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Bis{(*Z*)-*N*′-(2,4-dichlorobenzylidene)-2-hydroxybenzohydrazide-κ^2N',O}bis(pyridine-κN)cobalt(II)

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The title compound, $[Co(C_{14}H_{10}Cl_2N_2O_2)_2(C_5H_5N)_2]$, is a neutral mononuclear cobalt(II) complex. The Co atom in the compound is six-coordinated by two N atoms and two O atoms from two Schiff base ligands and two N atoms from two *cis*-pyridine molecules, giving an approximately octahedral coordination.

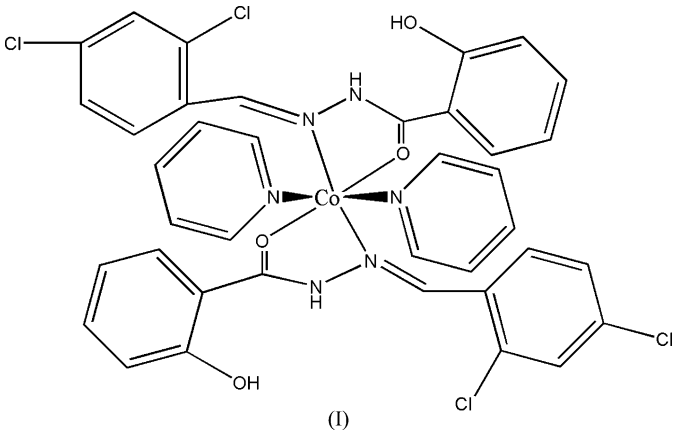
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.044
wR factor = 0.101
Data-to-parameter ratio = 16.1

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

Comment

Recently, we have reported a few Schiff base complexes (Qiu *et al.*, 2004; Zhu *et al.*, 2003), As an extension of our work on the structural characterization of Schiff base complexes, a mononuclear cobalt(II) complex, (I), is reported here (Fig. 1).



(I)

The Co atom in the compound is six-coordinated by two N atoms and two O atoms from two Schiff base ligands and two N atoms from two pyridine molecules, which are *cis* to each other. The Schiff base acts as a bidentate ligand and ligates to the Co atom through an O atom and an N atom. The three *trans* angles at Co are close to 180° (Table 1). The other angles are close 90°, varying from 75.17 (17) to 102.56 (7)°, which indicates a somewhat distorted octahedral geometry of the Co atom. The six bond distances around the Co atom are similar. The Co—O bond lengths are comparable with the value of 2.088 (4) Å we observed in a Schiff base–cobalt(II) compound (You *et al.*, 2004). The average Co—N bond distance of 2.208 (2) Å is a little longer than the value of 2.096 (4) Å observed in a similar Schiff base complex (Hu *et al.*, 2005). The comformation of the five-membered rings containing the Co, hydrazino N atoms, carbonyl O atom and C atom is a distorted plate. The mean deviation from the plane is 0.0863 (2) Å. The trans angles in the CoN_2O_2 are 177.50 (7) (O2—Co1—O4) and 163.70 (8)° (N2—Co1—N5), indicating a slightly distorted square-planar geometry of Co1. Atom Co1 deviates from the CoN_2O_2 square plane by 0.0496 (2) Å.

Experimental

The reagents were commercial products and were used without further purification. A methanol (10 ml) and pyridine (4 ml) solution of cobalt(II) acetate (0.5 mmol, 89 mg) was added to a methanol (10 ml) of (*Z*)-*N*′-(2,4-dichlorobenzylidene)-2-hydroxybenzohydrazide. The reaction mixture was stirred for 20 min. After allowing the resulting clear solution to stand at room temperature in the air for 12 d, large red crystals were formed by slow evaporation of the solvent. The crystals were isolated, washed three times with methanol and dried in a vacuum desiccator using anhydrous $CaCl_2$ (yield 56%).

Crystal data

$[Co(C_{14}H_{10}Cl_2N_2O_2)_2(C_5H_5N)_2]$
M_r = 835.41
Monoclinic, $P2_1/n$
a = 13.1832 (5) Å
b = 12.2799 (5) Å
c = 23.2108 (10) Å
β = 97.934 (2)°
V = 3721.6 (3) Å^3
Z = 4
D_x = 1.491 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.80 mm^{-1}
T = 298 (2) K
Block, red
0.36 × 0.26 × 0.14 mm

Data collection

Bruker SMART APEX area-detector diffractometer
ω scans
Absorption correction: multi-scan *SADABS* (Sheldrick, 1996)
T_{min} = 0.778, T_{max} = 0.889
21284 measured reflections
7675 independent reflections
5595 reflections with $I > 2\sigma(I)$
R_{int} = 0.033
θ_{max} = 26.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.101
S = 1.02
7675 reflections
478 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0365P)^2 + 1.8102P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—O2	2.0103 (16)	N1—N2	1.391 (3)
Co1—O4	2.0233 (17)	O2—C7	1.283 (3)
Co1—N6	2.173 (2)	N2—C8	1.280 (3)
Co1—N5	2.176 (2)	N3—C21	1.315 (3)
Co1—N4	2.223 (2)	N3—N4	1.392 (3)
Co1—N2	2.262 (2)	O4—C21	1.280 (3)
N1—C7	1.311 (3)	N4—C22	1.278 (3)
O2—Co1—O4	177.50 (7)	N6—Co1—N4	160.84 (8)
O2—Co1—N6	91.80 (8)	N5—Co1—N4	101.21 (8)
O4—Co1—N6	89.32 (7)	O2—Co1—N2	75.15 (7)
O2—Co1—N5	89.07 (8)	O4—Co1—N2	102.57 (7)
O4—Co1—N5	93.14 (8)	N6—Co1—N2	93.34 (8)
N6—Co1—N5	91.14 (8)	N5—Co1—N2	163.70 (8)
O2—Co1—N4	102.90 (7)	N4—Co1—N2	78.90 (7)
O4—Co1—N4	75.54 (7)		

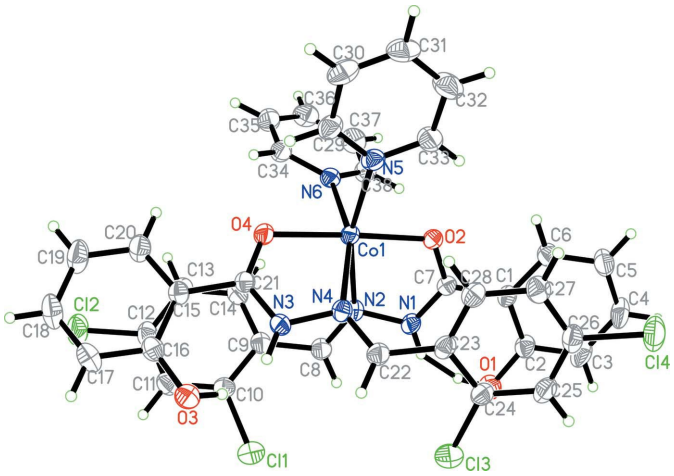


Figure 1
The structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H, N—H and O—H distances of 0.93, 0.86 and 0.82 Å, respectively, and with U_{iso}(H) = 1.2U_{eq}(C, N) or 1.5U_{eq}(O).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); 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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Bis{(*Z*)-*N*′-(2,4-dichlorobenzylidene)-2-hydroxybenzohydrazide-κ^2N',O}bis(pyridine-κN)cobalt(II). Corrigendum

Xiao-Yang Qiu,[a,b] Sen-Lin Yang,[b] Wei-Sheng Liu[a]* and Hai-Liang Zhu[c]*

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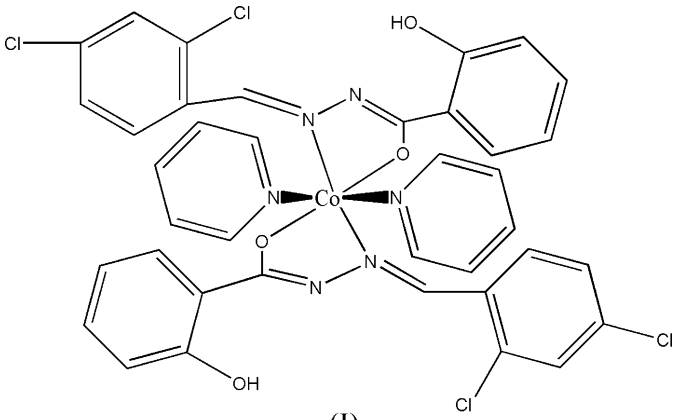
In the original paper by Qiu, Yang, Liu & Zhu [*Acta Cryst.* (2006), E**62**, m1320–m1231], the H atoms attached to N1 and N3 are positioned incorrectly. These have been deleted and the structure rerefined. The correct name of the structure is bis(2,4-dichlorobenzaldehyde 2-hydroxybenzoylhydrazonato-κ^2N,O)bis(pyridine-κN)cobalt(II). The scheme, figure, *Crystal data*, *Refinement* and hydrogen-bond table are corrected.



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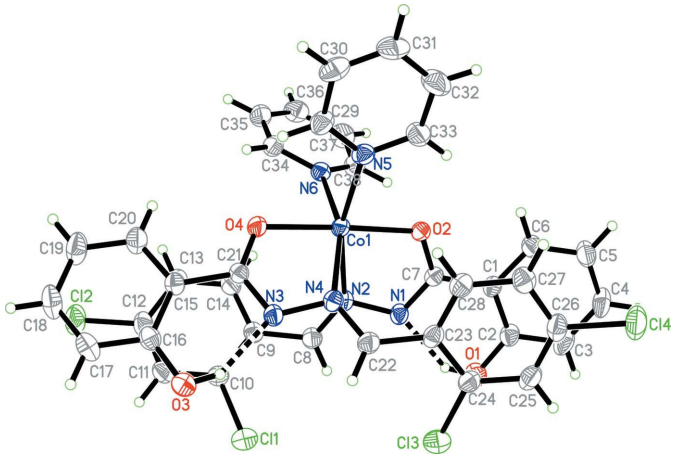

Figure 1
The structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme. The dashed lines indicate hydrogen bonds.

Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.043
wR factor = 0.092
Data-to-parameter ratio = 15.8

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

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.043$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.092$	
$S = 1.02$	$\Delta\rho_{max} = 0.34$ e Å^{-3}
7675 reflections	$\Delta\rho_{min} = -0.37$ e Å^{-3}
486 parameters	

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.80 (3)	1.87 (3)	2.566 (3)	144 (3)
O3—H16···N3	0.84 (4)	1.83 (4)	2.564 (3)	146 (3)