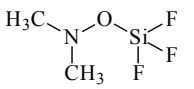
300 **$C_2H_6F_3NOSi$** ***N*-Methyl-*N*-[(trifluorosilyl)oxy]methanamine** **C_s** assumed

ED, *ab initio* and DFT calculations

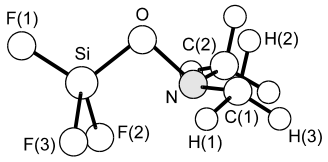
N,N-Dimethyl-*O*-trifluorosilylhydroxylamine



r_α	Å [a])
Si–F(1) [b])	1.566(4)
Si–F(2,3) [b]) [c])	1.564(2)
Si–O [c])	1.618(8)
O–N [c])	1.478(7)
N–C [c])	1.453(4)
C(1)–H(1) [b])	1.108(7)
C(1)–H(2) [b])	1.111(8)
C(1)–H(3) [b])	1.117(8)

θ_α	deg [a])
O–Si–F(1) [b])	104.1(10)
Si–O–N	94.3(9)
O–N–C [c])	107.1(6)
C–N–C [c])	114.1(9)
O–Si–F(2,3) [b])	111.8(10)
N–C(1)–H(1) [b])	107.6(8) [d])
N–C(1)–H(2) [b])	106.0(9)
N–C(1)–H(3) [b])	109.9(9)
C–N–C–H(1) [b])	–171.4(59)
C–N–C–H(2) [b])	71.1(59)
C–N–C–H(3) [b])	–50.9(61)
N–O–Si–F(2)	64.7(4)

The nozzle temperature was 20 °C.



[a]) Estimated standard errors.
[b]) Differences between the similar parameters were restrained to the values from MP2/6-311G** calculations.
[c]) Differences between the Si–O and Si–F(2,3) bond lengths, between the N–C and O–N bond lengths and between the C–N–C and O–N–C bond angles were restrained to the values from MP2/6-311G** calculations.
[d]) Value from MP2/6-311G** calculations was used as flexible restraint (SARACEN method).

Mitzel, N.W., Losehand, U., Wu, A., Cremer, D., Rankin, D.W.H.: J. Am. Chem. Soc. **122** (2000) 4471.