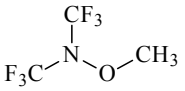
359 **$C_3H_3F_6NO$** **1,1,1-Trifluoro-*N*-methoxy-*N*-(trifluoromethyl)-methanamine** **C_s** (*syn*)

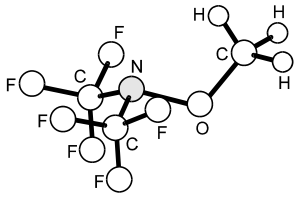
ED, *ab initio* calculations

1,1,1,1',1',1'-Hexafluoro-*N*-methoxydimethylamine
O-Methyl-*N,N*-bis(trifluoromethyl)hydroxylamine



r [a])	Å [b])	θ [a])	deg [b])
C–F	1.324(2)	C–N–C	118.0(9)
N–C	1.429(7)	C–N–O	108.1(17)
N–O	1.424(28)	N–O–C	109.4(17)
O–C	1.450(26)	F–C–F	108.3(3)
C–H	1.100 [c])	H–C–H	110.0 [c])
		tilt(CF_3) [d])	3.7(8)
		τ(CF_3) [e])	3.1(34)

The experimental intensities were reproduced by use of a single conformation with *syn* orientation of the C–O bond relative to the nitrogen lone pair. This was confirmed by *ab initio* calculations (HF/3-21G$^{(*)}$ (polarization functions only on nitrogen) and MP2/6-31G*) which predicted that the *anti* conformer is less stable by 7.6 kcal mol^{-1}.
The nozzle was at room temperature.



[a]) Unidentified, possibly r_a and θ_a.
[b]) Three times the estimated standard errors.
[c]) Assumed.
[d]) Tilt angle in the CNC plane between the C_3 axis of the CF_3 group and the N–C bond direction. The positive value corresponds to a tilt away from each other.
[e]) Torsional angle of the CF_3 groups; for $\tau = 0°$ the CF_3 groups are exactly staggered with respect to the opposite N–C bond.

Casper, B., Jakob, J., Minkwitz, R., Oberhammer, H.: Chem. Ber. **129** (1996) 653.