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

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Key indicators

Single-crystal X-ray study
T = 104 K
Mean σ(C–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.

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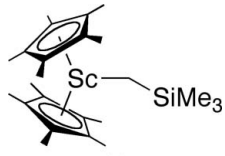
The geometric features of the title compound, $[Sc(C_5Me_5)_2(C_4H_{11}Si)]$, are similar to those found in related monomeric organometallic scandium compounds. It is of interest with respect to related systems which have achieved catalytic metathesis of olefins with methane.

Comment

Selective functionalization of saturated hydrocarbons to more valuable products has attracted considerable attention in organometallic research. Alkyl-, aryl-, and hydridometallocenes 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 $[Cp^*_2ScCH_2C(CH_3)_3]$ (Cp* is pentamethylcyclopentadienyl), (II), for the hydromethylation of olefins with methane. The known title compound $[Cp^*_2ScCH_2Si(CH_3)_3]$, (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)° similar to the Sc1—C21—C22 angle of 128.3 (3)° 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 [0.7–11.7°, average 6.2°) from the metal center of the complex.



(I)

Experimental

A solution of (trimethylsilyl)methyllithium (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

$[Sc(C_{10}H_{15})_2(C_4H_{11}Si)]$	$Z = 4$
$M_r = 402.62$	$D_x = 1.115$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 14.7186$ (15) Å	$\mu = 0.36$ mm^{-1}
$b = 11.1667$ (11) Å	$T = 104$ (2) K
$c = 15.2229$ (15) Å	Block, colorless
$\beta = 106.4930$ (10)°	0.33 × 0.19 × 0.18 mm
$V = 2399.1$ (4) Å^3	

Data collection

Siemens SMART CCD diffractometer	10986 measured reflections
	4353 independent reflections
ω scans	3619 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)	$R_{int} = 0.018$
	$\theta_{max} = 25.4°$
$T_{min} = 0.92$, $T_{max} = 1.00$ (expected range = 0.862–0.937)	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0597P)^2 + 0.888P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.037$	
$wR(F^2) = 0.103$	$(\Delta/\sigma)_{max} = 0.018$
$S = 1.08$	$\Delta\rho_{max} = 0.35$ e Å^{-3}
4353 reflections	$\Delta\rho_{min} = -0.29$ e Å^{-3}
248 parameters	
H-atom parameters constrained	

H atoms were positioned geometrically, with C–H = 0.97 Å for CH_2 groups or 0.96 Å for CH_3 groups, and constrained to ride on their parent atoms. U_{iso}(H) values were set at 1.2 times U_{eq}(C) for CH_2 groups and 1.5 times U_{eq}(C) for CH_3 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*.

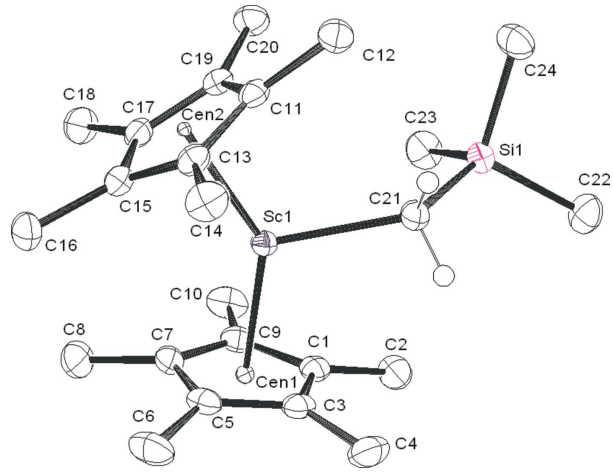


Figure 1
Displacement ellipsoid plot of (I) (50% probability level, methyl H atoms omitted for clarity) with the atom-numbering scheme.

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