

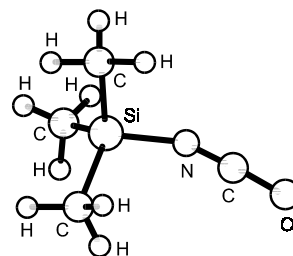
1793
ED

C₄H₉NOSi

Trimethylsilyl isocyanate

apparently C₃
(see remarks)
O=C=N-Si(CH₃)₃

r_a	\AA^a	θ_a	deg ^{a)}
C-H	1.099(5)	H-C-Si	109.0(9)
C=O	1.176(10)	C-Si-C	108.8(25)
N=C	1.202(16)	Si-N=C	156.9(30)
Si-N	1.740(4)	N=C=O	165.8(36)
Si-C	1.864(2)	twist (CH ₃) ^{b)}	26.9(35)
		C-Si-N=C	60 ^{c)}
		Si-N=C=O	0 ^{c)}
		tilt (Si(CH ₃) ₃) ^{d)}	5.7(24)



The apparent bends at N and C atoms, the twist about the Si-N bond and the tilt of the Si(CH₃)₃ group are to be ascribed to the effects of the large-amplitude, low-frequency bend at the N atom. See SiH₃NCO which is known to have a quasilinear skeleton. The measurements were made at room temperature.

^{a)} Uncertainties are unidentified, possibly estimated standard errors.

^{b)} Twist angle of the methyl groups from the position giving the Si(CH₃)₃ group C_{3v} symmetry in an (assumed) concerted fashion.

^{c)} Assumed.

^{d)} Away from the C=O group.

Cradock, S., Huntley, C.M., Durig, J.R.: J. Mol. Struct. **127** (1985) 319.

MW

effectively C_{3v}

r_0	\AA	θ_0	deg
C-H	1.093 ^{a)}	H-C-H	107.93 ^{a)}
C=O	1.179 ^{a)}	C-Si-C	110.17 ^{a)}
N=C	1.15 ^{a)}	Si-N=C	180
Si-N	1.690(50)		
Si-C	1.86 ^{a)}		
Si...(N)...C	2.845(20)		

^{a)} Assumed.

Careless, A.J., Green, M.C., Kroto, H.W.: Chem. Phys. Lett. **16** (1972) 414.