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Tetrakis(2-aminopyrazine-κN^4)-dichloridocobalt(II)

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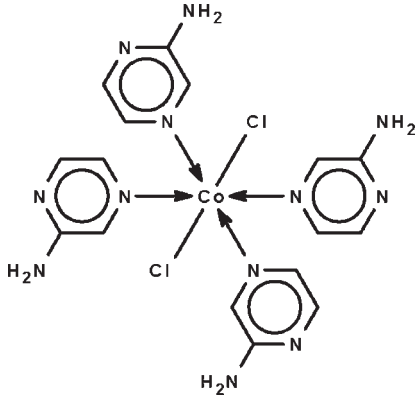
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.025; wR factor = 0.074; data-to-parameter ratio = 16.3.

The Co^{II} atom in the title complex, $[CoCl_2(C_4H_5N_3)_4]$, exists in an all-*trans* Cl_2N_4Co octahedral geometry. The Co^{II} atom lies on a special position of 2 site symmetry. Adjacent molecules are linked by N—H···N and N—H···Cl hydrogen bonds into a three-dimensional network.

Related literature

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



Experimental

Crystal data

$[CoCl_2(C_4H_5N_3)_4]$
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^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.04 mm^{-1}
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_{min} = 0.746, T_{max} = 0.860
20053 measured reflections
2553 independent reflections
2234 reflections with $I > 2\sigma(I)$
R_{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 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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···A	D—H	H···A	D···A	D—H···A
N3—H1···Cl1^{i}	0.85 (1)	2.36 (1)	3.209 (2)	175 (2)
N3—H2···N5^{ii}	0.86 (1)	2.43 (2)	3.134 (2)	140 (2)
N6—H3···Cl1^{iii}	0.85 (1)	2.42 (1)	3.265 (1)	171 (2)
N6—H4···N2^{iv}	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/MSC, 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: *publCIF* (Westrip, 2009).

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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). E**65**, m1502 [**doi:10.1107/S1600536809045309**]

Tetrakis(2-aminopyrazine-κN^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±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

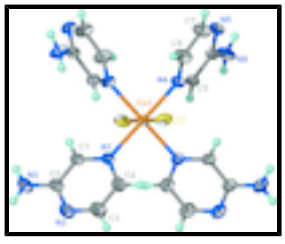

Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of $CoCl_2(C_2H_5N_3)_4$ at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

Tetrakis(2-aminopyrazine-κN^4)dichloridocobalt(II)

Crystal data

$[CoCl_2(C_4H_5N_3)_4]$	F_{000} = 1044
M_r = 510.27	D_x = 1.516 Mg m^{-3}
Orthorhombic, *Pccn*	Mo *K*α radiation, λ = 0.71073 Å
Hall symbol: -P 2ab 2ac	Cell parameters from 15790 reflections
a = 7.6347 (2) Å	θ = 2.3–27.5°
b = 15.7341 (4) Å	μ = 1.04 mm^{-1}
c = 18.6074 (4) Å	*T* = 293 K
V = 2235.22 (9) Å^3	Block, red
Z = 4	0.30 × 0.20 × 0.15 mm

Data collection

Rigaku RAXIS-RAPID IP	2553 independent reflections

diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

T = 293 K

ω 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_{int} = 0.024

θ_{max} = 27.5º

θ_{min} = 3.2º

h = −9→9

k = −20→20

l = −24→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 e Å^{-3}

$\Delta\rho_{min}$ = −0.25 e Å^{-3}

Extinction correction: none

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Co1	0.7500	0.2500	0.103443 (12)	0.02794 (9)
Cl1	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 (Å^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 (Å, °)

Co1—N1^{i}	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^{i}	2.1941 (11)	N6—H3	0.852 (9)
Co1—Cl1^{i}	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^{i}	87.12 (6)	C6—N6—H4	118.8 (14)
N4—Co1—N1^{i}	92.07 (4)	H3—N6—H4	121 (2)

$N4^{i}$—Co1—$N1^{i}$	176.67 (4)	N1—C1—C2	121.63 (13)
N4—Co1—N1	176.67 (4)	N1—C1—H1A	119.2
$N4^{i}$—Co1—N1	92.07 (4)	C2—C1—H1A	119.2
$N1^{i}$—Co1—N1	88.93 (6)	N2—C2—N3	117.51 (14)
N4—Co1—$Cl1^{i}$	91.77 (3)	N2—C2—C1	120.88 (15)
$N4^{i}$—Co1—$Cl1^{i}$	87.91 (3)	N3—C2—C1	121.59 (13)
$N1^{i}$—Co1—$Cl1^{i}$	88.89 (3)	N2—C3—C4	123.88 (15)
N1—Co1—$Cl1^{i}$	91.43 (3)	N2—C3—H3A	118.1
N4—Co1—Cl1	87.91 (3)	C4—C3—H3A	118.1
$N4^{i}$—Co1—Cl1	91.77 (3)	N1—C4—C3	120.47 (15)
$N1^{i}$—Co1—Cl1	91.43 (3)	N1—C4—H4A	119.8
N1—Co1—Cl1	88.89 (3)	C3—C4—H4A	119.8
$Cl1^{i}$—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)		
$N4^{i}$—Co1—N1—C1	45.73 (12)	C3—N2—C2—N3	−179.1 (2)
$N1^{i}$—Co1—N1—C1	−131.09 (13)	C3—N2—C2—C1	2.7 (3)
$Cl1^{i}$—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)
$N4^{i}$—Co1—N1—C4	−138.03 (13)	C2—N2—C3—C4	−1.6 (3)
$N1^{i}$—Co1—N1—C4	45.15 (12)	C1—N1—C4—C3	1.4 (3)
$Cl1^{i}$—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)
$N4^{i}$—Co1—N4—C5	−124.52 (13)	C8—N4—C5—C6	−1.1 (2)
$N1^{i}$—Co1—N4—C5	52.25 (11)	Co1—N4—C5—C6	172.58 (10)
$Cl1^{i}$—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)
$N4^{i}$—Co1—N4—C8	48.91 (11)	N4—C5—C6—N5	0.1 (2)
$N1^{i}$—Co1—N4—C8	−134.32 (13)	N4—C5—C6—N6	−178.74 (15)
$Cl1^{i}$—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···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H1···Cl1^{ii}	0.85 (1)	2.36 (1)	3.209 (2)	175 (2)
N3—H2···N5^{iii}	0.86 (1)	2.43 (2)	3.134 (2)	140 (2)
N6—H3···Cl1^{iv}	0.85 (1)	2.42 (1)	3.265 (1)	171 (2)
N6—H4···N2^{v}	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