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{6,6′-Dimethyl-2,2′-[propane-1,3-diylbis(nitrilomethylidyne)]diphenolato}cobalt(II)

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Key indicators

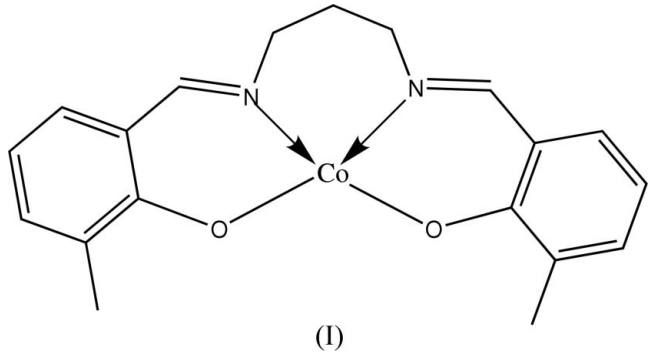
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
R factor = 0.034
wR factor = 0.083
Data-to-parameter ratio = 17.8

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

In the title mononuclear cobalt(II) compound, [Co($C_{19}H_{20}N_2O_2$)], the Co atom is coordinated by two N and two O atoms, giving a square-planar geometry.

Comment

Cobalt compounds have been of great interest in coordination chemistry (Billson *et al.*, 2000; Kotera *et al.*, 2003; Fritsky *et al.*, 2003). A new cobalt(II) compound, (I), derived from a tetradentate chelating Schiff base ligand, is described here.



(I)

In the crystal structure, (I) possesses mirror plane symmetry, as shown in Fig. 1. The coordination sites are occupied by the four donor atoms of the Schiff base ligand, giving a slightly distorted square-planar geometry. All the bond lengths (Table 1) around the metal centre are comparable with those in similar compounds (Cador *et al.*, 2003; Kennedy *et al.*, 1984). The crystal packing of (I) is shown in Fig. 2.

Experimental

All chemicals were of AR grade. 3-Methyl-2-hydroxybenzaldehyde (135.1 mg, 1.0 mmol), propane-1,3-diamine (36.9 mg, 0.5 mmol) and $Co(CH_3COO)_2{\cdot}4H_2O$ (125.1 mg, 0.5 mmol) were refluxed in methanol (50 ml) for 30 min. The mixture was cooled to room temperature and filtered. After keeping the filtrate in air for 5 d, brown block-shaped crystals suitable for X-ray analysis were obtained.

Crystal data

[Co($C_{19}H_{20}N_2O_2$)]
M_r = 367.30
Orthorhombic, $A2_1am$
a = 7.529 (1) Å
b = 10.398 (2) Å
c = 21.553 (3) Å
V = 1687.3 (4) Å^3
Z = 4
D_x = 1.446 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3132 reflections
θ = 2.7–24.5°
μ = 1.03 mm^{-1}
T = 298 (2) K
Block, brown
0.37 × 0.31 × 0.18 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.702, T_{max} = 0.836
9543 measured reflections
2014 independent reflections
1858 reflections with $I > 2\sigma(I)$
R_{int} = 0.036
θ_{max} = 28.3°
$h = -9 \rightarrow 9$
$k = -13 \rightarrow 13$
$l = -27 \rightarrow 27$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.083
S = 1.07
2014 reflections
113 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0344P)^2 + 0.5503P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}
Absolute structure: Flack (1983)
Flack parameter: 0.00 (2), with 859 Friedel pairs

Table 1
Selected geometric parameters (Å, °).

Co1—O1	1.846 (2)	Co1—N1	1.887 (2)
O1^{i}—Co1—O1	82.16 (12)	O1—Co1—N1	91.31 (9)
O1^{i}—Co1—N1	172.84 (10)	N1^{i}—Co1—N1	95.05 (15)

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

When using the $Cmc2_1$ space group, the structure is difficult to be sovled. However, it can be easily solved when using the unconventional space group $A2_1am$. H atoms were positioned geometrically and refined as riding atoms, with C—H distances of 0.93–0.97 Å and U_{iso}(H) = 1.2 or 1.5U_{eq}(C).

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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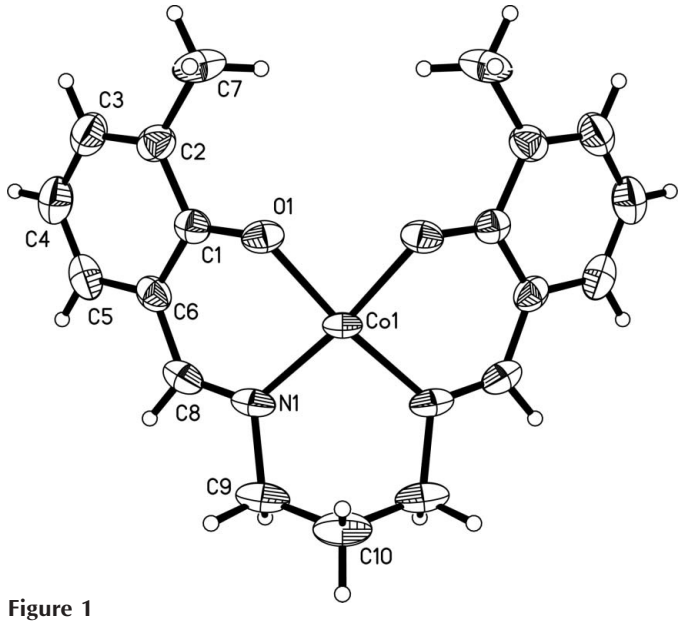

Figure 1
The molecular structure of (I), with anisotropic displacement ellipsoids drawn at the 30% probability level. Unlabelled atoms are related to labelled atoms by the symmetry operator $(x, y, 2-z)$.

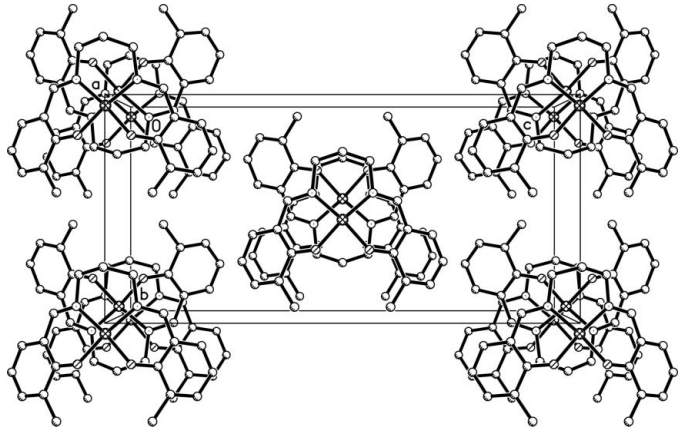

Figure 2
The molecular packing of (I). H atoms have been omitted.

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