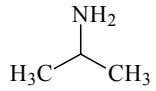
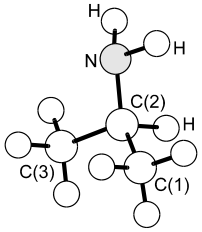
450 **C_3H_9N** **2-Propanamine** **C_s** assumed (*anti*)
ED, *ab initio* calculations
Isopropylamine



r_g	Å [a])	θ_α	deg [a])
C–C	1.529(5)	C–C–N	108.9(9)
C–N	1.469(13)	C–C–C	114.4(16)
C(1,3)–H	1.104(15)	C–C–H (methyl)	111.1(32)
C(2)–H	1.111 [b])	N–C–H	111.8 [c])
N–H	1.031 [d])	C–N–H	111.5 [d])
		H–N–H	106.0 [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(2)–H bond. Local C_{3v} symmetry, staggered conformation and no tilt were assumed for the methyl groups.
The nozzle was at room temperature.



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

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