Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Bis(2-hydroxyiminomethyl-6-methoxyphenolato-κ^2O^1,N)cobalt(II)

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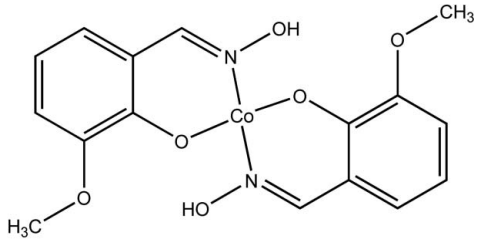
Received 10 November 2008; accepted 24 November 2008

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.025; wR factor = 0.065; data-to-parameter ratio = 12.2.

In the title compound, $[Co(C_8H_8NO_3)_2]$, the Co^{II} atom lies on a centre of inversion and is coordinated in a slightly distorted square-planar geometry by two N and two O atoms from the 2-hydroxyiminomethyl-6-methoxyphenolate ligands. Intramolecular O—H···O hydrogen bonds are formed and the complexes form stacks along the b axis, with an interplanar separation of 3.332 (1) Å between complexes. Pairs of C—H···O contacts are formed between complexes in neighbouring stacks.

Related literature

For recent related literature concerning Schiff-base compounds, see: Gupta & Sutar (2008); Sreenivasulu *et al.* (2005); Zhang *et al.* (2008); Raptopoulou *et al.* (2006); Milios *et al.* (2006); Yang *et al.* (2007).



Experimental

Crystal data

$[Co(C_8H_8NO_3)_2]$ M_r = 391.24
Monoclinic, $P2_1/n$
a = 8.4254 (19) Å
b = 4.9111 (11) Å
c = 18.951 (4) Å
β = 95.375 (3)°
V = 780.7 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.14 mm^{-1}
T = 293 (2) K
0.22 × 0.18 × 0.14 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: none
4577 measured reflections
1433 independent reflections
1216 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.065
S = 1.04
1433 reflections
117 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O1^{i}	0.82	1.91	2.5336 (19)	132
C7—H7···O2^{ii}	0.93	2.48	3.321 (2)	150

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

This work is financially supported by the Young Science Foundation of Guangxi Province of China (grant No. 0832085)

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BI2324).

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supporting information

Acta Cryst. (2008). E**64**, m1627 [doi:10.1107/S1600536808039512]

Bis(2-hydroxyiminomethyl-6-methoxyphenolato-κ^2O^1,N)cobalt(II)

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S1. Comment

Schiff-base complexes have been studied for many years (Gupta & Sutar, 2008; Sreenivasulu *et al.*, 2005; Zhang *et al.*, 2008) and have aroused increasing interest because of their antiviral, anticancer, catalytic and fluorescent properties. Most model studies of metal complexes of Schiff-base ligands containing salicylaldehyde derivatives and oxime have focused on the binding mode of the ligands (Raptopoulou *et al.*, 2006; Milios *et al.*, 2006; Yang *et al.*, 2007). The crystal structures of the complexes demonstrate that the Schiff-base ligands act in a bidentate, tridentate or mu^5^:eta^1^:etaî^:eta^3^ mode, coordinating through the phenolato O, imine N, or oxime O atoms. Our research group is interested in the Schiff-base derived from 2-hydroxy-3-methoxy-benzaldehyde and hydroxylammonium chloride.

S2. Experimental

A solution of (0.152 g, 1.0 mmol) 2-hydroxy-3-methoxy-benzaldehyde oxime and (0.056 g, 1 mmol) potassium hydroxide in 20 ml absolute methanol was added slowly to a solution of $CoNO_3.6H_2O$ (0.145 g, 0.5 mmol) in methanol. The mixture was stirred for 1 h at room temperature to give a red solution which was filtered and the filtrate was left to stand at room temperature. Red block crystals suitable for were obtained by slow evaporation Yield: 80.1 % (based on Co). Elemental analysis calculated: C 49.12, H 4.12, N 7.16 %; found: C 48.99, H 4.21, N 7.22 %.

S3. Refinement

H atoms were positioned geometrically and refined with a riding model, with distances 0.96 (CH_3) or 0.93 Å (aromatic ring), and with U_{iso}(H) = 1.2 U_{eq}(aromatic ring) or U_{iso}(H) = 1.5 U_{eq}(CH_3), and with O–H distance 0.82 Å and U_{iso}(H) = 1.5 U_{eq}(O).

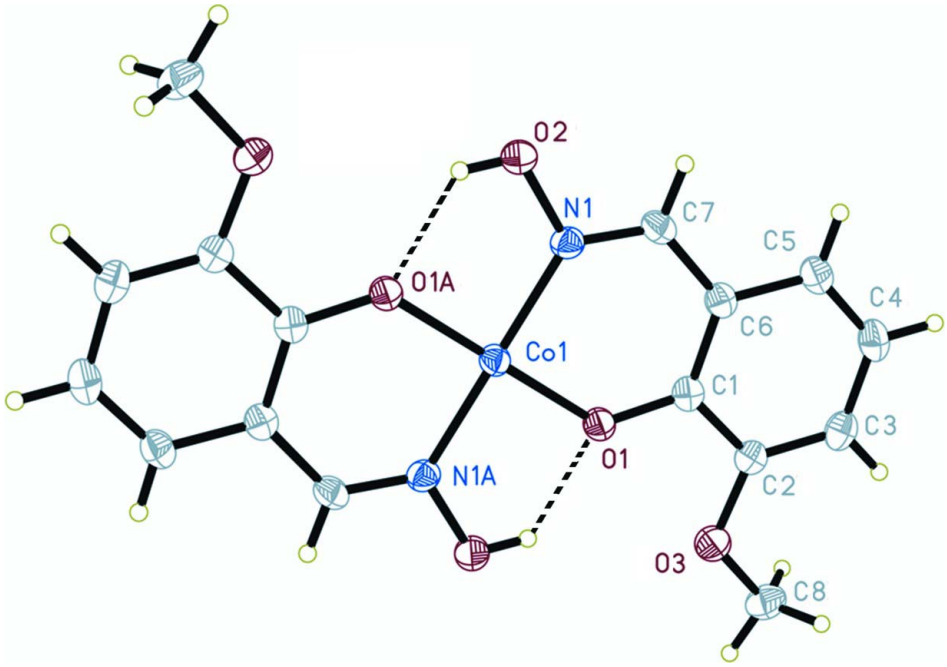

Figure 1

Molecular structure of the title compound, showing 30% probability displacement ellipsoids for non-H atoms. Dashed lines denote O—H···O hydrogen bonds. Symmetry code (A): -*x*, 1 - *y*, -*z*.

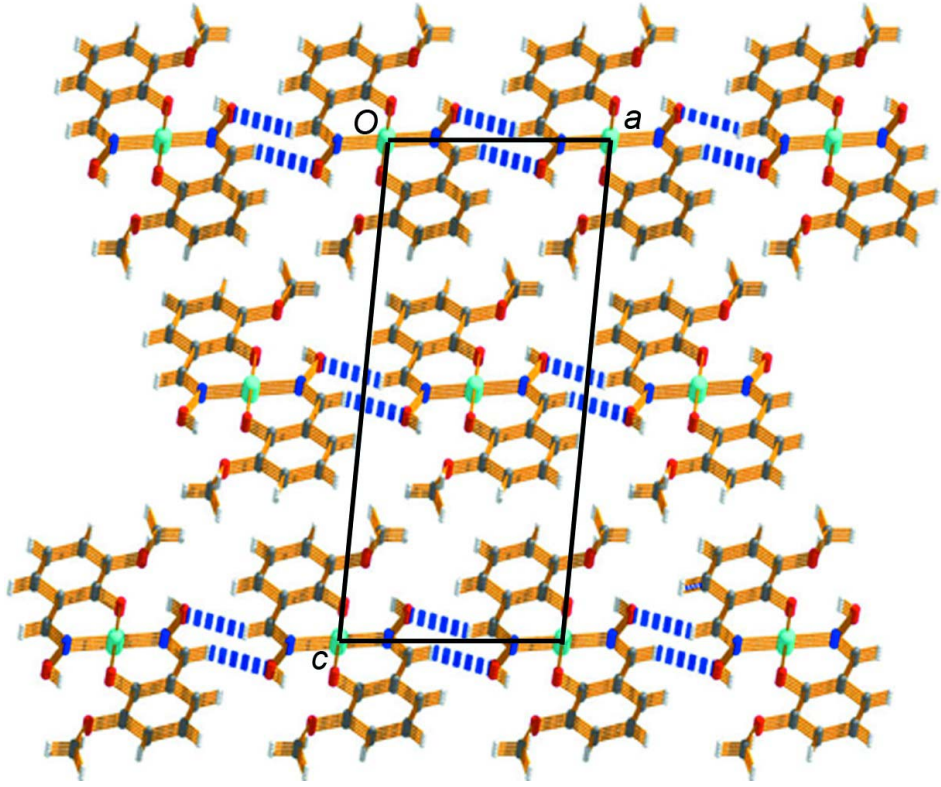

Figure 2

Packing diagram viewed down the *b* axis. Dasehd lines denote C—H···O contacts.

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Crystal data

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c = 18.951 (4) Å
β = 95.375 (3)°
V = 780.7 (3) Å^3
Z = 2
$F(000)$ = 402
D_x = 1.664 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4577 reflections
θ = 2.6–25.5°
μ = 1.14 mm^{-1}
T = 293 K
Block, red
0.22 × 0.18 × 0.14 mm

Data collection

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
4577 measured reflections
1433 independent reflections
1216 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
θ_{max} = 25.5°, θ_{min} = 2.6°
h = −10→10
k = −5→5
l = −22→22

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.065
S = 1.04
1433 reflections
117 parameters
0 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.0303P)^2 + 0.2885P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2$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	0.5000	0.0000	0.03262 (15)
C1	0.1093 (2)	0.0793 (4)	0.09770 (10)	0.0353 (4)

C2	0.0701 (2)	−0.1107 (4)	0.14960 (10)	0.0377 (5)
C3	0.1851 (3)	−0.2781 (4)	0.18262 (11)	0.0448 (5)
H3	0.1581	−0.4028	0.2164	0.054*
C4	0.3423 (3)	−0.2610 (4)	0.16538 (11)	0.0477 (6)
H4	0.4196	−0.3744	0.1880	0.057*
C5	0.3837 (3)	−0.0794 (4)	0.11564 (11)	0.0429 (5)
H5	0.4889	−0.0696	0.1048	0.052*
C6	0.2676 (2)	0.0939 (4)	0.08055 (10)	0.0361 (4)
C7	0.3153 (2)	0.2796 (4)	0.02809 (10)	0.0386 (5)
H7	0.4217	0.2799	0.0187	0.046*
C8	−0.1391 (3)	−0.3153 (5)	0.20761 (12)	0.0535 (6)
H8A	−0.1090	−0.4897	0.1902	0.080*
H8B	−0.2529	−0.3074	0.2077	0.080*
H8C	−0.0903	−0.2898	0.2550	0.080*
N1	0.21926 (19)	0.4465 (3)	−0.00691 (8)	0.0363 (4)
O1	−0.00708 (15)	0.2354 (3)	0.06754 (7)	0.0387 (3)
O2	0.29495 (16)	0.6086 (3)	−0.05443 (8)	0.0487 (4)
H2	0.2301	0.7143	−0.0744	0.073*
O3	−0.08737 (17)	−0.1063 (3)	0.16291 (8)	0.0494 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0291 (2)	0.0337 (2)	0.0348 (2)	−0.00160 (15)	0.00146 (15)	0.00203 (16)
C1	0.0385 (11)	0.0311 (10)	0.0354 (11)	0.0001 (8)	−0.0005 (9)	−0.0038 (8)
C2	0.0415 (11)	0.0352 (10)	0.0362 (11)	−0.0016 (9)	0.0025 (9)	−0.0015 (9)
C3	0.0566 (14)	0.0375 (11)	0.0392 (11)	−0.0009 (10)	−0.0007 (10)	0.0040 (9)
C4	0.0503 (13)	0.0425 (12)	0.0478 (13)	0.0103 (10)	−0.0080 (10)	−0.0001 (10)
C5	0.0384 (11)	0.0455 (12)	0.0436 (12)	0.0057 (9)	−0.0030 (9)	−0.0045 (10)
C6	0.0360 (10)	0.0350 (10)	0.0364 (11)	−0.0010 (8)	−0.0017 (8)	−0.0043 (8)
C7	0.0286 (10)	0.0438 (11)	0.0429 (11)	0.0001 (9)	0.0016 (8)	−0.0041 (9)
C8	0.0591 (14)	0.0510 (14)	0.0524 (13)	−0.0079 (11)	0.0160 (11)	0.0078 (11)
N1	0.0327 (9)	0.0410 (10)	0.0352 (9)	−0.0053 (7)	0.0040 (7)	0.0019 (7)
O1	0.0332 (7)	0.0397 (8)	0.0434 (8)	0.0005 (6)	0.0044 (6)	0.0083 (6)
O2	0.0346 (8)	0.0598 (10)	0.0523 (9)	−0.0032 (7)	0.0070 (7)	0.0185 (8)
O3	0.0452 (9)	0.0493 (8)	0.0547 (9)	−0.0010 (7)	0.0105 (7)	0.0153 (8)

Geometric parameters (Å, º)

Co1—O1	1.8290 (13)	C4—H4	0.930
Co1—O1^{i}	1.8290 (13)	C5—C6	1.414 (3)
Co1—N1	1.8826 (17)	C5—H5	0.930
Co1—N1^{i}	1.8826 (17)	C6—C7	1.434 (3)
C1—O1	1.331 (2)	C7—N1	1.290 (2)
C1—C6	1.404 (3)	C7—H7	0.930
C1—C2	1.417 (3)	C8—O3	1.425 (2)
C2—O3	1.374 (2)	C8—H8A	0.960
C2—C3	1.376 (3)	C8—H8B	0.960

C3—C4	1.396 (3)	C8—H8C	0.960
C3—H3	0.930	N1—O2	1.400 (2)
C4—C5	1.367 (3)	O2—H2	0.820
O1—Co1—O1^{i}	180.00 (8)	C6—C5—H5	119.8
O1—Co1—N1	92.64 (6)	C1—C6—C5	119.37 (19)
O1^{i}—Co1—N1	87.36 (6)	C1—C6—C7	121.78 (18)
O1—Co1—N1^{i}	87.36 (6)	C5—C6—C7	118.86 (18)
O1^{i}—Co1—N1^{i}	92.64 (6)	N1—C7—C6	123.89 (18)
N1—Co1—N1^{i}	180.00 (13)	N1—C7—H7	118.1
O1—C1—C6	123.29 (18)	C6—C7—H7	118.1
O1—C1—C2	117.87 (18)	O3—C8—H8A	109.5
C6—C1—C2	118.84 (17)	O3—C8—H8B	109.5
O3—C2—C3	125.24 (19)	H8A—C8—H8B	109.5
O3—C2—C1	114.13 (17)	O3—C8—H8C	109.5
C3—C2—C1	120.62 (19)	H8A—C8—H8C	109.5
C2—C3—C4	120.0 (2)	H8B—C8—H8C	109.5
C2—C3—H3	120.0	C7—N1—O2	112.97 (16)
C4—C3—H3	120.0	C7—N1—Co1	128.68 (14)
C5—C4—C3	120.65 (19)	O2—N1—Co1	118.33 (12)
C5—C4—H4	119.7	C1—O1—Co1	129.71 (13)
C3—C4—H4	119.7	N1—O2—H2	109.5
C4—C5—C6	120.5 (2)	C2—O3—C8	116.90 (17)
C4—C5—H5	119.8		

Symmetry code: (i) −*x*, −*y*+1, −*z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O1^{i}	0.82	1.91	2.5336 (19)	132
C7—H7···O2^{ii}	0.93	2.48	3.321 (2)	150

Symmetry codes: (i) −*x*, −*y*+1, −*z*; (ii) −*x*+1, −*y*+1, −*z*.