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Bis[2-(cyclopropyliminomethyl)-6-methoxyphenolato]cobalt(II)

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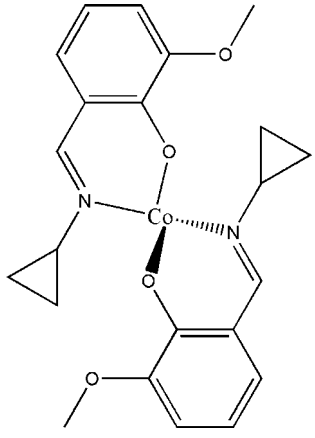
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.030; wR factor = 0.083; data-to-parameter ratio = 16.9.

In the title compound, $[Co(C_{11}H_{12}NO_2)_2]$, the Co^{II} atom, lying on a twofold rotation axis, is four-coordinated by two imine N and two phenolate O atoms from two Schiff base ligands in a distorted tetrahedral coordination gometry. The two Schiff base ligands are nearly perpendicular to each other, with a dihedral angle of 87.1 (2)° between their mean planes.

Related literature

For general background, see: Au-Yeung & Chan (2004); Lewiński *et al.* (2005); Liu *et al.* (2006); Robin & Fromm (2006); Salmon *et al.* (2005); Vicente & Arcas (2005); Xu *et al.* (2005). For related structures, see: Ni *et al.* (2005); Iyere *et al.* (2004); Peng & Hou (2006); Zhang, Yue *et al.* (2005); Zhou *et al.* (2004). For related literature, see: Zhang *et al.* (2006).



Experimental

Crystal data

$[Co(C_{11}H_{12}NO_2)_2]$
M_r = 439.36
Monoclinic, $C2/c$
a = 20.249 (2) Å
b = 9.2011 (11) Å
c = 13.1621 (16) Å
β = 126.193 (1)°
V = 1979.1 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.90 mm^{-1}
T = 298 (2) K
0.22 × 0.20 × 0.17 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.827, T_{max} = 0.862
8175 measured reflections
2254 independent reflections
2078 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.083
S = 1.09
2254 reflections
133 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—O1	1.8958 (10)	Co1—N1	2.0016 (13)
O1^i—Co1—O1	127.41 (7)	O1—Co1—N1	95.48 (5)
O1^i—Co1—N1	111.73 (5)	N1^i—Co1—N1	116.57 (8)

Symmetry code: (i) $-x, y, -z+\frac{1}{2}$.

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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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2429).

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supplementary materials

Acta Cryst. (2007). E**63**, m3185 [**doi:10.1107/S1600536807061880**]

Bis[2-(cyclopropyliminomethyl)-6-methoxyphenolato]cobalt(II)

S.-J. Peng and C.-S. Zhou

Comment

The design of O/N-donor multidentate ligands, their metallosupramolecular chemistry and the study of their physical properties have been of considerable recent interest (Robin & Fromm, 2006; Vicente & Arcas, 2005; Au-Yeung & Chan, 2004). A major goal in modern coordination chemistry is to synthesize molecules with a predefined geometry. Condensation of aromatic carbaldehydes with primary amines offers an easy and inexpensive way of forming a variety of polydentate Schiff base ligands, leading to the formation of a variety of complexes (Lewiński *et al.*, 2005; Salmon *et al.*, 2005; Xu *et al.*, 2005; Liu *et al.*, 2006). We report here the synthesis and structure of the title mononuclear cobalt(II) complex (I), Fig. 1, Table 1.

The Co^{II} atom in (I), lying on a twofold rotation axis, is four-coordinated by two imine N and two phenolate O atoms from two Schiff base ligand, forming a distorted tetrahedral coordination geometry. The metal-ligand bond lengths are comparable to the values in other similar cobalt(II) complexes (Zhou *et al.*, 2004; Iyere *et al.*, 2004; Zhang *et al.*, 2006; Yue *et al.*, 2005; Peng & Hou, 2006).

Experimental

3-Methoxysalicylaldehyde (0.2 mmol, 30.5 mg), cyclopropylamine (0.2 mmol, 11.5 mg), and cobalt(II) acetate tetrahydrate (0.1 mmol, 12.5 mg) were stirred at 318 K in methanol (20 ml) for 30 min. The filtrate was kept in air for twelve days depositing brown block-like crystals of (I).

Refinement

All H-atoms bound to carbon were refined using a riding model with d(C—H) = 0.93–0.98 Å, and with $U_{iso} = 1.2U_{eq}$(C) and $1.5U_{eq}$(methyl C).

Figures

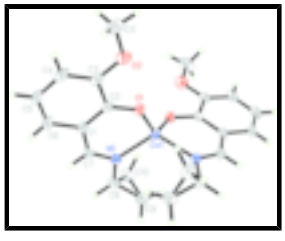

Fig. 1. The molecular structure of (I), showing the atom-numbering scheme and 30% probability displacement ellipsoids. Unlabelled atoms are at the symmetry position $-x, y, 1/2 - z$.

Bis[2-(cyclopropyliminomethyl)-6-methoxyphenolato]cobalt(II)

Crystal data

$[Co(C_{11}H_{12}NO_2)_2]$	$F_{000} = 916$
$M_r = 439.36$	$D_x = 1.475$ Mg m^{-3}
Monoclinic, $C2/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -C 2yc	Cell parameters from 5017 reflections
$a = 20.249$ (2) Å	$\theta = 2.4$–28.1º
$b = 9.2011$ (11) Å	$\mu = 0.90$ mm^{-1}
$c = 13.1621$ (16) Å	$T = 298$ (2) K
$\beta = 126.193$ (1)º	Block, brown
$V = 1979.1$ (4) Å^3	0.22 × 0.20 × 0.17 mm
$Z = 4$	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	2254 independent reflections
Radiation source: fine-focus sealed tube	2078 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.022$
$T = 298$(2) K	$\theta_{max} = 27.5$º
ω scans	$\theta_{min} = 2.5$º
Absorption correction: multi-scan (SADABS; Bruker, 2000)	$h = -26 \rightarrow 26$
$T_{min} = 0.827$, $T_{max} = 0.862$	$k = -11 \rightarrow 11$
8175 measured reflections	$l = -16 \rightarrow 17$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.030$	H-atom parameters constrained
$wR(F^2) = 0.083$	$w = 1/[\sigma^2(F_o^2) + (0.0486P)^2 + 0.7933P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.09$	$(\Delta/\sigma)_{max} = <0.001$
2254 reflections	$\Delta\rho_{max} = 0.20$ e Å^{-3}
133 parameters	$\Delta\rho_{min} = -0.38$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Co1	0.0000	0.71997 (3)	0.2500	0.03157 (11)
O1	0.08279 (7)	0.62869 (12)	0.24704 (10)	0.0369 (2)
O2	0.18014 (8)	0.43298 (15)	0.25833 (13)	0.0550 (3)
N1	−0.04711 (8)	0.83432 (14)	0.09181 (12)	0.0331 (3)
C1	0.03581 (10)	0.70545 (16)	0.04006 (15)	0.0334 (3)
C2	0.08396 (9)	0.61938 (16)	0.14909 (14)	0.0317 (3)
C3	0.13761 (9)	0.51622 (18)	0.15175 (16)	0.0385 (3)
C4	0.14302 (11)	0.5045 (2)	0.05247 (18)	0.0471 (4)
H4	0.1786	0.4370	0.0564	0.056*
C5	0.09592 (12)	0.5922 (2)	−0.05353 (18)	0.0502 (5)
H5	0.1004	0.5840	−0.1196	0.060*
C6	0.04346 (11)	0.6897 (2)	−0.05995 (17)	0.0441 (4)
H6	0.0118	0.7476	−0.1313	0.053*
C7	−0.02386 (10)	0.80863 (17)	0.02062 (15)	0.0354 (3)
H7	−0.0490	0.8640	−0.0524	0.043*
C8	−0.11140 (10)	0.94043 (19)	0.04572 (17)	0.0437 (4)
H8	−0.1237	0.9997	−0.0254	0.052*
C9	−0.12263 (12)	1.0133 (2)	0.1354 (2)	0.0559 (5)
H9A	−0.0857	0.9869	0.2236	0.067*
H9B	−0.1398	1.1142	0.1197	0.067*
C10	−0.18265 (11)	0.9026 (2)	0.0465 (2)	0.0530 (5)
H10A	−0.2363	0.9362	−0.0234	0.064*
H10B	−0.1822	0.8088	0.0805	0.064*
C11	0.23366 (14)	0.3262 (3)	0.2667 (2)	0.0714 (7)
H11A	0.2030	0.2592	0.1978	0.107*
H11B	0.2595	0.2746	0.3448	0.107*
H11C	0.2747	0.3725	0.2630	0.107*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.03802 (18)	0.03337 (18)	0.03506 (17)	0.000	0.02805 (14)	0.000

O1	0.0430 (6)	0.0423 (6)	0.0363 (6)	0.0069 (5)	0.0294 (5)	0.0025 (4)
O2	0.0552 (8)	0.0550 (8)	0.0609 (8)	0.0187 (6)	0.0376 (7)	0.0023 (6)
N1	0.0347 (6)	0.0325 (6)	0.0381 (6)	−0.0013 (5)	0.0247 (6)	0.0020 (5)
C1	0.0379 (8)	0.0366 (8)	0.0352 (7)	−0.0103 (6)	0.0269 (7)	−0.0070 (6)
C2	0.0343 (7)	0.0325 (7)	0.0381 (7)	−0.0086 (6)	0.0267 (6)	−0.0085 (6)
C3	0.0371 (8)	0.0377 (8)	0.0485 (9)	−0.0051 (6)	0.0295 (7)	−0.0101 (7)
C4	0.0491 (9)	0.0467 (9)	0.0670 (11)	−0.0124 (8)	0.0462 (9)	−0.0230 (8)
C5	0.0647 (11)	0.0569 (11)	0.0550 (10)	−0.0191 (9)	0.0497 (10)	−0.0207 (9)
C6	0.0539 (10)	0.0521 (10)	0.0397 (9)	−0.0137 (8)	0.0350 (8)	−0.0091 (7)
C7	0.0393 (8)	0.0369 (8)	0.0339 (7)	−0.0061 (6)	0.0237 (7)	0.0016 (6)
C8	0.0452 (9)	0.0430 (9)	0.0501 (9)	0.0095 (7)	0.0320 (8)	0.0129 (7)
C9	0.0592 (11)	0.0492 (10)	0.0672 (12)	0.0154 (9)	0.0417 (10)	0.0035 (9)
C10	0.0393 (9)	0.0599 (11)	0.0634 (11)	0.0079 (8)	0.0323 (9)	0.0100 (9)
C11	0.0540 (12)	0.0672 (14)	0.0746 (15)	0.0223 (11)	0.0278 (11)	−0.0132 (12)

Geometric parameters (Å, °)

Co1—O1^{i}	1.8958 (10)	C5—C6	1.354 (3)
Co1—O1	1.8958 (10)	C5—H5	0.9300
Co1—N1^{i}	2.0016 (13)	C6—H6	0.9300
Co1—N1	2.0016 (13)	C7—H7	0.9300
O1—C2	1.3063 (17)	C8—C9	1.487 (3)
O2—C3	1.367 (2)	C8—C10	1.490 (2)
O2—C11	1.418 (2)	C8—H8	0.9800
N1—C7	1.295 (2)	C9—C10	1.485 (3)
N1—C8	1.443 (2)	C9—H9A	0.9700
C1—C2	1.409 (2)	C9—H9B	0.9700
C1—C6	1.421 (2)	C10—H10A	0.9700
C1—C7	1.436 (2)	C10—H10B	0.9700
C2—C3	1.427 (2)	C11—H11A	0.9600
C3—C4	1.379 (2)	C11—H11B	0.9600
C4—C5	1.392 (3)	C11—H11C	0.9600
C4—H4	0.9300		
O1^{i}—Co1—O1	127.41 (7)	C1—C6—H6	119.3
O1^{i}—Co1—N1^{i}	95.48 (5)	N1—C7—C1	128.25 (15)
O1—Co1—N1^{i}	111.73 (5)	N1—C7—H7	115.9
O1^{i}—Co1—N1	111.73 (5)	C1—C7—H7	115.9
O1—Co1—N1	95.48 (5)	N1—C8—C9	119.61 (15)
N1^{i}—Co1—N1	116.57 (8)	N1—C8—C10	118.42 (15)
C2—O1—Co1	125.52 (10)	C9—C8—C10	59.83 (13)
C3—O2—C11	117.19 (17)	N1—C8—H8	115.8
C7—N1—C8	116.26 (14)	C9—C8—H8	115.8
C7—N1—Co1	120.21 (11)	C10—C8—H8	115.8
C8—N1—Co1	123.39 (10)	C10—C9—C8	60.17 (13)
C2—C1—C6	119.86 (15)	C10—C9—H9A	117.8
C2—C1—C7	123.83 (14)	C8—C9—H9A	117.8
C6—C1—C7	116.29 (16)	C10—C9—H9B	117.8

O1—C2—C1	124.30 (13)	C8—C9—H9B	117.8
O1—C2—C3	118.46 (14)	H9A—C9—H9B	114.9
C1—C2—C3	117.24 (13)	C9—C10—C8	60.00 (13)
O2—C3—C4	125.05 (15)	C9—C10—H10A	117.8
O2—C3—C2	114.00 (14)	C8—C10—H10A	117.8
C4—C3—C2	120.95 (16)	C9—C10—H10B	117.8
C3—C4—C5	120.91 (16)	C8—C10—H10B	117.8
C3—C4—H4	119.5	H10A—C10—H10B	114.9
C5—C4—H4	119.5	O2—C11—H11A	109.5
C6—C5—C4	119.66 (15)	O2—C11—H11B	109.5
C6—C5—H5	120.2	H11A—C11—H11B	109.5
C4—C5—H5	120.2	O2—C11—H11C	109.5
C5—C6—C1	121.35 (18)	H11A—C11—H11C	109.5
C5—C6—H6	119.3	H11B—C11—H11C	109.5

Symmetry codes: (i) $-x$, y, $-z+1/2$.

Fig. 1