

[*N,N'*-Bis(2-hydroxynaphthylmethyl-imino)-1,2-ethanediaminato]cobalt(II)

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Key indicators

Single-crystal X-ray study

T = 293 K

Mean $\sigma(\text{C}-\text{C}) = 0.006 \text{ \AA}$

R factor = 0.062

wR factor = 0.134

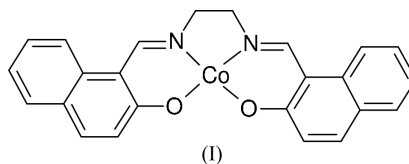
Data-to-parameter ratio = 13.7

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

The title compound, $[\text{Co}(\text{C}_{24}\text{H}_{18}\text{N}_2\text{O}_2)]$, is mononuclear. The Co^{II} atom is coordinated by two N atoms and two O atoms from a bis-Schiff base ligand in a slightly distorted square-planar geometry.

Comment

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



The title compound, (I), is an electronically neutral mononuclear cobalt(II) compound (Fig. 1). The Co atom in the compound is four-coordinated by two O atoms and by two N atoms from the bis-Schiff base ligand. This CoO_2N_2 coordination forms a slightly distorted square-planar geometry, as is usually observed in the structures of cobalt(II) complexes (You, Zhu & Liu, 2004; Lyon *et al.*, 1998). The Co atom is 0.011 (1) \AA out of the square plane defined by the four donor atoms in the complex. The average $\text{Co}-\text{O}(\text{phenolate})$ bond length of 1.852 (3) \AA (Table 1) is not significantly longer than the corresponding value of 1.846 (3) \AA observed in a similar Schiff base cobalt(II) complex (You, Zhu & Liu, 2004). The average $\text{Co}-\text{N}(\text{imine})$ bond distance of 1.846 (3) \AA is essentially the same as the value of 1.850 (2) \AA observed in the same complex. The *trans* angles in the CoN_2O_2 square plane are 176.29 (12) ($\text{N1}-\text{Co1}-\text{O2}$) and 177.55 (12) ($\text{N2}-\text{Co1}-\text{O1}$), indicating a slightly distorted square-planar geometry of

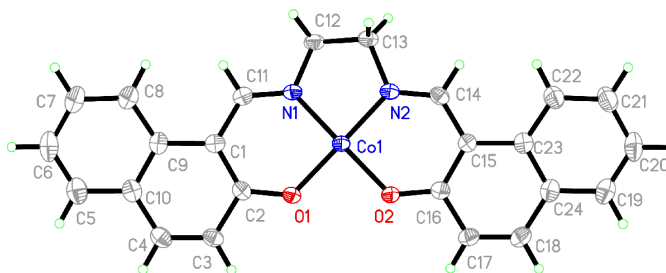


Figure 1

The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

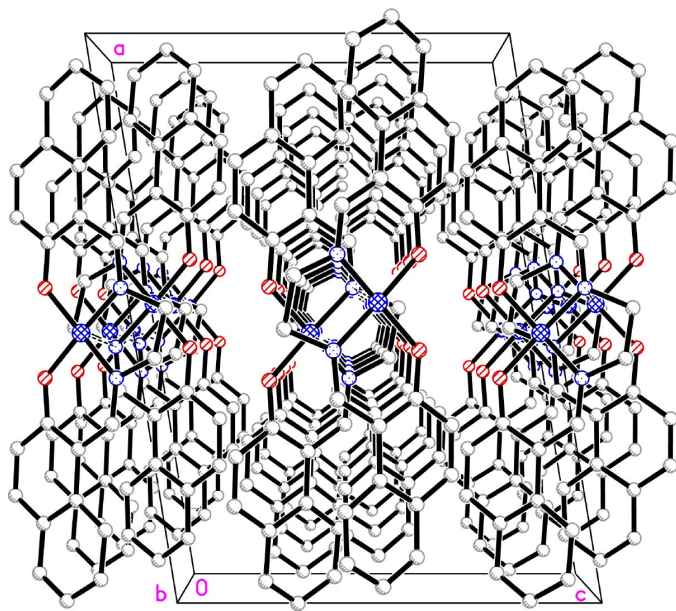


Figure 2
The crystal packing of (I), viewed along the *b* axis. H atoms have been omitted.

Co1. Atom C12 deviates from the CoN_2O_2 square plane by 0.380 (4) Å, whereas C13 deviates from it on the opposite side by 0.108 (4) Å. The CoN_2O_2 square plane forms dihedral angles of 4.9 (2) and 5.2 (2)°, respectively, with the two naphthalene ring systems, which are inclined at 5.6 (2)° to each other.

Experimental

2-Hydroxy-1-naphthaldehyde (0.2 mmol, 34.4 mg) and 1,2-diaminoethane (0.1 mmol, 6.0 mg) were dissolved in MeOH (10 ml). The mixture was stirred for 1 h to give a clear yellow solution of *L* (0.1 mmol), where *L* is *N,N'*-bis(2-hydroxynaphthylmethylimino)-1,2-diaminoethane. To the solution of *L* was added a MeOH solution (10 ml) of $\text{Co}(\text{CH}_3\text{COO})_2 \cdot 4\text{H}_2\text{O}$, with stirring. After keeping the resulting solution at room temperature in air for 11 d, red crystals were formed at the bottom of the vessel on slow evaporation of the solvent. The crystals were isolated, washed three times with MeOH and dried in a vacuum desiccator using anhydrous CaCl_2 (yield 71.2%). Analysis found: C 68.0, H 4.4, N 6.8%; calculated for $\text{C}_{24}\text{H}_{18}\text{CoN}_2\text{O}_2$: C 67.8, H 4.3, N 6.6%. Selected IR data: 3430 (*w*), 1611 (*s*), 1291 (*s*), 541 (*m*), 482 cm^{-1} (*m*).

Crystal data

$[\text{Co}(\text{C}_{24}\text{H}_{18}\text{N}_2\text{O}_2)]$
 $M_r = 425.33$
Monoclinic, $P2_1/c$
 $a = 17.667$ (4) Å
 $b = 8.140$ (2) Å
 $c = 12.992$ (3) Å
 $\beta = 99.21$ (3)°
 $V = 1844.3$ (8) Å³
 $Z = 4$

$D_x = 1.532$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1873 reflections
 $\theta = 2.7$ – 25.6 °
 $\mu = 0.96$ mm^{-1}
 $T = 293$ (2) K
Plate, red
 $0.41 \times 0.32 \times 0.03$ mm

Data collection

Siemens SMART CCD area-detector diffractometer
 φ and ω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.696$, $T_{\max} = 0.972$
8032 measured reflections

3593 independent reflections
2797 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.040$
 $\theta_{\max} = 26.0$ °
 $h = -21 \rightarrow 21$
 $k = -7 \rightarrow 10$
 $l = -11 \rightarrow 16$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.062$
 $wR(F^2) = 0.134$
 $S = 1.05$
3593 reflections
262 parameters

H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.062P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.69$ e Å⁻³
 $\Delta\rho_{\min} = -0.31$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Co1–N1	1.845 (3)	Co1–O2	1.850 (3)
Co1–N2	1.847 (3)	Co1–O1	1.854 (2)
N1–Co1–N2	86.68 (13)	N1–Co1–O1	92.71 (12)
N1–Co1–O2	176.29 (12)	N2–Co1–O1	177.55 (12)
N2–Co1–O2	92.78 (12)	O2–Co1–O1	87.98 (11)

After checking their presence in a difference map, all the H atoms were placed in geometrically idealized positions and allowed to ride on their parent atoms, with $U_{\text{iso}}(\text{H})$ values fixed at 0.08 Å². The highest peak in the difference map was found at 0.95 Å from Co1.

Data collection: SMART (Siemens, 1996); cell refinement: SMART; data reduction: SAINT (Siemens, 1996); program(s) used to solve structure: SHELXS97 (Sheldrick, 1997a); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997a); molecular graphics: SHELXTL (Sheldrick, 1997b); software used to prepare material for publication: SHELXTL.

The authors thank the Education Office of Anhui Province, People's Republic of China, for research grant No. 2004kj300zd.

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