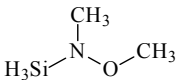


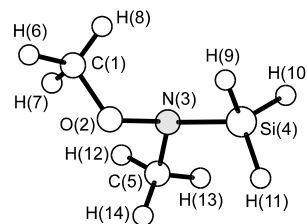
**318** **C<sub>2</sub>H<sub>9</sub>NOSi**ED, *ab initio*  
calculations***N*-Methoxy-*N*-methylsilanamine***N*,*O*-Dimethyl-*N*-silylhydroxylamine**C<sub>1</sub>**

$r_a$	Å <sup>a)</sup>	$\theta_a$	deg <sup>a)</sup>	
Si(4)–N(3)	1.742(1)	O(2)–N(3)–Si(4)	104.3(4)	
C(5)–N(3)	1.460(3)	O(2)–N(3)–C(5)	106.2(12)	
N(3)–O(2)	1.449(4)	N(3)–O(2)–C(1)	103.2(12)	
O(2)–C(1)	1.425(4)	N(3)–Si(4)–H(9)	107.3(13)	
Si(4)–H(9)	1.483(8)	N(3)–Si(4)–H(10)	106.3(14)	
Si(4)–H(10)	1.488(9)	N(3)–Si(4)–H(11)	109.8(6)	
Si(4)–H(11)	1.490(9)	O(2)–C(1)–H(6)	105.7(4)	
C(1)–H(6)	1.115(2)	O(2)–C(1)–H(7)	111.3(6)	
C(1)–H(7)	1.117(5)	O(2)–C(1)–H(8)	111.0(6)	
C(1)–H(8)	1.117(5)	N(3)–C(5)–H(12)	109.8(6)	
C(5)–H(12)	1.116(5)	N(3)–C(5)–H(13)	108.2(6)	
C(5)–H(13)	1.117(5)	N(3)–C(5)–H(14)	112.9(6)	
C(5)–H(14)	1.121(5)	Si(4)–N(3)–C(5) <sup>b)</sup>	121.8(5)	
		C(1)–O(2)–N(3)–Si(4)	127.9(17)	
		C(1)–O(2)–N(3)–C(5)	–102.4(15)	
		O(2)–N(3)–Si(4)–H(9)	–31.5(64)	
		O(2)–N(3)–Si(4)–H(10)	209.5(64)	
		O(2)–N(3)–Si(4)–H(11)	89.8(67)	
		O(2)–N(3)–C(5)–H(12)	73.7(114)	
		O(2)–N(3)–C(5)–H(13)	–167.6(111)	
		O(2)–N(3)–C(5)–H(14)	–47.5(118)	
		N(3)–O(2)–C(1)–H(6)	168.0(83)	
		N(3)–O(2)–C(1)–H(7)	–71.4(85)	
		N(3)–O(2)–C(1)–H(8)	49.4(88)	

The values from MP2/6-311G\*\* calculations were used as constraints in the flexibly restrained ED analysis. The configuration at the N atom was found to be steeply pyramidal. The nozzle temperature was 20 °C.

<sup>a)</sup> Uncertainties were unidentified, possibly estimated standard errors including a systematic error. The restraint uncertainties were estimated to be 0.005 Å for differences in distances, 1.5° for the angles, 0.5° for differences between angles (both to H atoms) and 3.0° for differences between torsional angles.

<sup>b)</sup> Dependent parameter.



Mitzel, N.W., Oberhammer, H.: Inorg. Chem. **37** (1998) 3593.