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trans-Bis{2-[1-(hydroxyimino)ethyl]phenolato}-cobalt(II)

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Key indicators

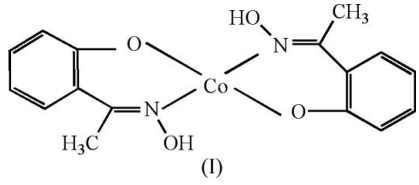
Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.005 Å
R factor = 0.042
wR factor = 0.130
Data-to-parameter ratio = 14.9

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

In the title compound, $[Co(C_8H_8NO_2)_2]$, the Co atom has a distorted square-planar coordination involving two N atoms and two O atoms from two ethanone 1-(2-hydroxyphenyl)oximato ligands. The molecular structure and packing are stabilized by intramolecular O—H···O hydrogen bonds and C—H···π intermolecular interaction.

Comment

Hydroxyoximates constitute a class of organonitrogen compounds with strong coordinating properties that are known to have significant and extensive use in solvent extraction systems, in hydrometallurgy and as analytical reagents (Keeney *et al.*, 1984). Several transition metal complexes with 2-hydroxyaryloximes have been reported previously (Kantouri & Hartophylles, 1992). We report here a new cobalt(II) complex with the ethanone 1-(2-hydroxyphenyl)oximato ligand.



(I)

In the title compound, which is isostructural with the corresponding nickel(II) (Hatzidimitriou *et al.*, 1997) and copper(II) (Zhou *et al.*, 1985) complexes, the geometry of the cobalt(II) ion is best described as distorted square-planar. The Co—N bond lengths of 1.889 (3) and 1.892 (3) Å are in agreement with the corresponding distances found in other four-coordinated Co complexes (Fachinetti *et al.*, 1979; Rudolf *et al.*, 1988). The Co—O bond lengths are slightly shorter than those found in other structures (Horrocks *et al.*, 1982; Larkworthy & Povey, 1983).

The crystal packing is stabilized by intramolecular O—H···O hydrogen bonds (Table 2) and intermolecular C—H···π interactions [C9···*Cg*1 = 3.624 (2) Å; H9*B*···*Cg*1 = 2.76 Å; C9—H9*B*···*Cg*1 = 150°; *Cg*1 is the centroid of the benzene ring C11^{i}—C16^{i}; symmetry code: (i) $1-x, 2-y, -z$].

Experimental

The title compound was prepared by the reaction of $CoCl_2$ (0.02 mol) with ethanone 1-(2-hydroxyphenyl)oxime (0.04 mol) in ethanol with a few drops of aqueous ammonia (6.0 *N*). The precipitate was filtered off and washed with ethanol and water (yield 68%). Single crystals suitable for X-ray measurements were obtained by slow evaporation of a tetrahydrofuran solution at room temperature.

Crystal data

$[Co(C_8H_8NO_2)_2]$
M_r = 359.24
Monoclinic, $P2_1/c$
a = 7.8420 (16) Å
b = 9.913 (2) Å
c = 19.344 (4) Å
β = 94.43 (3)°
V = 1499.3 (5) Å^3
Z = 4
D_x = 1.592 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 1.17 mm^{-1}
T = 295 (2) K
Block, blue
0.25 × 0.20 × 0.18 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω scans
Absorption correction: none
3496 measured reflections
3257 independent reflections
2614 reflections with $I > 2\sigma(I)$
R_{int} = 0.068
θ_{max} = 27.0°
3 standard reflections
every 100 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.130
S = 1.09
3257 reflections
219 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0702P)^2 + 1.1322P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.94 e Å^{-3}
$\Delta\rho_{min}$ = −0.79 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0049 (10)

Table 1
Selected geometric parameters (Å, °).

Co1—O3	1.819 (2)	Co1—N2	1.889 (3)
Co1—O1	1.821 (2)	Co1—N1	1.892 (3)
O3—Co1—O1	178.95 (12)	O3—Co1—N1	88.31 (11)
O3—Co1—N2	92.07 (11)	O1—Co1—N1	91.91 (11)
O1—Co1—N2	87.69 (11)	N2—Co1—N1	178.49 (11)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2A···O3	0.86 (4)	1.75 (3)	2.493 (3)	144 (4)
O4—H4A···O1	0.86 (4)	1.75 (4)	2.475 (4)	141 (6)

C-bound H atoms were positioned geometrically and refined as riding, with C—H = 0.93–0.96 Å, and with U_{iso}(H) = 1.2–1.5U_{eq}(C). The H atoms attached to O atoms were located in a difference Fourier map and freely refined.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *NRCVAX* (Gabe *et al.*, 1989); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 1990); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

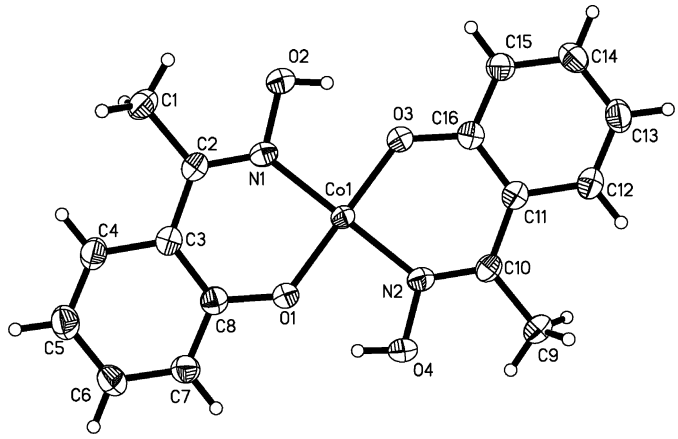


Figure 1
The structure of the title compound, showing 30% probability displacement ellipsoids and the atom-numbering scheme.

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