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Bis[4-chloro-2-(cyclohexyliminomethyl)-phenolato]cobalt(II)

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Key indicators

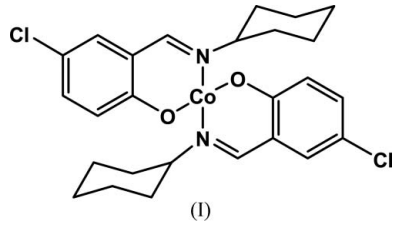
Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.004 Å
R factor = 0.034
wR factor = 0.069
Data-to-parameter ratio = 15.6

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

In the mononuclear title compound, $[Co(C_{13}H_{15}ClNO)_2]$, the Co atom is four-coordinated by two N atoms and two O atoms from two Schiff base ligands in a slightly distorted tetrahedral geometry.

Comment

Cobalt complexes are of great interest in coordination chemistry in relation to catalysis and enzymatic reactions, magnetism and molecular architectures (Billson *et al.*, 2000; Fritsky *et al.*, 2003; Kotera *et al.*, 2003). As an extension of work on the structural characterization of cobalt(II) compounds, the crystal structure of the title compound, (I), is reported here.



(I)

Compound (I) is a mononuclear Co^{II} complex (Fig. 1). The Co^{II} ion is coordinated by two O and two N atoms from two Schiff base ligands. This CoN_2O_2 coordination forms a distorted tetrahedral geometry, with angles subtended at the Co^{II} atom in the range 94.41 (8)–122.87 (8)° (Table 1). The bond lengths around the Co atom range from 1.9092 (18) to 2.0055 (19) Å.

Experimental

5-Chlorosalicylaldehyde (0.1 mmol, 15.7 mg), $Co(CH_3COO)_2\cdot 4H_2O$ (0.1 mmol, 24.9 mg) and cyclohexylamine (0.1 mmol, 9.3 mg) were dissolved in methanol (10 ml). The mixture was stirred for 30 min at room temperature to give a clear brown solution. After allowing the resulting solution to stand in air for 11 d, brown block-shaped crystals of (I) were formed on slow evaporation of the solvent. The crystals were collected, washed with methanol and dried in a vacuum desiccator using anhydrous $CaCl_2$ (yield 54%). Analysis found: C 58.64, H 5.63%; calculated for $C_{26}H_{30}Cl_2CoN_2O_2$: C 58.64%, H 5.64%.

Crystal data

$[Co(C_{13}H_{15}ClNO)_2]$
M_r = 532.35
Orthorhombic, *Pbca*
a = 14.860 (3) Å
b = 13.560 (2) Å
c = 24.959 (5) Å
V = 5029.3 (16) Å^3
Z = 8
D_x = 1.406 Mg m^{-3}
D_m = ? Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 26 reflections
θ = 2.6–13.5°
μ = 0.92 mm^{-1}
T = 296 (2) K
Block, brown
0.54 × 0.50 × 0.46 mm

Data collection

Siemens *P*4 diffractometer	R_{int} = 0.016
ω scans	θ_{max} = 25.5°
Absorption correction: ψ scan (*XSCANS*; Siemens, 1995)	$h = 0 \rightarrow 18$
	$k = 0 \rightarrow 16$
T_{min} = 0.614, T_{max} = 0.655	$l = -30 \rightarrow 1$
5644 measured reflections	3 standard reflections
4679 independent reflections	every 97 reflections
2714 reflections with $I > 2\sigma(I)$	intensity decay: 3.1%

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0289P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.035	$(\Delta/\sigma)_{max}$ = 0.001
$wR(F^2)$ = 0.069	$\Delta\rho_{max}$ = 0.24 e Å^{-3}
S = 0.85	$\Delta\rho_{min}$ = −0.25 e Å^{-3}
4679 reflections	Extinction correction: *SHELXL97*
299 parameters	Extinction coefficient: 0.00173 (11)
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Co—O2	1.9092 (18)	Co—N2	1.997 (2)
Co—O1	1.9149 (16)	Co—N1	2.0055 (19)
O2—Co—O1	121.42 (8)	O2—Co—N1	112.57 (8)
O2—Co—N2	95.18 (8)	O1—Co—N1	94.41 (8)
O1—Co—N2	112.63 (8)	N2—Co—N1	122.87 (8)

All H atoms were placed in idealized positions and allowed to ride on their parent atoms, with C—H distances in the range 0.93–0.98 Å, and with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *XSCANS* (Siemens, 1995); cell refinement: *XSCANS*; data reduction: *SHELXTL* (Siemens, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXL97*.

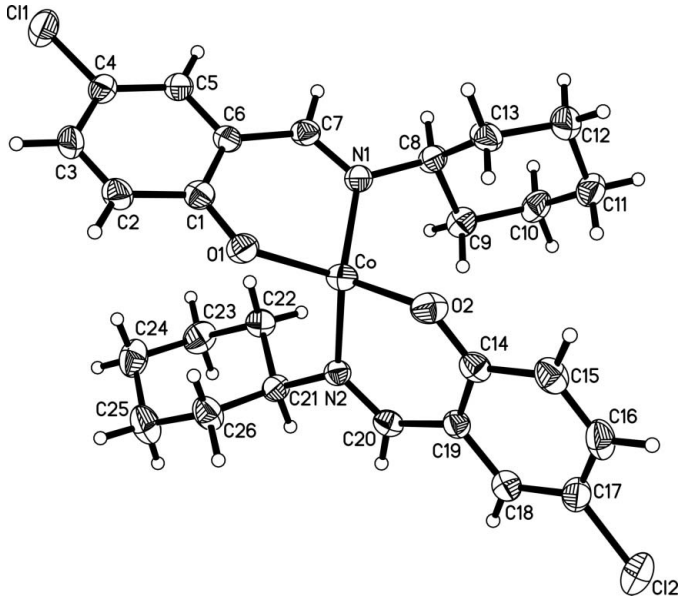


Figure 1
The structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

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