

## Bis{2-[(*E*)-benzyliminomethyl]-4-methylphenolato- $\kappa^2$ N,O}cobalt(II)

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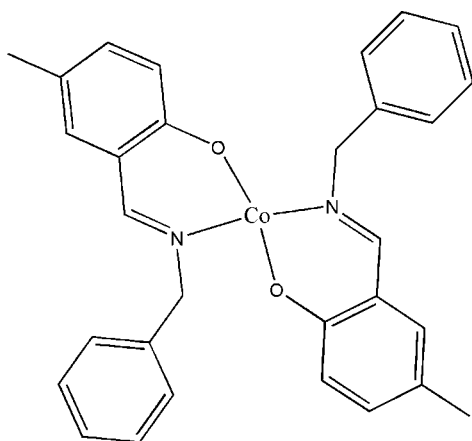
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Key indicators: single-crystal X-ray study;  $T = 296$  K; mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å;  $R$  factor = 0.027;  $wR$  factor = 0.080; data-to-parameter ratio = 17.4.

In the title complex,  $[\text{Co}(\text{C}_{15}\text{H}_{14}\text{NO})_2]$ , the  $\text{Co}^{\text{II}}$  atom, situated on an inversion centre, is coordinated by two O and two N atoms from two symmetry-related bidentate Schiff base ligands in a slightly distorted square-planar geometry. The two phenolate rings form a dihedral angle of  $10.53(2)^\circ$ .

### Related literature

For background on complexes of Schiff bases with transition metals, see: Rodriguez Barbarin *et al.* (1994).



### Experimental

#### Crystal data

$[\text{Co}(\text{C}_{15}\text{H}_{14}\text{NO})_2]$   
 $M_r = 507.47$   
Monoclinic,  $P2_1/c$   
 $a = 13.735(3)$  Å  
 $b = 10.625(2)$  Å  
 $c = 8.7926(17)$  Å  
 $\beta = 107.394(2)^\circ$

$V = 1224.5(4)$  Å<sup>3</sup>  
 $Z = 2$   
Mo  $K\alpha$  radiation  
 $\mu = 0.73$  mm<sup>-1</sup>  
 $T = 296(2)$  K  
 $0.37 \times 0.30 \times 0.25$  mm

#### Data collection

Bruker SMART APEXII  
diffractometer  
Absorption correction: multi-scan  
(*SADABS*; Sheldrick, 1997)  
 $T_{\text{min}} = 0.765$ ,  $T_{\text{max}} = 0.825$

10315 measured reflections  
2807 independent reflections  
2404 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.022$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.027$   
 $wR(F^2) = 0.080$   
 $S = 1.08$   
2807 reflections

161 parameters  
H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.22$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.24$  e Å<sup>-3</sup>

**Table 1**

Selected geometric parameters (Å, °).

Co1—O1	1.8259 (11)	Co1—N1	1.9258 (11)
O1 <sup>i</sup> —Co1—O1	180.0	O1—Co1—N1	93.01 (5)
O1 <sup>i</sup> —Co1—N1	86.99 (5)		

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *XP* in *SHELXTL*.

We are grateful to the Starting Fund for the Doctoral Program of Xi'an University of Architecture and Technology (grant No. RC0737) for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GW2053).

### References

- Bruker (2004). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.  
Rodriguez Barbarin, C. O., Bailey, N. A., Fenton, D. E. & He, Q. (1994). *Inorg. Chim. Acta*, **219**, 205–207.  
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.  
Sheldrick, G. M. (2008). *Acta Cryst. A* **64**, 112–122.

**supplementary materials**

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## Bis{2-[(*E*)-benzyliminomethyl]-4-methylphenolato- $\kappa^2$ N,O}cobalt(II)

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### Comment

Schiff bases have played an important role in the development of coordination chemistry as they readily form stable complexes with most of the transition metals (Rodriguez Barbarin *et al.*, 1994). Salicylaldehyde and its derivatives are useful carbonyl precursors for the synthesis of a large variety of Schiff bases. Here we report on a new cobalt(II) complex (I).

The molecular structure of (I) as illustrated in Fig. 1 has the  $\text{Co}^{2+}$  center in a square geometry as it is coordinated by two O atoms and two N atoms from two 2-[(*E*)-benzylimino)methyl]-4-methylphenol bidentate chelating ligand. The Co1—O1 distance of 1.8259 (11) Å is shorter than the distance of Co1—N1 (1.9258 (11)) (Table 1). The dihedral angle between the plane of O1, N1,  $\text{Co}^{2+}$  and two parallel phenol rings with the distance of 0.484 Å is 10.53 °.

### Experimental

1 mmol of  $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$  (0.238 g) were added to a 15 ml ethanol solution containing 2 mmol (0.450 g) 2-[(*E*)-benzylimino)methyl]-4-methylphenol. The resulting mixture was stirred for about 0.5 h. The slow vaporization of the solvent yielded after about 5 d dark brown single crystals. Yield: 68.8%. Calcd. for  $\text{C}_{30}\text{H}_{28}\text{CoN}_2\text{O}_2$ : C, 71.00; H, 5.56; N, 5.52; Found: C, 71.31; H, 5.60; N, 5.47%.

### Refinement

All H atoms were located from difference Fourier syntheses, H atoms from the C—H groups were placed in geometrically idealized positions and constrained to ride on their parent atoms (C—H = 0.93Å, 0.96Å, 0.97Å;) and  $U_{\text{iso}}(\text{H})$  values equal to 1.2  $U_{\text{eq}}(\text{C})$ .

### Figures

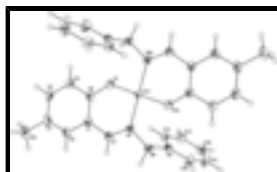


Fig. 1. The structure of (I), showing displacement ellipsoids drawn at the 30% probability level. [Symmetry code: (A)  $-x + 1, -y + 2, -z$ ]

## Bis{2-[(*E*)-benzyliminomethyl]-4-methylphenolato- $\kappa^2$ N,O}cobalt(II)

### Crystal data

$[\text{Co}(\text{C}_{15}\text{H}_{14}\text{NO})_2]$

$F_{000} = 530.0$

# supplementary materials

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$M_r = 507.47$

Monoclinic,  $P2_1/c$

Hall symbol: -P 2ybc

$a = 13.735$  (3) Å

$b = 10.625$  (2) Å

$c = 8.7926$  (17) Å

$\beta = 107.394$  (2)°

$V = 1224.5$  (4) Å<sup>3</sup>

$Z = 2$

$D_x = 1.376$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation

$\lambda = 0.71073$  Å

Cell parameters from 2457 reflections

$\theta = 1.0$ – $27.6$ °

$\mu = 0.73$  mm<sup>-1</sup>

$T = 296$  (2) K

Block, dark brown

$0.37 \times 0.30 \times 0.25$  mm

## Data collection

Bruker SMART APEXII  
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 296$ (2) K

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan  
(SADABS; Sheldrick, 1997)

$T_{\min} = 0.765$ ,  $T_{\max} = 0.825$

10315 measured reflections

2807 independent reflections

2404 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.022$

$\theta_{\max} = 27.6$ °

$\theta_{\min} = 1.0$ °

$h = -17 \rightarrow 17$

$k = -11 \rightarrow 13$

$l = -11 \rightarrow 11$

## Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.027$

$wR(F^2) = 0.080$

$S = 1.08$

2807 reflections

161 parameters

Primary atom site location: structure-invariant direct  
methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring  
sites

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0449P)^2 + 0.166P]$$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.22$  e Å<sup>-3</sup>

$\Delta\rho_{\min} = -0.24$  e Å<sup>-3</sup>

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  $F^2 > \sigma(F^2)$  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 ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Co1	0.5000	1.0000	0.0000	0.03135 (9)
N1	0.50882 (8)	0.85049 (10)	0.12722 (13)	0.0361 (2)
O1	0.63563 (8)	1.03507 (11)	0.08454 (14)	0.0505 (3)
C9	0.35213 (9)	0.85593 (12)	0.21649 (15)	0.0350 (3)
C1	0.69440 (10)	0.84697 (13)	0.23467 (16)	0.0398 (3)
C8	0.41511 (10)	0.78371 (12)	0.13166 (16)	0.0384 (3)
H8A	0.4341	0.7033	0.1845	0.046*
H8B	0.3735	0.7670	0.0233	0.046*
C7	0.59332 (10)	0.80109 (13)	0.21412 (16)	0.0398 (3)
H7A	0.5877	0.7280	0.2691	0.048*
C14	0.39142 (11)	0.95166 (14)	0.32390 (16)	0.0402 (3)
H14A	0.4589	0.9767	0.3425	0.048*
C2	0.77878 (11)	0.77682 (15)	0.32681 (18)	0.0486 (3)
H2A	0.7671	0.7011	0.3715	0.058*
C6	0.71010 (11)	0.96291 (15)	0.16800 (17)	0.0408 (3)
C3	0.87726 (11)	0.81665 (17)	0.35251 (19)	0.0534 (4)
C10	0.25147 (11)	0.82053 (16)	0.19115 (18)	0.0501 (4)
H10A	0.2237	0.7565	0.1192	0.060*
C4	0.89188 (11)	0.93208 (18)	0.2855 (2)	0.0546 (4)
H4A	0.9581	0.9612	0.3018	0.065*
C11	0.19180 (12)	0.87956 (19)	0.2719 (2)	0.0608 (4)
H11A	0.1244	0.8545	0.2541	0.073*
C13	0.33122 (14)	1.01077 (14)	0.4041 (2)	0.0495 (4)
H13A	0.3586	1.0751	0.4759	0.059*
C12	0.23131 (14)	0.97510 (17)	0.3785 (2)	0.0554 (4)
H12A	0.1910	1.0149	0.4322	0.066*
C5	0.81198 (13)	1.00369 (15)	0.1967 (2)	0.0511 (4)
H5A	0.8250	1.0800	0.1548	0.061*
C15	0.96691 (15)	0.7397 (2)	0.4506 (3)	0.0824 (6)
H15A	0.9442	0.6822	0.5171	0.124*
H15B	1.0177	0.7949	0.5161	0.124*
H15C	0.9957	0.6933	0.3808	0.124*

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Co1	0.02864 (14)	0.03280 (15)	0.03417 (14)	0.00058 (9)	0.01176 (10)	0.00084 (9)
N1	0.0347 (5)	0.0355 (6)	0.0411 (6)	-0.0002 (4)	0.0158 (5)	-0.0030 (5)
O1	0.0353 (5)	0.0509 (6)	0.0613 (7)	-0.0012 (4)	0.0085 (5)	0.0136 (5)
C9	0.0351 (6)	0.0364 (7)	0.0347 (6)	-0.0026 (5)	0.0120 (5)	0.0031 (5)
C1	0.0369 (7)	0.0438 (7)	0.0403 (7)	0.0051 (5)	0.0143 (5)	-0.0024 (6)
C8	0.0393 (7)	0.0329 (6)	0.0447 (7)	-0.0037 (5)	0.0150 (6)	-0.0022 (5)

## supplementary materials

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C7	0.0430 (7)	0.0356 (7)	0.0437 (7)	0.0034 (5)	0.0173 (6)	0.0003 (5)
C14	0.0383 (7)	0.0410 (7)	0.0426 (7)	-0.0049 (6)	0.0144 (6)	-0.0023 (6)
C2	0.0454 (8)	0.0500 (8)	0.0520 (8)	0.0105 (6)	0.0169 (7)	0.0052 (7)
C6	0.0361 (7)	0.0466 (7)	0.0403 (7)	0.0034 (6)	0.0126 (6)	0.0003 (6)
C3	0.0395 (8)	0.0686 (10)	0.0526 (9)	0.0140 (7)	0.0146 (7)	0.0047 (8)
C10	0.0412 (8)	0.0631 (10)	0.0476 (8)	-0.0144 (7)	0.0158 (6)	-0.0118 (7)
C4	0.0332 (7)	0.0732 (12)	0.0589 (9)	0.0031 (7)	0.0162 (7)	0.0012 (8)
C11	0.0390 (8)	0.0865 (13)	0.0625 (10)	-0.0105 (8)	0.0237 (7)	-0.0095 (9)
C13	0.0578 (10)	0.0470 (9)	0.0475 (8)	-0.0029 (7)	0.0215 (8)	-0.0085 (6)
C12	0.0531 (10)	0.0660 (10)	0.0556 (9)	0.0064 (8)	0.0292 (8)	-0.0027 (8)
C5	0.0378 (8)	0.0589 (10)	0.0574 (10)	-0.0016 (6)	0.0157 (7)	0.0068 (7)
C15	0.0461 (9)	0.1026 (17)	0.0950 (14)	0.0244 (11)	0.0154 (10)	0.0311 (14)

### Geometric parameters ( $\text{\AA}$ , $^\circ$ )

Co1—O1 <sup>i</sup>	1.8259 (11)	C2—C3	1.370 (2)
Co1—O1	1.8259 (11)	C2—H2A	0.9300
Co1—N1	1.9258 (11)	C6—C5	1.414 (2)
Co1—N1 <sup>i</sup>	1.9258 (11)	C3—C4	1.401 (2)
N1—C7	1.2946 (17)	C3—C15	1.514 (2)
N1—C8	1.4804 (16)	C10—C11	1.385 (2)
O1—C6	1.3129 (19)	C10—H10A	0.9300
C9—C14	1.3831 (19)	C4—C5	1.371 (2)
C9—C10	1.3851 (18)	C4—H4A	0.9300
C9—C8	1.5096 (17)	C11—C12	1.378 (3)
C1—C6	1.408 (2)	C11—H11A	0.9300
C1—C2	1.412 (2)	C13—C12	1.376 (2)
C1—C7	1.4311 (19)	C13—H13A	0.9300
C8—H8A	0.9700	C12—H12A	0.9300
C8—H8B	0.9700	C5—H5A	0.9300
C7—H7A	0.9300	C15—H15A	0.9600
C14—C13	1.387 (2)	C15—H15B	0.9600
C14—H14A	0.9300	C15—H15C	0.9600
O1 <sup>i</sup> —Co1—O1	180.0	O1—C6—C1	123.56 (13)
O1 <sup>i</sup> —Co1—N1	86.99 (5)	O1—C6—C5	119.02 (14)
O1—Co1—N1	93.01 (5)	C1—C6—C5	117.41 (13)
O1 <sup>i</sup> —Co1—N1 <sup>i</sup>	93.01 (5)	C2—C3—C4	117.37 (14)
O1—Co1—N1 <sup>i</sup>	86.99 (5)	C2—C3—C15	121.46 (17)
N1—Co1—N1 <sup>i</sup>	180.00 (4)	C4—C3—C15	121.17 (16)
C7—N1—C8	115.04 (11)	C11—C10—C9	120.66 (14)
C7—N1—Co1	124.53 (9)	C11—C10—H10A	119.7
C8—N1—Co1	120.43 (8)	C9—C10—H10A	119.7
C6—O1—Co1	129.64 (11)	C5—C4—C3	122.29 (15)
C14—C9—C10	118.45 (12)	C5—C4—H4A	118.9
C14—C9—C8	123.16 (12)	C3—C4—H4A	118.9
C10—C9—C8	118.32 (12)	C12—C11—C10	120.60 (14)
C6—C1—C2	119.94 (13)	C12—C11—H11A	119.7

C6—C1—C7	120.59 (12)	C10—C11—H11A	119.7
C2—C1—C7	119.44 (13)	C12—C13—C14	120.58 (15)
N1—C8—C9	113.61 (10)	C12—C13—H13A	119.7
N1—C8—H8A	108.8	C14—C13—H13A	119.7
C9—C8—H8A	108.8	C13—C12—C11	119.04 (15)
N1—C8—H8B	108.8	C13—C12—H12A	120.5
C9—C8—H8B	108.8	C11—C12—H12A	120.5
H8A—C8—H8B	107.7	C4—C5—C6	120.84 (15)
N1—C7—C1	126.95 (13)	C4—C5—H5A	119.6
N1—C7—H7A	116.5	C6—C5—H5A	119.6
C1—C7—H7A	116.5	C3—C15—H15A	109.5
C9—C14—C13	120.66 (13)	C3—C15—H15B	109.5
C9—C14—H14A	119.7	H15A—C15—H15B	109.5
C13—C14—H14A	119.7	C3—C15—H15C	109.5
C3—C2—C1	122.15 (15)	H15A—C15—H15C	109.5
C3—C2—H2A	118.9	H15B—C15—H15C	109.5
C1—C2—H2A	118.9		

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

Fig. 1

