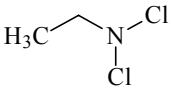
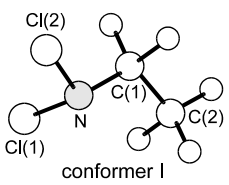
280 **$C_2H_5Cl_2N$** ***N*,*N*-Dichloroethanamine** **C_1** (conformer I)
ED, *ab initio* calculations *N*,*N*-Dichloroethylamine **C_s** (conformer II)

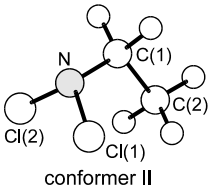


r_g	Å [a])	θ_α	deg [a])
N–C(1)	1.479(6)	N–C(1)–C(2)	108.2(8)
C(1)–C(2)	1.542(7)	C(1)–N–Cl(1)	108.7(3) [b])
N–Cl(1)	1.759(2) [b])	C(1)–N–Cl(2)	107.7(3) [b])
N–Cl(2)	1.760(2) [b])	Cl(1)–N–Cl(2)	106.9(2)
C–H (average)	1.107(8)	τ [c])	–76(2)

It was assumed that the molecule exists as a mixture of two conformers with symmetry C_1 (conformer I) and C_s (conformer II). The ratio of conformers I and II was determined to be 79(9):21. The differences between the corresponding parameters of these conformers were assumed at the values from MP2/6-31G** calculations.
The parameters are listed for conformer I.
The nozzle was at room temperature.



conformer I



conformer II

[a]) Three times the estimated standard errors.
[b]) Differences between the N–Cl(1) and N–Cl(2) bond lengths and between the C(1)–N–Cl(1) and C(1)–N–Cl(2) bond angles were assumed at the values from MP2/6-31G** calculations.
[c]) Torsional angle Cl(1)–N–C(1)–C(2) from the *syn* position.

Egawa, T., Ohtsubo, M., Nakagawa, H., Kuze, N., Fujiwara, H., Konaka, S.: J. Phys. Chem. A **104** (2000) 1311.