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Key indicators

Single-crystal X-ray study
 $T = 104$ K
 Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.037
 wR factor = 0.103
 Data-to-parameter ratio = 17.6

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

Bis(pentamethylcyclopentadienyl)[(trimethylsilyl)methyl]scandium(III)

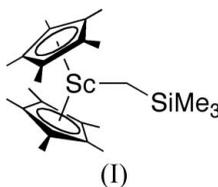
The geometric features of the title compound, $[\text{Sc}(\text{C}_5\text{Me}_5)_2(\text{C}_4\text{H}_{11}\text{Si})]$, are similar to those found in related monomeric organometallic scandium compounds. It is of interest with respect to related systems which have achieved catalytic metathesis of olefins with methane.

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Comment

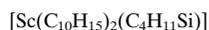
Selective functionalization of saturated hydrocarbons to more valuable products has attracted considerable attention in organometallic research. Alkyl-, aryl-, and hydridometallobenes of d^0 metals have shown potential utility in this regard, as their ability to activate aromatic and aliphatic C–H bonds has been demonstrated in several instances, with Thompson *et al.* (1987) the first to show that permethylscandocene alkyls are capable of σ -bond metathesis of hydrocarbon C–H bonds. Recently, Sadow & Tilley (2003) have achieved catalytic metathesis using the scandium neopentyl species $[\text{Cp}^*_2\text{ScCH}_2\text{C}(\text{CH}_3)_3]$ (Cp^* is pentamethylcyclopentadienyl), (II), for the hydromethylation of olefins with methane. The known title compound $[\text{Cp}^*_2\text{ScCH}_2\text{Si}(\text{CH}_3)_3]$, (I), has been synthesized by the method of Thompson *et al.* (1987) and has been used by Piers *et al.* (1993) for the insertion reaction of chalcogenides into Sc–C bonds. The single-crystal X-ray diffraction analysis of (I) shows geometric features comparable to those found in (II) (Sadow & Tilley, 2003), with the Sc1–C21–Si1 angle of $129.83(9)^\circ$ similar to the Sc1–C21–C22 angle of $128.3(3)^\circ$ in (II); while the Sc1–C21 bond lengths of 2.286(4) and 2.278(2) Å for (II) and (I), respectively, are essentially equivalent. The Cp^* rings of (I) are essentially planar, with the methyl groups bent slightly away $[0.7\text{--}11.7^\circ, \text{average } 6.2^\circ]$ from the metal center of the complex.



Experimental

A solution of (trimethylsilyl)methyl lithium (234 mg, 2.49 mmol) in toluene (7 ml) was added to a solution of bis(pentamethylcyclopentadienyl)scandium(III) chloride (1.00 g, 2.85 mmol) in toluene (12 ml). The resulting mixture was stirred at room temperature for 4 h. The solvent was removed *in vacuo*, the title compound was extracted with *n*-pentane (15 ml), and the solution filtered through Celite. Colorless crystals (489 mg, 49%) were grown from a saturated solution of *n*-pentane cooled to 238 K.

Crystal data



M_r = 402.62

Monoclinic, *P*2₁/*c*

a = 14.7186 (15) Å

b = 11.1667 (11) Å

c = 15.2229 (15) Å

β = 106.4930 (10)°

V = 2399.1 (4) Å³

Z = 4

D_x = 1.115 Mg m⁻³

Mo *K*α radiation

μ = 0.36 mm⁻¹

T = 104 (2) K

Block, colorless

0.33 × 0.19 × 0.18 mm

Data collection

Siemens SMART CCD

diffractometer

ω scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2005)

T_{min} = 0.92, *T_{max}* = 1.00

(expected range = 0.862–0.937)

10986 measured reflections

4353 independent reflections

3619 reflections with *I* > 2σ(*I*)

R_{int} = 0.018

θ_{max} = 25.4°

Refinement

Refinement on *F*²

R[*F*² > 2σ(*F*²)] = 0.037

wR(*F*²) = 0.103

S = 1.08

4353 reflections

248 parameters

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0597P)^2 + 0.888P]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

(Δ/*σ*)_{max} = 0.018

Δρ_{max} = 0.35 e Å⁻³

Δρ_{min} = -0.29 e Å⁻³

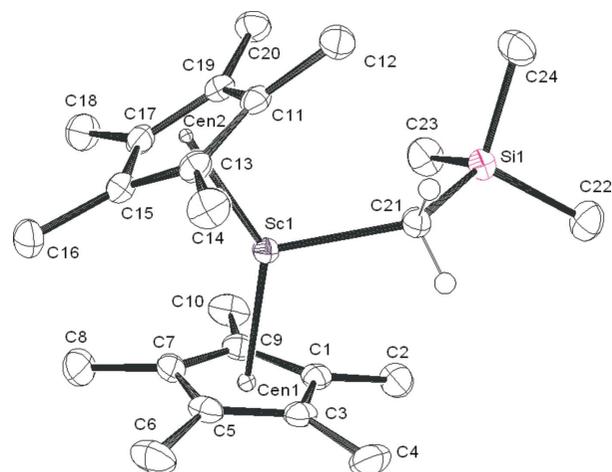


Figure 1

Displacement ellipsoid plot of (I) (50% probability level, methyl H atoms omitted for clarity) with the atom-numbering scheme.

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H atoms were positioned geometrically, with C–H = 0.97 Å for CH₂ groups or 0.96 Å for CH₃ groups, and constrained to ride on their parent atoms. *U*_{iso}(H) values were set at 1.2 times *U*_{eq}(C) for CH₂ groups and 1.5 times *U*_{eq}(C) for CH₃ groups.

Data collection: *SMART* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.