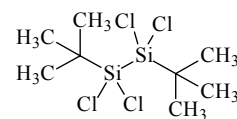


**854**      **C<sub>8</sub>H<sub>18</sub>Cl<sub>4</sub>Si<sub>2</sub>**ED, *ab initio*  
calculations**1,1,2,2-Tetrachloro-1,2-bis(1,1-dimethylethyl)disilane****C<sub>2</sub>**

$r_a$	Å <sup>a)</sup>	$\theta_a$	deg <sup>a)</sup>
C–H <sup>b)</sup>	1.142(4)	C–C–H	109.2(9)
C–C <sup>b)</sup>	1.543(2)	C–C–C	109.1(3)
Si–Si	2.380(7)	Si–Si–C	119.8(6)
Si–C	1.872(7)	Si–Si–Cl <sup>b)</sup>	105.2(3)
Si–Cl <sup>b)</sup>	2.071(1)	$\Delta(\text{Si–Si–Cl})$ <sup>c)</sup>	1.8(5)
		Si–C–C(1')	109.3(4)
		Si–C–C(1'')	112.0(8)
		Si–C–C(2)	108.2(7)
		Cl–Si–Cl	105.5(8)
		twist(CH <sub>3</sub> ) <sup>d)</sup>	176.6(21)
		tilt(CH <sub>3</sub> ) <sup>e)</sup>	2.5(19)
		twist( <i>t</i> -butyl) <sup>f)</sup>	167.5(17)
		tilt( <i>t</i> -butyl) <sup>g)</sup>	2.3(8)
		Cl torsion <sup>h)</sup>	124.4(5)
		$\Delta[\text{Cl torsion}]$ <sup>i)</sup>	2.8(11)
		C–Si–Si–C <sup>j)</sup>	167.7(11)

Local C<sub>3v</sub> symmetry was assumed for the methyl groups, and local C<sub>3</sub> symmetry was assumed for the *t*-butyl groups. Some differences between similar bond lengths and bond angles were restrained to the values from MP2/6-31G\* calculations.

The nozzle temperature was *ca.* 455 K.

<sup>a)</sup> Estimated standard errors.

<sup>b)</sup> Mean value.

<sup>c)</sup> [Si–Si–Cl(1)] – [Si–Si–Cl(2)].

<sup>d)</sup> Torsional angle Si–C(1)–C(1')–H from the *syn* position.

<sup>e)</sup> Positive if the H atoms are displaced toward the Si atom.

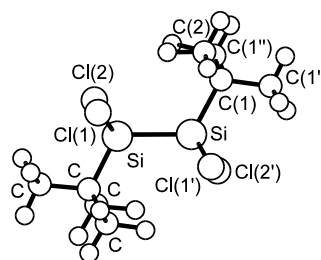
<sup>f)</sup> Torsional angle Si–Si–C(1)–C(1') from the *syn* position.

<sup>g)</sup> Positive if the *t*-butyl groups are displaced away from each other.

<sup>h)</sup> Average value of the dihedral angles between the C–Si–Si plane and the C–Si–Cl(1,2) planes.

<sup>i)</sup> Difference in the absolute values of [C(1)–Si–Si–Cl(1)] – [C(1)–Si–Si–Cl(2)], *i.e.*, the difference in the dihedral angles defined in footnote <sup>h)</sup>.

<sup>j)</sup> Torsional angle from the *syn* position.



Hinchley, S.L., Smart, B.A., Morrison, C., Robertson, H.E., Rankin, D.W.H., Coxall, R.A., Parsons, S., Zink, R., Siegl, H., Hassler, K., Mawhorter, R.: J. Chem. Soc., Dalton Trans. (2001) 2916.