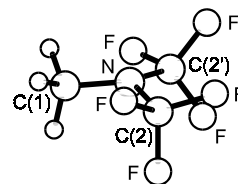


1107 **C₃H₃F₆N****1,1,1-Trifluoro-*N*-methyl-*N*-(trifluoromethyl)methanamine C₁**ED, *ab initio* calculations
(HF/3-21G*)*N,N*-Bis(trifluoromethyl)methylamineH₃C–N(CF₃)₂

r_a	Å ^{a)}	θ_α	deg ^{a)}
C–F	1.333(3)	C(2)–N–C(2')	117.8(11)
N–C(1)	1.478(13)	C(1)–N–C(2)	116.8(13)
N–C(2)	1.420(8)	F–C–F	107.6(3)
C–H	1.114(25)	H–C–H	110.0 ^{b)}
		ϕ (CF ₃) ^{c)}	1.8 ^{b)}
		τ_1 ^{d)}	25 ^{b)}
		τ_2 ^{d)}	13 ^{b)}



Local C_{3v} symmetry for the CH₃ and CF₃ groups were assumed.
The nozzle was at room temperature.

^{a)} Three times the estimated standard errors including the scale error.

^{b)} Fixed at *ab initio* value.

^{c)} Tilt angle between the C₃ axis of the CF₃ group and the N–C bond direction towards the nitrogen lone pair.

^{d)} Torsional angles of the two CF₃ groups; for $\tau=0^\circ$ the CF₃ group staggers exactly the opposite N–C(2) bond.

Jin, A., Zhu, X.-L., Kirchmeier, R.L., Shreeve, J.M., Patel, N.R., Oberhammer, H.: J. Mol. Struct. **323** (1994) 129.