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{2,2′-[Ethane-1,2-diylbis(nitrilomethylidene)]-diphenolato}cobalt(II)

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Key indicators

Single-crystal X-ray study
T = 297 K
Mean σ(C–C) = 0.005 Å
R factor = 0.037
wR factor = 0.082
Data-to-parameter ratio = 13.1

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

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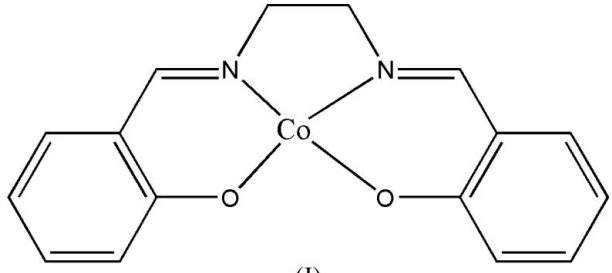
The Co^{II} atom in the title compound, $[Co(C_{16}H_{14}N_2O_2)]$, has a square-planar coordination.

Comment

Cobalt(II) Schiff base complexes have been extensively utilized as catalysts for the oxidation of organic molecules (Mukaiyama & Yamada, 1995; Fiammengo *et al.*, 2002). We have previously reported some lanthanide complexes with Schiff base ligands (Yuan *et al.*, 2004). The title mononuclear cobalt(II) complex, (I), is a further contribution in this area. The Co^{II} atom is four-coordinate, chelated by two O and two N atoms in a square-planar geometry (Fig. 1).



(I)

Experimental

Red crystals of (I) were obtained by slow evaporation of a solution in ethyl acetate–methanol (1:1 *v*/*v*) of a mixture (10 ml) of *N*,*N*′-bis(-salicylidene)-1,2-ethylenediamine (0.048 g, 0.2 mmol) and cobalt diacetate tetrahydrate (0.050 g, 0.2 mmol).

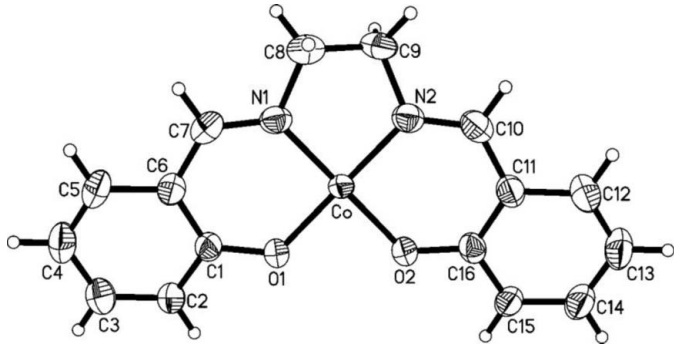


Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

Crystal data

$[Co(C_{16}H_{14}N_2O_2)]$	$Z = 8$
$M_r = 325.22$	$D_x = 1.605$ Mg m^{-3}
Orthorhombic, *Pbca*	Mo $K\alpha$ radiation
$a = 7.471$ (1) Å	$\mu = 1.28$ mm^{-1}
$b = 13.805$ (2) Å	$T = 297$ (2) K
$c = 26.096$ (5) Å	Prism, red
$V = 2691.5$ (7) Å^3	0.58 × 0.44 × 0.12 mm

Data collection

Siemens P4 diffractometer	1605 reflections with $I > 2\sigma(I)$
ω scans	$R_{int} = 0.013$
Absorption correction: ψ scan (North *et al.*, 1968)	$\theta_{max} = 25.5°$
$T_{min} = 0.514$, $T_{max} = 0.858$	3 standard reflections every 97 reflections
3059 measured reflections	intensity decay: 2.0%
2497 independent reflections	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.035P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.037$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.082$	$\Delta\rho_{max} = 0.31$ e Å^{-3}
$S = 0.97$	$\Delta\rho_{min} = -0.31$ e Å^{-3}
2497 reflections	Extinction correction: *SHELXL97*
191 parameters	Extinction coefficient: 0.0062 (3)
H-atom parameters constrained	

Table 1
Selected bond lengths (Å).

Co—N2	1.838 (3)	Co—O1	1.845 (2)
Co—N1	1.844 (3)	Co—O2	1.850 (2)

All H atoms were positioned geometrically and refined as riding, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *XSCANS* (Siemens, 1994); cell refinement: *XSCANS*; data reduction: *SHELXTL* (Sheldrick, 1997*b*); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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