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(*E*)-1,2-Bis(diphenylmethylsilyl)ethene

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Key indicators

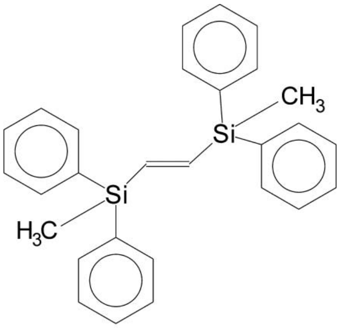
Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.007 Å
R factor = 0.055
wR factor = 0.192
Data-to-parameter ratio = 19.1

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

The molecule of the title compound, $C_{28}H_{28}Si_2$, occupies a special position on a centre of symmetry. It adopts an *E* configuration about the central C═C bond, with an Si—C═C—Si torsion angle of exactly 180°. Weak C—H$\cdots\pi$ hydrogen bonds and van der Waals interactions determine the crystal structure.

Comment

In the last two decades, we have developed silylative coupling reactions of vinylsilane derivatives in the presence of transition metal complexes (*e.g.* ruthenium, rhodium); in which the the *M*—H and *M*—Si bonds were either initially introduced or generated in the solution (Marciniec, 2005; Marciniec & Pietraszuk, 2003). Under optimal conditions (catalyst: $[RuCl_2(CO)_3]_2$ or $[RuHCl(CO)(PCy_3)_2]$), this process has become an excellent method for the selective synthesis of (*E*)-1,2-bis(silyl)ethenes (Majchrzak *et al.*, 2005; Marciniec & Lewandowski, 1997), and macromolecular organosilicon compounds containing (*E*)-1,2-bis(silyl) fragments (Marciniec & Małecka, 1999; Majchrzak *et al.*, 2000; Marciniec *et al.*, 2003). The number of reported structures of 1,2-unsubstituted and substituted bis(silyl)ethene is limited and most of them possess *trans* configurations.



(I)

In the Cambridge Structural Database (Allen, 2002), there are only six examples of 1,2-unsubstituted 1,2-bis(silyl)ethenes, of which three are metal complexes. All the uncomplexed molecules are in *trans* configurations; the change into a *cis* configuration might be realised by connecting the terminal silyl groups *via* a metallocene fragment (Finckh *et al.*, 1992; Majchrzak *et al.*, 2005). Therefore, the data for (I) might be of interest as reference data. The molecules of (I) occupy the special positions in the space group $P2_1/c$. The mid-point of the central C═C double bond lies at the center of symmetry, and the molecule has overall C_i symmetry (Fig. 1). This symmetry enforces the *E* configuration around the central bond and causes the Si—C—C—Si torsion angle to have a

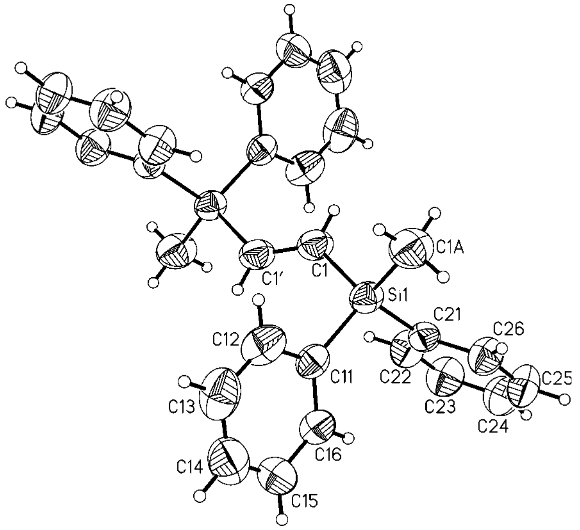


Figure 1
A view of (I), with displacement ellipsoids drawn at the 50% probability level. H atoms are drawn as spheres of arbitrary radii. [Symmetry code: (′) $1 - x, -y, -z$].

value of exactly 180°. A similar *E* disposition was observed, for example, in 1-diphenylsilyl-2-triphenylsilylethene (Lee *et al.*, 2001) and in 1,2-bis[di-*tert*-butyl(trimethylsilyl)silyl]ethene (Schmohl *et al.*, 2001). The phenyl rings are almost perpendicular one to another, the dihedral angle between their least-squares planes being 87.35 (14)°. The mean Si—C bond length is 1.867 (7) Å, and the disposition of the substituents around the Si atom is close to tetrahedral [the mean value of C—Si—C angles is 109.5 (10)°]. The *ipso* angles of both phenyl rings are significantly narrowed [116.3 (4) and 116.3 (3)°, respectively] as a result of the presence of silyl substituents. Crystal packing is determined mainly by van der Waals interactions.

Experimental

(*E*)-1,2-Bis(methyldiphenylsilyl)ethene has been synthesized *via* [RuHCl(CO)(PCy$_3$)$_2$]-catalysed selective silylative homo-coupling of methyldiphenylvinylsilane. Methyldiphenylvinylsilane (2.0 g, 8.9 mmol) was added to a solution of [RuHCl(CO)(PCy$_3$)$_2$] (128 mg, 0.18 mmol) in dry and deoxygenated toluene (10 ml) in a 50 ml two-necked flask equipped with a magnetic stirring bar, a reflux condenser and argon bubbling tube. The reaction mixture was heated under a flow of argon for 48 h at 393 K with stirring. The solvent was removed using a rotatory evaporator and the product was isolated by distillation under reduced pressure to give 3.37 g of (I) in 90% yield as white colourless crystals.

Crystal data

$C_{28}H_{28}Si_2$
$M_r = 420.68$
Monoclinic, $P2_1/c$
$a = 8.1929$ (16) Å
$b = 21.189$ (3) Å
$c = 7.192$ (2) Å
$\beta = 96.196$ (19)°
$V = 1241.2$ (5) Å^3
$Z = 2$
$D_x = 1.126$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.16$ mm^{-1}
$T = 295$ (1) K
Block, colourless
0.2 × 0.1 × 0.08 mm

Data collection

Kuma KM-4 diffractometer
ω–2θ scans
Absorption correction: none
2856 measured reflections
2619 independent reflections
1118 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.066$
$\theta_{\rm max} = 27.0°$
2 standard reflections
every 100 reflections
intensity decay: 1.5%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.055$
$wR(F^2) = 0.192$
$S = 0.99$
2619 reflections
137 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0974P)^2 + 0.0739P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.002$
$\Delta\rho_{\rm max} = 0.31$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.26$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Si1—C1	1.860 (4)	Si1—C11	1.875 (4)
Si1—C1*A*	1.866 (4)	C1—C1$^{\rm i}$	1.320 (8)
Si1—C21	1.870 (4)		
C1—Si1—C1*A*	110.5 (2)	C21—Si1—C11	109.33 (16)
C1—Si1—C21	108.66 (18)	C1$^{\rm i}$—C1—Si1	127.3 (4)
C1*A*—Si1—C21	110.7 (2)	C12—C11—C16	116.4 (4)
C1—Si1—C11	108.08 (18)	C22—C21—C26	116.3 (4)
C1*A*—Si1—C11	109.6 (2)		

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

All H atoms were located in a difference map, but they were repositioned geometrically, with C—H = 0.93–0.98 Å, and constrained to ride on their parent atoms, with $U_{\rm iso}$(H)= $1.2U_{\rm eq}$(C) for the phenyl and methylene groups and $1.5U_{\rm eq}$(C) for the methyl group.

Data collection: *KM-4 Software* (Kuma, 1991); cell refinement: *KM-4 Software*; data reduction: *KM-4 Software*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: Stereochemical Workstation Operation Manual (Siemens, 1989); software used to prepare material for publication: *SHELXL97*.

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