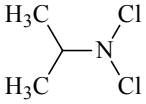
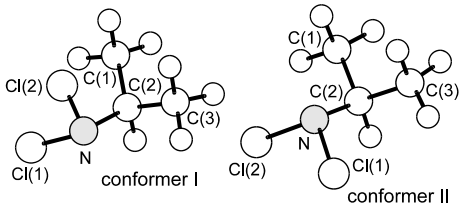
417 **$C_3H_7Cl_2N$** ***N,N*-Dichloro-2-propanamine** **C_1** (conformer I)
ED, *ab initio* calculations *N,N*-Dichloroisopropylamine **C_s** (conformer II)



r_g	Å [a])	θ_α	deg [a])
N–C(2)	1.496(11)	N–C(2)–C(3)	107.6(8) [b])
C(2)–C(3)	1.532(6) [b])	N–C(2)–C(1)	117.1(8) [b])
C(1)–C(2)	1.530(6) [b])	C(1)–C(2)–C(3)	108.3(18)
N–Cl(1)	1.762(2) [b])	C(2)–N–Cl(1)	108.5(6) [b])
N–Cl(2)	1.762(2) [b])	C(2)–N–Cl(2)	109.7(6) [b])
C–H (average)	1.119(5)	Cl(1)–N–Cl(2)	106.7(4)
		τ [c])	63(3)

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 88(12):12. 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.



[a]) Three times the estimated standard errors.
[b]) Differences between the C(2)–C(3) and C(1)–C(2), N–Cl(1) and N–Cl(2), N–C(2)–C(3) and N–C(2)–C(1), C(2)–N–Cl(1) and C(2)–N–Cl(2) were assumed at the values from MP2/6-31G** calculations.
[c]) Torsional angle Cl(1)–N–C(2)–C(1) from the *syn* position.

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