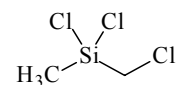


281 **C₂H₅Cl₃Si**ED, *ab initio*
calculations**Dichloro(chloromethyl)methylsilane****C₁ (*gauche*)****C_s (*anti*)**

r_g	\AA^a		θ_α	deg^a	
	<i>gauche</i>	<i>anti</i>		<i>gauche</i>	<i>anti</i>
Si–C(1)	1.877(5)	1.876(5)	C–Si–C	113.6(23)	109.7(23)
Si–C(3)	1.854(5)	1.856(5)	Si–C–Cl	110.4(6)	113.1(6)
C(1)–Cl	1.787(7)	1.773(7)	Si–C(1)–H	114.3(24)	113.1(24)
C(1)–H	1.090(15)	1.088(15)	Cl–Si–Cl	107.9(12)	108.6(12)
C(3)–H	1.100(15)	1.099(15)	C(1)–Si–Cl ^b	108.8(5)	109.6(5)
Si–Cl(2)	2.041(3)	2.040(3)	C(3)–Si–Cl ^b	108.8(5)	109.6(5)
Si–Cl(3)	2.051(3)	2.040(3)	Cl–C–H ^b	106.5(13)	105.6(14)
			H–C(1)–H ^b	106.0(27)	105.6(27)
			H–C(3)–H ^b	104.8(28)	104.6(28)
			Si–C(3)–H ^b	113.8(24)	114.0(24)
			τ^c	51(5)	180 ^d

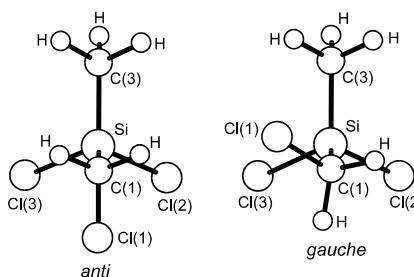
The molecule exists as a mixture of *gauche* (84(15)% and *anti* (16(15)%) conformers. The energy difference $\Delta E^\circ = E^\circ(\textit{anti}) - E^\circ(\textit{gauche}) = 0.6(7) \text{ kcal mol}^{-1}$ was estimated from the experimental conformational composition and $\Delta S^\circ(\textit{anti-gauche})$ calculated from the *ab initio* (MP2(fc)/6-311+G(d,p)//HF/6-31G(d)) results. Local C_{3v} symmetry and staggered conformation were assumed for the methyl group. The nozzle was at 296...297 K.

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

^b) Dependent parameter.

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

^d) Assumed.



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