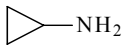
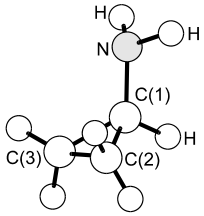
424 **C_3H_7N** **Cyclopropanamine** **C_s** assumed (*anti*)
ED, *ab initio* calculations
Cyclopropylamine



r_g	Å [a])	θ_α	deg [a])
C(1)–C(2,3)	1.514(3)	C–C–N	117.2(6)
Δ(C–C) [b])	0.005 [c])	C–N–H	111.5 [d])
C–N	1.429(8)	H–C–H	114.5 [e])
C(2,3)–H	1.099 [e])	N–C–H	117.8 [c])
C(1)–H	1.104 [f])	H–N–H	106.0 [d])
N–H	1.031 [d])		

It was assumed that the molecule has C_s overall symmetry and *anti* conformation, where the nitrogen lone pair is *anti* with respect to the C(1)–H bond. The CCC and HCH planes were assumed to bisect each other.
The nozzle was at room temperature.



[a]) Three times the estimated standard errors including a systematic error.
[b]) [C(2)–C(3)] – [C(1)–C(2,3)].
[c]) Assumed at the value from HF/4-31G(N*) calculations.
[d]) Assumed at the value of methylamine.
[e]) Assumed at the value of cyclopropane.
[f]) Difference between the C(2,3)–H and C(1)–H bond lengths was assumed at the value from HF/4-31G(N*) calculations.

Iijima, T., Kondou, T., Takenaka, T.: J. Mol. Struct. **445** (1998) 23.

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