

cis-Dichloridobis(1,10-phenanthroline)-cobalt(II) dimethylformamide solvate

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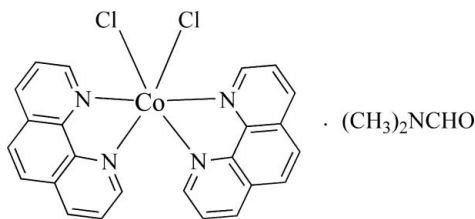
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; disorder in solvent or counterion; R factor = 0.026; wR factor = 0.063; data-to-parameter ratio = 12.2.

In the title complex, $[\text{CoCl}_2(\text{C}_{12}\text{H}_8\text{N}_2)_2] \cdot \text{C}_3\text{H}_7\text{NO}$, which has twofold rotation symmetry, the Co^{II} cation is coordinated by two 1,10-phenanthroline (phen) molecules and two chloride ligands in a distorted octahedral geometry. In the crystal structure, a cavity is created by six complex molecules connected by $\text{C}-\text{H} \cdots \pi$ interactions and non-classical $\text{C}-\text{H} \cdots \text{Cl}$ hydrogen bonds. The cavities are occupied by the disordered dimethylformamide solvent molecule. The C and N atoms of the C—N bond in the solvent molecule also lie on a crystallographic twofold rotation axis; the remaining atoms of the solvent are statistically disordered (ratio 0.5:0.5) about this axis.

Related literature

For general background, see: Forster *et al.* (2000); Holder *et al.* (2007); Ma *et al.* (2002). Matsumoto *et al.* (2002); Xie *et al.* (2006). For a related structure, see: Hazell *et al.* (1997).



Experimental

Crystal data

$[\text{CoCl}_2(\text{C}_{12}\text{H}_8\text{N}_2)_2] \cdot \text{C}_3\text{H}_7\text{NO}$
 $M_r = 563.33$
 Orthorhombic, *Pbcn*
 $a = 16.345$ (3) Å
 $b = 12.342$ (2) Å
 $c = 12.342$ (2) Å

$V = 2489.8$ (8) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.94$ mm⁻¹
 $T = 293$ (2) K
 $0.20 \times 0.20 \times 0.20$ mm

Data collection

Rigaku Mercury70 CCD diffractometer
 Absorption correction: multi-scan (*CrystalClear*; Rigaku & Molecular Structure Corporation,
 2000)
 $T_{\text{min}} = 0.829$, $T_{\text{max}} = 0.829$
 14711 measured reflections
 2204 independent reflections
 2168 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.017$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.026$
 $wR(F^2) = 0.063$
 $S = 1.09$
 2204 reflections
 180 parameters
 2 restraints
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.34$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.21$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Co1—N2	2.1517 (13)	Co1—Cl1	2.4099 (5)
Co1—N1	2.1636 (13)		
N2—Co1—N2 ⁱ	176.70 (7)	N2 ⁱ —Co1—Cl1	90.43 (4)
N2—Co1—N1	76.81 (5)	N1—Co1—Cl1	162.67 (4)
N2—Co1—N1 ⁱ	100.65 (5)	N1 ⁱ —Co1—Cl1	87.23 (4)
N1—Co1—N1 ⁱ	82.44 (7)	Cl1—Co1—Cl1 ⁱ	105.91 (2)
N2—Co1—Cl1	91.56 (4)		

Symmetry code: (i) $-x + 1, y, -z + \frac{1}{2}$.

Table 2

Hydrogen-bond geometry (Å, °).

$D-\text{H} \cdots A$	$D-\text{H}$	$\text{H} \cdots A$	$D \cdots A$	$D-\text{H} \cdots A$
C10—H10A [·] ···Cl1	0.93	2.74	3.3408 (17)	124
C6—H6A [·] ···Cl1 ⁱⁱ	0.93	2.80	3.6743 (18)	158
C5—H5A [·] ···Cl1 ⁱⁱⁱ	0.93	2.85	3.6375 (17)	144
C2—H2A [·] ···Cg1 ^{iv}	0.93	2.99	3.768 (2)	142
C8—H8A [·] ···Cg2 ^v	0.93	2.90	3.608 (2)	134

Symmetry codes: (ii) $x + \frac{1}{2}, -y + \frac{3}{2}, -z$; (iii) $x + \frac{1}{2}, y + \frac{1}{2}, -z + \frac{1}{2}$; (iv) $x, -y + 1, z - \frac{1}{2}$; (v) $-x + \frac{3}{2}, -y + \frac{1}{2}, z - \frac{1}{2}$.

Data collection: *CrystalClear* (Rigaku & Molecular Structure Corporation, 2000); cell refinement: *CrystalClear*; data reduction: *CrystalClear* program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2005); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008) and *PLATON* (Spek; 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2538).

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supplementary materials

Acta Cryst. (2008). E64, m1328-m1329 [doi:10.1107/S1600536808030341]

***cis*-Dichloridobis(1,10-phenanthroline)cobalt(II) dimethylformamide solvate**

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Comment

ML_mX_n coordination compounds ($L = \alpha, \alpha'$ -diimine chelate ligands, such as 2,2'-bipyridine, 1,10-phenanthroline, and their derivatives; $X =$ halide or pseudohalide ligands) have been receiving extensive attention due to their importance in crystal engineering and supramolecular chemistry. They also serve as models to aid the understanding of phenomena such as photosensitization and crystallization (Forster *et al.*, 2000; Holder *et al.*, 2007; Ma *et al.*, 2002). In such molecules a variety of weak intermolecular interactions involving the halide anions, aromatic ligands and solvent molecules can stabilise and regulate the supramolecular architecture in different aggregation states (Matsumoto *et al.*, 2002; Xie *et al.*, 2006). Herein, we report the crystal structure of a new cobalt(II) chloride complex with a phenanthroline ligand, Fig 1.

The crystallographic asymmetric unit of (I) consists of one half occupancy Co^{II} atom that lies on a two-fold rotation axis, one phenanthroline molecule, one Cl^- anion, and half a molecule of dimethylformamide. In the complex, the Co^{II} atom is in a distorted octahedral coordination environment provided by four N atoms from two bidentate phen ligands and two terminal Cl^- anions. The $Co-N$ and $Co-Cl$ bond lengths (Table 1) are normal, and are comparable to those found in a related octahedral cobalt(II) complex $[CoCl_2(C_{12}H_8N_2)_2] \cdot 1.5CH_3CN$ [Hazell *et al.*, 1997].

Interestingly in the crystal structure, a cavity is created by six complex molecules connected by $C-H \cdots \pi$ interactions and non-classical $C-H \cdots Cl$ hydrogen bonds (Table 2, Fig. 2) which is occupied by the disordered dmf solvate molecule. The solvate lies with the C14 and N3 on a crystallographic 2-fold rotation axis; the remaining atoms of the solvate are statistically disordered about this axis. The calculated void space of the cavity was estimated to be 557.6 \AA^3 per unit cell, which corresponds to 23.2% of the total volume (2489.8 \AA^3) (Fig 2) (Spek, 2003).

Experimental

$[CoCl_2 \cdot 6(H_2O)]$ (238 mg) was dissolved in a mixture of dimethylformamide (10 ml) and tetrahydrofuran (10 ml) with stirring. A color change from blue to dark blue was observed after the phenanthroline (40 mg) was added to the solution. The mixture was cooled down to room temperature after stirring for 1 h at $90^\circ C$. The resulting mixture was then filtered, and the filtrate was concentrated to *ca* 13 ml by rotary evaporation and left in a refrigerator at $4^\circ C$. Transparent blue prismatic crystals suitable for X-ray diffraction were produced in a few days (yield 21%). Analysis calculated for $C_{27}H_{23}Cl_2CoN_5O$: C 57.57, N 12.43, H 4.12%; found: C 57.72, N 12.56, H 3.97%.

Refinement

The H atoms bonded to C atoms were placed in calculated positions and treated using a riding-model approximation ($C-H = 0.96 \text{ \AA}$ and $U_{iso}(H) = 1.5U_{eq}(C)$ for the methyl group; $C-H = 0.93 \text{ \AA}$ and $U_{iso}(H) = 1.2U_{eq}(C)$ for the 1,10-phenanthroline and aldehyde groups).

Figures

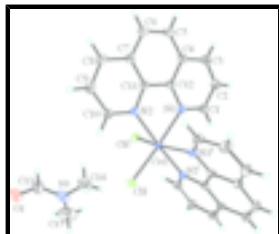


Fig. 1. The structure of the title compound showing the atom numbering. Thermal ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii. Only one of the disorder components of the dmf molecule is shown. [Symmetry codes: (i) $1 - x + 1, y, 1/2 - z.$]

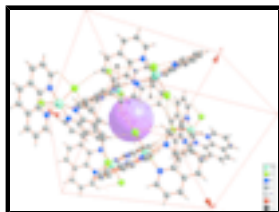


Fig. 2. Crystal packing of (I) showing the cavity (represented by the pink sphere) created by the C—H...Cl and C—H... π interactions with hydrogen bonds drawn as dashed lines.

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Crystal data

$[\text{CoCl}_2(\text{C}_{12}\text{H}_8\text{N}_2)_2] \cdot \text{C}_3\text{H}_7\text{NO}$

$M_r = 563.33$

Orthorhombic, *Pbcn*

Hall symbol: $-P\ 2n\ 2ab$

$a = 16.345\ (3)\ \text{\AA}$

$b = 12.342\ (2)\ \text{\AA}$

$c = 12.342\ (2)\ \text{\AA}$

$V = 2489.8\ (8)\ \text{\AA}^3$

$Z = 4$

$F_{000} = 1156$

$D_x = 1.503\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation

$\lambda = 0.71073\ \text{\AA}$

Cell parameters from 6370 reflections

$\theta = 2.1\text{--}25.0^\circ$

$\mu = 0.94\ \text{mm}^{-1}$

$T = 293\ (2)\ \text{K}$

Block, colorless

$0.20 \times 0.20 \times 0.20\ \text{mm}$

Data collection

Rigaku Mercury70 CCD
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 293\ (2)\ \text{K}$

ω scans

Absorption correction: multi-scan

(CrystalClear; Rigaku & Molecular Structure Corporation, 2000)

$T_{\min} = 0.829, T_{\max} = 0.829$

14711 measured reflections

2204 independent reflections

2168 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.017$

$\theta_{\max} = 25.0^\circ$

$\theta_{\min} = 2.1^\circ$

$h = -17 \rightarrow 19$

$k = -14 \rightarrow 14$

$l = -13 \rightarrow 14$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.026$	H-atom parameters constrained
$wR(F^2) = 0.063$	$w = 1/[\sigma^2(F_o^2) + (0.0288P)^2 + 1.9948P]$
$S = 1.09$	where $P = (F_o^2 + 2F_c^2)/3$
2204 reflections	$(\Delta/\sigma)_{\max} < 0.001$
180 parameters	$\Delta\rho_{\max} = 0.34 \text{ e } \text{\AA}^{-3}$
2 restraints	$\Delta\rho_{\min} = -0.21 \text{ e } \text{\AA}^{-3}$
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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Co1	0.5000	0.71666 (2)	0.2500	0.01272 (10)	
Cl1	0.41390 (2)	0.59903 (3)	0.14376 (3)	0.01956 (11)	
N2	0.59089 (8)	0.72168 (10)	0.12398 (11)	0.0151 (3)	
C11	0.65206 (9)	0.79462 (12)	0.14122 (12)	0.0141 (3)	
N1	0.57879 (8)	0.84851 (11)	0.29957 (11)	0.0162 (3)	
C7	0.72069 (9)	0.80426 (13)	0.07300 (13)	0.0171 (3)	
C12	0.64445 (9)	0.86417 (12)	0.23421 (13)	0.0148 (3)	
C3	0.69394 (10)	1.00860 (14)	0.34665 (14)	0.0228 (4)	
H3A	0.7317	1.0626	0.3628	0.027*	
C10	0.59726 (10)	0.65659 (13)	0.03895 (13)	0.0187 (3)	
H10A	0.5558	0.6065	0.0264	0.022*	
C1	0.57135 (10)	0.91093 (14)	0.38597 (14)	0.0215 (4)	
H1A	0.5264	0.9007	0.4311	0.026*	
C6	0.78081 (10)	0.88565 (14)	0.09568 (14)	0.0209 (4)	
H6A	0.8261	0.8924	0.0507	0.025*	
C5	0.77263 (10)	0.95285 (14)	0.18162 (14)	0.0218 (4)	
H5A	0.8120	1.0059	0.1940	0.026*	

supplementary materials

C2	0.62797 (10)	0.99184 (15)	0.41280 (15)	0.0253 (4)	
H2A	0.6208	1.0336	0.4748	0.030*	
C8	0.72538 (11)	0.73320 (13)	-0.01602 (14)	0.0210 (4)	
H8A	0.7699	0.7360	-0.0629	0.025*	
C9	0.66376 (10)	0.65987 (14)	-0.03293 (14)	0.0222 (4)	
H9A	0.6660	0.6126	-0.0916	0.027*	
C4	0.70425 (10)	0.94361 (13)	0.25393 (13)	0.0176 (3)	
O1	0.5517 (2)	0.0842 (2)	0.1510 (3)	0.0433 (7)	0.50
N3	0.5000	0.2344 (2)	0.2500	0.0453 (7)	
C13	0.5478 (6)	0.1828 (7)	0.1772 (8)	0.048 (3)	0.50
H13A	0.5840	0.2276	0.1400	0.057*	0.50
C14	0.5000	0.3523 (3)	0.2500	0.0553 (10)	
H14A	0.5551	0.3783	0.2427	0.083*	0.50
H14B	0.4772	0.3783	0.3168	0.083*	0.50
H14C	0.4677	0.3783	0.1904	0.083*	0.50
C15	0.5421 (7)	0.1760 (10)	0.1657 (9)	0.067 (4)	0.50
H15A	0.5375	0.2151	0.0987	0.100*	0.50
H15B	0.5180	0.1055	0.1575	0.100*	0.50
H15C	0.5988	0.1685	0.1846	0.100*	0.50

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.01000 (16)	0.01385 (16)	0.01430 (17)	0.000	-0.00028 (11)	0.000
Cl1	0.0170 (2)	0.0213 (2)	0.0203 (2)	-0.00516 (15)	-0.00274 (15)	-0.00162 (16)
N2	0.0134 (6)	0.0161 (6)	0.0159 (7)	-0.0002 (5)	-0.0015 (5)	0.0012 (5)
C11	0.0124 (7)	0.0146 (7)	0.0152 (8)	0.0011 (6)	-0.0018 (6)	0.0033 (6)
N1	0.0131 (6)	0.0174 (7)	0.0181 (7)	0.0004 (5)	-0.0004 (5)	-0.0016 (6)
C7	0.0148 (8)	0.0187 (8)	0.0177 (8)	0.0012 (6)	0.0003 (6)	0.0036 (6)
C12	0.0130 (7)	0.0147 (7)	0.0168 (8)	0.0012 (6)	-0.0027 (6)	0.0023 (6)
C3	0.0203 (8)	0.0208 (8)	0.0272 (9)	-0.0047 (7)	-0.0045 (7)	-0.0045 (7)
C10	0.0185 (8)	0.0180 (8)	0.0195 (8)	-0.0006 (6)	-0.0012 (7)	-0.0031 (7)
C1	0.0176 (8)	0.0252 (9)	0.0218 (9)	0.0001 (7)	0.0035 (7)	-0.0054 (7)
C6	0.0156 (8)	0.0263 (8)	0.0208 (8)	-0.0033 (7)	0.0022 (7)	0.0047 (7)
C5	0.0181 (8)	0.0236 (8)	0.0238 (9)	-0.0078 (7)	-0.0018 (7)	0.0036 (7)
C2	0.0227 (9)	0.0270 (9)	0.0262 (9)	-0.0020 (7)	0.0003 (7)	-0.0109 (8)
C8	0.0185 (8)	0.0249 (8)	0.0197 (8)	0.0025 (7)	0.0055 (7)	0.0018 (7)
C9	0.0240 (9)	0.0224 (8)	0.0203 (8)	0.0012 (7)	0.0022 (7)	-0.0048 (7)
C4	0.0155 (8)	0.0179 (8)	0.0194 (8)	-0.0003 (7)	-0.0034 (6)	0.0015 (6)
O1	0.0492 (19)	0.0294 (16)	0.0512 (19)	0.0003 (14)	-0.0046 (15)	-0.0048 (14)
N3	0.0390 (15)	0.0223 (12)	0.075 (2)	0.000	-0.0214 (14)	0.000
C13	0.065 (7)	0.018 (4)	0.060 (5)	-0.007 (4)	0.030 (5)	0.001 (3)
C14	0.049 (2)	0.0259 (16)	0.090 (3)	0.000	-0.0091 (19)	0.000
C15	0.047 (5)	0.057 (7)	0.095 (7)	0.001 (5)	-0.041 (5)	-0.028 (5)

Geometric parameters (\AA , $^\circ$)

Co1—N2	2.1517 (13)	C6—C5	1.353 (2)
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Co1—N2 ⁱ	2.1517 (13)	C6—H6A	0.9300
Co1—N1	2.1636 (13)	C5—C4	1.435 (2)
Co1—N1 ⁱ	2.1636 (13)	C5—H5A	0.9300
Co1—C11	2.4099 (5)	C2—H2A	0.9300
Co1—C11 ⁱ	2.4099 (5)	C8—C9	1.370 (2)
N2—C10	1.326 (2)	C8—H8A	0.9300
N2—C11	1.362 (2)	C9—H9A	0.9300
C11—C7	1.408 (2)	O1—C13	1.260 (9)
C11—C12	1.439 (2)	N3—C13	1.351 (7)
N1—C1	1.321 (2)	N3—C15	1.441 (8)
N1—C12	1.356 (2)	N3—C14	1.456 (4)
C7—C8	1.408 (2)	N3—C13 ⁱ	1.351 (7)
C7—C6	1.433 (2)	N3—C15 ⁱ	1.441 (8)
C12—C4	1.406 (2)	C13—H13A	0.9300
C3—C2	1.368 (2)	C14—H14A	0.9600
C3—C4	1.408 (2)	C14—H14B	0.9600
C3—H3A	0.9300	C14—H14C	0.9600
C10—C9	1.404 (2)	C15—H15A	0.9600
C10—H10A	0.9300	C15—H15B	0.9600
C1—C2	1.401 (2)	C15—H15C	0.9600
C1—H1A	0.9300		
N2—Co1—N2 ⁱ	176.70 (7)	C5—C6—C7	121.01 (15)
N2—Co1—N1	76.81 (5)	C5—C6—H6A	119.5
N2 ⁱ —Co1—N1	100.65 (5)	C7—C6—H6A	119.5
N2—Co1—N1 ⁱ	100.65 (5)	C6—C5—C4	121.05 (15)
N2 ⁱ —Co1—N1 ⁱ	76.81 (5)	C6—C5—H5A	119.5
N1—Co1—N1 ⁱ	82.44 (7)	C4—C5—H5A	119.5
N2—Co1—C11	91.56 (4)	C3—C2—C1	119.15 (16)
N2 ⁱ —Co1—C11	90.43 (4)	C3—C2—H2A	120.4
N1—Co1—C11	162.67 (4)	C1—C2—H2A	120.4
N1 ⁱ —Co1—C11	87.23 (4)	C9—C8—C7	119.36 (15)
N2—Co1—C11 ⁱ	90.43 (4)	C9—C8—H8A	120.3
N2 ⁱ —Co1—C11 ⁱ	91.56 (4)	C7—C8—H8A	120.3
N1—Co1—C11 ⁱ	87.23 (4)	C8—C9—C10	119.48 (15)
N1 ⁱ —Co1—C11 ⁱ	162.67 (4)	C8—C9—H9A	120.3
C11—Co1—C11 ⁱ	105.91 (2)	C10—C9—H9A	120.3
C10—N2—C11	117.80 (14)	C12—C4—C3	117.06 (15)
C10—N2—Co1	127.52 (11)	C12—C4—C5	119.30 (15)
C11—N2—Co1	114.39 (10)	C3—C4—C5	123.62 (15)
N2—C11—C7	123.19 (14)	C13 ⁱ —N3—C13	123.8 (8)
N2—C11—C12	117.10 (14)	C13—N3—C15 ⁱ	121.4 (4)
C7—C11—C12	119.71 (14)	C13 ⁱ —N3—C15	121.4 (4)
C1—N1—C12	118.02 (14)	C15 ⁱ —N3—C15	120.0 (11)
C1—N1—Co1	127.74 (11)	C13—N3—C14	118.1 (4)

supplementary materials

C12—N1—Co1	114.20 (10)	C15—N3—C14	120.0 (6)
C11—C7—C8	117.23 (15)	O1—C13—N3	130.9 (6)
C11—C7—C6	119.27 (15)	O1—C13—H13A	114.6
C8—C7—C6	123.49 (15)	N3—C13—H13A	114.6
N1—C12—C4	123.13 (14)	N3—C14—H14A	109.5
N1—C12—C11	117.25 (14)	N3—C14—H14B	109.5
C4—C12—C11	119.62 (14)	H14A—C14—H14B	109.5
C2—C3—C4	119.56 (16)	N3—C14—H14C	109.5
C2—C3—H3A	120.2	H14A—C14—H14C	109.5
C4—C3—H3A	120.2	H14B—C14—H14C	109.5
N2—C10—C9	122.94 (15)	N3—C15—H15A	109.5
N2—C10—H10A	118.5	N3—C15—H15B	109.5
C9—C10—H10A	118.5	H15A—C15—H15B	109.5
N1—C1—C2	123.06 (16)	N3—C15—H15C	109.5
N1—C1—H1A	118.5	H15A—C15—H15C	109.5
C2—C1—H1A	118.5	H15B—C15—H15C	109.5
N1—Co1—N2—C10	178.15 (14)	N2—C11—C12—N1	2.6 (2)
N1 ⁱ —Co1—N2—C10	-102.31 (13)	C7—C11—C12—N1	-177.44 (14)
C11—Co1—N2—C10	-14.83 (13)	N2—C11—C12—C4	-177.75 (14)
C11 ⁱ —Co1—N2—C10	91.10 (13)	C7—C11—C12—C4	2.2 (2)
N1—Co1—N2—C11	4.54 (10)	C11—N2—C10—C9	0.1 (2)
N1 ⁱ —Co1—N2—C11	84.08 (11)	Co1—N2—C10—C9	-173.37 (12)
C11—Co1—N2—C11	171.56 (10)	C12—N1—C1—C2	-0.1 (2)
C11 ⁱ —Co1—N2—C11	-82.51 (10)	Co1—N1—C1—C2	177.45 (13)
C10—N2—C11—C7	0.5 (2)	C11—C7—C6—C5	0.2 (2)
Co1—N2—C11—C7	174.73 (12)	C8—C7—C6—C5	179.06 (16)
C10—N2—C11—C12	-179.63 (14)	C7—C6—C5—C4	1.1 (3)
Co1—N2—C11—C12	-5.35 (17)	C4—C3—C2—C1	-0.8 (3)
N2—Co1—N1—C1	179.24 (15)	N1—C1—C2—C3	0.6 (3)
N2 ⁱ —Co1—N1—C1	1.40 (15)	C11—C7—C8—C9	0.7 (2)
N1 ⁱ —Co1—N1—C1	76.37 (14)	C6—C7—C8—C9	-178.19 (16)
C11—Co1—N1—C1	130.31 (14)	C7—C8—C9—C10	-0.2 (2)
C11 ⁱ —Co1—N1—C1	-89.67 (14)	N2—C10—C9—C8	-0.2 (3)
N2—Co1—N1—C12	-3.15 (10)	N1—C12—C4—C3	0.1 (2)
N2 ⁱ —Co1—N1—C12	179.00 (10)	C11—C12—C4—C3	-179.44 (14)
N1 ⁱ —Co1—N1—C12	-106.02 (12)	N1—C12—C4—C5	178.67 (15)
C11—Co1—N1—C12	-52.08 (19)	C11—C12—C4—C5	-0.9 (2)
C11 ⁱ —Co1—N1—C12	87.94 (10)	C2—C3—C4—C12	0.4 (2)
N2—C11—C7—C8	-0.8 (2)	C2—C3—C4—C5	-178.04 (17)
C12—C11—C7—C8	179.25 (14)	C6—C5—C4—C12	-0.7 (2)
N2—C11—C7—C6	178.10 (14)	C6—C5—C4—C3	177.71 (16)
C12—C11—C7—C6	-1.8 (2)	C13 ⁱ —N3—C13—O1	9.9 (10)
C1—N1—C12—C4	-0.3 (2)	C15 ⁱ —N3—C13—O1	18 (2)
Co1—N1—C12—C4	-178.17 (12)	C15—N3—C13—O1	-62 (7)
C1—N1—C12—C11	179.28 (14)	C14—N3—C13—O1	-170.1 (10)
Co1—N1—C12—C11	1.42 (17)		

Symmetry codes: (i) $-x+1, y, -z+1/2$.

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C10—H10A \cdots C11	0.93	2.74	3.3408 (17)	124
C6—H6A \cdots C11 ⁱⁱ	0.93	2.80	3.6743 (18)	158
C5—H5A \cdots C11 ⁱⁱⁱ	0.93	2.85	3.6375 (17)	144
C2—H2A \cdots Cg1 ^{iv}	0.93	2.99	3.768 (2)	142
C8—H8A \cdots Cg2 ^v	0.93	2.90	3.608 (2)	134

Symmetry codes: (ii) $x+1/2, -y+3/2, -z$; (iii) $x+1/2, y+1/2, -z+1/2$; (iv) $x, -y+1, z-1/2$; (v) $-x+3/2, -y+1/2, z-1/2$.

Fig. 1

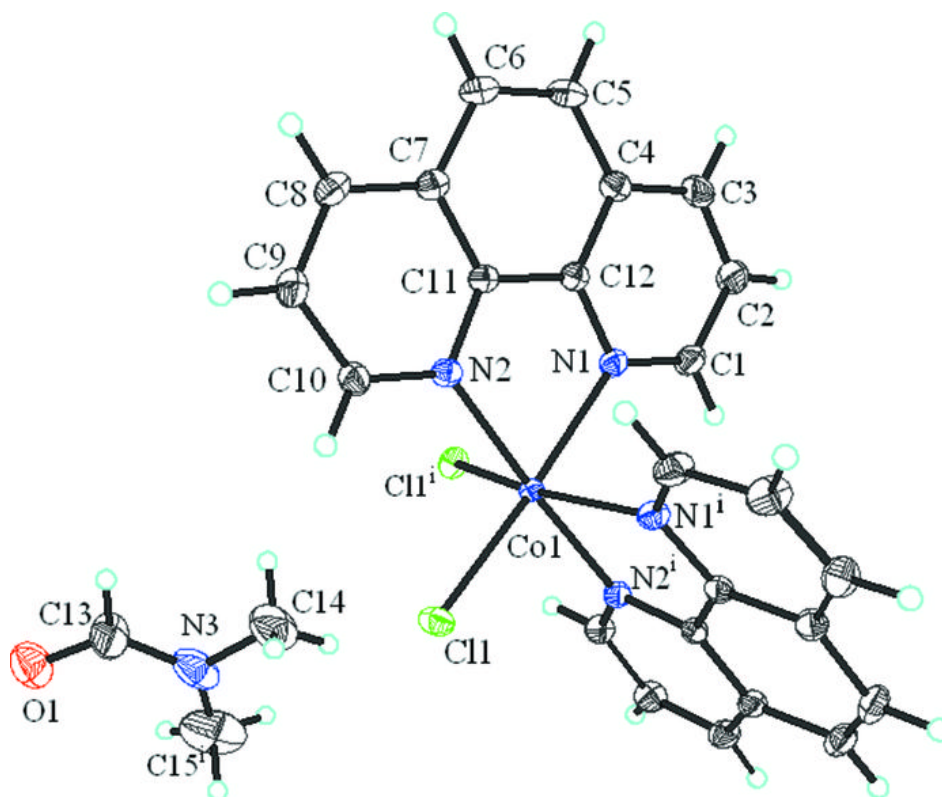


Fig. 2

