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A polymorph of *cis*-dichloridobis(1,10-phenanthroline-κ^2N,N')cobalt(II)

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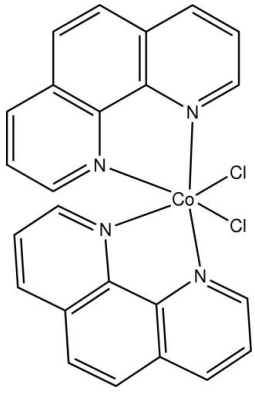
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.003 Å; R factor = 0.022; wR factor = 0.055; data-to-parameter ratio = 17.2.

A new polymorph of the title cobalt(II) complex, $[CoCl_2(C_{12}H_8N_2)_2]$, is reported here. A previous study reported a monoclinic form of this complex [Zhong, Zeng & Luo (2006), *Acta Cryst.* E**62**, m3330–m3332]. In the present orthorhombic structure, the Co^{II} ion is located in a distorted octahedral geometry and coordinated by four N atoms from two 1,10-phenanthroline ligands and two Cl^- anions. The molecules are linked into a two-dimensional framework *via* weak C—H···Cl hydrogen bonding.

Related literature

For related structures, see: Zhong *et al.* (2006); Liu *et al.* (2004); Fu *et al.* (2006); Zhong *et al.* (2007).



Experimental

Crystal data

$[CoCl_2(C_{12}H_8N_2)_2]$
M_r = 490.24
Orthorhombic, $Pna2_1$
a = 21.2371 (14) Å
b = 7.7364 (5) Å
c = 12.6733 (9) Å
V = 2082.2 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.10 mm^{-1}
T = 273 (2) K
0.43 × 0.21 × 0.13 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1990)
T_{min} = 0.649, T_{max} = 0.870
8974 measured reflections
4821 independent reflections
4496 reflections with $I > 2\sigma(I)$
R_{int} = 0.012

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.055
S = 1.02
4821 reflections
280 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}
Absolute structure: Flack (1983), with 2121 Friedel pairs
Flack parameter: 0.028 (9)

Table 1
Selected bond lengths (Å).

Co1—N1	2.1703 (14)	Co1—N4	2.2043 (15)
Co1—N2	2.1395 (14)	Co1—Cl1	2.3928 (6)
Co1—N3	2.1615 (14)	Co1—Cl2	2.4348 (5)

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···Cl1^{i}	0.93	2.74	3.665 (2)	171
C9—H9···Cl1^{ii}	0.93	2.80	3.561 (3)	140

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

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); 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: XU2267).

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supplementary materials

Acta Cryst. (2007). E**63**, m1880 [**doi:10.1107/S1600536807028073**]

A polymorph of *cis*-dichloridobis(1,10-phenanthroline-κ^2N,N')cobalt(II)

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Comment

Herein, we report a polymorph of the title complex. This complex was determined with monoclinic P 21/c space group by Zhong *et al.* (2006). The corresponding six-coordinate complex with water and carbonate anion have been reported (Liu *et al.*, 2004; Fu *et al.*, 2006; Zhong *et al.*, 2007).

In the present structure, the Co^{II} ion is located in a distorted octahedral geometry (Fig. 1) and coordinated by four N atoms from two 1,10-phenanthroline ligands and two Cl^- anions. The average Co—Cl bond distance of 2.168 (2) Å and Co—N bond distance of 2.4138 (5) Å (Table 1) are somewhat shorter than those found in the reported monoclinic structure [average 2.326 (2) Å and 2.4435 (8) Å].

The molecules are linked into a two-dimensional framework (Fig. 2) *via* weak intermolecular C—H···Cl hydrogen bonding (Table 2). But in the reported monoclinic structure, the molecules are linked into a three-dimensional framework by C—H···Cl hydrogen bonding and the π-π stacking.

Experimental

A methanol solution (5 ml) of 1,10-phenanthroline (0.5 mmol) was added to an aqueous solution (10 ml) of cobalt dichloride (1.0 mmol) with stirring. The mixture was stirred continuously for 2 h at room temperature, and then filtered. Slow evaporation of the solution gave single crystals of the title compound.

Refinement

H atoms were placed in calculated positions with C—H = 0.93 Å and refined in riding mode with $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

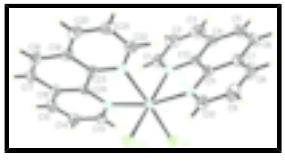

Fig. 1. The molecular structure of the title compound, displacement ellipsoids are drawn at the 30% probability.

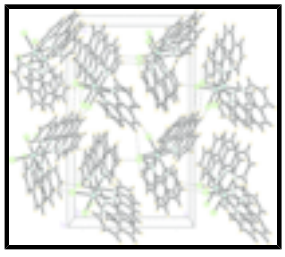

Fig. 2. The unit cell packing diagram.

cis-dichloridobis(1,10-phenanthroline-κ^2N,N')cobalt(II)

Crystal data

$[CoCl_2(C_{12}H_8N_2)_2]$	$F_{000} = 996$
$M_r = 490.24$	$D_x = 1.564$ Mg m^{-3}
Orthorhombic, $Pna2_1$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: P 2c -2n	Cell parameters from 5332 reflections
$a = 21.2371$ (14) Å	$\theta = 2.5$–28.2º
$b = 7.7364$ (5) Å	$\mu = 1.10$ mm^{-1}
$c = 12.6733$ (9) Å	$T = 273$ (2) K
$V = 2082.2$ (2) Å^3	Block, red
$Z = 4$	0.43 × 0.21 × 0.13 mm

Data collection

Bruker CCD area-detector diffractometer	4821 independent reflections
Radiation source: fine-focus sealed tube	4496 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.012$
$T = 273$(2) K	$\theta_{max} = 28.3$º
φ and ω scans	$\theta_{min} = 2.5$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1990)	$h = -8\rightarrow28$
$T_{min} = 0.649$, $T_{max} = 0.870$	$k = -9\rightarrow10$
8974 measured reflections	$l = -15\rightarrow16$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.022$	$w = 1/[\sigma^2(F_o^2) + (0.0247P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.055$	$(\Delta/\sigma)_{max} = 0.003$
$S = 1.02$	$\Delta\rho_{max} = 0.20$ e Å^{-3}
4821 reflections	$\Delta\rho_{min} = -0.15$ e Å^{-3}
280 parameters	Extinction correction: none
1 restraint	Absolute structure: Flack (1983), with 2121 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.028 (9)
Secondary atom site location: difference Fourier map	

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	0.836180 (9)	0.68890 (3)	0.71778 (2)	0.03249 (6)
Cl2	0.92419 (2)	0.85110 (6)	0.64460 (4)	0.04752 (11)
Cl1	0.81796 (2)	0.51066 (6)	0.56653 (4)	0.04825 (11)
C11	0.70676 (7)	0.8328 (2)	0.71241 (17)	0.0357 (3)
N4	0.85782 (7)	0.82299 (17)	0.86690 (12)	0.0360 (3)
N3	0.90037 (6)	0.51456 (18)	0.79647 (11)	0.0344 (3)
N2	0.76570 (6)	0.87682 (19)	0.68047 (11)	0.0369 (3)
C23	0.91076 (7)	0.7581 (2)	0.91265 (14)	0.0344 (3)
C12	0.69965 (8)	0.6750 (2)	0.77073 (14)	0.0365 (4)
N1	0.75226 (6)	0.58222 (18)	0.79065 (12)	0.0379 (3)
C22	0.83464 (9)	0.9694 (3)	0.90508 (17)	0.0466 (5)
H22	0.7976	1.0128	0.8763	0.056*
C19	0.94340 (9)	0.8446 (2)	0.99313 (14)	0.0411 (4)
C7	0.65355 (9)	0.9379 (3)	0.69216 (16)	0.0493 (5)
C10	0.77303 (10)	1.0268 (2)	0.63089 (17)	0.0484 (5)
H10	0.8132	1.0587	0.6092	0.058*
C24	0.93201 (7)	0.5905 (2)	0.87816 (13)	0.0335 (3)
C15	0.99882 (10)	0.3426 (3)	0.89786 (19)	0.0527 (5)
H15	1.0315	0.2841	0.9312	0.063*
C4	0.63959 (9)	0.6242 (3)	0.80633 (17)	0.0504 (5)
C6	0.59281 (9)	0.8773 (3)	0.7262 (2)	0.0653 (6)
H6	0.5572	0.9427	0.7107	0.078*
C21	0.86354 (11)	1.0611 (3)	0.98676 (17)	0.0550 (5)
H21	0.8452	1.1618	1.0126	0.066*
C9	0.72273 (13)	1.1385 (3)	0.61005 (19)	0.0627 (6)
H9	0.7296	1.2427	0.5753	0.075*
C2	0.68866 (13)	0.3801 (3)	0.8858 (2)	0.0669 (7)
H2	0.6863	0.2785	0.9248	0.080*
C13	0.91756 (8)	0.3573 (2)	0.76871 (15)	0.0418 (4)
H13	0.8963	0.3043	0.7133	0.050*
C8	0.66375 (11)	1.0931 (3)	0.6412 (2)	0.0639 (6)
H8	0.6301	1.1670	0.6282	0.077*
C20	0.91877 (11)	1.0023 (3)	1.02858 (16)	0.0510 (5)

H20	0.9398	1.0660	1.0799	0.061*
C16	0.98266 (8)	0.5114 (3)	0.92949 (15)	0.0418 (4)
C5	0.58623 (9)	0.7304 (4)	0.7792 (2)	0.0667 (7)
H5	0.5461	0.6951	0.7993	0.080*
C14	0.96628 (10)	0.2657 (3)	0.81833 (16)	0.0505 (5)
H14	0.9762	0.1539	0.7971	0.061*
C1	0.74660 (11)	0.4377 (3)	0.84612 (17)	0.0537 (5)
H1	0.7824	0.3720	0.8592	0.064*
C3	0.63605 (12)	0.4745 (3)	0.8664 (2)	0.0683 (7)
H3	0.5975	0.4389	0.8935	0.082*
C18	0.99832 (9)	0.7653 (3)	1.03787 (16)	0.0500 (5)
H18	1.0221	0.8262	1.0870	0.060*
C17	1.01607 (9)	0.6046 (3)	1.01017 (17)	0.0521 (5)
H17	1.0503	0.5532	1.0435	0.063*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.02694 (9)	0.03490 (11)	0.03564 (11)	−0.00102 (7)	−0.00133 (10)	0.00495 (11)
Cl2	0.0369 (2)	0.0532 (3)	0.0524 (3)	−0.01210 (18)	0.0080 (2)	0.0052 (2)
Cl1	0.0511 (2)	0.0495 (3)	0.0442 (2)	−0.0074 (2)	−0.0059 (2)	−0.0020 (2)
C11	0.0306 (7)	0.0412 (8)	0.0354 (8)	0.0027 (6)	−0.0049 (8)	−0.0030 (8)
N4	0.0356 (7)	0.0363 (8)	0.0363 (8)	0.0000 (6)	−0.0002 (6)	−0.0007 (6)
N3	0.0340 (7)	0.0355 (7)	0.0336 (7)	0.0000 (5)	0.0012 (6)	0.0005 (6)
N2	0.0342 (7)	0.0376 (8)	0.0390 (8)	−0.0024 (6)	−0.0049 (6)	0.0078 (6)
C23	0.0350 (8)	0.0353 (9)	0.0328 (9)	−0.0035 (7)	0.0024 (7)	0.0020 (7)
C12	0.0314 (8)	0.0449 (10)	0.0333 (9)	−0.0058 (6)	0.0013 (7)	−0.0038 (7)
N1	0.0361 (7)	0.0384 (8)	0.0391 (8)	−0.0052 (6)	0.0000 (6)	0.0075 (6)
C22	0.0472 (10)	0.0444 (11)	0.0483 (12)	0.0092 (8)	0.0040 (9)	−0.0037 (9)
C19	0.0457 (10)	0.0451 (10)	0.0323 (9)	−0.0117 (8)	−0.0020 (7)	0.0031 (8)
C7	0.0411 (9)	0.0571 (12)	0.0497 (13)	0.0139 (8)	−0.0093 (8)	−0.0115 (9)
C10	0.0540 (11)	0.0422 (10)	0.0490 (12)	−0.0047 (8)	−0.0059 (9)	0.0122 (9)
C24	0.0293 (7)	0.0391 (9)	0.0321 (9)	−0.0019 (6)	0.0001 (6)	0.0030 (7)
C15	0.0498 (11)	0.0555 (12)	0.0527 (13)	0.0194 (9)	−0.0034 (10)	0.0087 (10)
C4	0.0380 (9)	0.0663 (13)	0.0469 (11)	−0.0157 (9)	0.0096 (9)	−0.0109 (10)
C6	0.0345 (9)	0.0851 (15)	0.0764 (16)	0.0168 (9)	−0.0009 (12)	−0.0137 (17)
C21	0.0740 (14)	0.0408 (11)	0.0501 (12)	0.0028 (10)	0.0056 (11)	−0.0091 (9)
C9	0.0804 (16)	0.0418 (11)	0.0659 (15)	0.0045 (11)	−0.0179 (12)	0.0141 (10)
C2	0.0836 (17)	0.0579 (14)	0.0592 (15)	−0.0278 (12)	0.0075 (13)	0.0191 (12)
C13	0.0454 (10)	0.0406 (9)	0.0394 (10)	0.0034 (7)	0.0009 (8)	0.0006 (8)
C8	0.0679 (15)	0.0544 (13)	0.0695 (15)	0.0256 (10)	−0.0208 (13)	0.0012 (12)
C20	0.0676 (13)	0.0447 (11)	0.0408 (11)	−0.0100 (9)	−0.0028 (9)	−0.0059 (8)
C16	0.0364 (9)	0.0499 (11)	0.0391 (10)	0.0018 (7)	−0.0022 (7)	0.0040 (8)
C5	0.0284 (10)	0.0954 (18)	0.0762 (17)	−0.0009 (10)	0.0113 (9)	−0.0159 (15)
C14	0.0606 (12)	0.0438 (10)	0.0471 (12)	0.0153 (9)	0.0029 (10)	0.0015 (9)
C1	0.0614 (12)	0.0493 (11)	0.0504 (12)	−0.0080 (10)	−0.0044 (10)	0.0154 (9)
C3	0.0603 (14)	0.0819 (17)	0.0627 (15)	−0.0322 (13)	0.0154 (12)	0.0036 (13)
C18	0.0473 (10)	0.0597 (12)	0.0428 (11)	−0.0119 (9)	−0.0148 (9)	0.0023 (9)

C17	0.0403 (10)	0.0709 (15)	0.0450 (12)	−0.0009 (9)	−0.0140 (8)	0.0051 (10)

Geometric parameters (Å, °)

Co1—N1	2.1703 (14)	C24—C16	1.398 (2)
Co1—N2	2.1395 (14)	C15—C14	1.359 (3)
Co1—N3	2.1615 (14)	C15—C16	1.409 (3)
Co1—N4	2.2043 (15)	C15—H15	0.9300
Co1—Cl1	2.3928 (6)	C4—C3	1.388 (3)
Co1—Cl2	2.4348 (5)	C4—C5	1.441 (3)
C11—N2	1.359 (2)	C6—C5	1.327 (4)
C11—C7	1.416 (2)	C6—H6	0.9300
C11—C12	1.435 (2)	C21—C20	1.365 (3)
N4—C22	1.326 (2)	C21—H21	0.9300
N4—C23	1.361 (2)	C9—C8	1.360 (4)
N3—C13	1.318 (2)	C9—H9	0.9300
N3—C24	1.367 (2)	C2—C3	1.357 (4)
N2—C10	1.328 (2)	C2—C1	1.402 (3)
C23—C19	1.403 (2)	C2—H2	0.9300
C23—C24	1.441 (2)	C13—C14	1.403 (3)
C12—N1	1.352 (2)	C13—H13	0.9300
C12—C4	1.409 (2)	C8—H8	0.9300
N1—C1	1.326 (2)	C20—H20	0.9300
C22—C21	1.397 (3)	C16—C17	1.438 (3)
C22—H22	0.9300	C5—H5	0.9300
C19—C20	1.401 (3)	C14—H14	0.9300
C19—C18	1.435 (3)	C1—H1	0.9300
C7—C8	1.380 (3)	C3—H3	0.9300
C7—C6	1.439 (3)	C18—C17	1.346 (3)
C10—C9	1.400 (3)	C18—H18	0.9300
C10—H10	0.9300	C17—H17	0.9300
N2—Co1—N3	165.28 (5)	C16—C24—C23	119.57 (15)
N2—Co1—N1	77.17 (5)	C14—C15—C16	119.53 (18)
N3—Co1—N1	94.83 (5)	C14—C15—H15	120.2
N2—Co1—N4	90.89 (5)	C16—C15—H15	120.2
N3—Co1—N4	76.51 (5)	C3—C4—C12	117.2 (2)
N1—Co1—N4	89.16 (6)	C3—C4—C5	124.3 (2)
N2—Co1—Cl1	95.82 (4)	C12—C4—C5	118.4 (2)
N3—Co1—Cl1	96.43 (4)	C5—C6—C7	121.67 (18)
N1—Co1—Cl1	89.37 (4)	C5—C6—H6	119.2
N4—Co1—Cl1	172.63 (4)	C7—C6—H6	119.2
N2—Co1—Cl2	95.89 (4)	C20—C21—C22	119.74 (19)
N3—Co1—Cl2	90.76 (4)	C20—C21—H21	120.1
N1—Co1—Cl2	171.28 (4)	C22—C21—H21	120.1
N4—Co1—Cl2	85.64 (4)	C8—C9—C10	119.2 (2)
Cl1—Co1—Cl2	96.66 (2)	C8—C9—H9	120.4
N2—C11—C7	122.52 (17)	C10—C9—H9	120.4
N2—C11—C12	117.60 (14)	C3—C2—C1	119.1 (2)
C7—C11—C12	119.86 (16)	C3—C2—H2	120.4

C22—N4—C23	117.78 (16)	C1—C2—H2	120.4
C22—N4—Co1	129.59 (13)	N3—C13—C14	123.42 (18)
C23—N4—Co1	111.34 (11)	N3—C13—H13	118.3
C13—N3—C24	117.56 (15)	C14—C13—H13	118.3
C13—N3—Co1	128.87 (13)	C9—C8—C7	120.35 (19)
C24—N3—Co1	113.04 (11)	C9—C8—H8	119.8
C10—N2—C11	117.87 (15)	C7—C8—H8	119.8
C10—N2—Co1	128.02 (12)	C21—C20—C19	119.10 (18)
C11—N2—Co1	114.11 (11)	C21—C20—H20	120.4
N4—C23—C19	122.83 (15)	C19—C20—H20	120.4
N4—C23—C24	117.47 (15)	C24—C16—C15	117.42 (18)
C19—C23—C24	119.67 (15)	C24—C16—C17	119.43 (18)
N1—C12—C4	122.70 (17)	C15—C16—C17	123.14 (19)
N1—C12—C11	117.45 (14)	C6—C5—C4	121.75 (18)
C4—C12—C11	119.85 (17)	C6—C5—H5	119.1
C1—N1—C12	118.15 (16)	C4—C5—H5	119.1
C1—N1—Co1	128.36 (13)	C15—C14—C13	119.11 (19)
C12—N1—Co1	113.41 (11)	C15—C14—H14	120.4
N4—C22—C21	122.74 (19)	C13—C14—H14	120.4
N4—C22—H22	118.6	N1—C1—C2	122.5 (2)
C21—C22—H22	118.6	N1—C1—H1	118.7
C20—C19—C23	117.63 (17)	C2—C1—H1	118.7
C20—C19—C18	123.31 (18)	C2—C3—C4	120.2 (2)
C23—C19—C18	119.01 (17)	C2—C3—H3	119.9
C8—C7—C11	117.33 (18)	C4—C3—H3	119.9
C8—C7—C6	124.36 (19)	C17—C18—C19	121.32 (17)
C11—C7—C6	118.3 (2)	C17—C18—H18	119.3
N2—C10—C9	122.6 (2)	C19—C18—H18	119.3
N2—C10—H10	118.7	C18—C17—C16	120.67 (18)
C9—C10—H10	118.7	C18—C17—H17	119.7
N3—C24—C16	122.87 (16)	C16—C17—H17	119.7
N3—C24—C23	117.55 (14)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···Cl1^{i}	0.93	2.74	3.665 (2)	171
C9—H9···Cl1^{ii}	0.93	2.80	3.561 (3)	140

Symmetry codes: (i) −*x*+3/2, *y*−1/2, *z*+1/2; (ii) *x*, *y*+1, *z*.

Fig. 1

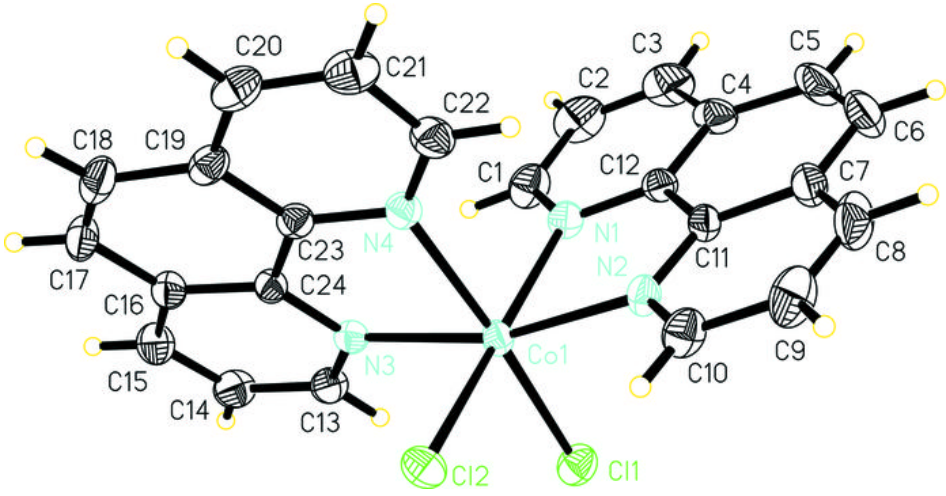
C20
C21
C22
C18
C19
C17
C16
C23
C24
N4
N3
C15
C14
C13
C3
C5
C2
C4
C6
C1
C12
C7
N1
N2
C11
C8
C10
C9
Co1
Cl2
Cl1

Fig. 2