Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Methyltriphenylsilane

Theresa Kückmann, Hans-Wolfram Lerner and Michael Bolte*

Institut für Anorganische Chemie, J. W. Goethe-Universität Frankfurt, Marie-Curie-Strasse 11, 60439 Frankfurt/Main, Germany

Correspondence e-mail:
bolte@chemie.uni-frankfurt.de

Received 16 August 2005
Accepted 17 August 2005
Online 27 August 2005

Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.002 Å
R factor = 0.036
wR factor = 0.091
Data-to-parameter ratio = 15.5

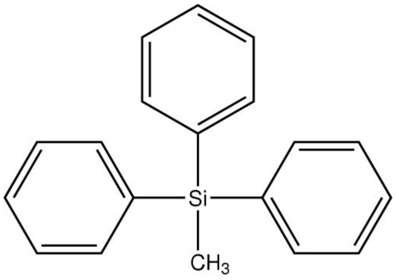
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, $C_{19}H_{18}Si$, crystallizes with two almost identical molecules in the asymmetric unit, which are related by a non-crystallographic translation. The phenyl rings show a propeller-like conformation, with significant deviation from C_3 symmetry.

Comment

Organosilicon compounds have found widespread use in chemistry. In this context, we are interested in the chemistry of silyl anions. A convenient method that gives alkali metal silanides in good yield is the cleavage of Si—C bonds by alkali metals (Lerner, 2005). Recently, we have shown that $(Me_3Si)_4C$ can be synthesized by the reaction of $(Me_3Si)_3CLi$ with Me_3SiCl (Lerner & Bolte, 2005). We report here the X-ray crystal structure analysis of Ph_3SiMe, (I). The synthesis of (I) was achieved by treatment of the silyl chloride Ph_3SiCl with MeLi, as indicated in the reaction scheme below.

$$(C_6H_5)_3SiCl + CH_3Li \xrightarrow{195\ K} (C_6H_5)_3SiCH_3 + LiCl$$



(I)

A perspective view of the two molecules of (I) is shown in Fig. 1. There are two almost identical molecules in the asymmetric unit. A least-squares fit of both is shown in Fig. 2. The two molecules adopt the same orientation in the crystal and they are related by a translation of x ~0.51, y ~0.27, z ~0.52, but no crystallographic symmetry element relating them can be detected. Bond lengths and angles can be regarded as normal (Cambridge Structural Database, Version 1.7 plus three updates; *MOGUL* Version 1.0; Allen, 2002). Two angles between the Si—CH_3 vector and the phenyl rings are almost equal [53.88 (7) and 50.46 (7)° for C11–C16 and C21–C26; 46.66 (7) and 51.00 (7)° for C11*A*–C16*A* and C21*A*–C26*A*], whereas the third one differs markedly [12.94 (8)° for C31–C36 and 15.19 (8)° for C31*A*–C36*A*]. As a result, no threefold rotation axis can be observed.

doi:10.1107/S1600536805026310

Experimental

To a stirred solution of Ph_3SiCl (32.7 mmol) in Et_2O (10 ml), MeLi (32 mmol) in Et_2O (20 ml) was added at 195 K. After stirring for 12 h at 195 K, the solution was treated with *t*BuOH. Filtration and concentration of the filtrate yielded crystals of Ph_3SiMe (yield: 7.34 g, 84%) suitable for X-ray structure analysis. ^{1}H NMR (C_6D_6, internal TMS): δ 0.73 (*s*, 3H, Me), 7.15 (*m*, 9H, Ph), 7.52 (*m*, 6H, Ph). ^{13}C{^{1}H} NMR (C_6D_6, internal TMS): δ 3.2 (Me), 128.2 (*m*-Ph), 129.6 (*p*-Ph), 135.7 (*o*-Ph), 136.5 (*i*-Ph).

Crystal data

$C_{19}H_{18}Si$
$M_r = 274.42$
Monoclinic, $P2_1/c$
$a = 18.5888$ (12) Å
$b = 9.5697$ (5) Å
$c = 18.3776$ (13) Å
$\beta = 107.883$ (5)°
$V = 3111.2$ (4) Å^3
$Z = 8$
$D_x = 1.172$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 31037 reflections
$\theta = 2.2$–25.1°
$\mu = 0.14$ mm^{-1}
$T = 173$ (2) K
Block, colourless
0.52 × 0.48 × 0.46 mm

Data collection

Stoe IPDS-II two-circle diffractometer
ω scans
Absorption correction: multi-scan (*MULABS*; Spek, 2003; Blessing, 1995)
$T_{\min} = 0.928$, $T_{\max} = 0.940$
37476 measured reflections
5587 independent reflections
4463 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.070$
$\theta_{\max} = 25.3°$
$h = -21 \rightarrow 22$
$k = -11 \rightarrow 11$
$l = -22 \rightarrow 22$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.091$
$S = 1.00$
5587 reflections
361 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0578P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.41$ e Å^{-3}
$\Delta\rho_{\min} = -0.24$ e Å^{-3}

All H atoms were located in a difference electron-density map and refined with fixed individual displacement parameters [$U_{\rm iso}(H) = 1.2U_{\rm eq}(C)$ or $1.5U_{\rm eq}(C_{\rm methyl})$], using a riding model, with C—H = 0.95 and 0.98 Å, for aromatic and methyl C atoms, respectively.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2003).

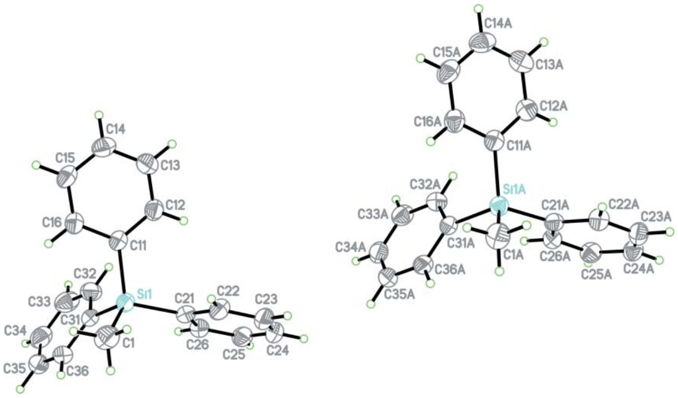


Figure 1
Perspective view of the two molecules in the asymmetric unit of the title compound with the atom numbering. Displacement ellipsoids are drawn at the 50% probability level.

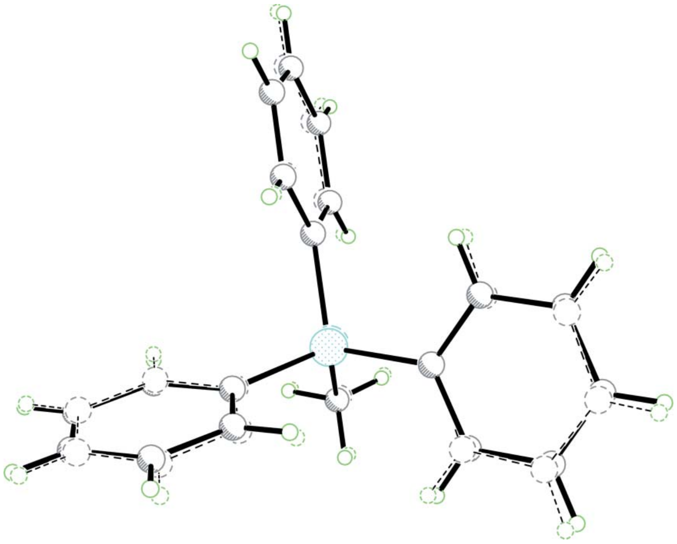


Figure 2
Least-squares fit of the two molecules in the asymmetric unit (r.m.s. deviation = 0.0913 Å). The molecule containing Si1*A* is drawn with full bonds, while that containing Si1 is drawn with dashed lines.

References

Allen, F. H. (2002). *Acta Cryst.* B**58**, 380–388.
Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–38.
Lerner, H.-W. (2005). *Coord. Chem. Rev.* **249**, 781–798.
Lerner, H.-W. & Bolte, M. (2005). *Acta Cryst.* E**61**, o2326–o2327.
Sheldrick, G. M. (1990). *Acta Cryst.* A**46**, 467–473.
Sheldrick, G. M. (1991). *SHELXTL-Plus*. Release 4.1. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Stoe & Cie (2001). *X-AREA*. Version 1.15. Stoe & Cie, Darmstadt, Germany.