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## Structure Reports

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Tetrakis(2-aminopyrazine- $\kappa N^4$ )-dichloridocobalt(II)Wei Kang,<sup>a</sup> Li-Hua Huo,<sup>a</sup> Shan Gao<sup>a</sup> and Seik Weng Ng<sup>b\*</sup><sup>a</sup>College of Chemistry and Materials Science, Heilongjiang University, Harbin 150080, People's Republic of China, and <sup>b</sup>Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia

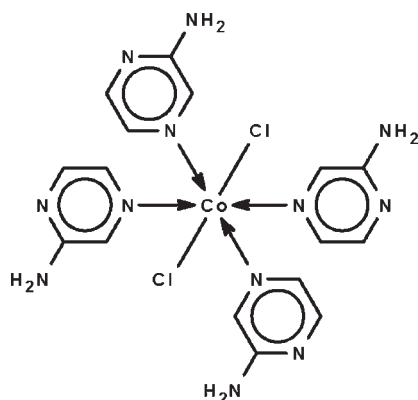
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Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å;  $R$  factor = 0.025;  $wR$  factor = 0.074; data-to-parameter ratio = 16.3.

The  $\text{Co}^{\text{II}}$  atom in the title complex,  $[\text{CoCl}_2(\text{C}_4\text{H}_5\text{N}_3)_4]$ , exists in an all-*trans*  $\text{Cl}_2\text{N}_4\text{Co}$  octahedral geometry. The  $\text{Co}^{\text{II}}$  atom lies on a special position of 2 site symmetry. Adjacent molecules are linked by  $\text{N}-\text{H}\cdots\text{N}$  and  $\text{N}-\text{H}\cdots\text{Cl}$  hydrogen bonds into a three-dimensional network.

## Related literature

For the triclinic modification, see: Csöregi *et al.* (2000).

## Experimental

## Crystal data

 $[\text{CoCl}_2(\text{C}_4\text{H}_5\text{N}_3)_4]$  $M_r = 510.27$ Orthorhombic, *Pccn* $a = 7.6347$  (2) Å $b = 15.7341$  (4) Å $c = 18.6074$  (4) Å $V = 2235.22$  (9) Å<sup>3</sup> $Z = 4$ Mo  $K\alpha$  radiation $\mu = 1.04$  mm<sup>-1</sup> $T = 293$  K

0.30 × 0.20 × 0.15 mm

## Data collection

Rigaku R-Axis RAPID IP diffractometer  
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)  
 $T_{\text{min}} = 0.746$ ,  $T_{\text{max}} = 0.860$ 20053 measured reflections  
2553 independent reflections  
2234 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.024$ 

## Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.025$   
 $wR(F^2) = 0.074$   
 $S = 1.06$   
2553 reflections  
157 parameters  
4 restraintsH atoms treated by a mixture of independent and constrained refinement  
 $\Delta\rho_{\text{max}} = 0.29$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.25$  e Å<sup>-3</sup>

Table 1

Selected bond lengths (Å).

Co1—N1	2.2068 (11)	Co1—Cl1	2.4206 (4)
Co1—N4	2.1941 (11)		

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N3—H1 $\cdots$ Cl1 <sup>i</sup>	0.85 (1)	2.36 (1)	3.209 (2)	175 (2)
N3—H2 $\cdots$ N5 <sup>ii</sup>	0.86 (1)	2.43 (2)	3.134 (2)	140 (2)
N6—H3 $\cdots$ Cl1 <sup>iii</sup>	0.85 (1)	2.42 (1)	3.265 (1)	171 (2)
N6—H4 $\cdots$ N2 <sup>iv</sup>	0.86 (1)	2.33 (2)	3.045 (2)	142 (2)

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalClear* (Rigaku/MSK, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *pubCIF* (Westrip, 2009).

We thank the Natural Science Foundation of Heilongjiang Province (No. B200501), Heilongjiang University, China, and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2656).

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**supplementary materials**

*Acta Cryst.* (2009). E65, m1502 [ doi:10.1107/S1600536809045309 ]

## Tetrakis(2-aminopyrazine- $\kappa N^4$ )dichloridocobalt(II)

W. Kang, L.-H. Huo, S. Gao and S. W. Ng

### Experimental

Cobalt(II) chloride hexahydrate (0.48 g, 2 mmol) and 2-aminopyrazine (0.19 g, 2 mmol) were dissolved in a small volume of water. Red crystals of the adduct separated from the filtered solution after several days. CH&N elemental analysis. Calc. for  $C_{16}H_{20}Cl_2N_{12}Co$ : C 37.66, H 3.95, N 32.94%; found: C 37.63, H 3.89, N 32.97%.

### Refinement

Amino-H atoms were located in a difference Fourier map and refined isotropically with a distance restraint of N–H =  $0.86 \pm 0.01$  Å. Carbon-bound H-atoms were placed in calculated positions (C–H = 0.93 Å) and were included in the refinement in the riding model approximation with  $U_{iso}(H)$  set to  $1.2U_{eq}(C)$ .

### Figures

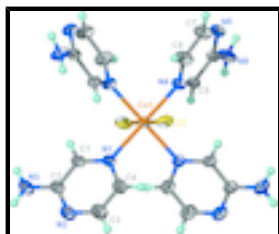


Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of  $CoCl_2(C_2H_5N_3)_4$  at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

## Tetrakis(2-aminopyrazine- $\kappa N^4$ )dichloridocobalt(II)

### Crystal data

$[CoCl_2(C_4H_5N_3)_4]$

$M_r = 510.27$

Orthorhombic, *Pccn*

Hall symbol: -P 2ab 2ac

$a = 7.6347$  (2) Å

$b = 15.7341$  (4) Å

$c = 18.6074$  (4) Å

$V = 2235.22$  (9) Å<sup>3</sup>

$Z = 4$

$F_{000} = 1044$

$D_x = 1.516$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 15790 reflections

$\theta = 2.3$ – $27.5^\circ$

$\mu = 1.04$  mm<sup>-1</sup>

$T = 293$  K

Block, red

$0.30 \times 0.20 \times 0.15$  mm

### Data collection

Rigaku RAXIS-RAPID IP

2553 independent reflections

# supplementary materials

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diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 293$  K

$\omega$  scans

Absorption correction: Multi-scan  
(ABSCOR; Higashi, 1995)

$T_{\min} = 0.746$ ,  $T_{\max} = 0.860$

20053 measured reflections

2234 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.024$

$\theta_{\max} = 27.5^\circ$

$\theta_{\min} = 3.2^\circ$

$h = -9 \rightarrow 9$

$k = -20 \rightarrow 20$

$l = -24 \rightarrow 24$

## Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.025$

$wR(F^2) = 0.074$

$S = 1.06$

2553 reflections

157 parameters

4 restraints

Primary atom site location: structure-invariant direct  
methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring  
sites

H atoms treated by a mixture of  
independent and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.0439P)^2 + 0.4514P]$$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.29 \text{ e } \text{\AA}^{-3}$

$\Delta\rho_{\min} = -0.25 \text{ e } \text{\AA}^{-3}$

Extinction correction: none

## Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Co1	0.7500	0.2500	0.103443 (12)	0.02794 (9)
C11	0.98632 (5)	0.14744 (2)	0.103952 (17)	0.03970 (11)
N1	0.61989 (16)	0.17473 (8)	0.01880 (6)	0.0348 (3)
N2	0.46194 (19)	0.08976 (11)	-0.09614 (7)	0.0553 (4)
N3	0.1968 (2)	0.09877 (14)	-0.03954 (8)	0.0686 (5)
N4	0.88907 (16)	0.31841 (7)	0.18890 (6)	0.0339 (3)
N5	1.03169 (17)	0.40550 (8)	0.30631 (6)	0.0387 (3)
N6	0.9535 (2)	0.53209 (8)	0.25231 (7)	0.0527 (4)
C1	0.45050 (19)	0.15892 (9)	0.01846 (7)	0.0357 (3)
H1A	0.3823	0.1771	0.0569	0.043*
C2	0.3693 (2)	0.11475 (10)	-0.03920 (7)	0.0413 (3)
C3	0.6338 (2)	0.10573 (14)	-0.09351 (9)	0.0625 (6)
H3A	0.7027	0.0878	-0.1318	0.075*
C4	0.7141 (2)	0.14683 (13)	-0.03790 (9)	0.0509 (4)
H4A	0.8345	0.1557	-0.0391	0.061*
C5	0.88843 (19)	0.40188 (8)	0.19189 (6)	0.0319 (3)
H5	0.8395	0.4324	0.1541	0.038*
C6	0.96002 (18)	0.44673 (8)	0.25094 (7)	0.0325 (3)
C7	1.0327 (2)	0.32043 (10)	0.30155 (8)	0.0453 (4)

H7	1.0823	0.2896	0.3390	0.054*
C8	0.9645 (2)	0.27664 (10)	0.24459 (8)	0.0452 (4)
H8	0.9700	0.2176	0.2440	0.054*
H1	0.136 (3)	0.1094 (14)	-0.0022 (8)	0.078 (7)*
H2	0.155 (3)	0.0704 (11)	-0.0753 (8)	0.063 (6)*
H3	0.978 (3)	0.5580 (12)	0.2913 (7)	0.060 (6)*
H4	0.909 (2)	0.5583 (11)	0.2164 (8)	0.061 (6)*

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Co1	0.03367 (16)	0.02901 (14)	0.02114 (14)	-0.00229 (9)	0.000	0.000
Cl1	0.0462 (2)	0.0432 (2)	0.02968 (18)	0.01013 (15)	0.00662 (13)	0.00476 (12)
N1	0.0337 (6)	0.0435 (6)	0.0271 (5)	-0.0030 (5)	0.0015 (5)	-0.0079 (5)
N2	0.0407 (8)	0.0851 (11)	0.0401 (7)	-0.0055 (7)	0.0052 (6)	-0.0322 (7)
N3	0.0366 (8)	0.1287 (16)	0.0407 (8)	-0.0134 (9)	0.0027 (6)	-0.0368 (9)
N4	0.0428 (7)	0.0326 (5)	0.0262 (5)	-0.0011 (5)	-0.0058 (5)	0.0003 (4)
N5	0.0447 (7)	0.0433 (6)	0.0281 (5)	-0.0005 (5)	-0.0095 (5)	-0.0004 (5)
N6	0.0912 (12)	0.0339 (6)	0.0331 (6)	-0.0092 (7)	-0.0211 (7)	0.0002 (5)
C1	0.0359 (7)	0.0464 (7)	0.0248 (6)	0.0013 (6)	0.0028 (5)	-0.0084 (6)
C2	0.0352 (8)	0.0588 (9)	0.0300 (6)	-0.0012 (7)	0.0005 (6)	-0.0124 (6)
C3	0.0416 (9)	0.1031 (16)	0.0429 (9)	-0.0042 (10)	0.0106 (7)	-0.0368 (9)
C4	0.0340 (8)	0.0789 (12)	0.0398 (8)	-0.0060 (7)	0.0075 (6)	-0.0206 (8)
C5	0.0399 (7)	0.0323 (6)	0.0236 (6)	-0.0039 (5)	-0.0055 (5)	0.0036 (5)
C6	0.0376 (7)	0.0349 (6)	0.0251 (6)	-0.0057 (5)	-0.0034 (5)	0.0008 (5)
C7	0.0582 (10)	0.0450 (8)	0.0326 (7)	0.0103 (7)	-0.0151 (7)	0.0028 (6)
C8	0.0650 (11)	0.0335 (7)	0.0371 (7)	0.0090 (7)	-0.0136 (7)	0.0015 (6)

Geometric parameters ( $\text{\AA}$ ,  $^\circ$ )

Co1—N1 <sup>i</sup>	2.2068 (11)	N5—C6	1.3348 (18)
Co1—N1	2.2068 (11)	N5—C7	1.341 (2)
Co1—N4	2.1941 (11)	N6—C6	1.3441 (18)
Co1—N4 <sup>i</sup>	2.1941 (11)	N6—H3	0.852 (9)
Co1—Cl1 <sup>i</sup>	2.4206 (4)	N6—H4	0.856 (9)
Co1—Cl1	2.4206 (4)	C1—C2	1.4207 (19)
N1—C1	1.3170 (19)	C1—H1A	0.9300
N1—C4	1.3501 (19)	C3—C4	1.366 (2)
N2—C2	1.3332 (19)	C3—H3A	0.9300
N2—C3	1.337 (2)	C4—H4A	0.9300
N3—C2	1.341 (2)	C5—C6	1.4157 (18)
N3—H1	0.853 (9)	C5—H5	0.9300
N3—H2	0.864 (9)	C7—C8	1.367 (2)
N4—C5	1.3145 (17)	C7—H7	0.9300
N4—C8	1.3556 (18)	C8—H8	0.9300
N4—Co1—N4 <sup>i</sup>	87.12 (6)	C6—N6—H4	118.8 (14)
N4—Co1—N1 <sup>i</sup>	92.07 (4)	H3—N6—H4	121 (2)

## supplementary materials

N4 <sup>i</sup> —Co1—N1 <sup>i</sup>	176.67 (4)	N1—C1—C2	121.63 (13)
N4—Co1—N1	176.67 (4)	N1—C1—H1A	119.2
N4 <sup>i</sup> —Co1—N1	92.07 (4)	C2—C1—H1A	119.2
N1 <sup>i</sup> —Co1—N1	88.93 (6)	N2—C2—N3	117.51 (14)
N4—Co1—Cl1 <sup>i</sup>	91.77 (3)	N2—C2—C1	120.88 (15)
N4 <sup>i</sup> —Co1—Cl1 <sup>i</sup>	87.91 (3)	N3—C2—C1	121.59 (13)
N1 <sup>i</sup> —Co1—Cl1 <sup>i</sup>	88.89 (3)	N2—C3—C4	123.88 (15)
N1—Co1—Cl1 <sup>i</sup>	91.43 (3)	N2—C3—H3A	118.1
N4—Co1—Cl1	87.91 (3)	C4—C3—H3A	118.1
N4 <sup>i</sup> —Co1—Cl1	91.77 (3)	N1—C4—C3	120.47 (15)
N1 <sup>i</sup> —Co1—Cl1	91.43 (3)	N1—C4—H4A	119.8
N1—Co1—Cl1	88.89 (3)	C3—C4—H4A	119.8
Cl1 <sup>i</sup> —Co1—Cl1	179.552 (18)	N4—C5—C6	121.97 (12)
C1—N1—C4	117.25 (12)	N4—C5—H5	119.0
C1—N1—Co1	123.15 (9)	C6—C5—H5	119.0
C4—N1—Co1	119.50 (10)	N5—C6—N6	119.10 (12)
C2—N2—C3	115.85 (13)	N5—C6—C5	121.00 (12)
C2—N3—H1	119.6 (16)	N6—C6—C5	119.89 (12)
C2—N3—H2	117.9 (14)	N5—C7—C8	123.50 (13)
H1—N3—H2	122 (2)	N5—C7—H7	118.2
C5—N4—C8	116.97 (12)	C8—C7—H7	118.2
C5—N4—Co1	121.27 (9)	N4—C8—C7	120.67 (14)
C8—N4—Co1	121.45 (10)	N4—C8—H8	119.7
C6—N5—C7	115.87 (12)	C7—C8—H8	119.7
C6—N6—H3	119.0 (14)		
N4 <sup>i</sup> —Co1—N1—C1	45.73 (12)	C3—N2—C2—N3	-179.1 (2)
N1 <sup>i</sup> —Co1—N1—C1	-131.09 (13)	C3—N2—C2—C1	2.7 (3)
Cl1 <sup>i</sup> —Co1—N1—C1	-42.23 (11)	N1—C1—C2—N2	-1.9 (2)
Cl1—Co1—N1—C1	137.45 (11)	N1—C1—C2—N3	-179.93 (17)
N4 <sup>i</sup> —Co1—N1—C4	-138.03 (13)	C2—N2—C3—C4	-1.6 (3)
N1 <sup>i</sup> —Co1—N1—C4	45.15 (12)	C1—N1—C4—C3	1.4 (3)
Cl1 <sup>i</sup> —Co1—N1—C4	134.01 (13)	Co1—N1—C4—C3	-175.03 (16)
Cl1—Co1—N1—C4	-46.30 (13)	N2—C3—C4—N1	-0.5 (4)
N4 <sup>i</sup> —Co1—N4—C5	-124.52 (13)	C8—N4—C5—C6	-1.1 (2)
N1 <sup>i</sup> —Co1—N4—C5	52.25 (11)	Co1—N4—C5—C6	172.58 (10)
Cl1 <sup>i</sup> —Co1—N4—C5	-36.70 (11)	C7—N5—C6—N6	179.54 (15)
Cl1—Co1—N4—C5	143.61 (11)	C7—N5—C6—C5	0.7 (2)
N4 <sup>i</sup> —Co1—N4—C8	48.91 (11)	N4—C5—C6—N5	0.1 (2)
N1 <sup>i</sup> —Co1—N4—C8	-134.32 (13)	N4—C5—C6—N6	-178.74 (15)
Cl1 <sup>i</sup> —Co1—N4—C8	136.73 (12)	C6—N5—C7—C8	-0.5 (3)
Cl1—Co1—N4—C8	-42.96 (12)	C5—N4—C8—C7	1.4 (2)
C4—N1—C1—C2	-0.3 (2)	Co1—N4—C8—C7	-172.29 (13)
Co1—N1—C1—C2	176.01 (11)	N5—C7—C8—N4	-0.6 (3)

Symmetry codes: (i)  $-x+3/2, -y+1/2, z$ .

Hydrogen-bond geometry (Å, °)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N3—H1 $\cdots$ C11 <sup>ii</sup>	0.85 (1)	2.36 (1)	3.209 (2)	175 (2)
N3—H2 $\cdots$ N5 <sup>iii</sup>	0.86 (1)	2.43 (2)	3.134 (2)	140 (2)
N6—H3 $\cdots$ C11 <sup>iv</sup>	0.85 (1)	2.42 (1)	3.265 (1)	171 (2)
N6—H4 $\cdots$ N2 <sup>v</sup>	0.86 (1)	2.33 (2)	3.045 (2)	142 (2)

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

Fig. 1

