(*E*)-1,2-Bis{4-[dimethyl(vinyl)silyl]-phenyl}ethene

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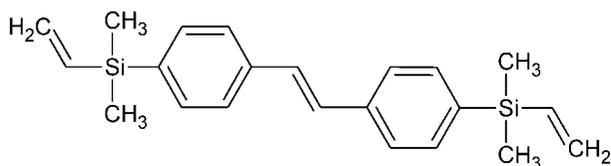Correspondence e-mail: mkubicki@amu.edu.pl

The molecule of the title compound, $C_{32}H_{34}Si_2$, is situated about a centre of symmetry. The whole diphenylethene fragment is planar and the C_{ar}—Si—C_3 group is rotated by *ca* 30° with respect to the plane of the benzene ring. The crystal structure is stabilized by some C—H···π contacts as well as van der Waals interactions.

Related literature

For related literature, see: JanBen & Krause (2005); Maciejewski *et al.* (2003); Majchrzak *et al.* (2005, 2007).

Experimental

Crystal data

$C_{22}H_{28}Si_2$	V = 2172.2 (7) Å³
M_r = 348.62	Z = 4
Monoclinic, $C2/c$	Mo $K\alpha$ radiation
a = 21.762 (2) Å	μ = 0.16 mm⁻¹
b = 6.2880 (9) Å	T = 295 (2) K
c = 19.159 (2) Å	0.3 × 0.2 × 0.15 mm
β = 124.05 (2)°	

Data collection

Kuma KM4CCD four-circle diffractometer	2116 independent reflections
Absorption correction: none	1441 reflections with $I > 2\sigma(I)$
5962 measured reflections	R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045	165 parameters
$wR(F^2)$ = 0.120	All H-atom parameters refined
S = 0.99	$\Delta\rho_{max}$ = 0.25 e Å⁻³
2116 reflections	$\Delta\rho_{min}$ = −0.22 e Å⁻³

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C12—H12A···$Cg1^i$	0.88 (3)	2.99 (3)	3.872 (3)	174 (2)
C13—H13C···$Cg1^{ii}$	0.97 (3)	3.03 (3)	3.912 (4)	152 (2)

Symmetry codes: (i) $-x + 1, y, -z + \frac{1}{2}$; (ii) $-x + 1, -y + 1, -z + 1$. $Cg1$ is the centroid of the C1–C6 ring.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* (Siemens, 1989); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2222).

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supporting information

(*E*)-1,2-Bis{4-[dimethyl(vinyl)silyl]phenyl}ethene

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S1. Comment

The synthesis of {(*E*)-1,2-bis(4-(dimethyl(vinyl)silyl)phenyl)}ethene, (I), consisted of two steps. During first step, the well know metathesis reaction of 4-bromostyrene was applied to obtain {(*E*)-1,2-bis(4-bromophenyl)}ethene which was used as a substrate for the second step, the typical reaction between an aryl-halide derivative of an olefin, a Grignard reagent generated *in situ* and vinylchlorosilane. This kind of vinylsilane-stilbene can be used as a very efficient monomer for the synthesis of arylene-silylene-vinylene polymers, polycarbosilanes or co-polymers with suitable aromatic olefin *via* silylative coupling polycondensation (SCP) or polyhydrosilylation reactions (Majchrzak *et al.*, 2005, 2007; Maciejewski *et al.*, 2003).

   The molecule of (I) is centrosymmetric with the mid-point of the central C41?C41A bond lying on a centre of symmetry (Fig. 1). The phenyl rings (planar within 0.0046 (14) Å) are, from symmetry, co-planar. As the C41 and Si1 atoms are almost co-planar with these rings (deviation from the least-squares plane = 0.009 (3)Å and 0.054 (3) Å, respectively), the whole diphenylethene fragment is planar. The C(ar)—Si—C$_3$ group is rotated by *ca* 30° with respect to to the plane of the phenyl ring, as can be seen from the values of C2—C1—Si—C(X) torsion angles: 28.5 (2)° for X = 13, -92.5 (2)° for X = 12, and 148.0 (2)° for X = 11. The crystal structure is stabilized by some relatively directional C—H···π contacts as well as van der Waals interactions.

S2. Experimental

First Step: A solution of 4-bromostyrene (6.095 g, 33.30 mmol) in THF (35 ml) was placed in a 50 ml glass two-neck mini reactor which was fitted with a condenser connected with an inert gas line. The Hoveyda–Grubbs catalyst 1st generation (10 mg, 0.017 mmol) was added and the reaction mixture was heated at 316–318 K and left for 5 h. The crude product was precipitated partially from solution. After the reaction was completed, the mixture was cooled to room temperature and the excess of organic solvent was evaporated under high vacuum. The mix of yellowish crystals was recovered by filtration and washed with cold hexane (3 *x* 10 ml). The residue was recrystallized from ethanol to provide 5.46 g (16.15 mmol, yield 97%) (*E*)-4,4′-dibromostilbene as a colorless solid. ^{1}H NMR (CDCl$_3$, δ (p.p.m.)): 7.06 (*s*, 2H, –C*H*=C*H*-), 7.42 (d, J$_{HH}$ = 8.80 Hz, 4H, *o*-C$_6$*H*$_4$-Br), 7.52 (d, J$_{HH}$ = 8.75 Hz, 4H, *m*-C$_6$*H*$_4$-Br). ^{13}C NMR (CDCl$_3$, δ (p.p.m.)): 122.6 (Br—C$_i$<), 127.3 (-CH=CH–), 129.8 (Br-*m*-C$_6$H$_4$–), 132.6 (Br-*o*-C$_6$H$_4$–), 137.1 (>C$_i$-CH=). MS—EI (*M/z* (%)) 338 (100) [*M*[+]], 258 (17), 178 (85), 152 (8), 89 (6). HRMS (*m/z*) calcd. for C$_{14}$H$_{10}$Br$_2$: 335.91493, found: 335.91374. m. p. 481–489 K, Lit. (JanBen & Krause, 2005): 483 K.

   Second Step: A solution of (*E*)-4,4′-dibromostilbene (3 g, 8.87 mmol) in THF (15 ml) was added dropwise to a suspension of Mg (0.518 g, 21.30 mmol, whose surface was activated by use of 1,2-dibromomethane (50 μL) and vinyldi-methylchlorosilane (2.35 g, 19.51 mmol) in slighly warm THF (15 ml). After the addition was completed, the reaction mixture was heated at 318 K for 4 h. The mixture was cooled to room temperature, water (2 ml) was added, and the whole was filtered. The organic phase was left overnight with magnesium sulfate. The solvent was then evaporated and

the residual solid was washed by cold hexane (2 x 15 ml). The isolated compound was recrystallized from ethanol to yield 2.1 g of (I) (6.02 mmol, yield 68%) as a colourless solid. ^{1}H NMR (CDCl$_3$, δ(p.p.m.)): 0.29 (s, 12H, –CH_3), 5.82 (dd, 2H, J$_{HH}$ = 3.8, 20.1 Hz, –CH=CH_2), 6.11 (dd, 2H, J$_{HH}$ = 3.8, 15.1 Hz, –CH=CH_2), 6.34 (dd, 2H, J$_{HH}$ = 14.6, 20.1 Hz, –CH=CH$_2$), 7.11 (s, 2H, –CH=CH-), 7.48 (d, 4H, o-C$_6$$H_4$-Si), 7.54 (d, 4H, m-C$_6$$H_4$-Si). ^{13}C NMR (CDCl$_3$, δ(p.p.m.)): -2.8, 127.3, 129.8, 135.9, 136.3, 137.8, 139.3, 140.1. ^{29}Si NMR (CDCl$_3$, δ(p.p.m.)): -10.60. HRMS (m/z) calcd. for C$_{22}$H$_{28}$Si$_2$: 348.17295, found 348.17284. Analysis: found C 75.72, H 8.09%. C$_{22}$H$_{28}$Si$_2$ requires: C 75.79, H 8.1%.

S3. Refinement

Hydrogen atoms were found in difference Fourier maps and freely refined so that the range of C= H = 0.88 (3) to 1.09 (4) Å.
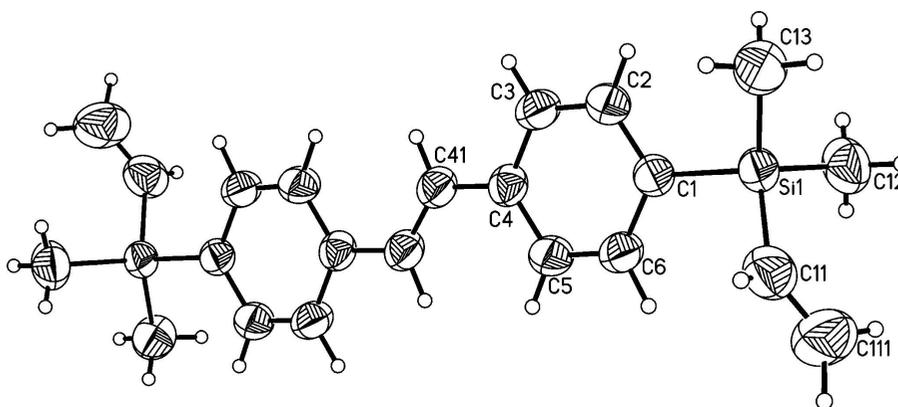

Figure 1

Molecular structure of (I) showing displacement ellipsoids at the 50% probability level and the atom numbering scheme. The hydrogen atoms are drawn as spheres with arbitrary radii. The unlabelled half of the molecule is related by the symmetry operation: 1/2 - x, 5/2 - y, -z.

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Crystal data

C$_{22}$H$_{28}$Si$_2$	$F(000) = 752$
$M_r = 348.62$	$D_x = 1.066$ Mg m^{-3}
Monoclinic, $C2/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -C 2yc	Cell parameters from 2322 reflections
$a = 21.762$ (2) Å	$\theta = 5$–22°
$b = 6.2880$ (9) Å	$\mu = 0.16$ mm^{-1}
$c = 19.159$ (2) Å	$T = 295$ K
$\beta = 124.05$ (2)°	Prism, colourless
$V = 2172.2$ (7) Å^3	0.3 × 0.2 × 0.15 mm
$Z = 4$	

Data collection

Kuma KM4CCD four-circle diffractometer	1441 reflections with $I > 2\sigma(I)$
	$R_{int} = 0.028$
Radiation source: fine-focus sealed tube	$\theta_{max} = 26.0°$, $\theta_{min} = 3.4°$
Graphite monochromator	$h = -26 \rightarrow 25$
ω scans	$k = -7 \rightarrow 5$
5962 measured reflections	$l = -19 \rightarrow 23$
2116 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.045$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.120$	
$S = 0.99$	All H-atom parameters refined
2116 reflections	$w = 1/[\sigma^2(F_o^2) + (0.07P)^2]$
165 parameters	where $P = (F_o^2 + 2F_c^2)/3$
0 restraints	$(\Delta/\sigma)_{max} = 0.011$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{max} = 0.25$ e Å^{-3}
	$\Delta\rho_{min} = -0.22$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.51385 (10)	0.4316 (3)	0.38537 (10)	0.0464 (4)
Si1	0.41638 (3)	0.33021 (8)	0.33072 (3)	0.0486 (2)
C11	0.35377 (13)	0.5625 (4)	0.30334 (19)	0.0733 (7)
H11	0.3499 (16)	0.626 (4)	0.3411 (18)	0.118 (12)*
C111	0.30599 (16)	0.6356 (5)	0.2302 (2)	0.1040 (10)
H11A	0.2932 (18)	0.546 (5)	0.175 (2)	0.163 (14)*
H11B	0.2738 (19)	0.779 (6)	0.221 (2)	0.161 (12)*
C12	0.3915 (2)	0.1875 (5)	0.23335 (17)	0.0760 (7)
H12A	0.3940 (15)	0.270 (4)	0.1977 (17)	0.108 (9)*
H12B	0.3425 (16)	0.138 (4)	0.2051 (17)	0.114 (10)*
H12C	0.4199 (16)	0.075 (4)	0.2443 (18)	0.123 (12)*
C13	0.41000 (17)	0.1498 (5)	0.40318 (18)	0.0709 (7)
H13A	0.4377 (16)	0.032 (5)	0.4133 (17)	0.118 (11)*
H13B	0.3635 (16)	0.098 (4)	0.3774 (16)	0.105 (9)*
H13C	0.4297 (14)	0.219 (4)	0.4570 (18)	0.110 (9)*
C2	0.57489 (11)	0.3167 (3)	0.44767 (13)	0.0557 (5)
H2	0.5684 (11)	0.186 (3)	0.4625 (13)	0.074 (6)*
C3	0.64669 (11)	0.3892 (3)	0.48563 (13)	0.0573 (5)
H3	0.6870 (11)	0.309 (3)	0.5288 (13)	0.070 (6)*
C4	0.66139 (9)	0.5860 (3)	0.46398 (10)	0.0479 (4)
C41	0.73897 (11)	0.6599 (3)	0.50658 (12)	0.0523 (5)
H41	0.7708 (11)	0.565 (3)	0.5483 (12)	0.070 (6)*
C5	0.60055 (11)	0.7024 (3)	0.40152 (12)	0.0561 (5)
H5	0.6066 (10)	0.837 (3)	0.3870 (11)	0.053 (5)*
C6	0.52923 (11)	0.6282 (3)	0.36415 (12)	0.0540 (5)

H6	0.4892 (11)	0.720 (3)	0.3224 (13)	0.068 (6)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0505 (10)	0.0467 (10)	0.0418 (9)	−0.0040 (8)	0.0258 (8)	0.0000 (8)
Si1	0.0483 (3)	0.0469 (3)	0.0455 (3)	−0.0072 (2)	0.0232 (3)	−0.0017 (2)
C11	0.0626 (14)	0.0618 (14)	0.0896 (18)	−0.0025 (11)	0.0389 (14)	0.0000 (13)
C111	0.0713 (18)	0.094 (2)	0.123 (3)	0.0154 (16)	0.0397 (19)	0.026 (2)
C12	0.093 (2)	0.0719 (17)	0.0589 (15)	−0.0191 (16)	0.0399 (15)	−0.0137 (13)
C13	0.0662 (16)	0.0803 (18)	0.0668 (16)	−0.0121 (14)	0.0376 (14)	0.0092 (14)
C2	0.0566 (12)	0.0506 (11)	0.0546 (12)	−0.0064 (9)	0.0279 (10)	0.0076 (9)
C3	0.0523 (12)	0.0584 (12)	0.0508 (11)	0.0010 (9)	0.0226 (10)	0.0137 (9)
C4	0.0479 (10)	0.0543 (10)	0.0404 (10)	−0.0045 (8)	0.0241 (8)	0.0013 (8)
C41	0.0504 (11)	0.0580 (12)	0.0427 (10)	−0.0026 (10)	0.0225 (9)	0.0048 (10)
C5	0.0565 (12)	0.0522 (12)	0.0550 (12)	−0.0068 (9)	0.0285 (10)	0.0119 (9)
C6	0.0490 (11)	0.0536 (11)	0.0508 (11)	0.0005 (9)	0.0227 (9)	0.0110 (9)

Geometric parameters (Å, º)

C1—C2	1.391 (3)	C13—H13B	0.90 (3)
C1—C6	1.399 (2)	C13—H13C	0.97 (3)
C1—Si1	1.8748 (18)	C2—C3	1.380 (3)
Si1—C12	1.857 (2)	C2—H2	0.91 (2)
Si1—C13	1.857 (2)	C3—C4	1.398 (2)
Si1—C11	1.862 (2)	C3—H3	0.95 (2)
C11—C111	1.275 (4)	C4—C5	1.395 (3)
C11—H11	0.87 (3)	C4—C41	1.480 (2)
C111—H11A	1.08 (3)	C41—C41ⁱ	1.309 (3)
C111—H11B	1.09 (4)	C41—H41	0.923 (19)
C12—H12A	0.88 (3)	C5—C6	1.377 (3)
C12—H12B	0.94 (3)	C5—H5	0.924 (17)
C12—H12C	0.88 (3)	C6—H6	0.97 (2)
C13—H13A	0.90 (3)		
C2—C1—C6	116.06 (17)	H13A—C13—H13B	103 (2)
C2—C1—Si1	122.72 (13)	Si1—C13—H13C	110.2 (16)
C6—C1—Si1	121.21 (14)	H13A—C13—H13C	107 (2)
C12—Si1—C13	110.72 (15)	H13B—C13—H13C	116 (2)
C12—Si1—C11	109.90 (15)	C3—C2—C1	122.40 (18)
C13—Si1—C11	109.92 (14)	C3—C2—H2	117.6 (14)
C12—Si1—C1	109.15 (12)	C1—C2—H2	120.0 (14)
C13—Si1—C1	108.97 (11)	C2—C3—C4	121.02 (19)
C11—Si1—C1	108.13 (9)	C2—C3—H3	120.5 (12)
C111—C11—Si1	127.6 (3)	C4—C3—H3	118.4 (12)
C111—C11—H11	110.4 (19)	C5—C4—C3	117.00 (17)
Si1—C11—H11	121.5 (19)	C5—C4—C41	123.39 (16)
C11—C111—H11A	119.2 (17)	C3—C4—C41	119.61 (17)

C11—C111—H11B	122.3 (17)	C41ⁱ—C41—C4	126.4 (2)
H11A—C111—H11B	118 (2)	C41ⁱ—C41—H41	123.1 (13)
Si1—C12—H12A	112.7 (18)	C4—C41—H41	110.3 (12)
Si1—C12—H12B	109.7 (17)	C6—C5—C4	121.37 (18)
H12A—C12—H12B	107 (2)	C6—C5—H5	117.6 (11)
Si1—C12—H12C	112.1 (19)	C4—C5—H5	120.9 (11)
H12A—C12—H12C	108 (3)	C5—C6—C1	122.13 (19)
H12B—C12—H12C	107 (2)	C5—C6—H6	117.1 (12)
Si1—C13—H13A	109.9 (18)	C1—C6—H6	120.8 (12)
Si1—C13—H13B	109.9 (16)		

Symmetry code: (i) −*x*+3/2, −*y*+3/2, −*z*+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C12—H12*A*···*Cg*1ⁱⁱ	0.88 (3)	2.99 (3)	3.872 (3)	174 (2)
C13—H13*C*···*Cg*1ⁱⁱⁱ	0.97 (3)	3.03 (3)	3.912 (4)	152 (2)

Symmetry codes: (ii) −*x*+1, *y*, −*z*+1/2; (iii) −*x*+1, −*y*+1, −*z*+1.