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(*E*)-1-Diphenylsilyl-2-triphenylsilylethene

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In the title compound, $C_{32}H_{28}Si_2$, the configuration at the C═C double bond is *E* [−179.1 (2)°], and two Si atoms in diphenylsilyl and triphenylsilyl groups bridged by the C═C double bond [1.292 (5) Å] retain the overall tetrahedral environment of the C and H atoms with an average Si—C bond length of 1.864 (1) Å and Si—H length of 1.35 (3) Å.

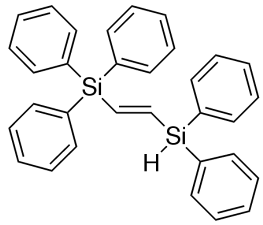
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.007 Å
R factor = 0.063
wR factor = 0.146
Data-to-parameter ratio = 14.8

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

Comment

Transition metal-catalyzed hydrosilylation of alkynes provides the most straightforward method for the preparation of vinylsilanes. In the course of our studies (Lee & Han, 1998; Lee *et al.*, 1996), we recently synthesized various (*E*)-vinylsilanes *via* stereoselective hydrosilylation using an Rh/CO catalytic system. These vinylsilanes have synthetic value because they are very versatile intermediates in organic synthesis, as well as in organosilicon chemistry. Particularly, the title (*E*)-vinylsilane, (I), containing an Si—H bond has the possibilities of further transformations. We present here the synthesis and the X-ray structure of (I).



(I)

Compound (I) consists of diphenylsilyl and triphenylsilyl groups connected by C═C double bond, as shown in Fig. 1.

The Si—C bond lengths range from 1.852 (4) to 1.875 (3) Å, with a mean value of 1.864 (1) Å and the C—Si—C angles range from 108.66 (16) to 111.20 (19)°, with a mean value of 109.75 (6)° (see Table 1). All these values are similar to those found in platinum-catalyzed hydrosilylation of alkynes (Lewis *et al.*, 1991). The geometries of the five phenyl rings are very similar to one another; the C—C bond lengths average to a value of 1.374 (1) Å and the rings are all planar with a maximum deviation of 0.012 (3) Å from the mean plane. The dihedral angles between neighbouring phenyl rings range from 72.91 (14) to 74.12 (11)°, with an average of 73.58 (6)°. The C19═C20 bond length [1.292 (5) Å] bridging the two silyl groups clearly displays double-bond character, and a similar bond length 1.294 (7) Å was found in platinum-catalyzed hydrosilylation products of alkynes (Lewis *et al.*, 1991). The four atoms Si1, C19, C20 and Si2, are coplanar within

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0.007 (2) Å, with a torsion angle Si1—C19—C20—Si2 of −179.1 (2)°.

The Si2—H length is 1.35 (3) Å which is somewhat shorter than the value of 1.42 (6) Å in tris[8-(dimethylamino)naphthyl]silane (Breliere *et al.*, 1994), but only 1σ different from it.

The closest intermolecular distance H24···H30($-1 + x$, $1 + y$, z) of 2.52 Å suggests that the molecular packing is governed only by van der Waals forces.

Experimental

The title compound, (I), was prepared using the stereoselective hydrosilylation of triphenylsilylacetylene with diphenylsilane catalyzed by rhodium metal in the presence of carbon monoxide at atmospheric pressure. The details of the synthesis will be reported elsewhere. Colorless crystals (I) (m.p. 413.2 K) were obtained by slow evaporation from a solution in *n*-hexane–dichloromethane (3:1 *v*/*v*) at room temperature.

Crystal data

$C_{32}H_{28}Si_2$
$M_r = 468.72$
Triclinic, $P\overline{1}$
$a = 11.1046$ (12) Å
$b = 11.4205$ (11) Å
$c = 12.7004$ (9) Å
$\alpha = 72.632$ (7)°
$\beta = 78.905$ (7)°
$\gamma = 62.198$ (11)°
$V = 1357.1$ (2) Å^3

$Z = 2$
$D_x = 1.147$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 10.0$–14.3°
$\mu = 0.15$ mm^{-1}
$T = 293$ (2) K
Plate, colorless
0.40 × 0.26 × 0.13 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Non-profiled $\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{\min} = 0.944$, $T_{\max} = 0.981$
4973 measured reflections
4739 independent reflections
2575 reflections with $I > 2\sigma(I)$

$R_{\rm int} = 0.024$
$\theta_{\max} = 25.0°$
$h = -12 \rightarrow 13$
$k = -12 \rightarrow 13$
$l = 0 \rightarrow 15$
3 standard reflections frequency: 300 min intensity decay: 1%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.063$
$wR(F^2) = 0.146$
$S = 1.02$
4739 reflections
321 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0497P)^2 + 0.2159P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.23$ e Å^{-3}
$\Delta\rho_{\min} = -0.18$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Si1—C19	1.852 (4)	Si2—C20	1.865 (4)
Si1—C1	1.864 (3)	Si2—C27	1.869 (4)
Si1—C13	1.868 (3)	Si2—H1	1.35 (3)
Si1—C7	1.875 (3)	C19—C20	1.292 (5)
Si2—C21	1.855 (4)		
C19—Si1—C1	108.84 (18)	C21—Si2—C20	111.20 (19)
C19—Si1—C13	111.04 (18)	C21—Si2—C27	110.76 (17)
C1—Si1—C13	108.81 (15)	C20—Si2—C27	109.02 (18)
C19—Si1—C7	108.66 (16)	C21—Si2—H1	108.6 (11)
C1—Si1—C7	109.48 (15)	C20—Si2—H1	108.4 (11)
C13—Si1—C7	109.98 (15)	C27—Si2—H1	108.8 (11)

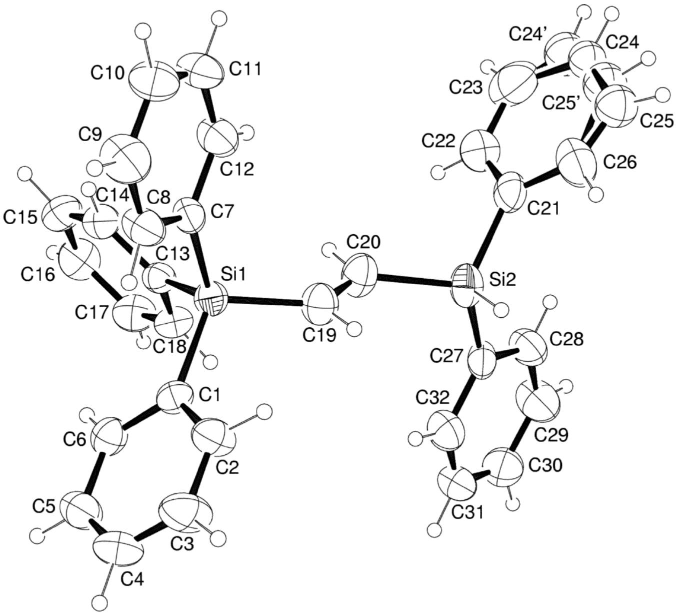

Figure 1
View of (I) with the atom-numbering scheme and displacement ellipsoids at the 35% probability level.

Three H atoms H1, H19 and H20 bound to Si2, C19 and C20 were found from a difference Fourier synthesis and refined isotropically, and the other H atoms were assigned to calculated positions and allowed to ride on their attached C atoms.

Data collection: *CAD*-4 *EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD*-4 *EXPRESS*; data reduction: *XCAD*4 (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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