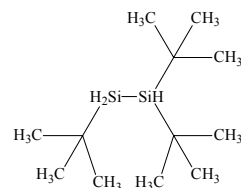


**913** **C<sub>12</sub>H<sub>30</sub>Si<sub>2</sub>**ED, *ab initio*  
calculations**1,1,2-Tris(1,1-dimethylethyl)disilane**1,1,2-Tri-*t*-butyldisilane**C<sub>1</sub>**

$r_a$	Å <sup>a</sup>	$\theta_a$	deg <sup>a</sup>
C–H	1.124(1)	C–C–H	110.1(6)
C–C	1.545(1)	C–C–C	108.5(2)
Si–Si	2.363(8)	Si–Si–H <sup>b</sup>	109.3(11)
Si–C <sup>b</sup>	1.910(3)	Si–Si–C <sup>b</sup>	112.0(6)
Si–H <sup>b</sup>	1.497(10)	$\Delta_1(\text{Si–Si–C})^c$	4.8(10)
		$\Delta_2(\text{Si–Si–C})^d$	7.3(11)
		twist(CH <sub>3</sub> ) <sup>e</sup>	58.4(22)
		tilt(CH <sub>3</sub> ) <sup>e</sup>	–4.4(11)
		rock(CH <sub>3</sub> ) <sup>e</sup>	2.0(21)
		twist( <i>t</i> -butyl) <sup>f</sup>	62.0(14)
		$\Delta_1[\text{twist}(\textit{t}\text{-butyl})]^g$	–12.3(20)
		$\Delta_2[\text{twist}(\textit{t}\text{-butyl})]^h$	–0.3(16)
		rock( <i>t</i> -butyl at C(21)) <sup>i</sup>	2.4(11)
		rock( <i>t</i> -butyl at C(11)) <sup>j</sup>	4.0(10)
		rock( <i>t</i> -butyl at C(12)) <sup>j</sup>	–4.7(9)
		tilt( <i>t</i> -butyl at C(21)) <sup>j</sup>	–3.0(10)
		tilt( <i>t</i> -butyl at C(11)) <sup>j</sup>	–2.0(9)
		tilt( <i>t</i> -butyl at C(12)) <sup>j</sup>	–2.4(10)
		C twist <sup>k</sup>	112.1(7)
		$\Delta(\text{C twist})^l$	–0.3(11)
		H twist <sup>m</sup>	122.0(11)
		H–Si–Si–C <sup>n</sup>	–6.2(11)

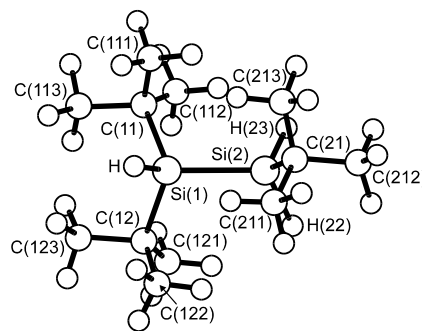


It was confirmed by a joint analysis of ED and vibrational spectroscopy data that the *syn* arrangement, in which each of the *t*-butyl groups eclipses an Si–H bond, was essentially a single conformer in the gas phase. This observation was supported by calculations of the MP2/D95\* level, which also identified the less stable (by *ca.* 10 kJ mol<sup>–1</sup>) *gauche* and *antiperiplanar* conformers. In the ED analysis, the *t*-butyl and methyl groups were assumed to have local C<sub>3</sub> and C<sub>3v</sub> symmetry, respectively. The nozzle temperature was *ca.* 411 K.

<sup>a</sup>) Estimated standard errors.<sup>b</sup>) Average value.<sup>c</sup>) [Si(1)–Si(2)–C(21)] – [Si(2)–Si(1)–C(11)].<sup>d</sup>) [Si(1)–Si(2)–C(21)] – [Si(2)–Si(1)–C(12)].

<sup>e</sup>) Torsion, tilt and rock angles of methyl groups are rotations about the local *x*, *z* and *y* axes, respectively. The *x* axis is the C–CH<sub>3</sub> vector, zero position when one H atom lies in the *xy* plane in the positive *x* and *y* directions. The *y* axis is in the plane formed by the C<sub>3</sub> axis of the *t*-butyl group and the *x* axis.

<sup>f</sup>) Average value of C(211)–C(21)–Si(2)–Si(1), C(111)–C(11)–Si(1)–Si(2) and C(121)–C(12)–Si(1)–Si(2) torsional angles.

<sup>g</sup>) [C(211)–C(21)–Si(2)–Si(1)] – [C(111)–C(11)–Si(1)–Si(2)].<sup>h</sup>) [C(211)–C(21)–Si(2)–Si(1)] – [C(121)–C(12)–Si(1)–Si(2)].*syn*

- <sup>i)</sup> Positive rock moves the *t*-butyl group at C(21) away from that at C(12) whilst the *t*-butyl group at C(11) moves towards C(12) and C(12) moves away from C(11).
- <sup>j)</sup> Positive tilts move the *t*-butyl groups at one end of the molecule towards the group at the other end.
- <sup>k)</sup> Average value of the two dihedral angles (DHs): DH between the C(11)–Si(1)–Si(2) and H–Si(1)–Si(2) planes and DH between the C(12)–Si(1)–Si(2) and H–Si(1)–Si(2) planes.
- <sup>l)</sup> Difference between the two DHs defined in <sup>k)</sup>.
- <sup>m)</sup> Average value of the two DHs: DH between the H(22)–Si(2)–Si(1) and C(21)–Si(2)–Si(1) planes and DH between the H(23)–Si(2)–Si(1) and C(21)–Si(2)–Si(1) planes; the difference between these angles was assumed at the value from *ab initio* calculations.
- <sup>n)</sup> Zero degree for the *syn* position.

Hinchley, S.L., Smart, B.A., Morrison, C.A., Robertson, H.E., Rankin, D.W.H., Zink, R., Hassler, K.: J. Chem. Soc., Dalton Trans. (1999) 2303.