591 [**doi:10.1107/S1600536807021393**]

Diaquabis[5-(pyrazin-2-yl)tetrazolato]cobalt(II)

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Comment

The design, synthesis, characterization, and properties of supramolecular networks formed by using functionalized organic molecules as bridges between metal centers are of great interest (Rizk *et al.*, 2005; Eddaoudi *et al.*, 2001). The reports on tetrazoles is expanding rapidly, since tetrazoles have an important role in coordination chemistry as a ligand (Deng *et al.*, 2006). Recently, 5-substituted 1*H*-tetrazoles have been synthesized by a facile approach (Demko & Sharpless, 2001a, 2001 b). In the general reaction, the tetrazoles are prepared by the addition of azide to nitriles in water with the aid of a lewis acid such a Zn^{2+}. In this paper, we selected 2-cyanopyrazine, NaN_3 and a Lewis acid $CoCl_2$ as reagent, to yield in one step the mononuclear structure (I) under hydrothermal condition.

In (I), the Co^{II} atom, located on an inversion center, is coordinated by four N atoms from two 5-(2-pyrazinyl)tetrazolate ligands and two water molecules in a distorted octahedral geometry (Fig. 1; Table 1). In the ligand, the pyrazinyl and tetrazolyl rings are almost coplanar, with a dihedral angle of 3.53 (4)°. Intermolecular O—H···N hydrogen bonds (Table 2) form a supramolecular network (Fig. 2).

Experimental

Hydrothermal treatment of $CoCl_2.6H_2O$ (1.0 mmol, 0.237 g), 2-cyanopyrazine (1 mmol, 0.105 g), Na_{N3} (1 mmol, 0.065 g), and water (3 ml) over 50 h at 422 K yielded red prisms of (I) (yield 78%).

Refinement

The water H atoms were located in a difference Fourier map and their positions were freely refined with $U_{iso}(H) = 1.2U_{eq}(O)$. The other H atoms were placed

in calculated positions (C—H = 0.93 Å) refined using a riding model with $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

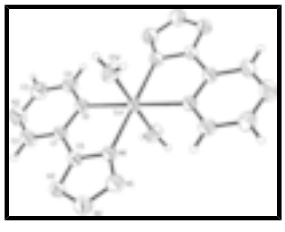

Fig. 1. The structure of (I), showing the atomic numbering scheme. Non-H atoms are shown as 50% probability displacement ellipsoids. Unlabelled atoms are related to the labelled atoms by the symmetry operator (1-x, 1-y, -z).

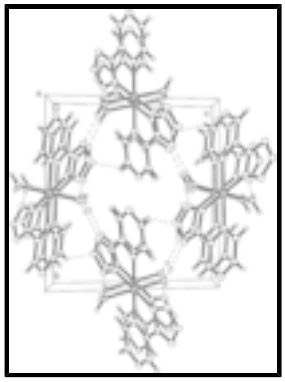

Fig. 2. A packing diagram of (I). Hydrogen bonds are depicted as broken lines.

Diaquabis[5-(pyrazin-2-yl)tetrazolate]cobalt(II)

Crystal data

$[Co(C_5H_3N_3)_2(H_2O)_2]$	F_{000} = 394
M_r = 389.23	D_x = 1.809 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 5700 reflections
a = 6.0676 (1) Å	θ = 1.7–28.0º
b = 11.4221 (2) Å	μ = 1.24 mm^{-1}
c = 10.7096 (2) Å	T = 293 (2) K
β = 105.652 (1)º	Prism, red
V = 714.70 (2) Å^3	0.18 × 0.16 × 0.15 mm
Z = 2	

Data collection

Bruker APEXII area-detector diffractometer	1693 independent reflections
Radiation source: fine-focus sealed tube	1325 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.035
T = 293(2) K	θ_{max} = 27.9º
φ and ω scans	θ_{min} = 2.7º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −7→7
T_{min} = 0.808, T_{max} = 0.836	k = −15→14
6011 measured reflections	l = −14→12

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)]$ = 0.034	$w = 1/[\sigma^2(F_o^2) + (0.0392P)^2 + 0.1286P]$

	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.083$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.06$	$\Delta\rho_{max} = 0.33$ e Å^{-3}
1693 reflections	$\Delta\rho_{min} = -0.30$ e Å^{-3}
121 parameters	Extinction correction: none
3 restraints	
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.5209 (3)	0.24786 (18)	0.0722 (2)	0.0292 (5)
C2	0.4676 (4)	0.13095 (19)	0.0833 (3)	0.0422 (6)
H2	0.5804	0.0813	0.1314	0.051*
C3	0.1084 (4)	0.1622 (2)	−0.0407 (3)	0.0437 (6)
H3	−0.0379	0.1351	−0.0813	0.052*
C4	0.1588 (4)	0.2787 (2)	−0.0534 (2)	0.0355 (5)
H4	0.0459	0.3277	−0.1025	0.043*
C5	0.7458 (3)	0.29806 (18)	0.1328 (2)	0.0292 (5)
Co1	0.5000	0.5000	0.0000	0.02720 (14)
H1W	0.305 (3)	0.5142 (18)	0.182 (2)	0.053*
H2W	0.457 (4)	0.5988 (15)	0.212 (2)	0.053*
N1	0.3655 (3)	0.32279 (14)	0.00284 (17)	0.0286 (4)
N2	0.2619 (3)	0.08721 (18)	0.0278 (2)	0.0507 (6)
N3	0.9254 (3)	0.24591 (16)	0.21020 (19)	0.0355 (4)
N4	1.0867 (3)	0.32889 (18)	0.2402 (2)	0.0427 (5)
N5	1.0062 (3)	0.42684 (17)	0.1815 (2)	0.0393 (5)
N6	0.7895 (3)	0.41001 (15)	0.11191 (18)	0.0306 (4)
O1W	0.4169 (3)	0.53856 (16)	0.17002 (18)	0.0428 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0287 (11)	0.0243 (10)	0.0337 (12)	0.0012 (8)	0.0066 (9)	0.0007 (9)

C2	0.0394 (13)	0.0269 (12)	0.0563 (17)	0.0021 (10)	0.0057 (12)	0.0062 (11)
C3	0.0346 (12)	0.0398 (14)	0.0532 (16)	−0.0101 (10)	0.0061 (12)	−0.0053 (12)
C4	0.0295 (11)	0.0368 (12)	0.0378 (13)	−0.0004 (9)	0.0053 (10)	−0.0005 (10)
C5	0.0292 (11)	0.0241 (10)	0.0343 (12)	0.0034 (8)	0.0086 (9)	0.0032 (9)
Co1	0.0264 (2)	0.0196 (2)	0.0336 (2)	−0.00012 (16)	0.00481 (16)	0.00184 (17)
N1	0.0296 (9)	0.0247 (9)	0.0310 (10)	0.0007 (7)	0.0072 (8)	0.0009 (7)
N2	0.0447 (12)	0.0308 (11)	0.0706 (16)	−0.0105 (9)	0.0055 (11)	0.0010 (11)
N3	0.0286 (9)	0.0329 (10)	0.0419 (11)	0.0020 (8)	0.0041 (8)	0.0081 (9)
N4	0.0323 (10)	0.0448 (12)	0.0461 (12)	−0.0013 (9)	0.0024 (9)	0.0063 (10)
N5	0.0310 (10)	0.0365 (11)	0.0465 (12)	−0.0049 (8)	0.0039 (9)	0.0003 (9)
N6	0.0249 (9)	0.0261 (9)	0.0382 (11)	−0.0014 (7)	0.0042 (8)	0.0007 (8)
O1W	0.0455 (10)	0.0381 (9)	0.0503 (11)	−0.0154 (8)	0.0225 (9)	−0.0143 (8)

Geometric parameters (Å, °)

C1—N1	1.340 (2)	Co1—O1W	2.0638 (18)
C1—C2	1.386 (3)	Co1—O1W^{i}	2.0638 (18)
C1—C5	1.461 (3)	Co1—N6^{i}	2.1076 (17)
C2—N2	1.327 (3)	Co1—N6	2.1076 (17)
C2—H2	0.9300	Co1—N1^{i}	2.1856 (16)
C3—N2	1.330 (3)	Co1—N1	2.1856 (16)
C3—C4	1.381 (3)	N3—N4	1.338 (3)
C3—H3	0.9300	N4—N5	1.311 (3)
C4—N1	1.335 (3)	N5—N6	1.339 (2)
C4—H4	0.9300	O1W—H1W	0.777 (15)
C5—N3	1.320 (3)	O1W—H2W	0.819 (15)
C5—N6	1.337 (3)		
N1—C1—C2	121.15 (19)	O1W^{i}—Co1—N1^{i}	90.25 (7)
N1—C1—C5	115.39 (18)	N6^{i}—Co1—N1^{i}	78.31 (6)
C2—C1—C5	123.46 (19)	N6—Co1—N1^{i}	101.69 (6)
N2—C2—C1	122.5 (2)	O1W—Co1—N1	90.25 (7)
N2—C2—H2	118.8	O1W^{i}—Co1—N1	89.75 (7)
C1—C2—H2	118.8	N6^{i}—Co1—N1	101.69 (6)
N2—C3—C4	122.3 (2)	N6—Co1—N1	78.31 (6)
N2—C3—H3	118.9	N1^{i}—Co1—N1	180.0
C4—C3—H3	118.9	C4—N1—C1	116.36 (18)
N1—C4—C3	121.7 (2)	C4—N1—Co1	130.69 (15)
N1—C4—H4	119.2	C1—N1—Co1	112.94 (13)
C3—C4—H4	119.2	C2—N2—C3	116.0 (2)
N3—C5—N6	111.69 (19)	C5—N3—N4	104.92 (17)
N3—C5—C1	128.00 (19)	N5—N4—N3	109.61 (17)
N6—C5—C1	120.31 (18)	N4—N5—N6	109.10 (17)
O1W—Co1—O1W^{i}	180.0	C5—N6—N5	104.68 (17)
O1W—Co1—N6^{i}	91.90 (7)	C5—N6—Co1	112.91 (13)
O1W^{i}—Co1—N6^{i}	88.10 (7)	N5—N6—Co1	142.10 (14)
O1W—Co1—N6	88.10 (7)	Co1—O1W—H1W	120.3 (18)

O1W^{i}—Co1—N6	91.90 (7)	Co1—O1W—H2W	123.5 (16)
N6^{i}—Co1—N6	180.0	H1W—O1W—H2W	111 (2)
O1W—Co1—N1^{i}	89.75 (7)		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1W···N5^{ii}	0.777 (15)	2.067 (15)	2.832 (2)	168 (2)
O1W—H2W···N3^{iii}	0.819 (15)	1.928 (15)	2.740 (2)	171 (2)

Symmetry codes: (ii) *x*−1, *y*, *z*; (iii) −*x*+3/2, *y*+1/2, −*z*+1/2.

Fig. 1

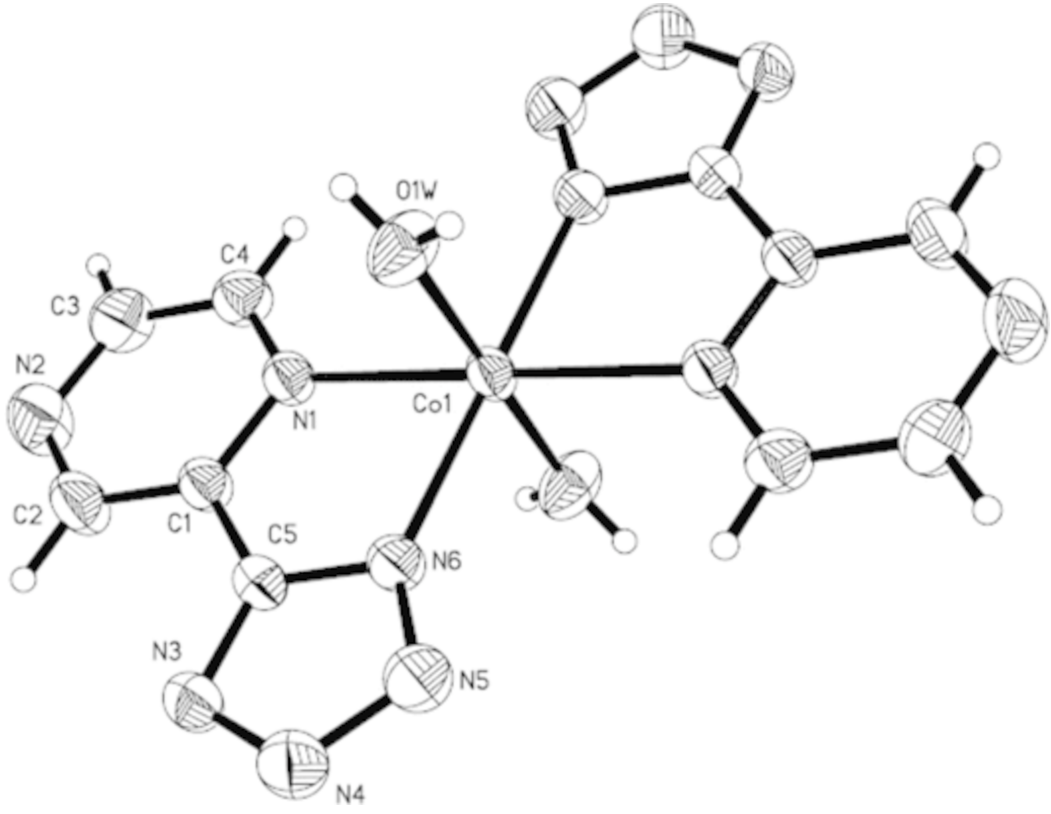

Fig. 2