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Bis(3-*tert*-butyl-*N*,5-dimethylsalicylaldiminato)-cobalt(II)

Xiaoyan Li,* Liye Huang, Shuli Dong, Mu Li and Hongjian Sun

School of Chemistry and Chemical Engineering, Shandong University, Shanda Nanlu 27, Jinan 250100, People's Republic of China

Correspondence e-mail: xli63@sdu.edu.cn

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Key indicators

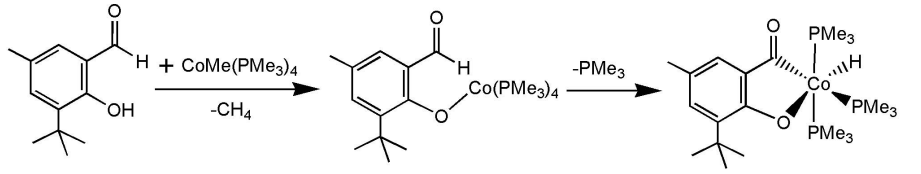
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.043
wR factor = 0.142
Data-to-parameter ratio = 15.9

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

The title compound, $[Co(C_{13}H_{18}NO)_2]$, was synthesized by the disproportionation of methyl–tetrakis(trimethylphosphine)-cobalt with 3-*tert*-butyl–N,5-dimethylsalicylaldimine in diethyl ether. The cobalt center in the structure is in a distorted tetrahedral geometry.

Comment

Reaction of 3-*tert*-butyl-5-methylsalicylaldehyde with $CoMe(PMe_3)_4$ was reported by Klein *et al.* (1998). In this reaction, the oxidative addition of the C—H bond of a formyl group at the cobalt centre, gives the stable octahedral hydridocobalt(III) complex. 3-*tert*-Butyl-*N*,5-dimethylsalicyl-aldimine is isoelectronic with 3-*tert*-butyl-5-methyl salicyl-aldehyde. However, the expected analogous reaction did not occur and the corresponding hydridocobalt(III) complex with an imine group could not be obtained. Instead, the reaction led to the formation of the title complex, (I), involving a disproportionation reaction (see scheme). Single crystals suitable for X-ray diffraction analysis were obtained. A view of the molecular structure is given in Fig. 1.



(I)

The cobalt centre is in a distorted tetrahedral geometry. Two equivalent ligands have Co—N and Co—O bond lengths Co1—O1 = 1.902 (2) Å, Co1—O2 = 1.898 (2) Å, Co1—N1 = 1.975 (3) Å and Co1—N2 = 1.967 (3) Å.

Experimental

Standard techniques were used in manipulations of volatile and air-sensitive material. Literature methods were applied in the preparation of methyltetrakis(trimethylphosphine)cobalt (Klein & Karsch, 1975), 3-*tert*-butyl-5-methylsalicylaldehyde (Hess, 1987) and 3-*tert*-butyl-*N*,5-dimethylsalicylaldimine (Law, 1912). Methyltetra(tri-

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methylphosphine)cobalt (870 mg, 2.3 mmol) was dissolved in pentane (50 ml), followed by the addition of 3-*tert*-butyl-*N*,5-dimethylsalicylaldimine (470 mg, 2.3 mmol). The resulting solution was stirred at ambient temperature for 18 h. During this period, the reaction solution turned orange. The mixture was then filtered. Crystallization at 269 K afforded red crystals of the title compound, which were suitable for X-ray diffraction analysis.

Crystal data

$[Co(C_{13}H_{18}NO)_2]$	D_x = 1.188 Mg m^{-3}
M_r = 467.50	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 3300 reflections
a = 13.122 (2) Å	θ = 2.3–24.2°
b = 12.943 (2) Å	μ = 0.68 mm^{-1}
c = 15.893 (3) Å	T = 293 (2) K
β = 104.517 (3)°	Block, red
V = 2613.1 (8) Å^3	0.28 × 0.18 × 0.10 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	4615 independent reflections
	3070 reflections with $I > 2\sigma(I)$
φ and ω scans	R_{int} = 0.044
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	θ_{max} = 25.0°
	$h = -15 \rightarrow 15$
T_{min} = 0.821, T_{max} = 0.934	$k = -12 \rightarrow 15$
13408 measured reflections	$l = -18 \rightarrow 14$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.043	$w = 1/[\sigma^2(F_o^2) + (0.0764P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.142	$(\Delta/\sigma)_{max}$ = 0.003
S = 1.06	$\Delta\rho_{max}$ = 0.35 e Å^{-3}
4615 reflections	$\Delta\rho_{min}$ = −0.40 e Å^{-3}
290 parameters	

H atoms were placed in idealized positions (C—H = 0.96 Å) and allowed to ride on their parent C atoms, with U_{iso}(H) = 1.2 or 1.5 times U_{eq}(C).

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2001); software used to prepare material for publication: *SHELXTL*.

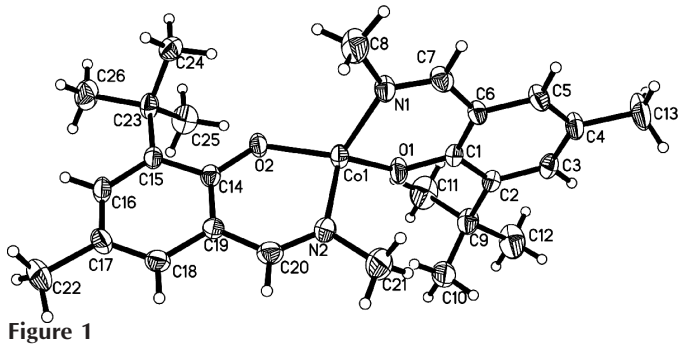

Figure 1
The molecular structure of the title complex. Displacement ellipsoids are drawn at the 50% probability level.

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