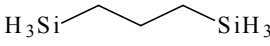


**463**      **C<sub>3</sub>H<sub>12</sub>Si<sub>2</sub>**  
ED, *ab initio*  
calculations

**1,3-Propanediylbissilane**  
1,5-Disilapentane  
1,3-Disilylpropane

**C<sub>2v</sub>** (*anti-anti*) assumed  
**C<sub>1</sub>** (*anti-gauche*)  
**C<sub>2</sub>** (*gauche<sup>+</sup>-gauche<sup>-</sup>*)

$r_g$	$\text{\AA}^a)$				
	AA	AG		G <sup>+</sup> G <sup>-</sup>	
C–C	1.537(2)	1.536(2) <sup>b) c)</sup>	1.537(2) <sup>c) d)</sup>	1.539(2) <sup>c)</sup>	
C–Si	1.886(1)	1.889(1) <sup>b) c)</sup>	1.886(1) <sup>c) d)</sup>	1.888(1) <sup>c)</sup>	
C–H <sup>e)</sup>	1.140(2)	1.140(2)		1.140(2)	
Si–H <sup>e)</sup>	1.487(4)	1.487(4)		1.487(4)	

$\theta_g$	deg <sup>a)</sup>				
	AA	AG		G <sup>+</sup> G <sup>-</sup>	
C–C–C	114.8(7)	116.2(9) <sup>f)</sup>		118.8(7) <sup>f)</sup>	
C–C–Si	114.1(4)	112.7(7) <sup>b) f)</sup>	115.2(6) <sup>d) f)</sup>	116.8(7) <sup>f)</sup>	
C–Si–H <sup>e)</sup>	110.5(12)	110.5(12)		110.5(12)	
Si–C–H	107.4(6)	107.7(6) <sup>b)</sup>	107.1(6) <sup>d)</sup>	106.6(6)	
H–C–H <sup>e)</sup>	107.2(14)	107.2(14)		107.2(14)	
Si–C–C–C	180 <sup>g)</sup>	176.3(17) <sup>b) f)</sup>	63.7(22) <sup>d) f)</sup>	60.9(10)	
twist(SiH <sub>3</sub> ) <sup>h)</sup>	180 <sup>g)</sup>	180 <sup>b) g)</sup>	25.3(40) <sup>c) d)</sup>	29.5(40)	

The molecule was assumed to exist as a mixture of *anti-anti*, *anti-gauche* and *gauche<sup>+</sup>-gauche<sup>-</sup>* conformers. Their ratio was found to be 28(4):40(5):32(6). Local C<sub>3v</sub> symmetry was assumed for the CSiH<sub>3</sub> groups. The CH<sub>2</sub> units were assumed to lie in the planes perpendicular to the CCSi or CCC planes. The structural analysis of ED data was carried out by applying flexible restraints based on the results of MP2/6-31G\* calculations. The nozzle was at 293 K.

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

<sup>b)</sup> *Anti* part of the *anti-gauche* conformer.

<sup>c)</sup> Difference assumed.

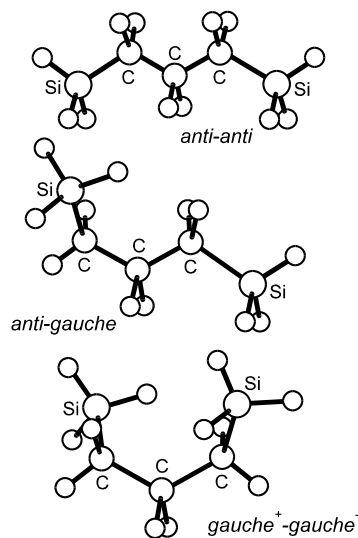
<sup>d)</sup> *Gauche* part of the *anti-gauche* conformer.

<sup>e)</sup> An equal value was assumed for all conformers.

<sup>f)</sup> Difference was flexibly constrained.

<sup>g)</sup> Assumed.

<sup>h)</sup> H–Si–C–C torsional angle from the *syn* position.



Mitzel, N.W., Smart, B.A., Blake, A.J., Robertson, H.E., Rankin, D.W.H.: J. Phys. Chem. **100** (1996) 9339.