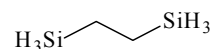


320 **C₂H₁₀Si₂**
ED, *ab initio*
calculations

1,2-Ethanedibisilane
1,4-Disilabutane
1,2-Disilylethane

C_{2h} assumed (*anti*)
C₂ (*gauche*)



r_g	\AA^a		θ_g	deg^a	
	<i>anti</i>	<i>gauche</i>		<i>anti</i>	<i>gauche</i>
C–C	1.563(5)	1.563(5) ^{b)}	C–C–Si	110.7(2)	114.4(5) ^{c)}
C–Si	1.882(1)	1.885(1) ^{b)}	H–C–H	108.1(16)	108.1(5)
C–H	1.141(2)	1.141(2)	C–Si–H	112.1(7)	112.4(6)
Si–H	1.499(3)	1.499(3)	Si–C–H	108.2(5)	108.2(4)
			τ^d	180 ^{e)}	78.5(21)
			twist(SiH ₃) ^{f)}	180 ^{e)}	153.9 ^{g)}

The molecule exists as a mixture of *gauche* (24(2)%) and *anti* (76(2)%) conformers with a Gibbs energy difference of 4.6(2) kJ mol^{−1}. Local C_{3v} symmetry was assumed for the CSiH₃ groups.

The nozzle was at 293 K.

^{a)} Estimated standard errors.

^{b)} Difference to the *anti* conformer was assumed at the value from MP2/6-311G* calculations.

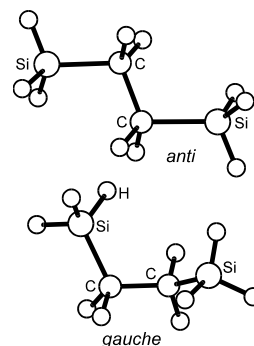
^{c)} Difference to the *anti* conformer refined, then fixed.

^{d)} Si–C–C–Si torsional angle, $\tau = 0^\circ$ for the *syn* position.

^{e)} Assumed.

^{f)} H–Si–C–C torsional angle from the *syn* position.

^{g)} Refined, then fixed.



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