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Key indicators

Single-crystal X-ray study
$T = 150$ K
Mean σ(C–C) = 0.007 Å
R factor = 0.039
wR factor = 0.098
Data-to-parameter ratio = 16.2

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.
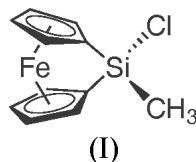
Methylchlorosila[1]ferrocenophane

In the title compound, [Fe(C$_{11}$H$_{11}$ClSi)], the cyclopentadienyl ligands are tilted towards the bridging Si atom, with a tilt angle of 19.4 (3)°.

Comment

The title compound, (I), is an important precursor to sila[1]-ferrocenophanes with unsymmetric substitution at the Si atom. The chlorine substituent in (I) can be replaced through reaction with a variety of lithium salts (Jäkle *et al.*, 2000; Berenbaum *et al.*, 2002). When lithium acetylides are used, the C≡C bond in the functionalized sila[1]ferrocenophanes can further react with dinuclear metal complexes to form highly metallized sila[1]ferrocenophanes with pendant metal clusters (Chan *et al.*, 2003).

In (I), the cyclopentadienyl (Cp) ligands are tilted towards the bridging Si atom. The angle between the least-squares planes formed by the Cp ligands bonded to Fe is 19.37 (32)°. The Fe—C distances range from 2.002 (5) to 2.078 (5) Å. The coordination geometry of the Si atom is approximately tetrahedral, with bond angles ranging from 98.0 (2) to 114.4 (2)°. The tilting of the Cp ligands leads to a compression of the C1—Si1—C6 angle [98.0 (2)°] compared to other bond angles around Si.

In the crystal structure, molecules of (I) related by *C*-centering are linked into *C*(6) chains (Bernstein *et al.*, 1995) by weak C—H···Cl interactions (see Table 2 and Fig. 2).

Experimental

Compound (I) was synthesized according to a published procedure (Zechel *et al.*, 1996). Crystals of (I) were obtained by slow evaporation of a solution in hexanes at 298 K under N$_2$.

Crystal data

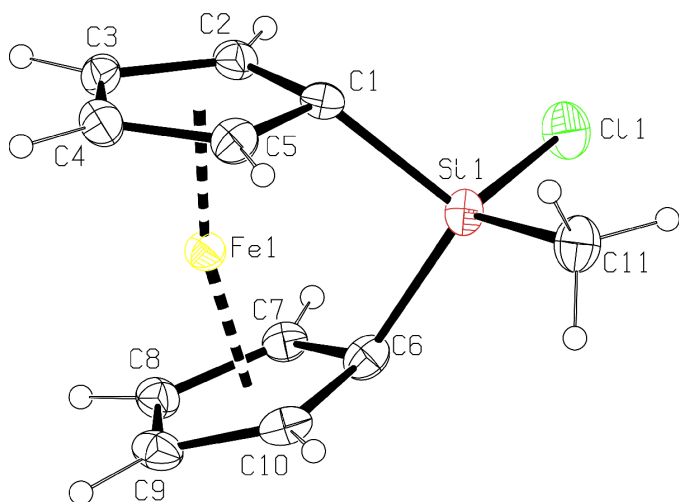|	
[Fe(C$_{11}$H$_{11}$ClSi)]	$D_x = 1.626$ Mg m^{-3}
$M_r = 262.59$	Mo $K\alpha$ radiation
Monoclinic, Cc	Cell parameters from 4024
$a = 13.4146$ (9) Å	reflections
$b = 10.2135$ (8) Å	$\theta = 2.6$–27.5°
$c = 7.8627$ (6) Å	$\mu = 1.72$ mm^{-1}
$\beta = 95.295$ (5)°	$T = 150$ (1) K
$V = 1072.67$ (14) Å^3	Block, orange
$Z = 4$	$0.20 \times 0.18 \times 0.14$ mm

Figure 1
View of (I), with displacement ellipsoids drawn at the 30% probability level (arbitrary spheres for the H atoms).

Data collection

Nonius KappaCCD diffractometer	1859 reflections with $I > 2\sigma(I)$
φ scans and ω scans with κ offsets	$R_{int} = 0.040$
Absorption correction: multi-scan	$\theta_{max} = 27.5°$
(*SORTAV*; Blessing, 1995)	$h = -17 \rightarrow 15$
$T_{min} = 0.585$, $T_{max} = 0.783$	$k = -12 \rightarrow 13$
4024 measured reflections	$l = -10 \rightarrow 10$
2078 independent reflections	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0418P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.039$	$+ 2.256P]$
$wR(F^2) = 0.098$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{max} < 0.001$
2078 reflections	$\Delta\rho_{max} = 0.48$ e Å^{-3}
128 parameters	$\Delta\rho_{min} = -0.50$ e Å^{-3}
H-atom parameters constrained	Absolute structure: Flack (1983),
	845 Friedel pairs
	Flack parameter = -0.02 (2)

Table 1
Selected geometric parameters (Å, °).

Cl1—Si1	2.0746 (18)	Si1—C1	1.871 (5)
Si1—C11	1.849 (5)	Si1—C6	1.872 (5)
C11—Si1—C1	114.4 (2)	C11—Si1—Cl1	110.5 (2)
C11—Si1—C6	116.0 (3)	C1—Si1—Cl1	107.90 (16)
C1—Si1—C6	98.0 (2)	C6—Si1—Cl1	109.18 (16)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C9—H9A···Cl1^i	1.00	2.81	3.641 (5)	141

Symmetry code: (i) $x - \frac{1}{2}, \frac{1}{2} + y, z$.

All H atoms were placed in calculated positions, with C—H distances of 0.95 (methyl) and 1.00 Å (Cp) and included in the refinement in the riding-model approximation, with U_{iso}(H) = $1.2U_{eq}$(Cp) or $1.5U_{eq}$(methyl).
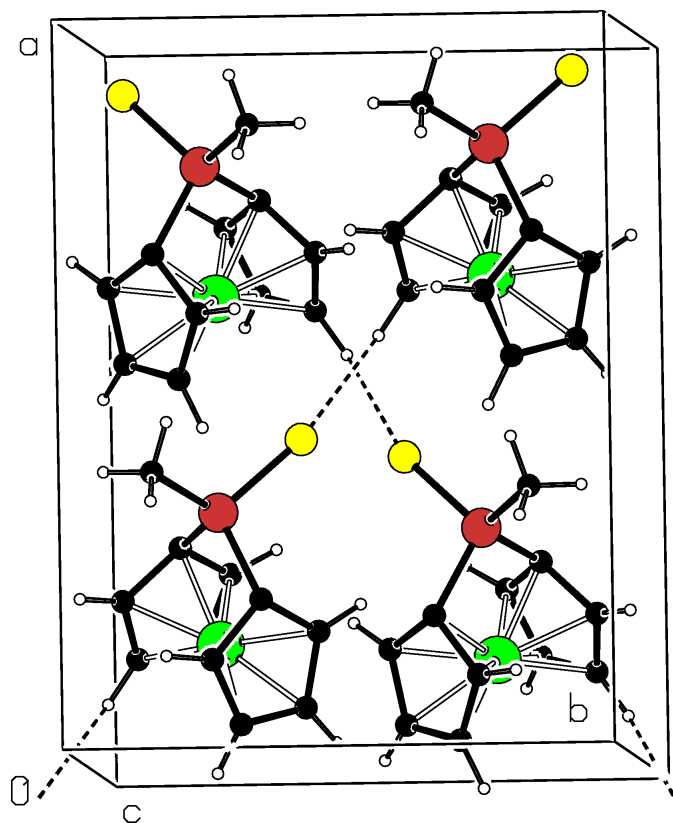

Figure 2
The unit cell contents in (I), viewed approximately along the *c* axis, showing weak C—H···Cl interactions as dashed lines. Colour codes: green Fe, red Si, yellow Cl and black C.

Data collection: *COLLECT* (Nonius, 2002); cell refinement: *DENZO-SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO-SMN*; program(s) used to solve structure: *SHELXTL/PC* (Sheldrick, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL/PC* and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL/PC*.

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