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Tetrakis(trimethylsilyl)methane

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(Si–C) = 0.011 Å
R factor = 0.094
wR factor = 0.237
Data-to-parameter ratio = 12.8

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

The crystal structure of the title compound, $C_{13}H_{36}Si_4$, originally determined by powder diffraction methods, has been redetermined using single-crystal data. The molecule is located on a threefold rotation axis with the methane C and one of the Si atoms located on this axis. All other atoms occupy general positions.

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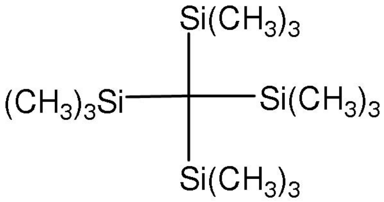
Comment

Molecules that feature symmetrical structures are always fascinating to chemists. Therefore, the molecular structure of $(Me_3Si)_4C$ is of particular interest to us. The reaction of lithium tris(trimethylsilyl)methanide $(Me_3Si)_3CLi$ and chlorotrimethylsilylsilane Me_3SiCl in diethyl ether gave tetrakis(trimethylsilyl)methane, $(Me_3Si)_4C$, (I), almost quantitatively. The crystal structure of the title compound, which undergoes a phase transition upon cooling, was originally determined by powder diffraction methods (Merker & Scott, 1964; Dinnebier *et al.*, 1999). We have redetermined the structure using single-crystal data. The molecule is located on a threefold rotation axis, with atoms C1 and Si1 located on this axis. All other atoms occupy general positions. The two structures agree quite well. The only notable difference is that the Si—Me distances are in a small range in the single crystal result [1.903 (11)–1.917 (10) Å], but vary significantly in the powder result (1.88–2.02 Å).



(I)

Experimental

Me_3SiCl (0.3 ml) was added to a solution of $(Me_3Si)_3CLi$ (0.5 mmol) in Et_2O at ambient temperature. After stirring for 3 h, all volatile compounds were removed *in vacuo* and the solid residue was extracted in benzene (10 ml). The NMR (^{1}H, ^{13}C, ^{29}Si) spectra showed only the signals of $(Me_3Si)_4C$ and thus indicated the formation of the title compound in quantitative yield. After filtration, X-ray quality crystals of $(Me_3Si)_4C$ were grown from a benzene solution at ambient temperature.

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Crystal data

$C_{13}H_{36}Si_4$
M_r = 304.78
Cubic, $P2_13$
a = 12.6529 (10) Å
V = 2025.7 (3) Å^3
Z = 4
D_x = 0.999 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 13605 reflections
θ = 2.7–25.1°
μ = 0.28 mm^{-1}
T = 173 (2) K
Block, colourless
0.43 × 0.34 × 0.24 mm

Data collection

Stoe IPDS-II two-circle diffractometer
ω scans
Absorption correction: multi-scan (*MULABS*; Spek, 2003; Blessing, 1995)
$T_{\min}$ = 0.890, $T_{\max}$ = 0.936
13605 measured reflections
679 independent reflections
670 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.073
$\theta_{\max}$ = 25.1°
$h = -14 \rightarrow 14$
$k = -14 \rightarrow 14$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.094
$wR(F^2)$ = 0.237
S = 1.18
679 reflections
53 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1815P)^2 + 1.6756P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max}$ = 1.17 e Å^{-3}
$\Delta\rho_{\min}$ = −0.50 e Å^{-3}

Table 1
Selected interatomic distances (Å).

C1—Si2	1.921 (5)	Si2—C21	1.903 (11)
C1—Si1	1.928 (14)	Si2—C23	1.906 (11)
Si1—C11	1.930 (12)	Si2—C22	1.917 (10)

All H atoms could be located by difference Fourier synthesis. They were refined with fixed individual displacement parameters [$U_{\rm iso}$(H) = 1.5$U_{\rm eq}$(C)] using a riding model with C—H = 0.98 Å. Since the absolute structure could not be determined reliably, Friedel pairs were merged. The structure is a racemic twin. The ratio of the two twin components refined to 0.489 (9)/0.511 (9). The highest peak in the final difference electron density map is located 1.78 Å from H22*A*. *PLATON* (Spek, 2003) suggests the space group $F\bar{4}3m$ for this structure, but it cannot be successfully refined in this space group.

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*.

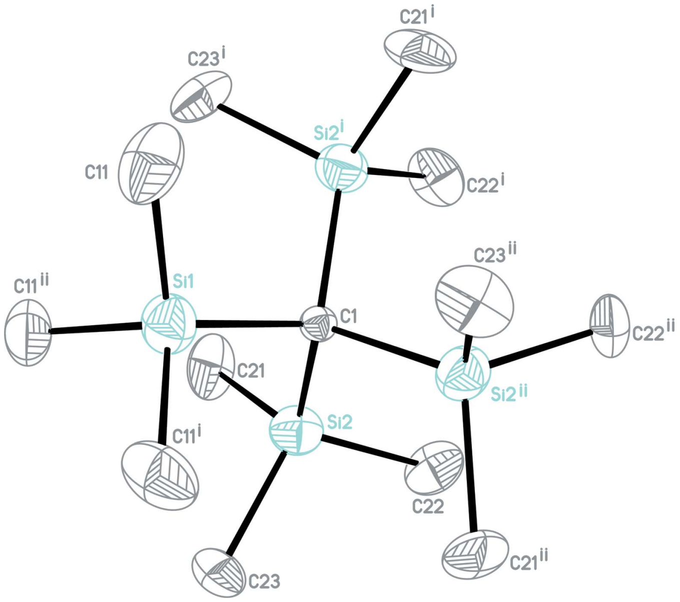

Figure 1
Perspective view of the title compound with the atom numbering; displacement ellipsoids are at the 50% probability level. H atoms have been omitted. [Symmetry codes: (i) $z - \frac{1}{2}, -x + \frac{1}{2}, -y + 1$; (ii) $-y + \frac{1}{2}, -z + 1, x + \frac{1}{2}$.]

References

Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–38.
Dinnebier, R. E., Dollase, W. A., Helluy, X., Kümmerlen, J., Sebald, A., Schmidt, M. U., Pagola, S., Stephens, P. W. & van Smaalen, S. (1999). *Acta Cryst.* B**55**, 1014–1029.
Merker, R. L. & Scott, M. J. (1964). *Acta Cryst.* **17**, 315.
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*. Stoe & Cie, Darmstadt, Germany.