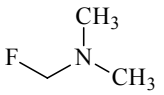
439 **C_3H_8FN** **1-Fluoro-*N*,*N*-dimethylmethanamine** **C_s**

ED, *ab initio* and DFT calculations

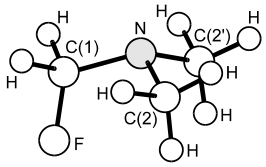
N-(Fluoromethyl)dimethylamine



r_a	Å [a])	θ_α	deg [a])
N–C (mean)	1.446(6)	C–N–C (mean)	111.6(10)
Δ(N–C) [b])	0.058(17)	Δ(C–N–C) [c])	1.5 [d])
N–C(1)	1.408(13)	C(1)–N–C(2)	112.1(11)
N–C(2)	1.466(9)	C(2)–N–C(2')	110.6(12)
C–F	1.410(5)	N–C–F	115.9(24)
C–H (mean)	1.112(3)	H–C–H (mean)	109.4(10)
		tilt(CH_3) [e])	2.2 [d])
		τ(C(2')–N–C(2)–H)	178.9 [d])

According to the ED data, the molecule exists as only *anti* conformer (C–F bond *antiperiplanar* to the nitrogen lone pair). The HF/3-21G(*) (polarization functions only at nitrogen) and VWN/TZVP (with polarized triple-ζ basis set) calculations predicted a second stable conformer with *synclinal* orientation of the C–F bond and 4.5…5.2 kcal mol^{-1} higher in energy.
Local C_{3v} symmetry was assumed for CH_3 groups in the ED analysis.
The nozzle was at room temperature.

[a]) Three times the estimated standard errors.
[b]) [N–C(2)] – [N–C(1)].
[c]) [C(1)–N–C(2)] – [C(2)–N–C(2′)].
[d]) Assumed at the MP2/6-311G(2d,p) value.
[e]) Tilt angle of the CH_3 groups towards the nitrogen lone pair.



Christen, D., Mack, H.-G., Rüdiger, S., Oberhammer, H.: J. Am. Chem. Soc. **118** (1996) 3720.