Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(Trimethylsilyl)acetylene

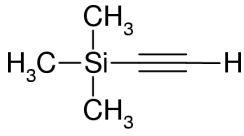
Andrew D. Bond* and John E. Davies

Department of Chemistry, University of Cambridge, Lensfield Road, Cambridge CB2 1EW, England

Correspondence e-mail: adb29@cam.ac.uk

Received 10 June 2002
Accepted 18 June 2002
Online 21 June 2002

The crystal structure of (trimethylsilyl)acetylene, $C_5H_{10}Si$, (I), has been determined at 150 K. In space group $P2_1$, there are three independent molecules in the asymmetric unit.



(I)

Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.009 Å
R factor = 0.096
wR factor = 0.273
Data-to-parameter ratio = 20.1

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

Experimental

The sample (98%) was obtained from the Aldrich Company and used without further purification. The crystal was grown in a 0.3 mm glass capillary tube at *ca* 265 K (a temperature only slightly less than the melting point of the solid in the capillary), using a technique described earlier (Davies & Bond, 2001). Once grown, the crystal was cooled to 150 (2) K for data collection. The length of the cylindrical crystal was not estimated, but it exceeded the diameter of the collimator (0.35 mm).

Crystal data

$C_5H_{10}Si$
M_r = 98.22
Monoclinic, $P2_1$
a = 10.868 (2) Å
b = 5.742 (1) Å
c = 17.190 (2) Å
β = 91.31 (1)°
V = 1072.4 (3) Å^3
Z = 6
D_x = 0.912 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 16948 reflections
θ = 1.0–27.5°
μ = 0.21 mm^{-1}
T = 150 (2) K
Cylinder, colourless
0.15 mm (radius)

Data collection

Nonius KappaCCD diffractometer
Thin-slice ω and φ scans
Absorption correction: none
5343 measured reflections
3566 independent reflections
2955 reflections with $I > 2\sigma(I)$
R_{int} = 0.069
θ_{max} = 27.5°
$h = -13 \rightarrow 9$
$k = -5 \rightarrow 7$
$l = -21 \rightarrow 22$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.096
$wR(F^2)$ = 0.273
S = 1.04
3566 reflections
177 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1617P)^2 + 1.4254P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.53 e Å^{-3}
$\Delta\rho_{min}$ = −0.52 e Å^{-3}
Absolute structure: Flack (1983), 860 Friedel pairs
Flack parameter = −0.1 (4)

The crystal used for data collection, although the best of several attempts, was of relatively poor quality, with a mosaic spread of *ca* 1.9°. This is reflected in the high values of R_{int} and the final R indices.

© 2002 International Union of Crystallography
Printed in Great Britain – all rights reserved

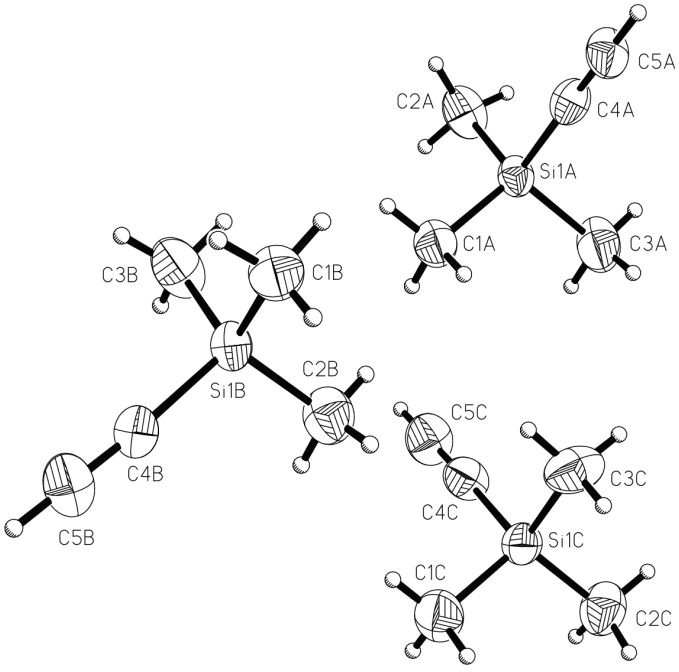


Figure 1
The asymmetric unit of (I) showing displacement ellipsoids at the 50% probability level.

H atoms were placed geometrically and refined with isotropic displacement parameters, with common parameters assigned to chemically equivalent H atoms (two parameters in total). The methyl groups were allowed to rotate about their local threefold axes. Chemically equivalent bonds in the three symmetry-independent molecules were restrained to be equal with standard uncertainties of 0.01 Å.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *HKL SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *HKL DENZO* and *SCALEPACK*; program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* (Sheldrick, 1993); software used to prepare material for publication: *SHELXL*97.

The authors thank the EPSRC for financial assistance towards the purchase of the diffractometer.

References

Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A., Burla, M. C., Polidori, G. & Camalli, M. (1994). *J. Appl. Cryst.* **27**, 435.
Davies, J. E. & Bond, A. D. (2001). *Acta Cryst.* E**57**, o947–o949.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Nonius (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.
Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr and R. M. Sweet, pp. 307–326. New York: Academic Press.
Sheldrick, G. M. (1993). *XP*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXL*97. University of Göttingen, Germany.