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Chloridobis(ethane-1,2-diamine-κ^2N,N')(3-methylpyridine-κN)cobalt(III) dichloride monohydrate

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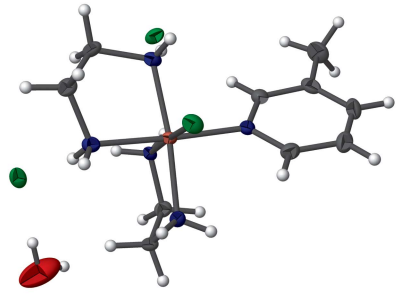
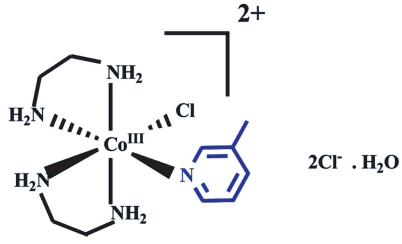
Structural data: full structural data are available from iucrdata.iucr.org

In the title hydrated salt, $[CoCl(C_6H_7N)(C_2H_8N_2)_2]Cl_2\cdot H_2O$, the Co^{III} ion exhibits a distorted octahedral coordination envirnoment defined by four N atoms of two ethane-1,2-diamine ligands, another N atom of the pyridine ligand and a Cl^- ligand. The pyridine N atom and the Cl^- ligand are in *cis* positions relative to each other. The crystal packing is dominated by intermolecular N—H···Cl, O—H···Cl and O—H···H hydrogen-bonding interactions involving the amino groups of the complex cation, the lattice water molecule and the non-coordinating Cl^- anions. Weak C—H···Cl interactions consolidate the three-dimensional hydrogen-bonded network structure.

3D view



Chemical scheme



Structure description

Cobalt is an essential and integral component of vitamin B_{12}. Hence it is found physiologically in most tissues. Complexes of cobalt are useful for nutritional supplementation to provide this element in a form that effectively increases the bioavailability, for instance, vitamin B_{12} by microorganisms present in the gut. Cobalt(III) complexes with ethane-1,2-diamine or with mixed ligands exhibit antitumor, antibacterial, antimicrobial, radiosenzitation and cytotoxicity activities (Sayed *et al.*, 1992; Teicher *et al.*, 1990; Arslan *et al.*, 2009; Delehanty *et al.*, 2008). In addition, cobalt(III) complexes are known for electron-transfer and ligand-substitution reactions. In this context, we have synthesized another cobalt(III) complex with mixed ligands, $[CoCl(C_6H_7N)(C_2H_8N_2)_2]Cl_2\cdot H_2O$, and report here its crystal structure.

The structural entities of the title compound are shown in Fig. 1. The Co^{III} cation is octahedrally surrounded by four N atoms of two ethane-1,2-diamine ligands, a pyridine N atom and a Cl^- ligand, whereby the pyridine N atom and the Cl^- ligand are *cis* to each

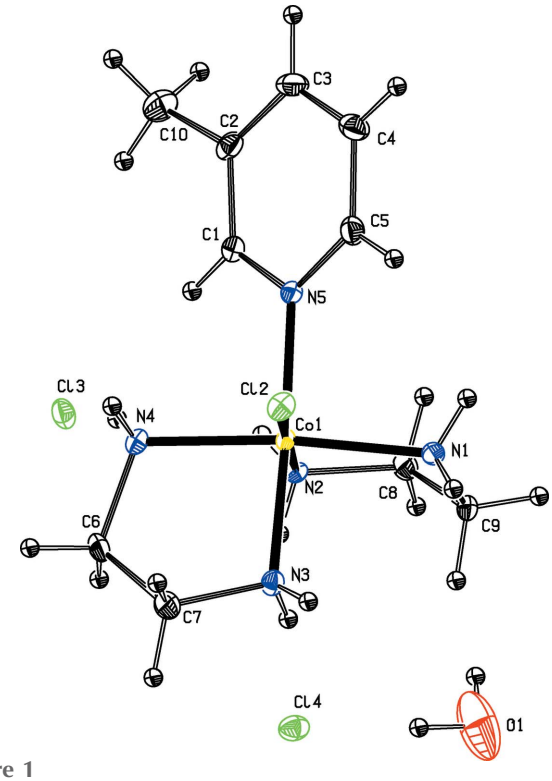


Figure 1
The molecular entities in the title structure with displacement ellipsoids at the 30% probability level.

other. The Co—N and Co—Cl bond lengths are typical for trivalent cobalt and comparable with related complexes comprising of N- and Cl-donating ligands (Anbalagan *et al.*, 2009; Ramesh *et al.*, 2008; Ravichandran *et al.*, 2009). The least-squares planes of the two ethane-1,2-diamine ligands make a dihedral angle of 78.0 (2)°. Puckering parameters for the Co1/N1/C9/C8/N2 and Co1/N3/C7/C6/N4 rings are: q_2 = 0.439 (3) Å, φ = 86.4 (3)° and q_2 = 0.422 (3)°, φ = 82.2 (3)°, respectively. According to Nardelli (1983), ring asymmetry parameters from out-of-plane displacements are Δ_2(Co1) = 3.6 (2)°for the first metalla ring and Δ_2(Co1) = 7.4 (2)° for the second ring.

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1···Cl3	0.93	2.66	3.585 (3)	174
C8—H8A···Cl3^{i}	0.97	2.90	3.395 (3)	113
C9—H9B···Cl3^{ii}	0.97	2.95	3.440 (3)	113
N1—H1A···Cl3^{ii}	0.85 (2)	2.41 (2)	3.194 (2)	153 (2)
N1—H1B···Cl4^{iii}	0.86 (2)	2.48 (2)	3.292 (2)	157 (2)
N2—H2A···Cl4	0.85 (2)	2.57 (2)	3.370 (2)	158 (2)
N2—H2B···Cl3	0.86 (2)	2.70 (2)	3.383 (2)	137 (2)
N2—H2B···Cl3^{i}	0.86 (2)	2.86 (2)	3.514 (3)	135 (2)
N3—H3A···Cl4	0.85 (2)	2.36 (2)	3.191 (2)	168 (3)
N3—H3B···Cl4^{iii}	0.86 (2)	2.67 (2)	3.406 (2)	144 (2)
N4—H4A···Cl3	0.84 (2)	2.38 (2)	3.178 (3)	160 (2)
N4—H4B···Cl2^{iv}	0.85 (2)	2.64 (2)	3.310 (2)	137 (2)
O1—H1C···Cl4	0.87 (2)	2.28 (2)	3.120 (3)	162 (4)
O1—H1D···O1^{v}	0.85 (2)	2.45 (1)	2.940 (7)	118 (1)

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

The complex cation, chloride anions and lattice water molecule are linked into a three-dimensional network by intermolecular N—H···Cl, O—H···Cl and O—H···O hydrogen-bonding interactions, supplemented by weaker C—H···Cl interactions (Table 1 and Fig. 2). This involves an $R_2^2(4)$ ring motif between two adjacent water molecules (Fig. 3).

Synthesis and crystallization

The complex was synthesized using dichloridobis(ethane-1,2-diamine)cobalt(III) chloride (Bailar & Clapp, 1945) as a precursor. *trans*-[Co^{III}(en)$_2$Cl$_2$]Cl (2 g) was suspended in 3–4

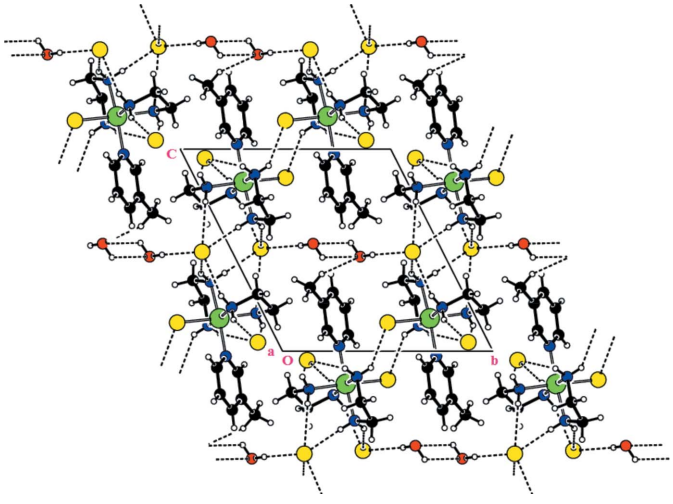


Figure 2
A view along the *a* axis of the title compound, emphasizing the molecular packing. N—H···Cl, O—H···O, O—H···Cl and C—H···Cl hydrogen bonds are shown as dashed lines (see Table 1 for numerical details).

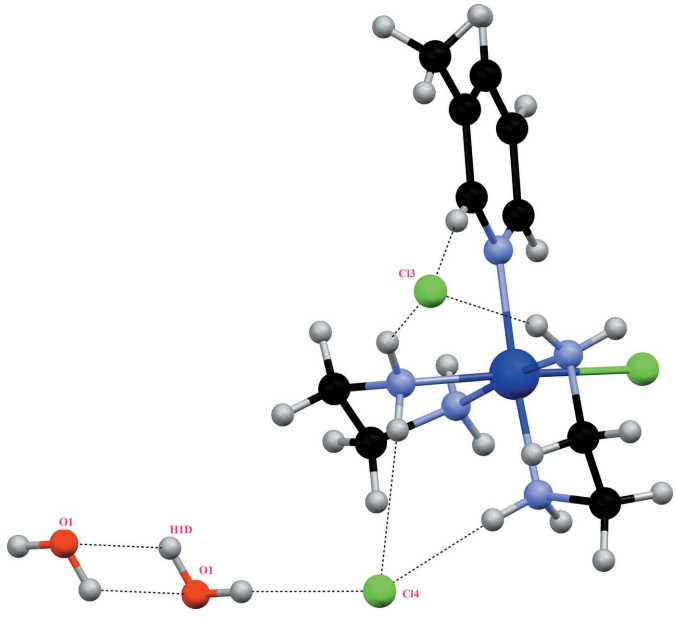


Figure 3
A partial of the crystal packing of the title compound, showing an $R_2^2(4)$ motif formed *via* an inversion-related pair of O—H···O hydrogen bonds (dashed lines).

Table 2
Experimental details.

Crystal data	
Chemical formula	$[CoCl(C_6H_7N)(C_2H_8N_2)_2]Cl_2·H_2O$
M_r	396.63
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	293
a, b, c (Å)	7.6771 (4), 10.8911 (5), 11.6132 (7)
α, β, γ (°)	113.439 (5), 99.872 (5), 102.384 (4)
V (Å^3)	833.67 (8)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	1.51
Crystal size (mm)	0.25 × 0.20 × 0.15
Data collection	
Diffractometer	Bruker SMART APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2008)
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	5316, 2929, 2456
R_{int}	0.025
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.594
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.032, 0.087, 1.09
No. of reflections	2929
No. of parameters	219
No. of restraints	16
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.61, −0.37

Computer programs: *APEX2* and *SAINT* (Bruker, 2008), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2009).

drops of deionized water. Then 3-methylpyridine (3 ml) was added dropwise for 20 min, resulting in a colour change from dull green to violet–red. The final mixture was stirred for 30 min and continued for another 30 min until no further change was observed. The mixture was allowed to stand overnight. Finally, the obtained solid was washed 3–4 times with ethanol and dissolved in 5–10 ml of deionized water that had been pre-heated to 343 K. The title cobalt(III) complex was recrystallized by cooling this solution to which a few drops of conc. HCl were added. The resulting crystals were filtered, washed with ethanol and dried under vacuum.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Funding information

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full crystallographic data

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Crystal data

$[CoCl(C_6H_7N)(C_2H_8N_2)_2]Cl_2\cdot H_2O$
M_r = 396.63
Triclinic, $P\overline{1}$
a = 7.6771 (4) Å
b = 10.8911 (5) Å
c = 11.6132 (7) Å
α = 113.439 (5)°
β = 99.872 (5)°
γ = 102.384 (4)°
V = 833.67 (8) Å^3
Z = 2
$F(000)$ = 412
D_x = 1.580 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2456 reflections
θ = 2.8–25.0°
μ = 1.51 mm^{-1}
T = 293 K
Block, violet-red
0.25 × 0.20 × 0.15 mm

Data collection

Bruker SMART APEXII CCD diffractometer
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
5316 measured reflections
2929 independent reflections
2456 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 25.0°, θ_{min} = 2.8°
h = −8→9
k = −12→12
l = −13→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.087
S = 1.09
2929 reflections
219 parameters
16 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0515P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.61 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

Special details

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

Refinement. H atoms of water molecules and amino groups were located from difference maps and refined with restraints on their bond lengths [(N,O)—H = 0.85 Å]).

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.3844 (3)	0.2624 (3)	1.1036 (3)	0.0201 (6)
H1	0.4616	0.2135	1.0660	0.024*
C2	0.4109 (4)	0.3106 (3)	1.2368 (3)	0.0234 (6)
C3	0.2932 (4)	0.3807 (3)	1.2909 (3)	0.0262 (7)
H3	0.3058	0.4145	1.3801	0.031*
C4	0.1575 (4)	0.4004 (3)	1.2127 (3)	0.0258 (7)
H4	0.0770	0.4468	1.2485	0.031*
C5	0.1409 (3)	0.3511 (3)	1.0809 (3)	0.0218 (6)
H5	0.0495	0.3658	1.0287	0.026*
C6	0.5567 (4)	0.2506 (3)	0.7483 (3)	0.0234 (6)
H6A	0.5676	0.1565	0.7171	0.028*
H6B	0.6754	0.3155	0.7618	0.028*
C7	0.4074 (4)	0.2550 (3)	0.6496 (3)	0.0249 (6)
H7A	0.4120	0.3515	0.6712	0.030*
H7B	0.4222	0.2111	0.5626	0.030*
C8	0.0579 (3)	−0.0546 (3)	0.7964 (3)	0.0205 (6)
H8A	0.0380	−0.0344	0.8815	0.025*
H8B	0.0465	−0.1537	0.7514	0.025*
C9	−0.0815 (3)	−0.0193 (3)	0.7177 (3)	0.0193 (6)
H9A	−0.0744	−0.0526	0.6283	0.023*
H9B	−0.2067	−0.0630	0.7162	0.023*
C10	0.5621 (4)	0.2841 (3)	1.3149 (3)	0.0361 (8)
H10A	0.6269	0.2340	1.2583	0.054*
H10B	0.6479	0.3724	1.3820	0.054*
H10C	0.5085	0.2290	1.3546	0.054*
N1	−0.0337 (3)	0.1366 (2)	0.7830 (2)	0.0169 (5)
N2	0.2452 (3)	0.0339 (2)	0.8119 (2)	0.0157 (5)
N3	0.2283 (3)	0.1755 (2)	0.6559 (2)	0.0174 (5)
N4	0.5063 (3)	0.2910 (2)	0.8731 (2)	0.0176 (5)
N5	0.2547 (3)	0.2816 (2)	1.0253 (2)	0.0162 (5)
Cl2	0.20805 (9)	0.43180 (7)	0.85882 (7)	0.02175 (17)
Cl3	0.69806 (8)	0.09570 (7)	0.95580 (7)	0.02316 (18)
Cl4	0.21383 (9)	−0.14314 (7)	0.49221 (6)	0.02355 (18)
Co1	0.23612 (4)	0.22144 (3)	0.83760 (3)	0.01406 (13)
O1	−0.0839 (4)	−0.4040 (3)	0.4680 (4)	0.0880 (12)
H1C	0.017 (5)	−0.341 (4)	0.477 (4)	0.106*
H1D	−0.061 (6)	−0.415 (3)	0.536 (2)	0.106*
H1A	−0.087 (3)	0.157 (3)	0.8438 (19)	0.021 (8)*
H1B	−0.088 (3)	0.159 (3)	0.727 (2)	0.011 (7)*
H2A	0.270 (3)	−0.007 (2)	0.7402 (16)	0.005 (6)*
H2B	0.324 (3)	0.033 (3)	0.8730 (18)	0.024 (8)*
H3A	0.207 (4)	0.0875 (19)	0.613 (3)	0.035 (9)*
H3B	0.149 (3)	0.201 (3)	0.617 (3)	0.035 (9)*
H4A	0.559 (3)	0.255 (2)	0.914 (2)	0.021 (8)*
H4B	0.545 (3)	0.3800 (17)	0.918 (3)	0.021 (8)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0157 (13)	0.0211 (14)	0.0193 (15)	0.0033 (11)	0.0038 (11)	0.0069 (12)
C2	0.0220 (15)	0.0205 (14)	0.0203 (15)	−0.0022 (12)	−0.0005 (12)	0.0091 (12)
C3	0.0342 (17)	0.0233 (15)	0.0155 (15)	0.0023 (13)	0.0085 (12)	0.0063 (13)
C4	0.0300 (16)	0.0222 (14)	0.0237 (16)	0.0076 (13)	0.0134 (13)	0.0070 (13)
C5	0.0168 (14)	0.0233 (14)	0.0251 (16)	0.0066 (12)	0.0066 (12)	0.0102 (13)
C6	0.0155 (14)	0.0317 (15)	0.0251 (16)	0.0046 (12)	0.0096 (12)	0.0146 (13)
C7	0.0222 (15)	0.0297 (15)	0.0232 (16)	0.0029 (12)	0.0084 (12)	0.0141 (13)
C8	0.0200 (14)	0.0208 (14)	0.0223 (15)	0.0044 (11)	0.0079 (11)	0.0117 (12)
C9	0.0135 (13)	0.0218 (14)	0.0184 (15)	0.0000 (11)	0.0037 (11)	0.0082 (12)
C10	0.0334 (17)	0.0446 (19)	0.0266 (18)	0.0097 (15)	0.0021 (14)	0.0162 (15)
N1	0.0144 (11)	0.0241 (12)	0.0141 (12)	0.0067 (10)	0.0034 (10)	0.0104 (11)
N2	0.0129 (11)	0.0204 (11)	0.0107 (12)	0.0032 (9)	0.0008 (9)	0.0061 (10)
N3	0.0155 (12)	0.0191 (12)	0.0180 (13)	0.0036 (10)	0.0030 (10)	0.0105 (11)
N4	0.0140 (11)	0.0182 (12)	0.0175 (13)	0.0036 (10)	0.0009 (9)	0.0071 (11)
N5	0.0143 (11)	0.0172 (11)	0.0145 (12)	0.0021 (9)	0.0033 (9)	0.0065 (10)
Cl2	0.0220 (3)	0.0182 (3)	0.0227 (4)	0.0065 (3)	0.0029 (3)	0.0082 (3)
Cl3	0.0162 (3)	0.0339 (4)	0.0271 (4)	0.0100 (3)	0.0087 (3)	0.0191 (3)
Cl4	0.0265 (4)	0.0270 (4)	0.0179 (4)	0.0121 (3)	0.0043 (3)	0.0099 (3)
Co1	0.0103 (2)	0.0168 (2)	0.0132 (2)	0.00278 (14)	0.00175 (14)	0.00627 (16)
O1	0.069 (2)	0.067 (2)	0.156 (4)	0.0194 (17)	0.063 (2)	0.066 (2)

Geometric parameters (Å, º)

C1—N5	1.339 (4)	C9—N1	1.485 (3)
C1—C2	1.381 (4)	C9—H9A	0.9700
C1—H1	0.9300	C9—H9B	0.9700
C2—C3	1.380 (4)	C10—H10A	0.9600
C2—C10	1.499 (4)	C10—H10B	0.9600
C3—C4	1.373 (4)	C10—H10C	0.9600
C3—H3	0.9300	N1—Co1	1.952 (2)
C4—C5	1.377 (4)	N1—H1A	0.852 (15)
C4—H4	0.9300	N1—H1B	0.859 (16)
C5—N5	1.357 (3)	N2—Co1	1.962 (2)
C5—H5	0.9300	N2—H2A	0.852 (15)
C6—N4	1.484 (3)	N2—H2B	0.858 (16)
C6—C7	1.499 (4)	N3—Co1	1.952 (2)
C6—H6A	0.9700	N3—H3A	0.847 (17)
C6—H6B	0.9700	N3—H3B	0.855 (17)
C7—N3	1.490 (3)	N4—Co1	1.957 (2)
C7—H7A	0.9700	N4—H4A	0.836 (16)
C7—H7B	0.9700	N4—H4B	0.848 (16)
C8—N2	1.485 (3)	N5—Co1	1.980 (2)
C8—C9	1.500 (4)	Cl2—Co1	2.2664 (7)
C8—H8A	0.9700	O1—H1C	0.874 (18)
C8—H8B	0.9700	O1—H1D	0.845 (19)

N5—C1—C2	124.2 (2)	H10B—C10—H10C	109.5
N5—C1—H1	117.9	C9—N1—Co1	109.48 (15)
C2—C1—H1	117.9	C9—N1—H1A	106.5 (18)
C3—C2—C1	117.3 (3)	Co1—N1—H1A	116.0 (18)
C3—C2—C10	123.2 (3)	C9—N1—H1B	106.8 (18)
C1—C2—C10	119.5 (3)	Co1—N1—H1B	111.6 (16)
C4—C3—C2	119.7 (3)	H1A—N1—H1B	106.0 (19)
C4—C3—H3	120.1	C8—N2—Co1	109.53 (16)
C2—C3—H3	120.1	C8—N2—H2A	105.7 (16)
C3—C4—C5	119.7 (3)	Co1—N2—H2A	109.5 (16)
C3—C4—H4	120.1	C8—N2—H2B	108.4 (19)
C5—C4—H4	120.1	Co1—N2—H2B	115.4 (19)
N5—C5—C4	121.6 (3)	H2A—N2—H2B	107.8 (19)
N5—C5—H5	119.2	C7—N3—Co1	110.22 (16)
C4—C5—H5	119.2	C7—N3—H3A	111 (2)
N4—C6—C7	108.4 (2)	Co1—N3—H3A	109 (2)
N4—C6—H6A	110.0	C7—N3—H3B	102 (2)
C7—C6—H6A	110.0	Co1—N3—H3B	115 (2)
N4—C6—H6B	110.0	H3A—N3—H3B	109 (2)
C7—C6—H6B	110.0	C6—N4—Co1	110.18 (16)
H6A—C6—H6B	108.4	C6—N4—H4A	107.2 (19)
N3—C7—C6	105.6 (2)	Co1—N4—H4A	110.4 (19)
N3—C7—H7A	110.6	C6—N4—H4B	110.0 (19)
C6—C7—H7A	110.6	Co1—N4—H4B	109.6 (17)
N3—C7—H7B	110.6	H4A—N4—H4B	109 (2)
C6—C7—H7B	110.6	C1—N5—C5	117.4 (2)
H7A—C7—H7B	108.8	C1—N5—Co1	121.98 (17)
N2—C8—C9	107.0 (2)	C5—N5—Co1	120.51 (19)
N2—C8—H8A	110.3	N1—Co1—N3	89.50 (9)
C9—C8—H8A	110.3	N1—Co1—N4	173.58 (9)
N2—C8—H8B	110.3	N3—Co1—N4	85.02 (9)
C9—C8—H8B	110.3	N1—Co1—N2	85.27 (9)
H8A—C8—H8B	108.6	N3—Co1—N2	91.85 (10)
N1—C9—C8	106.3 (2)	N4—Co1—N2	91.55 (10)
N1—C9—H9A	110.5	N1—Co1—N5	93.08 (9)
C8—C9—H9A	110.5	N3—Co1—N5	176.00 (9)
N1—C9—H9B	110.5	N4—Co1—N5	92.58 (9)
C8—C9—H9B	110.5	N2—Co1—N5	91.41 (9)
H9A—C9—H9B	108.7	N1—Co1—Cl2	91.55 (7)
C2—C10—H10A	109.5	N3—Co1—Cl2	86.76 (7)
C2—C10—H10B	109.5	N4—Co1—Cl2	91.49 (8)
H10A—C10—H10B	109.5	N2—Co1—Cl2	176.54 (7)
C2—C10—H10C	109.5	N5—Co1—Cl2	90.11 (7)
H10A—C10—H10C	109.5	H1C—O1—H1D	105 (3)

N5—C1—C2—C3	1.2 (4)	C8—C9—N1—Co1	41.2 (2)
N5—C1—C2—C10	−179.4 (3)	C9—C8—N2—Co1	38.1 (2)

C1—C2—C3—C4	−0.3 (4)	C6—C7—N3—Co1	40.9 (2)
C10—C2—C3—C4	−179.7 (3)	C7—C6—N4—Co1	34.9 (3)
C2—C3—C4—C5	−0.6 (4)	C2—C1—N5—C5	−1.0 (4)
C3—C4—C5—N5	0.7 (4)	C2—C1—N5—Co1	175.57 (19)
N4—C6—C7—N3	−48.6 (3)	C4—C5—N5—C1	0.0 (4)
N2—C8—C9—N1	−51.2 (3)	C4—C5—N5—Co1	−176.61 (19)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···Cl3	0.93	2.66	3.585 (3)	174
C8—H8*A*···Cl3^{i}	0.97	2.90	3.395 (3)	113
C9—H9*B*···Cl3^{ii}	0.97	2.95	3.440 (3)	113
N1—H1*A*···Cl3^{ii}	0.85 (2)	2.41 (2)	3.194 (2)	153 (2)
N1—H1*B*···Cl4^{iii}	0.86 (2)	2.48 (2)	3.292 (2)	157 (2)
N2—H2*A*···Cl4	0.85 (2)	2.57 (2)	3.370 (2)	158 (2)
N2—H2*B*···Cl3	0.86 (2)	2.70 (2)	3.383 (2)	137 (2)
N2—H2*B*···Cl3^{i}	0.86 (2)	2.86 (2)	3.514 (3)	135 (2)
N3—H3*A*···Cl4	0.85 (2)	2.36 (2)	3.191 (2)	168 (3)
N3—H3*B*···Cl4^{iii}	0.86 (2)	2.67 (2)	3.406 (2)	144 (2)
N4—H4*A*···Cl3	0.84 (2)	2.38 (2)	3.178 (3)	160 (2)
N4—H4*B*···Cl2^{iv}	0.85 (2)	2.64 (2)	3.310 (2)	137 (2)
O1—H1*C*···Cl4	0.87 (2)	2.28 (2)	3.120 (3)	162 (4)
O1—H1*D*···O1^{v}	0.85 (2)	2.45 (1)	2.940 (7)	118 (1)

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