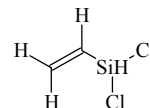


**265**      **C<sub>2</sub>H<sub>4</sub>Cl<sub>2</sub>Si**  
ED, *ab initio* and DFT  
calculations

**Dichloro(ethenyl)silane**  
Dichloro(vinyl)silane

**C<sub>s</sub> (*syn*)**  
**C<sub>1</sub> (*gauche*)**

$r_g$	Å <sup>a)</sup>	$\theta_a$	deg <sup>a)</sup>
C=C	1.357(7)	C–C–Si	121.8 <sup>b)</sup>
C–Si	1.847(5)	C–C–H	121.1 <sup>b)</sup>
		(average)	
Si–Cl	2.042(2)	Cl–Si–Cl	108.2(6)
Si–H	1.499 <sup>c)</sup>	C–Si–Cl	110.3(6)
C–H (average)	1.099 <sup>c)</sup>	C–C–H(1)	122.5 <sup>b)</sup>
		C–C–H(2)	121.9 <sup>b)</sup>
		C–C–H(3)	118.9 <sup>b)</sup>
		C–Si–H(4)	111.7 <sup>b)</sup>
		Si–C–H(3)	119.3 <sup>b)</sup>
		Cl–Si–H	108.1(7)
		H–C(1)–H	115.6 <sup>b)</sup>
		$\tau^d$	0.0 <sup>c)</sup>



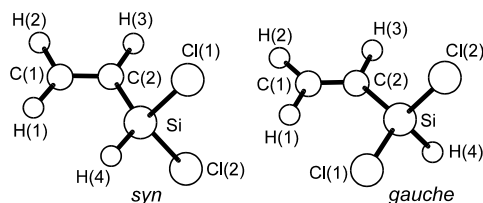
The molecule was found to exist as a mixture of *syn* (32%) and *gauche* (68%) conformers, no uncertainties being reported. A dynamic model of pseudoconformers was used to describe the internal rotation around the C–Si bond. Structural differences between all pseudoconformers were assumed at the values from HF/6-31G(d) and HF/6-311G(d) calculations. The structural parameters are listed for the *syn* conformer. The nozzle was at 296...298 K.

<sup>a)</sup> Twice the estimated standard errors including a systematic error.

<sup>b)</sup> Assumed at the value from HF/6-311G(d) calculations.

<sup>c)</sup> Assumed.

<sup>d)</sup> 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.