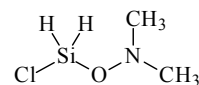


312 C₂H₈ClNOSiED, *ab initio*
calculations***N*-[(Chlorosilyl)oxy]-*N*-methylmethanamine**
(Dimethylaminoxy)chlorosilane
O-Chlorosilyl-*N,N*-dimethylhydroxylamine**C_s (*anti*)**
C₁ (*gauche*)

r_a	\AA^a		θ_a	deg^a	
	<i>anti</i>	<i>gauche</i>		<i>anti</i>	<i>gauche</i>
Si–O	1.654(4)	1.641(3)	Si–O–N	87.1(9)	104.7(11)
Si–Cl	2.050(4)	2.042(2)	O–Si–Cl	105.5(17)	109.4(9)
Si...N	2.160(7)	2.468(25)	O–Si–H(1)	112.0(11)	104.2(12)
N–O	1.475(6)	1.474(8)	O–Si–H(2)		111.7(13)
N–C(1)	1.460(5)	1.457(7)	O–N–C(1)	105.5(4)	104.5(5)
N–C(2)		1.460(7)	O–N–C(2)		104.8(5)
			C–N–C	109.8(10)	114.4(15)
			τ^b	180	72.9(28)

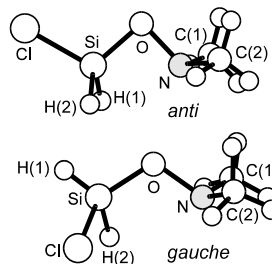
The molecule was found to exist as a mixture of *anti* (34(5) mol%) and *gauche* (66(5) mol%) conformers. The differences in the similar parameters were restrained flexibly by the values from MP2/6-311G** calculations.

The *gauche* conformer was estimated to be more stable by 0.17 kJ mol^{−1} than the *anti* conformer by the MP2/6-311G** method.

The nozzle temperature was 20 °C.

^a) Uncertainties were unidentified, possibly estimated standard errors.

^b) Cl–Si–O–N torsional angle, $\tau = 0^\circ$ for the *syn* position.



Mitzel, N.W., Losehand, U.: J. Am. Chem. Soc. **120** (1998) 7320.