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[*N*,*N*′-Bis(2-hydroxynaphthylmethylene)-1,3-propanediaminato]cobalt(II)

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.007 Å
R factor = 0.042
wR factor = 0.096
Data-to-parameter ratio = 10.2

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

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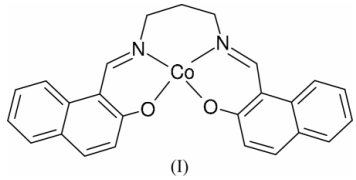
The title compound, $[Co(C_{25}H_{20}N_2O_2)]$, is mononuclear. The molecule has crystallographic mirror symmetry. The Co^{II} atom is coordinated by two N atoms and two O atoms from a bis-Schiff base ligand in a slightly distorted square-planar geometry.

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; You, Zhu & Liu, 2004). As an extension of our work on the structural characterization of Schiff base complexes, a mononuclear cobalt(II) complex is reported here.



(I)

The title compound, (I), is an electronically neutral mononuclear cobalt(II) compound (Fig. 1). The molecule of (I) possesses mirror symmetry, with atoms Co1 and C13 lying on the crystallographic mirror plane. The central 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 usually observed in the structures of cobalt(II) complexes (Lyon *et al.*, 1998). The Co atom is 0.0015 (3) Å out of the plane defined by the four donor atoms in the complex. The Co—O(phenolate) bond lengths of 1.846 (3) Å (Table 1) are comparable to the corresponding value of 1.846 (2) Å observed in a similar Schiff base cobalt(II) complex (Lyon *et al.*, 1998). The Co—N(imine) bond distances of 1.852 (3) Å

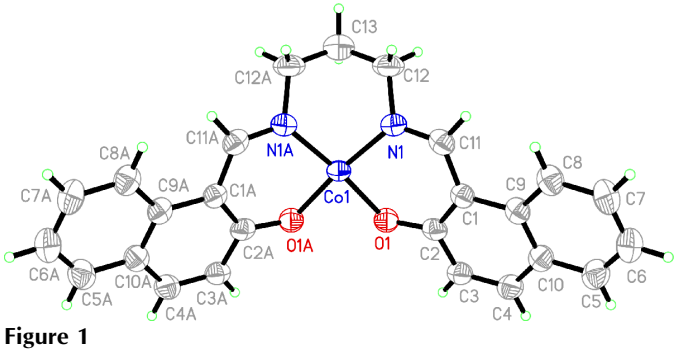


Figure 1
The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Atoms with the suffix *A* are related by the mirror symmetry (1 − *x*, *y*, *z*).

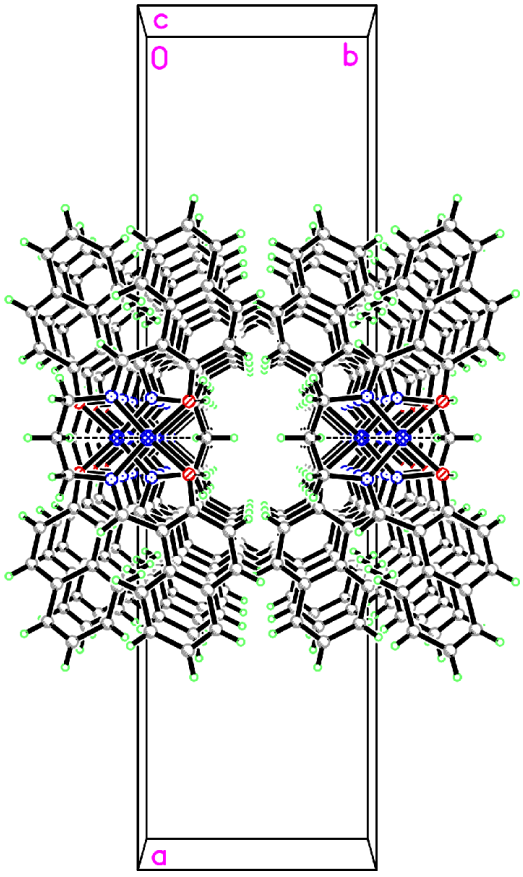


Figure 2
The crystal packing of (I), viewed along the *c* axis.

are also comparable to the value of 1.850 (2) Å observed in the same complex. Both the *trans* angles in the CoN_2O_2 square plane are 173.78 (14)°, indicating a slightly distorted square planar geometry of Co1. There is an overall butterfly shape to the molecule, as evidenced by a dihedral angle of 52.7 (5)° between the two naphthalene ring systems of the complex. The dihedral angle between the CoN_2O_2 square plane and the naphthalene ring system is 28.6 (3)°. The conformation of the six-membered ring containing the metal, azomethine N atoms and three C atoms of the connecting 1,3-diaminopropane is a symmetric boat. The distances of the two *para*-positioned boat atoms, Co1 and C13, from the mean plane of the other four atoms are 0.523 (3) and 0.599 (3) Å, respectively.

Experimental

All chemicals (reagent grade) used were commercially available. 2-Hydroxy-1-naphthaldehyde (0.2 mmol, 34.4 mg) and 1,3-diaminopropane (0.1 mmol, 7.4 mg) were dissolved in MeOH (10 ml). The mixture was stirred for 1 h to give a clear yellow solution of *L* (0.2 mmol), where *L* is *N*,*N*′–bis(2-hydroxynaphthylmethylene)-1,3-propanediamine. To the solution of *L* was added a MeOH solution (8 ml) of $Co(CH_3COO)_2{\cdot}4H_2O$ with stirring. After keeping the resulting solution at room temperature in air for 13 d, brown 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 68.3%). Analysis found: C 68.32, H 4.66, N 6.45%; calculated for $C_{25}H_{20}CoN_2O_2$: C 68.34, H 4.59, N 6.38%. Selected IR data (cm^{-1}): 3432 (*w*), 1613 (*s*), 1288 (*s*), 540 (*m*), 479 (*m*).

Crystal data

$[Co(C_{25}H_{20}N_2O_2)]$
M_r = 439.36
Orthorhombic, $Cmc2_1$
a = 30.554 (6) Å
b = 8.4240 (17) Å
c = 7.7270 (15) Å
V = 1988.8 (7) Å^3
Z = 4
D_x = 1.467 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2312 reflections
θ = 2.5–25.2°
μ = 0.89 mm^{-1}
T = 293 (2) K
Block, red
0.23 × 0.20 × 0.17 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.822, T_{max} = 0.864
3825 measured reflections
1414 independent reflections
1192 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 27.0°
$h = -37 \rightarrow 38$
$k = -10 \rightarrow 10$
$l = -9 \rightarrow 5$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.096
S = 1.00
1414 reflections
139 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0534P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}
Absolute structure: Flack (1983), 250 Friedel pairs
Flack parameter = 0.39 (3)

Table 1
Selected geometric parameters (Å, °).

Co1—O1	1.846 (3)	Co1—N1	1.852 (3)
O1^i—Co1—O1	82.30 (18)	O1—Co1—N1	91.48 (14)
O1—Co1—N1^i	173.78 (14)	N1^i—Co1—N1	94.7 (2)

Symmetry code: (i) $1-x, y, z$.

All H atoms were placed in geometrically idealized positions and allowed to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å, and U_{iso}(H) = 1.2U_{eq}(C). The Flack parameter is 0.39(3), which indicates a partial inversion twin.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1996); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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