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Bis(2-amino-3-methylpyridine)-dichloridocobalt(II)

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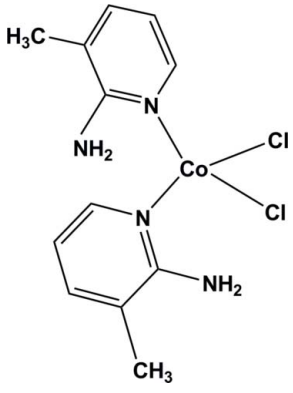
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.058; wR factor = 0.132; data-to-parameter ratio = 24.0.

In the title compound, $[CoCl_2(C_6H_8N_2)_2]$, the Co^{II} ion is four-coordinated by two pyridine N atoms from the 2-amino-3-methylpyridine ligands and two chloride ions in a distorted tetrahedral geometry. A weak intramolecular N—H···Cl interaction occurs. The crystal packing is stabilized by intermolecular N—H···Cl and C—H···Cl hydrogen-bond interactions.

Related literature

2-Amino-3-methylpyridine (ampy) can potentially coordinate to metal centers through the N atom of the amino group (Chen *et al.*, 2005) or the pyridyl nitrogen atom (Amani Komaei *et al.*, 1999; Ziegler *et al.*, 2000; Castillo *et al.*, 2001). For the structures of $[(ampyH)_2CoX_4]$ proton-transfer compounds (X = Cl, Br), see: Carnevale *et al.* (2010). Polar metal–halogen bonds are good hydrogen-bond acceptors, see: Aullón *et al.* (1998).



Experimental

Crystal data

$[CoCl_2(C_6H_8N_2)_2]$
M_r = 346.12
Monoclinic, $P2_1/n$
a = 9.3768 (19) Å
b = 13.841 (3) Å
c = 12.175 (2) Å
β = 100.31 (3)°
V = 1554.6 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.44 mm^{-1}
T = 298 K
0.50 × 0.38 × 0.30 mm

Data collection

Stoe IPDS II diffractometer
Absorption correction: numerical shape of crystal determined optically (*XRED* and *XSHAPE*; Stoe & Cie, 2005)
T_{min} = 0.517, T_{max} = 0.642
11996 measured reflections
4174 independent reflections
2803 reflections with $I > 2\sigma(I)$
R_{int} = 0.055

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.132
S = 1.07
4174 reflections
174 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.52 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—N3	2.034 (2)	Co1—Cl2	2.2303 (11)
Co1—N1	2.038 (3)	Co1—Cl1	2.2635 (11)
N3—Co1—N1	106.66 (10)	N3—Co1—Cl1	109.94 (8)
N3—Co1—Cl2	110.23 (8)	N1—Co1—Cl1	108.24 (8)
N1—Co1—Cl2	111.26 (9)	Cl2—Co1—Cl1	110.42 (5)

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2B···Cl1^{i}	0.86	2.72	3.427 (4)	140
N4—H4A···Cl1	0.86	2.67	3.363 (4)	138
N4—H4B···Cl2^{ii}	0.86	2.68	3.350 (4)	136
C3—H3···Cl2^{iii}	0.93	2.81	3.701 (4)	161

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

Data collection: *X-AREA* (Stoe & Cie, 2005); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: JJ2058).

References

Amani Komaei, S., Van Albada, G. A., Mutikainen, I., Turpeinen, U. & Reedijk, J. (1999). *Polyhedron*, **18**, 1991–1997.