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Dichloro(2,5-diphenyl-3,4-di-2-pyridylcyclopenta-2,4-dienone)cobalt(II)

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Key indicators

Single-crystal X-ray study
T = 180 K
Mean σ(C–C) = 0.003 Å
R factor = 0.038
wR factor = 0.106
Data-to-parameter ratio = 24.1

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

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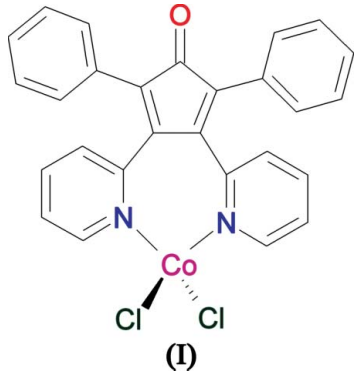
In the molecule of the title complex, $[CoCl_2(C_{27}H_{18}N_2O)]$, the coordination polyhedron about the cobalt(II) center is best described as a distorted tetrahedron. Weak intermolecular C—H···O hydrogen-bonding interactions link the molecules, forming infinite chains.

Comment

Cobalt compounds have been of great interest in coordination chemistry (Chen, 2006; Chen *et al.*, 2005; You *et al.*, 2004; Amirnasr *et al.*, 2001, 2002; Minardi *et al.*, 1999; Viossat *et al.*, 1994).



(I)

A new tetrahedral cobalt(II) compound, $[CoCl_2(\text{Red-}L)]$, (I), where Red-*L* is 2,5-diphenyl-3,4-di-2-pyridylcyclopenta-2,4-dienone, derived from a bidentate chelating ligand (Red-*L*) and two chloride anions, is described here. The title compound, (I), is an electronically neutral mononuclear cobalt(II) compound.

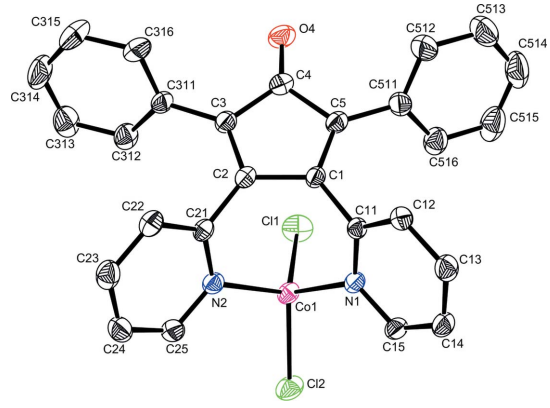


Figure 1
A drawing of the title molecular structure, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted for clarity.

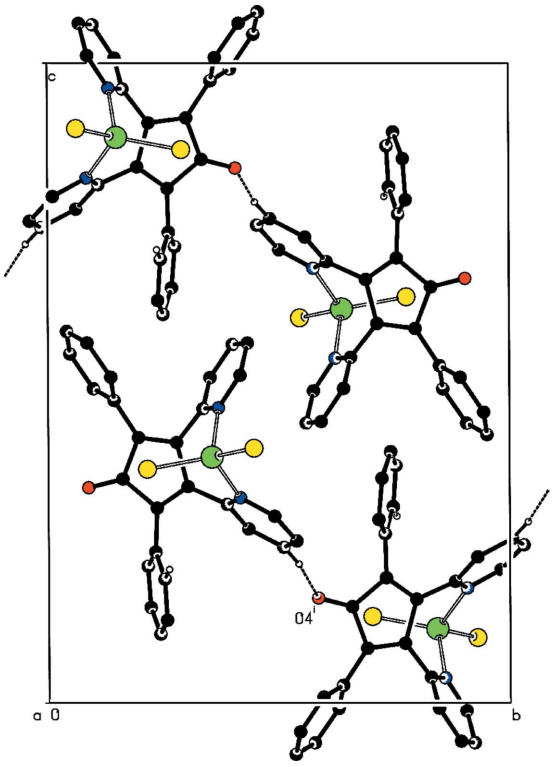


Figure 2
A packing diagram of (I), viewed down the *a* axis. H atoms not involved in hydrogen bonding (dashed lines) have been omitted for clarity.

The Co^{II} atom is in a tetrahedral geometry and is coordinated by one chelate ligand, and two chloride anions (Fig. 1). The Red-*L* ligand acts as a bidentate ligand and ligates to the Co atom through the two N atoms.

The average Co—N [2.042 (14) Å] and Co—Cl [2.2206 (5) Å] bond lengths (Table 1) in (I) are in good agreement with the corresponding mean distances of [2.048 (4) and 2.2273 (15) Å] in the related complex $CoCl_2$(Phca$_2$en), (II), where Phca$_2$en is *N*,*N*′-bis(*β*-phenylcinnamaldehyde)-1,2-diiminoethane, (Amirnasr *et al.*, 2002). The N1—Co1—N2 [97.30 (5)°] and Cl1—Co1—Cl2 [118.52 (2)°] angles (Table 1) in (I) are larger than the corresponding angles [84.07 (15) and 110.17 (6)°] in (II).

In the crystal packing, weak intermolecular C—H···O hydrogen-bonding interactions (Table 2) link the molecules, forming infinite chains (Fig. 2).

Experimental

The 2,5-diphenyl-3,4-di-2-pyridylcyclopenta-2,4-dienone (Red-*L*) ligand was prepared as reported elsewhere (Amirnasr *et al.*, 2000). Compound (I) was prepared by the reaction of $CoCl_2$ with Red-*L* (1:1) in an acetonitrile solution (5 ml) at 298 K. The dark-green precipitate was filtered off and dried under vacuum. Dark-green crystals of (I) were obtained by the slow diffusion of Et_2O vapor into an acetonitrile solution of the complex at 298 K (yield 0.0423 g, 82%; m.p. 503 K).

Crystal data

$[CoCl_2(C_{27}H_{18}N_2O)]$	D_x = 1.456 Mg m^{-3}
M_r = 516.26	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 8076 reflections
a = 7.2884 (3) Å	θ = 2.9–32.0°
b = 15.2580 (8) Å	μ = 0.98 mm^{-1}
c = 21.5709 (9) Å	T = 180 (2) K
β = 101.001 (4)°	Block, dark green
V = 2354.7 (2) Å^3	0.37 × 0.30 × 0.23 mm
Z = 4	

Data collection

Oxford Diffraction XCALIBUR diffractometer	7176 independent reflections
ω and φ scans	5404 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (Blessing, 1995)	R_{int} = 0.029
T_{min} = 0.704, T_{max} = 0.792	θ_{max} = 30.4°
22412 measured reflections	$h = -10 \rightarrow 10$
	$k = -21 \rightarrow 20$
	$l = -30 \rightarrow 30$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.055P)^2 + 0.0498P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.038	$(\Delta/\sigma)_{max}$ = 0.001
$wR(F^2)$ = 0.106	$\Delta\rho_{max}$ = 0.68 e Å^{-3}
S = 1.11	$\Delta\rho_{min}$ = −0.54 e Å^{-3}
7176 reflections	
298 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Co1—N1	2.0325 (13)	Co1—Cl1	2.2161 (5)
Co1—N2	2.0517 (14)	Co1—Cl2	2.2245 (5)
N1—Co1—N2	97.34 (5)	N1—Co1—Cl2	106.32 (4)
N1—Co1—Cl1	111.13 (4)	N2—Co1—Cl2	105.13 (4)
N2—Co1—Cl1	115.96 (4)	Cl1—Co1—Cl2	118.53 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
C23—H23···O4^{i}	0.95	2.53	3.432 (2)	158

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

H atoms were positioned geometrically (C—H = 0.95 Å) and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2003); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2003); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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