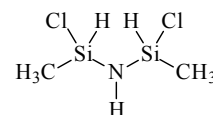


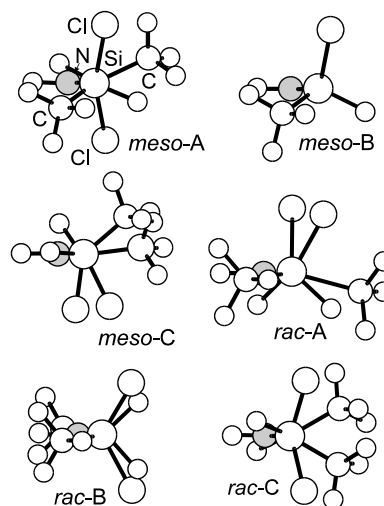
316 **C₂H₅Cl₂NSi₂**ED, *ab initio*
calculations**1,3-Dichloro-1,3-dimethyldisilazane**Bis[chloro(methyl)silyl]amine
1-Chloro-*N*-[chloro(methyl)silyl]-
1-methylsilanamineC₂ (*meso*-A)C_s (*meso*-B)C₁ (*meso*-C)C₁ (*rac*-A)C₂ (*rac*-B)C₂ (*rac*-C)

r_a	Å ^{a)}	θ_a	deg ^{a)}
N–Si	1.712(2)	a_1^b	128.8(12)
N–H	1.020 ^{c)}	a_2^b	1.1 ^{c)}
Si–H	1.488(17)	N–Si–Cl	112.9(4)
Si–Cl	2.062(1)	N–Si–H	107.6 ^{c)}
Si–C	1.845(3)	N–Si–C	115.7(9)
C–H	1.119(5)	C–Si–Cl	102.6(6)
		C–Si–H	113.5 ^{c)}
		Si–C–H	110.8 ^{c)}
		$\tau_{1,2}$ (<i>meso</i> -A) ^{d)}	–85(8)
		$\tau_{1,2}$ (<i>meso</i> -B) ^{d)}	–97(13)
		$\tau_{1,2}$ (<i>meso</i> -C) ^{d)}	114(11)
		$\tau_{1,2}$ (<i>rac</i> -A) ^{d)}	–81(9)
		$\tau_{1,2}$ (<i>rac</i> -B) ^{d)}	101(15)
		$\tau_{1,2}$ (<i>rac</i> -C) ^{d)}	102(4)
		τ^c	60 ^{f)}



According to ¹H NMR data, the molecule was assumed to exist as 1:1 mixture of *meso* and *rac* diastereomers. According to the results of MP2/6-311+G* calculations, it was assumed that the three conformers of each diastereomer, *meso*-A, *meso*-B, *meso*-C, *rac*-A, *rac*-B and *rac*-C, exist at the temperature of the ED experiment in the ratio of 0.325:0.090:0.085:0.110:0.165:0.225, respectively. The corresponding bond lengths and angles except for the Si–N–Si angle of these conformers were assumed to be equal. Planarity of the bonds at nitrogen was assumed according to the results of *ab initio* calculations. The two halves of the molecule were taken to be identical and each Si–CH₃ group was assumed to have local C_{3v} symmetry. The Si–Cl bonds in all conformers were found to be more or less orthogonal to the SiNSi plane.

The nozzle was at 343 K.



view along Si...Si

^{a)} Estimated standard errors.

^{b)} The Si–N–Si angle is given by a_1 – a_2 for *meso*-A and *rac*-A, by a_1 for *meso*-B and *rac*-B and by a_1 + $2a_2$ for *meso*-C and *rac*-C.

^{c)} Assumed at the average value from MP2/6-31G* calculations.

- ^{d)} Two torsional angles Cl–Si–N–H for each conformer were constrained together, so that only one parameter remained to describe them. The relationships between the two torsional angles τ_1 and τ_2 in each conformer were derived from the MP2/6-31G* results and were set as follows: *meso*-A, $\tau_1 = \tau_2$; *meso*-B, $\tau_1 = -\tau_2$; *meso*-C, $\tau_1 = -\tau_2 + 40^\circ$; *rac*-A, $\tau_1 = -\tau_2 - 33^\circ$; *rac*-B, $\tau_1 = \tau_2$; *rac*-C, $\tau_1 = \tau_2$.
- ^{e)} H–C–Si–N torsional angle.
- ^{f)} Assumed according to the *ab initio* results.

Fleischer, H., Brain, P.T., Rankin, D.W.H., Robertson, H.E., Bühl, M., Thiel, W.: J. Chem. Soc., Dalton Trans. (1998) 593.