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

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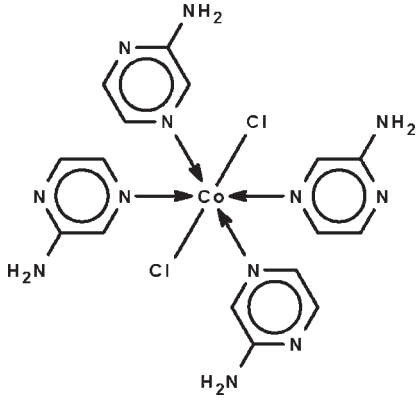
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.025; wR factor = 0.074; data-to-parameter ratio = 16.3.

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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supporting information

Acta Cryst. (2009). E**65**, m1502 [doi:10.1107/S1600536809045309]

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

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S1. 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%.

S2. 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).

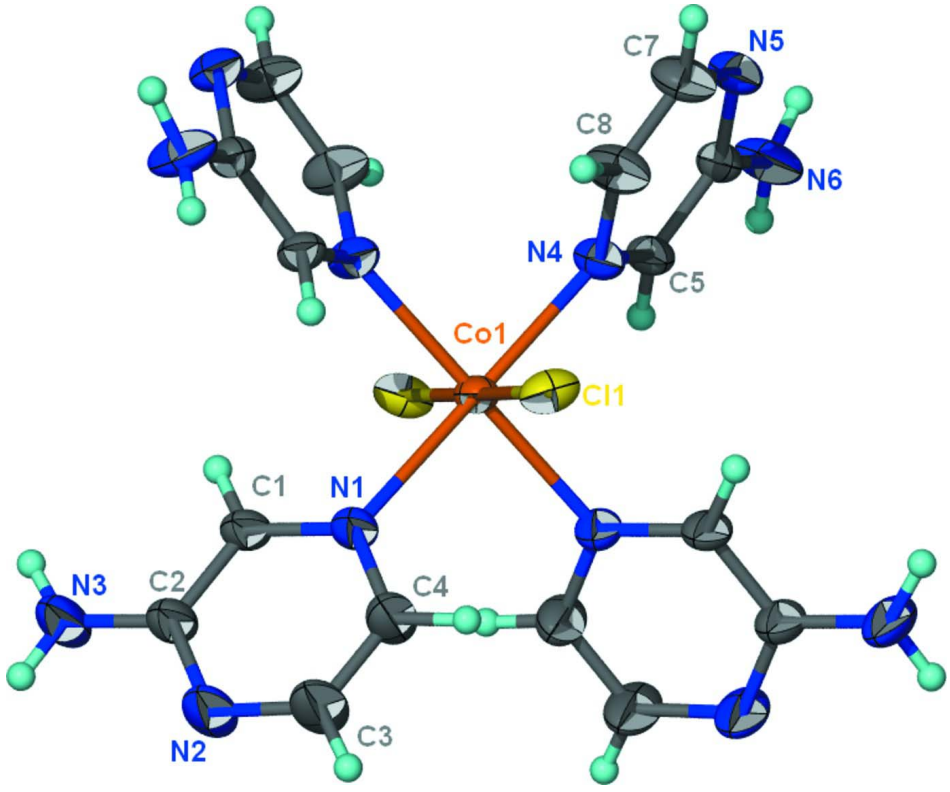

Figure 1

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

$[CoCl_2(C_4H_5N_3)_4]$
$M_r = 510.27$
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^3
$Z = 4$
$F(000) = 1044$
$D_x = 1.516$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 15790 reflections
$\theta = 2.3$–$27.5°$
$\mu = 1.04$ mm^{-1}
$T = 293$ K
Block, red
0.30 × 0.20 × 0.15 mm

Data collection

Rigaku RAXIS-RAPID IP diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.746$, $T_{max} = 0.860$
20053 measured reflections
2553 independent reflections
2234 reflections with $I > 2\sigma(I)$
$R_{int} = 0.024$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.2°$
$h = -9 \rightarrow 9$
$k = -20 \rightarrow 20$
$l = -24 \rightarrow 24$

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 $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.29$ e Å^{-3}
$\Delta\rho_{min} = -0.25$ e Å^{-3}

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 (Å²)

	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, º)

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 code: (i) −*x*+3/2, −*y*+1/2, *z*.

Hydrogen-bond geometry (Å, º)

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*.