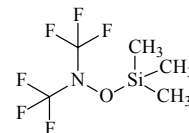


**654**      **C<sub>5</sub>H<sub>9</sub>F<sub>6</sub>NOSi**ED, *ab initio* and DFT  
calculations**1,1,1,1',1',1'-Hexafluoro-*N*-  
(trimethylsilyloxy)dimethylamine***N,N*-Bis(trifluoromethyl)-*O*-(trimethylsilyl)hydroxylamine1,1,1-Trifluoro-*N*-(trifluoromethyl)-*N*-  
[(trimethylsilyl)oxy]methanamine**C<sub>3</sub>**, assumed

$r_a$	Å <sup>a)</sup>
C–H	1.109(15)
C–F	1.328(2)
N–C	1.430[20] <sup>b)</sup>
N–O	1.450(18)
Si–O	1.724(8)
Si–C	1.858(4)

$\theta_a$	deg <sup>a)</sup>
C–Si–C	112.9(13)
Si–O–N	113.4(19)
O–N–C	102.2(12)
C–N–C	116.2(11)
F–C–F	107.7(2)
H–C–H	108.0 <sup>c)</sup>
tilt(SiMe <sub>3</sub> ) <sup>d)</sup>	6.2(29)
tilt(CF <sub>3</sub> ) <sup>e)</sup>	1.6 <sup>c)</sup>
$\tau$ (CF <sub>3</sub> ) <sup>f)</sup>	3.7(25)



Local C<sub>3v</sub> symmetry and no tilt were assumed for the methyl groups. Local C<sub>3v</sub> symmetry was also assumed for the Si(CH<sub>3</sub>)<sub>3</sub> and CF<sub>3</sub> groups. The Si–O bond is *syn* with respect to the nitrogen lone pair.

The nozzle was at room temperature.

<sup>a)</sup> Three times the estimated standard errors including a systematic error.

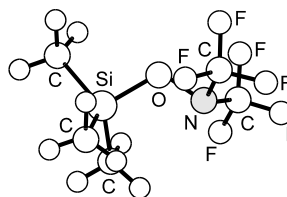
<sup>b)</sup> Not refined, but varied within the given range.

<sup>c)</sup> Estimated according to the results of HF/3-21G\* and B3LYP/6-31G\* calculations.

<sup>d)</sup> Angle between the C<sub>3</sub> axis of the Si(CH<sub>3</sub>)<sub>3</sub> group and the Si–O bond, away from the N atom.

<sup>e)</sup> Angle between the C<sub>3</sub> axis of the CF<sub>3</sub> group and the C–N bond in the CNC plane and toward the O atom.

<sup>f)</sup> Torsional angle of the CF<sub>3</sub> group around the C–N bond,  $\tau$ (CF<sub>3</sub>) = 0° when CF<sub>3</sub> group is staggered exactly with respect to the opposite N–C bond.



Hertel, T., Jakob, J., Minkwitz, R., Oberhammer, H.: Inorg. Chem. **37** (1998) 5092.