Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

The galla[1]ferrocenophane {[dimethyl(2-pyridyl)silyl]bis(trimethylsilyl)methyl-κ^2C,N}(ferrocene-1,1′-diyl)gallium(III)

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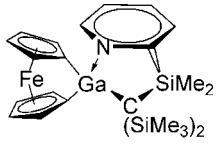
Received 20 February 2008; accepted 26 February 2008

Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.005 Å; R factor = 0.044; wR factor = 0.088; data-to-parameter ratio = 18.6.

The title compound, $[GaFe(C_5H_4)_2(C_{14}H_{28}NSi_3)]$ or $[\{(2\text{-}H_4C_5N)Me_2Si\}(Me_3Si)_2C]Ga(C_5H_4)_2Fe$, a galla[1]ferrocenophane, crystallizes with two independent molecules in the asymmetric unit. In these strained sandwich compounds, the angles between the planes of the two π-ligands are 15.4 (2) and 16.4 (2)°, with gallium in a distorted tetrahedral coordination environment.

Related literature

The synthesis of the title compound was described by Schachner *et al.* (2005*b*). A related galla[1]ferrocenophane was published by Lund *et al.* (2006). For related literature, see: Bellas & Rehahn (2007); Foucher *et al.* (1992); Herbert *et al.* (2007); Lund *et al.* (2007); Osborne & Whiteley (1975); Schachner *et al.* (2005*a*, 2007).



Experimental

Crystal data

$[GaFe(C_5H_4)_2(C_{14}H_{28}NSi_3)]$
M_r = 548.38
Monoclinic, $P2_1/c$
a = 9.64630 (10) Å
b = 35.2258 (4) Å
c = 15.4862 (2) Å
β = 92.5212 (7)°
V = 5257.10 (11) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.73 mm^{-1}
T = 173 (2) K
0.20 × 0.12 × 0.12 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: ψ scan (*SHELXTL*; Sheldrick, 2008)
T_{min} = 0.692, T_{max} = 0.811
58270 measured reflections
10370 independent reflections
7767 reflections with $I > 2\sigma(I)$
R_{int} = 0.079

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.088
S = 1.04
10370 reflections
557 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2003).

We thank the Natural Sciences and Engineering Research Council of Canada (NSERC Discovery Grant for JM), the Department of Chemistry and the University of Saskatchewan for their generous support. The authors also thank the Canadian Foundation for Innovation and the Government of Saskatchewan for funding of the X-ray and NMR facilities.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: OM2215).

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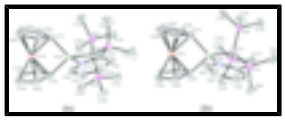

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