

Holger Braunschweig\* and  
Thomas KupferInstitut für Anorganische Chemie, Universität  
Würzburg, Am Hubland, 97074 Würzburg,  
GermanyCorrespondence e-mail:  
h.braunschweig@mail.uni-wuerzburg.de

## Key indicators

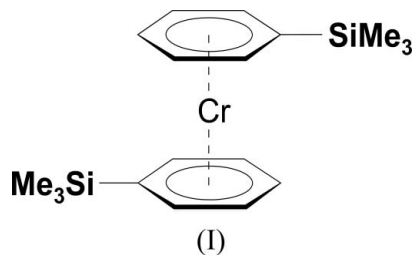
Single-crystal X-ray study  
 $T = 100$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å  
 $R$  factor = 0.024  
 $wR$  factor = 0.067  
Data-to-parameter ratio = 18.4For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.Bis( $\eta^6$ -trimethylsilylbenzene)chromium(0)

The molecule of the title compound,  $[\text{Cr}(\text{C}_6\text{H}_5\text{SiMe}_3)_2]$ , has approximate  $C_{2h}$  symmetry. The two aromatic ring systems are arranged almost ideally parallel to each other; the angle between the least-squares planes of the six-membered rings is  $0.75(12)^\circ$ . The two  $\text{Me}_3\text{Si}$  substituents exhibit an *anti* arrangement, with a pseudo-torsion angle of  $178.4(2)^\circ$ .

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## Comment

The title compound, (I), was originally prepared by Elschenbroich and co-workers in the 1970s by a salt elimination of dilithiated bis(benzene)chromium with  $\text{Me}_3\text{SiCl}$  (Elschenbroich *et al.*, 1970). In the course of our recent studies on substituted sandwich complexes (Braunschweig *et al.*, 2000, 2003, 2004, 2005, 2006), we became interested in (I) as a suitable precursor for the preparation of boron-containing metallocenes. For instance, related silyl-substituted benzene derivatives have been shown to react with bromoboranes with  $\text{Me}_3\text{SiBr}$  elimination to yield arylboranes (Haubold *et al.*, 1986; Kaufmann *et al.*, 1987).



The molecule of compound (I) has approximate  $C_{2h}$  symmetry. The  $\text{Cr}-\text{C}$  distances are comparable with those found in the unsubstituted bis(benzene)chromium (Keulen & Jellinek *et al.*, 1966). Both rings are planar and can be described as primarily  $\eta^6$ -coordinated. As expected, the two rings exhibit a parallel arrangement, with an angle of  $0.75(12)^\circ$  between the planes of the six-membered rings. In addition, the angle  $\delta$  ( $179.6^\circ$ ), defined by the ring centroids and the metal center, is essentially the same as in the parent compound. The geometry around the silyl groups and their expected *anti* arrangement [pseudo-torsion angle  $\text{Si}1-\text{C}11\cdots\text{C}21\cdots\text{Si}2 = 178.4(2)^\circ$ ] is in agreement with the analogous ferrocene derivative (Foucher *et al.*, 1995).

## Experimental

The title compound was prepared by a modified literature procedure (Elschenbroich *et al.*, 1970). A suspension of  $[\text{Cr}(\text{C}_6\text{H}_5\text{Li})_2]\cdot\text{tmeda}$  (0.51 g, 1.52 mmol; tmeda = *N,N,N',N'*-tetramethylethylenediamine) in hexanes (10 ml) was treated dropwise at 243 K with a solution of

Me<sub>3</sub>SiCl (0.41 g, 3.79 mmol) in hexanes (3 ml). The reaction was allowed to reach ambient temperature and was stirred for a further 48 h. All volatiles were removed under reduced pressure and the resulting solid was extracted with pentane (5 ml). Storage at 243 K yielded orange–brown crystals of (I) (0.38 g, 1.08 mmol, 71%).

#### Crystal data

[Cr(C<sub>9</sub>H<sub>14</sub>Si)<sub>2</sub>]

*M<sub>r</sub>* = 352.58

Orthorhombic, *P*2<sub>1</sub>2<sub>1</sub>2<sub>1</sub>

*a* = 6.4586 (2) Å

*b* = 16.7064 (6) Å

*c* = 17.0965 (6) Å

*V* = 1844.71 (11) Å<sup>3</sup>

*Z* = 4

*D<sub>x</sub>* = 1.270 Mg m<sup>-3</sup>

Mo *Kα* radiation

*μ* = 0.74 mm<sup>-1</sup>

*T* = 100 (2) K

Needle, orange

0.25 × 0.09 × 0.04 mm

#### Data collection

Bruker APEX2 area-detector

diffractometer

*φ* and *ω* scans

Absorption correction: multi-scan

(*SADABS*; Sheldrick, 1996)

*T<sub>min</sub>* = 0.836, *T<sub>max</sub>* = 0.975

8279 measured reflections

3490 independent reflections

3230 reflections with *I* > 2σ(*I*)

*R<sub>int</sub>* = 0.030

*θ<sub>max</sub>* = 26.0°

#### Refinement

Refinement on *F*<sup>2</sup>

*R* [*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.024

*wR* (*F*<sup>2</sup>) = 0.067

*S* = 1.08

3490 reflections

190 parameters

H-atom parameters constrained

*w* = 1/[σ<sup>2</sup>(*F<sub>o</sub>*<sup>2</sup>) + (0.0304*P*)<sup>2</sup> + 0.1864*P*]

where *P* = (*F<sub>o</sub>*<sup>2</sup> + 2*F<sub>c</sub>*<sup>2</sup>)/3

(Δ/σ)<sub>max</sub> = 0.002

Δρ<sub>max</sub> = 0.37 e Å<sup>-3</sup>

Δρ<sub>min</sub> = -0.22 e Å<sup>-3</sup>

Absolute structure: Flack (1983),

1446 Friedel pairs

Flack parameter: 0.003 (17)

**Table 1**

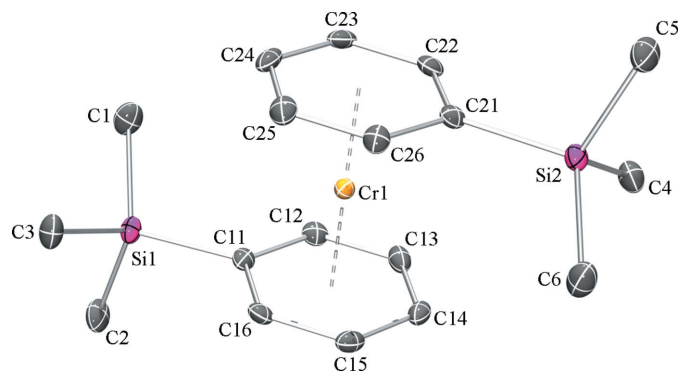
Selected bond lengths (Å).

Cr1—C11	2.1766 (19)	Cr1—C23	2.1441 (20)
Cr1—C12	2.1432 (20)	Cr1—C24	2.1484 (21)
Cr1—C13	2.1500 (22)	Cr1—C25	2.1400 (22)
Cr1—C14	2.1517 (21)	Cr1—C26	2.1405 (21)
Cr1—C15	2.1442 (22)	Cr1— <i>X</i> <sub>1</sub>	1.673
Cr1—C16	2.1449 (21)	Cr1— <i>X</i> <sub>2</sub>	1.664
Cr1—C21	2.1578 (19)	C11—Si1	1.8743 (20)
Cr1—C22	2.1378 (21)	C21—Si2	1.8728 (21)

Notes: (a) *X*<sub>1</sub> = centroid of the six-membered ring C11–C16; (b) *X*<sub>2</sub> = centroid of the six-membered ring C21–C26.

H atoms were placed at idealized positions and treated as riding atoms, with C–H = 0.98 (CH<sub>3</sub>) and 0.95 Å (aromatic CH), *U*<sub>iso</sub>(H) = 1.5*U*<sub>eq</sub>(primary C) or *U*<sub>iso</sub>(H) = 1.2*U*<sub>eq</sub>(aromatic C).

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT-Plus* (Bruker, 2004); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to



**Figure 1**

The molecular structure of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms have been omitted.

refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXL97*.

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