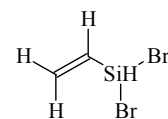


255 **C₂H₄Br₂Si**
ED, *ab initio* and DFT
calculations

Dibromo(ethenyl)silane
Dibromo(vinyl)silane

C_s (*syn*)
C₁ (*gauche*)

r_g	Å ^{a)}	θ_α	deg ^{a)}
C=C	1.366(10)	C–C–Si	121.7 ^{b)}
C–Si	1.827(9)	C–C–H	121.2 ^{b)}
		(average)	
Si–Br	2.206(2)	Br–Si–Br	109.0(2)
Si–H	1.501 ^{c)}	C–Si–Br	110.1(8)
C–H (average)	1.100 ^{c)}	C–C–H(1)	122.5 ^{b)}
		C–C–H(2)	121.9 ^{b)}
		C–C–H(3)	119.1 ^{b)}
		C–Si–H(4)	111.4 ^{b)}
		Si–C–H(3)	119.2 ^{b)}
		Br–Si–H	108.1(9)
		H–C–H	115.6 ^{b)}
		$\tau^d)$	0 ^{c)}



The molecule was found to exist as a mixture of *syn* (27%) and *gauche* (73%) conformers, no uncertainties being reported. A dynamic model of pseudoconformers was used to describe the internal rotation around the C–Si bond. Structural differences between all pseudoconformers were assumed at the values from HF/3-21G* and HF/6-311G(d) calculations. The structural parameters are listed for the *syn* conformer.

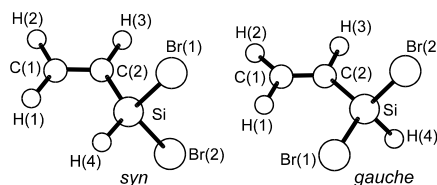
The nozzle was at 296...298 K.

^{a)} Twice the estimated standard errors including a systematic error.

^{b)} Assumed at the value from HF/6-311G(d) calculations.

^{c)} Assumed.

^{d)} Torsional angle C=C–Si–H. This angle was assumed to be 120° for the *gauche* conformer.



Johansen, T.H., Hagen, K., Hassler, K., Richardson, A.D., Pätzold, U., Stølevik, R.: J. Mol. Struct. **550-551** (2000) 257.