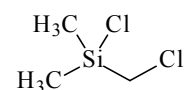


438 **C₃H₈Cl₂Si**ED, *ab initio*
calculations**Chloro(chloromethyl)dimethylsilane****C_s (*anti*)****C₁ (*gauche*)**

r_g	\AA^a		θ_α	deg^a	
	<i>anti</i>	<i>gauche</i>		<i>anti</i>	<i>gauche</i>
Si–C(1)	1.888(3)	1.890(3)	C(2)–Si–C(3)	111.5 ^b	111.0 ^b
Si–C(2)	1.865(3)	1.865(3)	Si–C–Cl	110.7(10)	113.5(10)
Si–C(3)	1.866(3)	1.871(3)	Si–C–H	112.3(15)	112.1(15)
Si–C(average)	1.873(3)	1.875(3)	Cl–Si–C(1)	104.0 ^b	107.5 ^b
Si–Cl	2.078(5)	2.068(5)	C(3)–Si–C(1) ^c	108.9 ^b	107.4 ^b
C–Cl	1.793(14)	1.782(14)	C(1)–Si–C(2) ^c	108.9 ^b	111.4 ^b
C(2,3)–H	1.105(9)	1.105(9)	Cl–Si–C(2,3) ^c	110.3 ^b	109.6 ^b
C(1)–H	1.087(9)	1.087(9)	Cl–C–H ^c	108.0(10)	108.0(10)
			H–C–H ^c	106.5(16)	106.5(16)
			τ^d	161(3) ^c	70(8)

The molecule exists as a mixture of *anti* (59(16)%) and *gauche* (41(16)%) conformers. The energy difference $\Delta E^\circ = E^\circ(\textit{gauche}) - E^\circ(\textit{anti}) = 0.6(4) \text{ kcal mol}^{-1}$ was estimated from the experimental conformational composition and $\Delta S^\circ(\textit{anti-gauche})$ calculated from the *ab initio* results (MP2(fc)/6-311+G(d,p)//HF/6-31G(d)). Local C_{3v} symmetry and staggered conformation were assumed for the methyl groups. The nozzle was at 296...297 K.

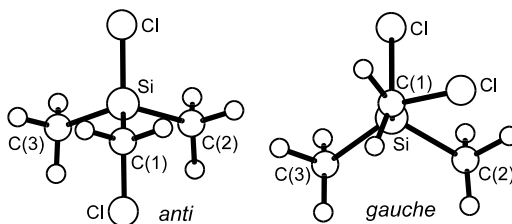
^a) Twice the estimated standard errors including a systematic error.

^b) Assumed.

^c) Dependent parameter.

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

^e) Average value, the deviation from 180° is not a real deviation, but a result of large-amplitude torsional motion about the Si–C bond.



Johansen, T.H., Wold, K.H., Hagen, K., Stølevik, R.: J. Mol. Struct. **384** (1996) 215.