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Bis(*N*-*tert*-butylsalicylaldiminato)iron(II)

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Key indicators

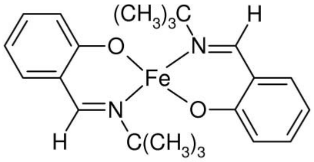
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.040
wR factor = 0.105
Data-to-parameter ratio = 17.0

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

The title compound {systematic name: bis[2-(*tert*-butyliminomethyl)phenolato-κ^2N,O]iron(II)}, [$Fe(C_{11}H_{14}NO)_2$], was synthesized by the reaction of tetrakis(trimethylphosphine)iron(0) and *N*-*tert*-butylsalicylaldimine in pentane. The Fe^{II} atom exhibits a distorted tetrahedral coordination geometry.

Comment

Reaction of 3-*tert*-butyl-*N*,5-dimethylsalicylaldimine with $CoMe(PMe_3)_4$ has been reported previously to lead to the formation of bis(3-*tert*-butyl-*N*,5-dimethylsalicylaldiminato)cobalt(II) *via* a disproportionation reaction (Li *et al.*, 2005). The ligand *N*-*tert*-butylsalicylaldimine is isoelectronic with 3-*tert*-butyl-*N*,5-dimethylsalicylaldimine, and reaction with $Fe(PMe_3)_4$ gave the expected title compound, (I), *via* an analogous reaction. In (I), the Fe^{II} centre exhibits a distorted tetrahedral coordination geometry (Fig. 1 and Table 1).



(I)

Experimental

Standard techniques were used for the manipulation of volatile and air-sensitive materials. Literature methods were applied for the preparation of tetrakis(trimethylphosphine)iron(0) (Klein & Karsch, 1975). $Fe(PMe_3)_4$ (0.82 g, 2.28 mmol) was then dissolved in pentane (80 ml), followed by the addition of *N*-*tert*-butylsalicylaldimine (0.31 g, 2.30 mmol). The resulting solution was stirred at ambient temperature for 12 h. During this period, the reaction solution turned dark red. The mixture was then filtered. Crystallization at 277 K afforded red crystals of the title compound.

Crystal data

[$Fe(C_{11}H_{14}NO)_2$]
M_r = 408.31
Orthorhombic, $P2_12_12_1$
a = 10.080 (2) Å
b = 10.219 (2) Å
c = 20.699 (4) Å
V = 2132.2 (7) Å^3
Z = 4
D_x = 1.272 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.73 mm^{-1}
T = 293 (2) K
Block, red
0.35 × 0.24 × 0.10 mm

Data collection

Bruker SMART CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.785, T_{max} = 0.931
9491 measured reflections
4238 independent reflections
3815 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
θ_{max} = 27.1°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.105$
$S = 1.10$
4238 reflections
250 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0634P)^2 + 0.2356P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.38$ e Å^{-3}
$\Delta\rho_{min} = -0.47$ e Å^{-3}
Absolute structure: Flack (1983), 1676 Friedel pairs
Flack parameter: −0.001 (18)

Table 1
Selected geometric parameters (Å, °).

Fe1—O2	1.914 (2)	Fe1—N1	2.062 (2)
Fe1—O1	1.920 (2)	Fe1—N2	2.064 (2)
O2—Fe1—O1	117.70 (10)	C1—O1—Fe1	130.12 (17)
O2—Fe1—N1	119.24 (9)	C18—O2—Fe1	129.2 (2)
O1—Fe1—N1	92.67 (8)	C7—N1—Fe1	121.49 (18)
O2—Fe1—N2	93.01 (9)	C8—N1—Fe1	120.63 (17)
O1—Fe1—N2	114.31 (9)	C12—N2—Fe1	121.3 (2)
N1—Fe1—N2	122.07 (10)	C19—N2—Fe1	119.48 (19)

H atoms were placed in idealized positions (C—H = 0.93 Å for aromatic or 0.96 Å for methyl H atoms) and allowed to ride on their parent C atoms, with $U_{iso}(H) = 1.2\,U_{eq}$(aromatic C) or $1.5\,U_{eq}$(methyl C). The methyl groups were allowed to rotate about their local threefold axes.

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*.

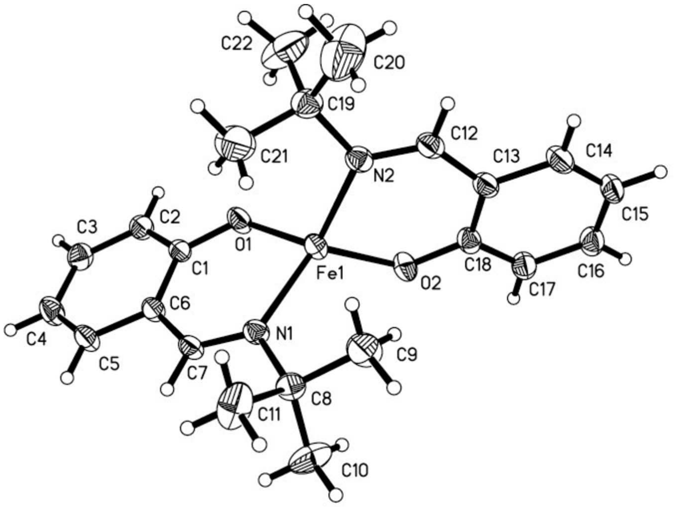


Figure 1
The molecular structure of (I) showing displacement ellipsoids drawn at the 50% probability level for non-H atoms.

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