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Dichloridobis(7-amino-2,4-dimethyl-1,8-naphthyridine-κ^2N,N')cobalt(II) methanol disolvate

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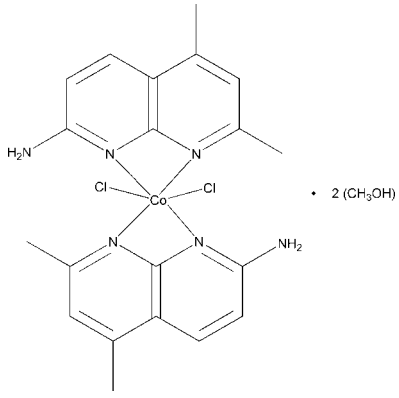
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.006 Å; R factor = 0.047; wR factor = 0.125; data-to-parameter ratio = 15.1.

The title compound, $[CoCl_2(C_{10}H_{11}N_3)_2]\cdot 2CH_3OH$, crystallizes with an elongated Co coordination polyhedron in a very distorted octahedral geometry. Both naphthyridine ligands coordinate to the Co atom *via* two N atoms in a bidentate chelating mode. The remaining coordination sites are occupied by two Cl atoms. Two uncoordinated solvent methanol molecules are hydrogen bonded to the Cl atoms. Additional N—H···O, C—H···Cl and N—H···Cl hydrogen bonds, and π–π stacking interactions [centroid–centroid distance 3.664 (4) Å], give rise to a three-dimensional network structure.

Related literature

For related literature, see: Bayer (1979); Che *et al.* (2001); Gavrilova & Bosnich (2004); Harvey *et al.* (2004); Jin *et al.* (2007); Kukrek *et al.* (2006); Mintert & Sheldrick (1995*a*,*b*); Oskui *et al.* (1999); Oskui & Sheldrick (1999).



Experimental

Crystal data

$[CoCl_2(C_{10}H_{11}N_3)_2]\cdot 2CH_4O$
M_r = 540.35
Triclinic, $P\overline{1}$
a = 9.694 (3) Å
b = 10.651 (3) Å
c = 14.154 (4) Å
α = 79.523 (4)°
β = 78.548 (4)°
γ = 65.697 (4)°
V = 1297.2 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.90 mm^{-1}
T = 298 (2) K
0.27 × 0.21 × 0.18 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.794, T_{max} = 0.855
6885 measured reflections
4521 independent reflections
2999 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.125
S = 1.04
4521 reflections
300 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···Cl1^{i}	0.82	2.35	3.162 (4)	172
O1—H1···Cl1^{ii}	0.82	2.44	3.194 (4)	154
N6—H6*B*···O2^{iii}	0.86	2.06	2.918 (4)	175
N6—H6*A*···Cl2	0.86	2.45	3.269 (4)	159
N3—H3*B*···O1^{iv}	0.86	2.09	2.947 (4)	175
N3—H3*A*···Cl1	0.86	2.51	3.309 (3)	156
C22—H22*B*···C17^{i}	0.96	2.91	3.789 (7)	154
C22—H22*B*···C18^{i}	0.96	2.71	3.575 (6)	150
C4—H4···Cl2^{v}	0.93	2.85	3.705 (4)	153
C7—H7···Cl1^{vi}	0.93	2.87	3.757 (4)	160
C13—H13···Cl1^{ii}	0.93	2.88	3.733 (4)	152

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZL2083).

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supplementary materials

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Dichloridobis(7-amino-2,4-dimethyl-1,8-naphthyridine-κ^2N,N')cobalt(II) methanol disolvate

S. Jin and Y. Sun

Comment

Molecular structures and chemical properties of transition metal complexes of 1,8-naphthyridine (napy) and its derivatives have received much attention (Kukrek *et al.*, 2006; Che *et al.*, 2001) as the ligands can link to metals *via* several coordination modes such as monodentate, chelating bidentate, and in a dinuclear bridging fashion (Gavrilova & Bosnich, 2004). 5,7-Dimethyl-1,8-naphthyridin-2-amine is a potentially tridentate ligand and is capable of linking two to four metal atoms together to form metal aggregates (Oskui *et al.*, 1999; Mintert & Sheldrick, 1995*a*; Oskui & Sheldrick, 1999; Mintert & Sheldrick, 1995*b*). The coordination chemistry of 5,7-dimethyl-1,8-naphthyridine-2-amine (*L*) has not been well studied before although a Co(II) complex ($Co(L)_2Cl_2$) was once described in a US patent (Bayer, 1979). As an extension of our study on naphthyridine coordination chemistry (Jin *et al.*, 2007), herein we report the synthesis and structure of the title complex as its bis methanol solvate, $(Co(L)_2(Cl)_2).2(CH_3OH)$.

The title compound was obtained as violet crystals by reacting cobalt chloride hexahydrate and *L* in methanol. The compound is air stable and light insensitive, and does not dissolve in water and most organic solvents. X-ray structural analysis shows that the complex is mononuclear, its molecular structure is shown in Fig. 1. The Co atom is positioned on an inversion center and is bonded to two *L* ligands and two chloride ions. Both of the two ligands coordinate to the metal center *via* two nitrogen atoms in a bidentate chelating fashion. The two chloride anions coordinated to the Co ion complete a very distorted octahedral geometry. With a N—Co—N bite angle of only 58.86 (11), and 60.39 (11) ° the structure can also be seen as a pseudotetrahedral complex with each of the naphthyridine ligands *L* counted as a singly bonded entity. The N—Co—N angle is of necessity quite small, thereby allowing for the Cl(2)—Co(1)—Cl(1) angle to expand to 96.99 (5) °. Perhaps as a result of the smaller spatial requirements of the chelating naphthyridine, the chloride ions are in *cis*-arrangement which is different from reported results (Harvey *et al.*, 2004).

The two naphthyridine rings are basically planar with an r.m.s. deviation of only 0.0098, and 0.0183 ° respectively, and both ligands are almost perpendicular to each other with an angle between the root mean square planes of the two ligands of 85.4 °.

The free methanol molecules are connected to the $(Co(L)_2(Cl)_2)$ moieties *via* O—H···Cl and N—H···O hydrogen bonds, and the $(Co(L)_2(Cl)_2)$ moieties themselves are connected with each other by N—H···Cl hydrogen bonds (see Table 1). The closest C—C distance between adjacent parallel naphthyridyl rings is 3.378 (4) Å, the corresponding centroid to centroid distance for the naphthyridyl rings is 3.664 Å, which implies the presence of π-π stacking interactions between the naphthyridyl rings. Via all these interactions the compound forms a three-dimensional network structure as shown in Fig. 2.

Experimental

All reagents and solvents were used as obtained without further purification. The CHN elemental analyses were performed on a Perkin-Elmer model 2400 elemental analyzer.

To a methanol solution of cobalt chloride hexahydrate (24 mg, 0.1 mmol), was added *L* (17.4 mg, 0.1 mmol) in 10 ml of methanol. The solution was stirred for three minutes, then the solution was filtered. The solution was left standing at room temperature for several days, and violet crystals were isolated after slow evaporation of the methanol solution in air. Yield: 38 mg, 70.3%. Anal. Calcd for $C_{22}H_{30}Cl_2CoN_6O_2$: C, 48.86; H, 5.55; N, 15.55; Found: C, 48.81; H, 5.52; N, 15.49.

Refinement

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with aromatic C—H = 0.93 Å, and methyl C—H = 0.96 Å. Hydrogen atoms bound to methanol molecules and amine groups were fixed, and restrained to O—H = 0.85 (1) Å, and N—H = 0.86 (1) Å.

Figures

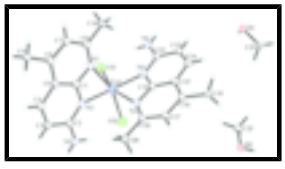


Fig. 1. The structure of the title compound, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

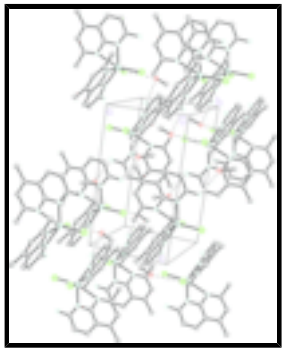


Fig. 2. The three dimensional network structure with π-π interactions and hydrogen bonds. The dashed lines present hydrogen bonds, the hydrogen atoms were omitted for clarity.

Dichloridobis(7-amino-2,4-dimethyl-1,8-naphthyridine-κ^2N,N')cobalt(II) methanol disolvate

Crystal data

$[CoCl_2(C_{10}H_{11}N_3)_2]\cdot 2CH_4O$	$Z = 2$
$M_r = 540.35$	$F_{000} = 562$
Triclinic, $P\overline{1}$	$D_x = 1.383$ Mg m^{-3}
$a = 9.694$ (3) Å	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$b = 10.651$ (3) Å	Cell parameters from 2019 reflections
$c = 14.154$ (4) Å	$\theta = 2.4$–$24.7°$
$\alpha = 79.523$ (4)°	$\mu = 0.90$ mm^{-1}
$\beta = 78.548$ (4)°	$T = 298$ (2) K
$\gamma = 65.697$ (4)°	Block, violet
$V = 1297.2$ (6) Å^3	0.27 × 0.21 × 0.18 mm

Data collection

Bruker SMART APEX CCD diffractometer	4521 independent reflections
Radiation source: fine-focus sealed tube	2999 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.021$
$T = 298(2)$ K	$\theta_{max} = 25.0°$
phi and ω scans	$\theta_{min} = 2.1°$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -9\rightarrow11$
$T_{min} = 0.794$, $T_{max} = 0.855$	$k = -12\rightarrow12$
6885 measured reflections	$l = -15\rightarrow16$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.047$	H-atom parameters constrained
$wR(F^2) = 0.125$	$w = 1/[\sigma^2(F_o^2) + (0.0565P)^2 + 0.2762P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} < 0.001$
4521 reflections	$\Delta\rho_{max} = 0.45$ e Å^{-3}
300 parameters	$\Delta\rho_{min} = -0.27$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Co1	0.96112 (6)	0.72223 (5)	0.23994 (3)	0.04516 (18)
Cl1	0.94391 (12)	0.51632 (9)	0.20816 (7)	0.0583 (3)
Cl2	1.22929 (11)	0.63991 (12)	0.21805 (8)	0.0690 (3)
N1	0.9345 (3)	0.9511 (3)	0.2182 (2)	0.0448 (7)
N2	0.8771 (3)	0.8510 (3)	0.1144 (2)	0.0426 (7)

N3	0.8215 (4)	0.7345 (3)	0.0155 (2)	0.0671 (10)
H3A	0.8541	0.6596	0.0544	0.080*
H3B	0.7872	0.7340	−0.0359	0.080*
N4	0.7015 (3)	0.7946 (3)	0.3218 (2)	0.0460 (7)
N5	0.9139 (3)	0.7129 (3)	0.3919 (2)	0.0437 (7)
N6	1.1406 (4)	0.6339 (4)	0.4536 (2)	0.0703 (10)
H6A	1.1885	0.6285	0.3955	0.084*
H6B	1.1906	0.6110	0.5021	0.084*
O1	0.7241 (4)	0.7211 (4)	0.8345 (2)	0.0855 (10)
H1	0.7914	0.6478	0.8186	0.089 (18)*
O2	0.2964 (4)	0.5474 (4)	0.6250 (2)	0.0891 (11)
H2	0.2413	0.5261	0.6713	0.12 (2)*
C1	0.8775 (4)	0.9703 (4)	0.1350 (3)	0.0425 (9)
C2	0.8242 (4)	0.8508 (4)	0.0350 (3)	0.0481 (9)
C3	0.7689 (4)	0.9765 (4)	−0.0293 (3)	0.0545 (10)
H3	0.7321	0.9762	−0.0851	0.065*
C4	0.7702 (4)	1.0942 (4)	−0.0091 (3)	0.0544 (10)
H4	0.7348	1.1748	−0.0513	0.065*
C5	0.8252 (4)	1.0972 (4)	0.0763 (3)	0.0463 (9)
C6	0.8331 (4)	1.2114 (4)	0.1076 (3)	0.0523 (10)
C7	0.8943 (5)	1.1897 (4)	0.1915 (3)	0.0584 (11)
H7	0.9018	1.2636	0.2132	0.070*
C8	0.9459 (4)	1.0583 (4)	0.2454 (3)	0.0492 (9)
C9	0.7767 (5)	1.3537 (4)	0.0519 (3)	0.0749 (13)
H9A	0.7672	1.4213	0.0919	0.112*
H9B	0.6789	1.3739	0.0337	0.112*
H9C	0.8481	1.3564	−0.0053	0.112*
C10	1.0178 (5)	1.0346 (5)	0.3348 (3)	0.0726 (13)
H10A	1.0493	0.9387	0.3603	0.109*
H10B	0.9451	1.0909	0.3824	0.109*
H10C	1.1052	1.0592	0.3189	0.109*
C11	0.7591 (4)	0.7613 (3)	0.4062 (3)	0.0423 (9)
C12	0.9893 (5)	0.6778 (4)	0.4685 (3)	0.0499 (9)
C13	0.9068 (5)	0.6885 (4)	0.5642 (3)	0.0590 (11)
H13	0.9596	0.6616	0.6174	0.071*
C14	0.7540 (5)	0.7371 (4)	0.5777 (3)	0.0593 (11)
H14	0.7017	0.7442	0.6404	0.071*
C15	0.6711 (4)	0.7778 (4)	0.4986 (3)	0.0486 (9)
C16	0.5117 (5)	0.8313 (4)	0.5007 (3)	0.0578 (11)
C17	0.4541 (5)	0.8647 (4)	0.4146 (3)	0.0638 (12)
H17	0.3488	0.9014	0.4149	0.077*
C18	0.5506 (5)	0.8449 (4)	0.3259 (3)	0.0548 (10)
C19	0.4055 (5)	0.8563 (5)	0.5956 (3)	0.0776 (14)
H19A	0.3138	0.9365	0.5854	0.116*
H19B	0.4552	0.8713	0.6423	0.116*
H19C	0.3802	0.7769	0.6192	0.116*
C20	0.4863 (5)	0.8810 (5)	0.2316 (3)	0.0796 (14)
H20A	0.4401	0.9799	0.2175	0.119*
H20B	0.4107	0.8427	0.2367	0.119*

H20C	0.5670	0.8432	0.1804	0.119*
C21	0.5865 (6)	0.7043 (6)	0.8635 (4)	0.1029 (18)
H21A	0.5910	0.6461	0.9241	0.154*
H21B	0.5687	0.6620	0.8152	0.154*
H21C	0.5047	0.7932	0.8712	0.154*
C22	0.4434 (6)	0.4976 (5)	0.6469 (5)	0.107 (2)
H22A	0.5042	0.5342	0.5971	0.161*
H22B	0.4866	0.3982	0.6509	0.161*
H22C	0.4416	0.5256	0.7080	0.161*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0519 (3)	0.0477 (3)	0.0353 (3)	−0.0186 (2)	−0.0107 (2)	−0.0001 (2)
Cl1	0.0749 (7)	0.0444 (5)	0.0566 (6)	−0.0238 (5)	−0.0118 (5)	−0.0039 (4)
Cl2	0.0498 (6)	0.0887 (8)	0.0553 (6)	−0.0175 (6)	−0.0085 (5)	0.0021 (6)
N1	0.0479 (18)	0.0481 (18)	0.0417 (18)	−0.0220 (15)	−0.0064 (14)	−0.0046 (14)
N2	0.0510 (19)	0.0451 (17)	0.0352 (17)	−0.0225 (15)	−0.0070 (14)	−0.0027 (13)
N3	0.100 (3)	0.064 (2)	0.056 (2)	−0.043 (2)	−0.032 (2)	0.0022 (17)
N4	0.0452 (19)	0.0450 (17)	0.0464 (19)	−0.0159 (15)	−0.0101 (15)	−0.0016 (14)
N5	0.0458 (19)	0.0458 (17)	0.0383 (17)	−0.0171 (15)	−0.0091 (14)	−0.0001 (13)
N6	0.053 (2)	0.103 (3)	0.051 (2)	−0.023 (2)	−0.0185 (17)	−0.004 (2)
O1	0.066 (2)	0.104 (3)	0.074 (2)	−0.010 (2)	−0.0108 (17)	−0.037 (2)
O2	0.066 (2)	0.135 (3)	0.067 (2)	−0.046 (2)	−0.0200 (18)	0.017 (2)
C1	0.042 (2)	0.046 (2)	0.040 (2)	−0.0202 (17)	0.0012 (16)	−0.0053 (17)
C2	0.053 (2)	0.055 (2)	0.041 (2)	−0.027 (2)	−0.0087 (18)	−0.0019 (18)
C3	0.057 (3)	0.067 (3)	0.039 (2)	−0.023 (2)	−0.0149 (18)	−0.0002 (19)
C4	0.057 (3)	0.048 (2)	0.047 (2)	−0.015 (2)	−0.0100 (19)	0.0091 (19)
C5	0.046 (2)	0.046 (2)	0.043 (2)	−0.0183 (18)	−0.0006 (17)	−0.0012 (17)
C6	0.057 (2)	0.043 (2)	0.054 (3)	−0.0209 (19)	0.002 (2)	−0.0043 (18)
C7	0.067 (3)	0.052 (2)	0.062 (3)	−0.029 (2)	0.003 (2)	−0.019 (2)
C8	0.046 (2)	0.057 (2)	0.049 (2)	−0.0237 (19)	−0.0045 (18)	−0.0111 (19)
C9	0.092 (4)	0.047 (2)	0.082 (3)	−0.028 (2)	−0.012 (3)	0.003 (2)
C10	0.078 (3)	0.088 (3)	0.067 (3)	−0.040 (3)	−0.017 (2)	−0.019 (3)
C11	0.050 (2)	0.0359 (19)	0.042 (2)	−0.0175 (17)	−0.0092 (17)	−0.0023 (16)
C12	0.059 (3)	0.049 (2)	0.044 (2)	−0.022 (2)	−0.0132 (19)	−0.0022 (18)
C13	0.077 (3)	0.062 (3)	0.038 (2)	−0.025 (2)	−0.020 (2)	0.0027 (19)
C14	0.076 (3)	0.059 (3)	0.041 (2)	−0.027 (2)	−0.002 (2)	−0.0054 (19)
C15	0.059 (3)	0.043 (2)	0.043 (2)	−0.0211 (19)	−0.0025 (19)	−0.0063 (17)
C16	0.061 (3)	0.052 (2)	0.057 (3)	−0.024 (2)	0.006 (2)	−0.011 (2)
C17	0.043 (2)	0.065 (3)	0.077 (3)	−0.016 (2)	−0.003 (2)	−0.012 (2)
C18	0.054 (3)	0.053 (2)	0.058 (3)	−0.020 (2)	−0.016 (2)	−0.0018 (19)
C19	0.070 (3)	0.082 (3)	0.070 (3)	−0.029 (3)	0.019 (2)	−0.015 (3)
C20	0.066 (3)	0.093 (4)	0.076 (3)	−0.025 (3)	−0.033 (3)	0.010 (3)
C21	0.081 (4)	0.111 (5)	0.113 (5)	−0.030 (3)	−0.013 (3)	−0.024 (4)
C22	0.083 (4)	0.075 (3)	0.168 (6)	−0.034 (3)	−0.036 (4)	0.009 (4)

Geometric parameters (Å, °)

Co1—N5	2.100 (3)	C7—C8	1.406 (5)
Co1—N2	2.115 (3)	C7—H7	0.9300
Co1—N1	2.312 (3)	C8—C10	1.497 (5)
Co1—Cl2	2.3508 (13)	C9—H9A	0.9600
Co1—Cl1	2.3936 (12)	C9—H9B	0.9600
Co1—N4	2.417 (3)	C9—H9C	0.9600
N1—C8	1.321 (5)	C10—H10A	0.9600
N1—C1	1.345 (4)	C10—H10B	0.9600
N2—C2	1.325 (4)	C10—H10C	0.9600
N2—C1	1.356 (4)	C11—C15	1.409 (5)
N3—C2	1.329 (5)	C12—C13	1.428 (5)
N3—H3A	0.8600	C13—C14	1.339 (6)
N3—H3B	0.8600	C13—H13	0.9300
N4—C18	1.328 (5)	C14—C15	1.408 (5)
N4—C11	1.346 (4)	C14—H14	0.9300
N5—C12	1.339 (5)	C15—C16	1.406 (5)
N5—C11	1.356 (4)	C16—C17	1.368 (6)
N6—C12	1.327 (5)	C16—C19	1.513 (5)
N6—H6A	0.8600	C17—C18	1.401 (5)
N6—H6B	0.8600	C17—H17	0.9300
O1—C21	1.391 (6)	C18—C20	1.505 (6)
O1—H1	0.8200	C19—H19A	0.9600
O2—C22	1.379 (5)	C19—H19B	0.9600
O2—H2	0.8200	C19—H19C	0.9600
C1—C5	1.403 (5)	C20—H20A	0.9600
C2—C3	1.439 (5)	C20—H20B	0.9600
C3—C4	1.341 (5)	C20—H20C	0.9600
C3—H3	0.9300	C21—H21A	0.9600
C4—C5	1.425 (5)	C21—H21B	0.9600
C4—H4	0.9300	C21—H21C	0.9600
C5—C6	1.403 (5)	C22—H22A	0.9600
C6—C7	1.372 (5)	C22—H22B	0.9600
C6—C9	1.507 (5)	C22—H22C	0.9600
N5—Co1—N2	140.51 (11)	C6—C9—H9B	109.5
N5—Co1—N1	94.22 (11)	H9A—C9—H9B	109.5
N2—Co1—N1	60.40 (11)	C6—C9—H9C	109.5
N5—Co1—Cl2	100.61 (9)	H9A—C9—H9C	109.5
N2—Co1—Cl2	109.61 (8)	H9B—C9—H9C	109.5
N1—Co1—Cl2	92.55 (8)	C8—C10—H10A	109.5
N5—Co1—Cl1	103.03 (8)	C8—C10—H10B	109.5
N2—Co1—Cl1	97.99 (8)	H10A—C10—H10B	109.5
N1—Co1—Cl1	158.32 (8)	C8—C10—H10C	109.5
Cl2—Co1—Cl1	96.99 (4)	H10A—C10—H10C	109.5
N5—Co1—N4	58.85 (10)	H10B—C10—H10C	109.5
N2—Co1—N4	88.79 (10)	N4—C11—N5	111.7 (3)
N1—Co1—N4	88.66 (10)	N4—C11—C15	124.9 (3)

Cl2—Co1—N4	159.45 (8)	N5—C11—C15	123.4 (3)
Cl1—Co1—N4	89.14 (8)	N6—C12—N5	118.9 (3)
C8—N1—C1	117.8 (3)	N6—C12—C13	121.1 (4)
C8—N1—Co1	152.4 (3)	N5—C12—C13	119.9 (4)
C1—N1—Co1	89.8 (2)	C14—C13—C12	120.4 (4)
C2—N2—C1	119.8 (3)	C14—C13—H13	119.8
C2—N2—Co1	141.9 (3)	C12—C13—H13	119.8
C1—N2—Co1	98.2 (2)	C13—C14—C15	121.1 (4)
C2—N3—H3A	120.0	C13—C14—H14	119.5
C2—N3—H3B	120.0	C15—C14—H14	119.5
H3A—N3—H3B	120.0	C16—C15—C14	127.9 (4)
C18—N4—C11	117.6 (3)	C16—C15—C11	116.2 (4)
C18—N4—Co1	154.6 (3)	C14—C15—C11	115.9 (4)
C11—N4—Co1	87.8 (2)	C17—C16—C15	118.5 (4)
C12—N5—C11	119.3 (3)	C17—C16—C19	120.5 (4)
C12—N5—Co1	139.0 (3)	C15—C16—C19	120.9 (4)
C11—N5—Co1	101.6 (2)	C16—C17—C18	121.3 (4)
C12—N6—H6A	120.0	C16—C17—H17	119.3
C12—N6—H6B	120.0	C18—C17—H17	119.3
H6A—N6—H6B	120.0	N4—C18—C17	121.5 (4)
C21—O1—H1	109.5	N4—C18—C20	117.6 (4)
C22—O2—H2	109.5	C17—C18—C20	120.9 (4)
N1—C1—N2	111.5 (3)	C16—C19—H19A	109.5
N1—C1—C5	124.7 (3)	C16—C19—H19B	109.5
N2—C1—C5	123.8 (3)	H19A—C19—H19B	109.5
N2—C2—N3	119.8 (3)	C16—C19—H19C	109.5
N2—C2—C3	119.9 (4)	H19A—C19—H19C	109.5
N3—C2—C3	120.3 (3)	H19B—C19—H19C	109.5
C4—C3—C2	120.2 (4)	C18—C20—H20A	109.5
C4—C3—H3	119.9	C18—C20—H20B	109.5
C2—C3—H3	119.9	H20A—C20—H20B	109.5
C3—C4—C5	120.8 (3)	C18—C20—H20C	109.5
C3—C4—H4	119.6	H20A—C20—H20C	109.5
C5—C4—H4	119.6	H20B—C20—H20C	109.5
C1—C5—C6	117.0 (3)	O1—C21—H21A	109.5
C1—C5—C4	115.5 (3)	O1—C21—H21B	109.5
C6—C5—C4	127.5 (3)	H21A—C21—H21B	109.5
C7—C6—C5	117.7 (3)	O1—C21—H21C	109.5
C7—C6—C9	120.5 (4)	H21A—C21—H21C	109.5
C5—C6—C9	121.8 (4)	H21B—C21—H21C	109.5
C6—C7—C8	121.6 (4)	O2—C22—H22A	109.5
C6—C7—H7	119.2	O2—C22—H22B	109.5
C8—C7—H7	119.2	H22A—C22—H22B	109.5
N1—C8—C7	121.2 (4)	O2—C22—H22C	109.5
N1—C8—C10	117.7 (4)	H22A—C22—H22C	109.5
C7—C8—C10	121.1 (4)	H22B—C22—H22C	109.5
C6—C9—H9A	109.5		
N5—Co1—N1—C8	32.8 (5)	N3—C2—C3—C4	179.3 (4)
N2—Co1—N1—C8	−179.2 (6)	C2—C3—C4—C5	−0.4 (6)

Cl2—Co1—N1—C8	−68.0 (5)	N1—C1—C5—C6	−0.3 (5)
Cl1—Co1—N1—C8	175.7 (4)	N2—C1—C5—C6	−180.0 (3)
N4—Co1—N1—C8	91.4 (5)	N1—C1—C5—C4	179.6 (3)
N5—Co1—N1—C1	−146.2 (2)	N2—C1—C5—C4	−0.1 (5)
N2—Co1—N1—C1	1.79 (19)	C3—C4—C5—C1	0.6 (5)
Cl2—Co1—N1—C1	112.95 (19)	C3—C4—C5—C6	−179.6 (4)
Cl1—Co1—N1—C1	−3.3 (3)	C1—C5—C6—C7	1.5 (5)
N4—Co1—N1—C1	−87.6 (2)	C4—C5—C6—C7	−178.3 (4)
N5—Co1—N2—C2	−121.2 (4)	C1—C5—C6—C9	−178.5 (3)
N1—Co1—N2—C2	−177.4 (4)	C4—C5—C6—C9	1.7 (6)
Cl2—Co1—N2—C2	101.1 (4)	C5—C6—C7—C8	−0.8 (6)
Cl1—Co1—N2—C2	0.7 (4)	C9—C6—C7—C8	179.2 (4)
N4—Co1—N2—C2	−88.3 (4)	C1—N1—C8—C7	2.6 (5)
N5—Co1—N2—C1	54.4 (3)	Co1—N1—C8—C7	−176.3 (4)
N1—Co1—N2—C1	−1.79 (19)	C1—N1—C8—C10	−176.5 (3)
Cl2—Co1—N2—C1	−83.3 (2)	Co1—N1—C8—C10	4.6 (7)
Cl1—Co1—N2—C1	176.32 (19)	C6—C7—C8—N1	−1.4 (6)
N4—Co1—N2—C1	87.4 (2)	C6—C7—C8—C10	177.7 (4)
N5—Co1—N4—C18	178.9 (6)	C18—N4—C11—N5	−179.3 (3)
N2—Co1—N4—C18	22.7 (6)	Co1—N4—C11—N5	0.3 (3)
N1—Co1—N4—C18	83.1 (6)	C18—N4—C11—C15	−1.1 (5)
Cl2—Co1—N4—C18	176.8 (5)	Co1—N4—C11—C15	178.5 (3)
Cl1—Co1—N4—C18	−75.3 (6)	C12—N5—C11—N4	178.6 (3)
N5—Co1—N4—C11	−0.21 (19)	Co1—N5—C11—N4	−0.4 (3)
N2—Co1—N4—C11	−156.4 (2)	C12—N5—C11—C15	0.4 (5)
N1—Co1—N4—C11	−96.0 (2)	Co1—N5—C11—C15	−178.6 (3)
Cl2—Co1—N4—C11	−2.3 (3)	C11—N5—C12—N6	−178.3 (3)
Cl1—Co1—N4—C11	105.60 (19)	Co1—N5—C12—N6	0.1 (6)
N2—Co1—N5—C12	−138.9 (3)	C11—N5—C12—C13	1.4 (5)
N1—Co1—N5—C12	−92.5 (4)	Co1—N5—C12—C13	179.8 (3)
Cl2—Co1—N5—C12	0.9 (4)	N6—C12—C13—C14	177.9 (4)
Cl1—Co1—N5—C12	100.7 (4)	N5—C12—C13—C14	−1.8 (6)
N4—Co1—N5—C12	−178.4 (4)	C12—C13—C14—C15	0.4 (6)
N2—Co1—N5—C11	39.7 (3)	C13—C14—C15—C16	−179.6 (4)
N1—Co1—N5—C11	86.1 (2)	C13—C14—C15—C11	1.2 (6)
Cl2—Co1—N5—C11	179.49 (19)	N4—C11—C15—C16	1.0 (5)
Cl1—Co1—N5—C11	−80.7 (2)	N5—C11—C15—C16	179.0 (3)
N4—Co1—N5—C11	0.22 (19)	N4—C11—C15—C14	−179.6 (3)
C8—N1—C1—N2	177.9 (3)	N5—C11—C15—C14	−1.7 (5)
Co1—N1—C1—N2	−2.6 (3)	C14—C15—C16—C17	179.9 (4)
C8—N1—C1—C5	−1.8 (5)	C11—C15—C16—C17	−0.9 (5)
Co1—N1—C1—C5	177.6 (3)	C14—C15—C16—C19	2.1 (6)
C2—N2—C1—N1	179.8 (3)	C11—C15—C16—C19	−178.7 (3)
Co1—N2—C1—N1	2.9 (3)	C15—C16—C17—C18	0.9 (6)
C2—N2—C1—C5	−0.5 (5)	C19—C16—C17—C18	178.7 (4)
Co1—N2—C1—C5	−177.4 (3)	C11—N4—C18—C17	0.9 (5)
C1—N2—C2—N3	−178.9 (3)	Co1—N4—C18—C17	−178.0 (4)
Co1—N2—C2—N3	−3.9 (6)	C11—N4—C18—C20	−179.5 (4)
C1—N2—C2—C3	0.7 (5)	Co1—N4—C18—C20	1.6 (8)

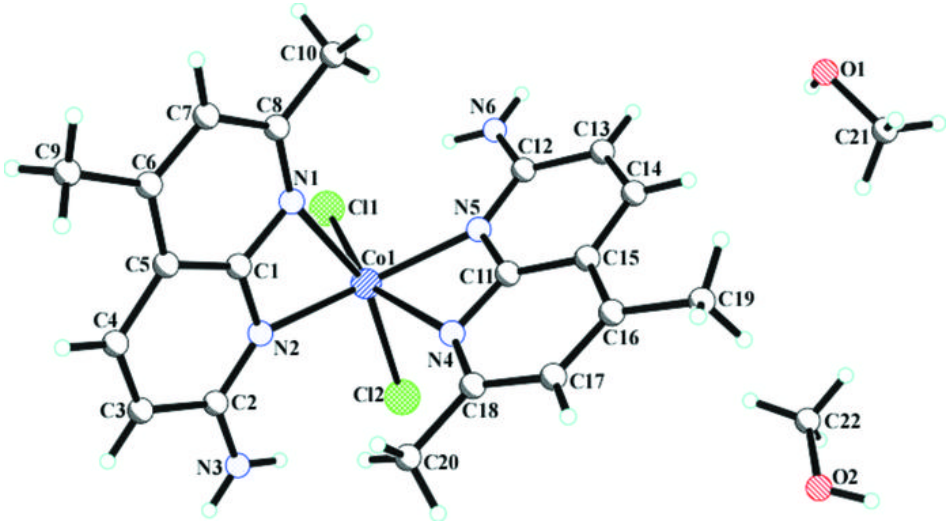
Co1—N2—C2—C3	175.7 (3)	C16—C17—C18—N4	−0.9 (6)
N2—C2—C3—C4	−0.2 (6)	C16—C17—C18—C20	179.5 (4)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···Cl1^{i}	0.82	2.35	3.162 (4)	172
O1—H1···Cl1^{ii}	0.82	2.44	3.194 (4)	154
N6—H6B···O2^{iii}	0.86	2.06	2.918 (4)	175
N6—H6A···Cl2	0.86	2.45	3.269 (4)	159
N3—H3B···O1^{iv}	0.86	2.09	2.947 (4)	175
N3—H3A···Cl1	0.86	2.51	3.309 (3)	156
C22—H22B···C17^{i}	0.96	2.91	3.789 (7)	154
C22—H22B···C18^{i}	0.96	2.71	3.575 (6)	150
C4—H4···Cl2^{v}	0.93	2.85	3.705 (4)	153
C7—H7···Cl1^{vi}	0.93	2.87	3.757 (4)	160
C13—H13···Cl1^{ii}	0.93	2.88	3.733 (4)	152

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) −*x*+2, −*y*+1, −*z*+1; (iii) *x*+1, *y*, *z*; (iv) *x*, *y*, *z*−1; (v) −*x*+2, −*y*+2, −*z*; (vi) *x*, *y*+1, *z*.

Fig. 1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C12
C13
C14
N5
C11
C15
C19
C16
C17
C18
O1
C21
C22
O2

Fig. 2