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Bis[2-(cyclohexyliminomethyl)-4-nitrophenolato]cobalt(II)

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Key indicators

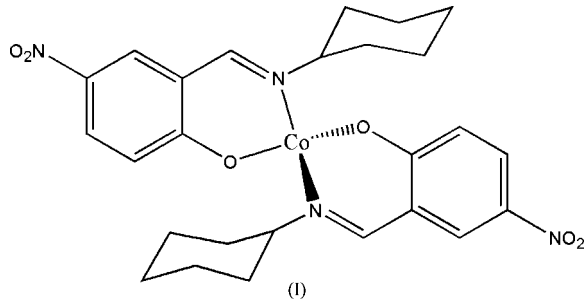
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.038
wR factor = 0.104
Data-to-parameter ratio = 17.5

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

The title compound, $[Co(C_{13}H_{15}N_2O_3)_2]$, is isostructural with the zinc(II) compound reported previously. The Co atom is coordinated by four donor atoms from two Schiff base ligands, forming a tetrahedral geometry.

Comment

Cobalt compounds are of great interest in coordination chemistry (Billson *et al.*, 2000; Kotera *et al.*, 2003; Fritsky *et al.*, 2003). As part of our investigations on non-covalent interactions in metal complexes (Chen, 2005), the new title Co^{II} complex, (I), has been prepared and its crystal structure is presented here.



(I)

Complex (I) is a mononuclear cobalt(II) compound (Fig. 1), which is isostructural with the zinc compound bis[2-(cyclohexyliminomethyl)-4-nitrophenolato]zinc(II) (You, 2005), and structurally similar to the cobalt compound bis[4-chloro-2-(cyclohexyliminomethyl)phenolato]cobalt(II) (Li & Zhang, 2005). In (I), the Co atom is coordinated by four donor atoms from two Schiff base ligands, forming a tetrahedral geometry.

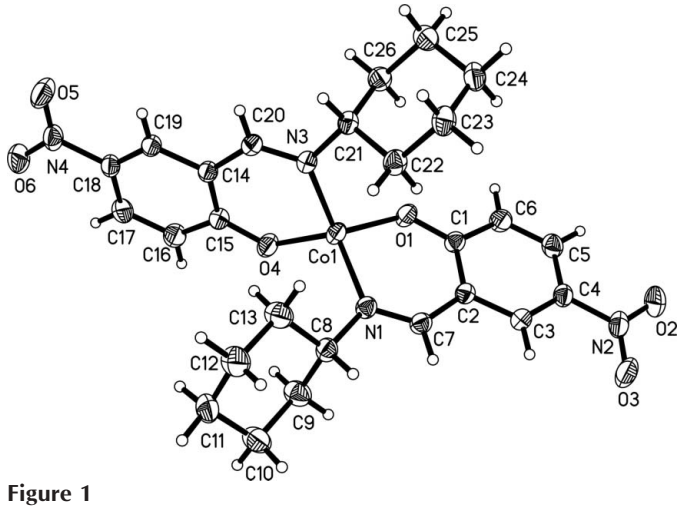


Figure 1
The molecular structure of compound (I), showing the labeling scheme and displacement ellipsoids drawn at the 30% probability level.

The Schiff base acts as a bidentate ligand and ligates to the metal *via* the phenolate O and imine N atoms. All the bond lengths (Table 1) around the metal center are comparable to those in similar complexes (Fun *et al.*, 1999; Iyere *et al.*, 2004; Elerman *et al.*, 1996).

Experimental

All the chemicals were of AR grade. 5-Nitro-2-hydroxybenzaldehyde (16.7 mg, 0.1 mmol), cyclohexylamine (9.9 mg, 0.1 mmol) and $CoCl_2{\cdot}4H_2O$ (20.2 mg, 0.1 mmol) were refluxed in 30 ml MeOH for 30 min. The mixture was cooled to room temperature and filtered. After keeping the filtrate in air for 11 d, red block crystals suitable for X-ray analysis were obtained.

Crystal data

$[Co(C_{13}H_{15}N_2O_3)_2]$	$Z = 2$
$M_r = 553.47$	$D_x = 1.423$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 10.765$ (1) Å	Cell parameters from 5677 reflections
$b = 11.135$ (1) Å	$\theta = 2.3$–$27.4°$
$c = 12.410$ (1) Å	$\mu = 0.71$ mm^{-1}
$\alpha = 113.698$ (1)°	$T = 298$ (2) K
$\beta = 104.064$ (1)°	Block, red
$\gamma = 95.105$ (1)°	0.20 × 0.16 × 0.10 mm
$V = 1291.84$ (19) Å^3	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	5834 independent reflections
	4950 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.022$
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)	$\theta_{max} = 27.5°$
	$h = -13 \rightarrow 13$
$T_{min} = 0.871$, $T_{max} = 0.932$	$k = -14 \rightarrow 14$
15016 measured reflections	$l = -15 \rightarrow 16$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0538P)^2 + 0.2812P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.038$	
$wR(F^2) = 0.104$	
$S = 1.03$	$(\Delta/\sigma)_{max} < 0.001$
5834 reflections	$\Delta\rho_{max} = 0.27$ e Å^{-3}
334 parameters	$\Delta\rho_{min} = -0.22$ e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Co1—O4	1.906 (2)	Co1—N1	1.994 (2)
Co1—O1	1.916 (2)	Co1—N3	1.994 (2)
O4—Co1—O1	120.86 (6)	O4—Co1—N3	95.93 (6)
O4—Co1—N1	113.14 (6)	O1—Co1—N3	110.11 (6)
O1—Co1—N1	95.95 (6)	N1—Co1—N3	122.81 (6)

All H atoms were positioned geometrically and refined as riding atoms, with C—H distances of 0.93–0.98 Å and $U_{iso}(H) = 1.2U_{eq}$(parent C atom).

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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