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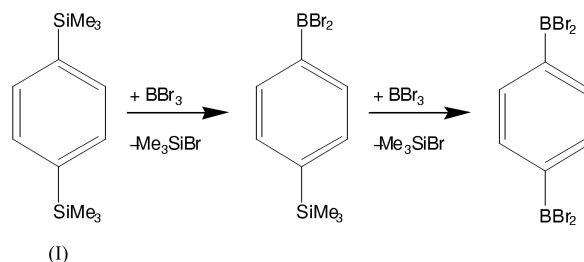
Key indicators

Single-crystal X-ray study
T = 173 K
Mean $\sigma(\text{C}-\text{C}) = 0.002 \text{ \AA}$
R factor = 0.038
wR factor = 0.092
Data-to-parameter ratio = 30.5For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.*p*-Bis(trimethylsilyl)benzene: rerefinement against new intensity data

The redetermination of the structure of the title compound, $\text{C}_{12}\text{H}_{22}\text{Si}_2$, agrees with the results previously reported by Menczel & Kiss [*Acta Cryst.* (1975). B31, 1787–1789], but with improved precision. The molecules are located on centres of inversion. As a result, there is just a half molecule in the asymmetric unit.

Comment

Dibromoboryl compounds with an aromatic ring system are conveniently accessible from trimethylsilylarenes and BBr_3 (see Scheme below) (Haberecht, 2002). π -Systems containing B atoms have attracted recent attention as a result of their potential applications. Therefore, we became interested in the reaction of bis(trimethylsilyl)benzene with BBr_3 . In this context, we recrystallized the title compound, (I), from hot toluene. The original synthesis and structure of (I) was reported by Menczel & Kiss (1975). The structure was determined using Weissenberg photographs and visual estimation of the intensities. In the present work, the structure was determined from data collected on a two-circle diffractometer equipped with an image-plate detector. Our results agree quite well with those of Menczel & Kiss; however, they are far more precise. The Si–CH₃ bonds are equal in length, applying the 3σ criterion, and the Si–C_{ar} bond is definitely longer. Furthermore, the aromatic C–C bonds are of the same length. These two results could not be deduced by Menczel & Kiss (1975).



Experimental

Colourless crystals of the title compound were obtained from a boiling solution of bis(trimethylsilyl)benzene in 10 ml toluene.

Crystal data

 $\text{C}_{12}\text{H}_{22}\text{Si}_2$
 $M_r = 222.48$
Monoclinic, $P2_1/n$
 $a = 6.5410 (7) \text{ \AA}$
 $b = 10.5452 (10) \text{ \AA}$
 $c = 10.3952 (12) \text{ \AA}$
 $\beta = 96.029 (9)^\circ$
 $V = 713.05 (13) \text{ \AA}^3$
 $Z = 2$ $D_x = 1.036 \text{ Mg m}^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 11837 reflections
 $\theta = 3.6\text{--}29.6^\circ$
 $\mu = 0.22 \text{ mm}^{-1}$
 $T = 173 (2) \text{ K}$
Block, colourless
 $0.39 \times 0.19 \times 0.17 \text{ mm}$

Data collection

Stoe IPDS II two-circle diffractometer

 ω scans

Absorption correction: multi-scan (MULABS; Spek, 1990; Blessing, 1995)

 $T_{\min} = 0.920$, $T_{\max} = 0.964$

9295 measured reflections

1955 independent reflections
1739 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.044$ $\theta_{\text{max}} = 29.4^\circ$ $h = -9 \rightarrow 8$ $k = -14 \rightarrow 14$ $l = -14 \rightarrow 14$ **Refinement**Refinement on F^2 $R[F^2 > 2\sigma(F^2)] = 0.038$ $wR(F^2) = 0.092$ $S = 1.08$

1955 reflections

64 parameters

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0421P)^2 + 0.2264P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\text{max}} < 0.001$ $\Delta\rho_{\text{max}} = 0.34 \text{ e } \text{\AA}^{-3}$ $\Delta\rho_{\text{min}} = -0.21 \text{ e } \text{\AA}^{-3}$ **Table 1**

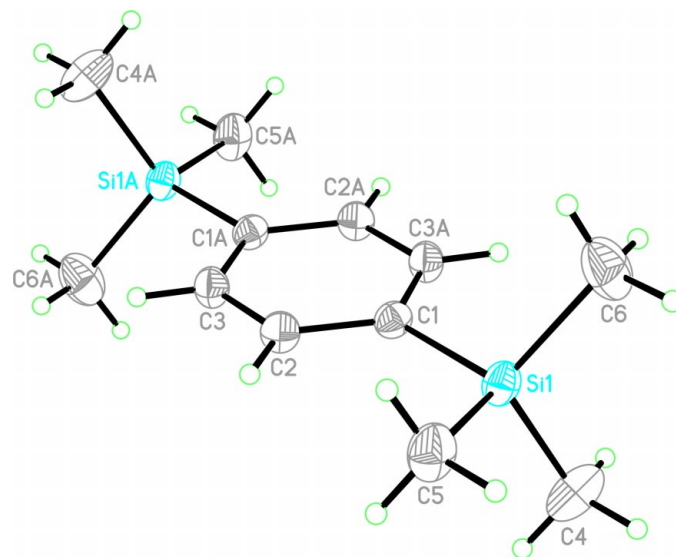
Selected geometric parameters (Å).

Si1–C6	1.8622 (17)	C1–C2	1.3994 (17)
Si1–C5	1.8633 (15)	C1–C3 ⁱ	1.4007 (17)
Si1–C4	1.8683 (17)	C2–C3	1.3946 (17)
Si1–C1	1.8817 (12)		

Symmetry code: (i) $1 - x, 1 - y, 1 - z$.

All H atoms could be located in a difference Fourier synthesis. They were refined with fixed individual displacement parameters [$U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$], using a riding model with C–H(aromatic) = 0.95 Å or C–H(methyl) = 0.98 Å.

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).

**Figure 1**

Perspective view of (I) with the atom numbering; displacement ellipsoids are drawn at the 50% probability level.

References

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