The *X*-Ray Crystal Structure of Tetramesityldisilene

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Tetramesityldisilene adopts a *trans*-bent geometry in the crystal, with an Si=Si bond length of 216.0 pm; two of the *cis* aromatic rings are only slightly twisted relative to the approximate plane of the two silicon and four neighbouring carbon atoms, while the other two rings are nearly perpendicular to this plane.

The synthesis of tetramesityldisilene (**1**) provided the first example of a molecule containing a silicon–silicon double bond.[1–3] This long-sought structural moiety is of obvious interest; a different synthesis of (**1**)[4] has been published and three additional disilenes are now known.[5,6] We report here the single crystal *X*-ray structure of (**1**).

Crystal data: crystals were grown by slowly cooling a saturated solution of (**1**) in toluene from room temperature to −20 °C. Crystals grown under these conditions incorporate one molecule of solvent per molecule of (**1**). $[C_{36}H_{44}Si_2 \cdot C_7H_8]$, $M = 629.1$, tetragonal, $a = 12.065(2)$, $b = 12.064(2)$, $c = 52.506(7)$ Å at 188 ± 5 K. $U = 7597$ Å^3, space group $I4_1/a$, $Z = 8$, $D_c = 1.10$, $\lambda(\text{Mo-}K_{\bar{\alpha}}) = 0.71073$ Å. The structure was solved by direct methods and refined by full-matrix least-squares refinement to a current $R_w = 0.077$, based on 2082 reflections with $F_o > 3\sigma(F_o)$.†

Figure 1 represents a molecule of (**1**), which contains a two-fold symmetry axis in the plane of the drawing passing through the centre of the Si–Si bond. The two silicon atoms and the four carbon atoms attached to them lie approximately in a plane. The two aromatic rings on one side of the Si=Si bond are almost orthogonal to this plane, whereas those on the other side are nearly parallel to the plane. The helical arrangement of the two latter groups and the Si=Si bond is reminiscent of the geometry of *cis*-stilbene. The deviations of the six central atoms from exact planarity can be described as resulting from moderate anti-pyramidalization at each silicon atom and a slight twist around the Si=Si bond. The angle between the

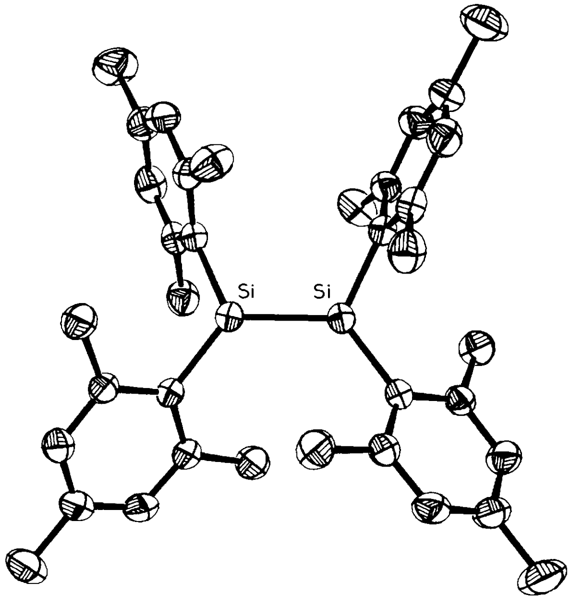

Figure 1. The structure of (**1**).

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† The atomic co-ordinates for this work are available on request from the Director of the Cambridge Crystallographic Data Centre, University Chemical Laboratory, Lensfield Road, Cambridge CB2 1EW. Any request should be accompanied by the full literature citation for this communication.

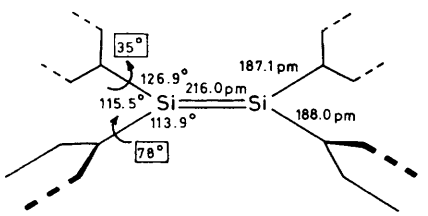

Figure 2. Bond lengths (right) and bond angles (left) in (**1**). Torsion angles between Si–Si–C planes and aromatic rings are shown in boxes.

C–Si–C plane and the line joining the two silicon atoms is 18° and the twist angle is 5°.

Interatomic distances and bond angles between heavy atoms are shown in Figure 2. The Si=Si bond length of 216.0 pm is about 18—20 pm shorter than the typical Si–Si single bond length [*e.g.*, the dihydro derivative (**2**) has two independent Si–Si distances of 235.0 and 236.2 pm[7]]. The decrease is greater than that going from a double to a single bond in carbon compounds; compare the central C–C distances of 135.5 pm for (**3**)[8] and 154 pm for (**4**),[9] respectively. On a percentage basis the bond shortening is 8—9% for silicon and 12% for carbon. These results indicate that there is a significant π-bonding component in the Si–Si double bond.[10] In contrast the strongly anti-pyramidalized tin compound (**5**) shows no shortening of the Sn–Sn bond relative to the normal single bond length.[11]

$(Me_3C_6H_2)_2Si{=}Si(C_6H_2Me_3)_2$ (**1**)

$(Me_3C_6H_2)_2HSi{-}SiH(C_6H_2Me_3)_2$ (**2**)

$Ph_2C{=}CPh_2$ (**3**)

$Ph_2CH{-}CHPh_2$ (**4**)

$\{[(Me_3Si)_2N]_2Sn\}_2$ (**5**)

The geometry of (**1**) is in accordance with quantum mechanical calculations[12–17] on the parent disilene, Si_2H_4, both with respect to the Si=Si distance and the slight anti-pyramidalization. However, the observed pyramidalization and torsion angle may be strongly affected by the crystal environment, especially since the calculations suggest that these types of deformations require very little energy. This is also suggested by the somewhat anisotropic thermal ellipsoids of the silicon atoms. In addition, the observed conformation of the aromatic rings in the crystal may well be only one of several present in solution.

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References

1 R. West, M. J. Fink, and J. Michl, 14th Organosilicon Symposium, Duke University, Durham, North Carolina, March, 1981.
2 A preliminary report of the *X*-ray structure of (**1**) was presented at the 6th International Symposium on Organosilicon Chemistry, Budapest, Hungary, August, 1981.
3 R. West, M. J. Fink, and J. Michl, *Science*, 1981, **214**, 1343.
4 H. Boudjouk, H. Byung-Hee, and K. R. Anderson, *J. Am. Chem. Soc.*, 1982, **104**, 4992.
5 S. Masamune, Y. Hanzawa, S. Murakami, T. Bally, and J. F. Blount, *J. Am. Chem. Soc.*, 1982, **104**, 1150.
6 M. J. Michalczyk, D. J. DeYoung, R. West, and J. Michl, Abstracts of Papers, 17th Organosilicon Symposium, Fargo, North Dakota, June 1983.
7 S. G. Baxter, K. Mislow, and J. F. Blount, *Tetrahedron*, 1980, **36**, 605.
8 A. Hoekstra and A. Vos, *Acta Crystallogr., Sect. B*, 1975, **31**, 1722.
9 D. A. Dougherty, K. Mislow, J. F. Blount, J. B. Wooten, and J. Jacobus, *J. Am. Chem. Soc.*, 1977, **99**, 6149.
10 K. W. Zilm, D. M. Grant, J. Michl, M. J. Fink, and R. West, *Organometallics*, 1983, **2**, 193.
11 P. J. Davidson, D. H. Harris, and M. F. Lappert, *J. Chem. Soc., Dalton Trans.*, 1976, 2268.
12 L. C. Snyder and Z. R. Wasserman, *J. Am. Chem. Soc.*, 1979, **101**, 5222.
13 R. Daudel, R. E. Kari, R. A. Poirier, J. D. Goddard, and I. G. Csizmadia, *J. Mol. Struct.*, 1978, **50**, 115.
14 R. A. Poirier and J. D. Goddard, *Chem. Phys. Lett.*, 1981, **80**, 37.
15 H. Lischka and H.-J. Kohler, *Chem. Phys. Lett.*, 1982, **85**, 467.
16 K. Krogh-Jespersen, *J. Phys. Chem.*, 1982, **86**, 1492.
17 T. Fjeldberg, A. Haaland, M. F. Lappert, B. E. R. Schilling, R. Seip, and A. J. Thorne, *J. Chem. Soc., Chem. Commun.*, 1982, 1408.