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Dichloro[tris(methylpyridyl)amine]cobalt(III) perchlorate hemihydrate

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The tris(methylpyridyl)amine (tpa, $C_{18}H_{18}N_4$) ligand in the title complex, $[Co(tpa)Cl_2]ClO_4\cdot0.5H_2O$, is bound to the Co^{III} centre in a tripodal fashion through the four N-donor atoms, allowing the two chloro ligands to occupy the remaining *cis* sites in the octahedral coordination sphere. Half a solvent water molecule is disordered over two sites. The metal–ligand bond lengths are typical for Co^{III} complexes.

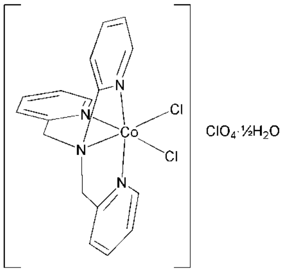
Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.002 Å
Disorder in solvent or counterion
R factor = 0.025
wR factor = 0.074
Data-to-parameter ratio = 26.9

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

The title complex, (I) (Fig. 1 and Table 1), is the first crystal structure of a Co^{III} complex containing the tris(methylpyridyl)amine (tpa) ligand. The complex is useful as a synthetic precursor to a wide variety of Co^{III}–tpa complexes, particularly those with bidentate chelating ligands. Furthermore, the structural parameters may be of use for molecular mechanics force fields, given the interest in studying Co^{III}–N systems with such methods.



(I)

Experimental

The complex was prepared according to a reported method (Hall *et al.*, 2003). Crystals of the complex were grown by slow cooling of an ethanol–methanol (1:1) solution of the complex.

Crystal data

$[CoCl_2(C_{18}H_{18}N_4)]ClO_4\cdot0.5H_2O$
M_r = 527.64
Monoclinic, $P2_1/c$
a = 10.2642 (14) Å
b = 15.166 (2) Å
c = 14.2695 (19) Å
β = 109.001 (3)°
V = 2100.2 (5) Å^3
Z = 4
D_x = 1.669 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 172 reflections
θ = 2.0–33.0°
μ = 1.24 mm^{-1}
T = 150 (2) K
Prism, purple
0.50 × 0.30 × 0.10 mm

Data collection

Bruker SMART CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min}$ = 0.577, $T_{\max}$ = 0.886
31 017 measured reflections
7781 independent reflections
6722 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.025
$\theta_{\max}$ = 33.0°
$h = -15 \rightarrow 15$
$k = -23 \rightarrow 23$
$l = -21 \rightarrow 21$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0426P)^2 + 0.434P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.025$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.074$	$\Delta\rho_{max} = 0.51$ e Å^{-3}
$S = 1.03$	$\Delta\rho_{min} = -0.41$ e Å^{-3}
7781 reflections	
289 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å).

Co1—N1	1.9450 (10)	Co1—N4	1.9624 (9)
Co1—N2	1.9553 (9)	Co1—Cl1	2.2374 (4)
Co1—N3	1.9357 (9)	Co1—Cl2	2.2630 (4)

The half-water molecule is disordered over two sites with occupancy factors fixed at 0.25 each. H atoms were placed in calculated positions using a riding model, with U_{eq} set at $1.2U_{eq}$ of the parent atom. H atoms of the disordered water molecule were not included.

Data collection: *SMART* (Bruker, 1995); cell refinement: *SMART*; data reduction: *SAINT-Plus* (Bruker, 1995); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* publication routines (Farrugia, 1999).

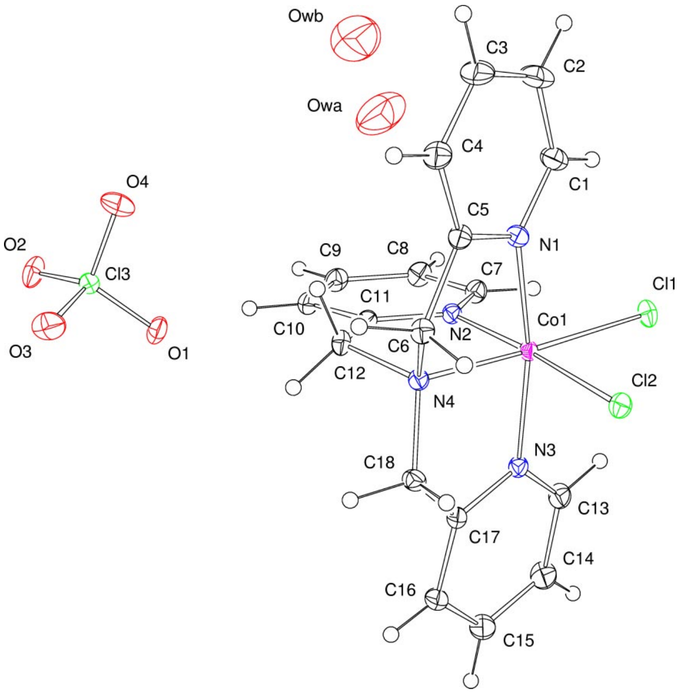


Figure 1
Displacement ellipsoid plot of (I), showing the crystallographic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

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