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ED

C₄H₉NSSi

Trimethylsilyl isothiocyanate

essentially C₃
S=C=N-Si(CH₃)₃

r_a	Å ^{a)}	θ_a	deg ^{a)}
Si-N	1.743(6)	N-Si-C	108.8(7)
Si-C	1.866(3)	H-C-Si	108.9(8)
C-H	1.100(5)	Si-N=C	158.2(10)
N=C	1.191(6)	twist (CH ₃) ^{b) c)}	-21(8)
C=S	1.587(4)	twist (Si(CH ₃) ₃) ^{b) d)}	34(4)
		Si-N=C=S	0 ^{e)}
		tilt (Si(CH ₃) ₃)	0 ^{e)}

The Si(CH₃)₃ and CH₃ groups were assumed to have C₃ and C_{3v} local symmetry, respectively. The SiNCS skeleton is likely to be pseudolinear; a small apparent deviation from linearity ($\approx 4^\circ$) in the NCS group is probably caused by the shrinkage effect. The nozzle was at room temperature.

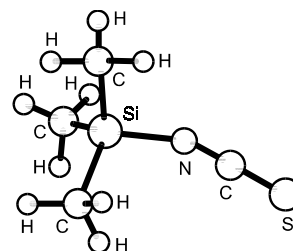
^{a)} Estimated standard errors including a systematic error.

^{b)} For a zero twist the groups are all in staggered positions.

^{c)} A positive twist represents a clockwise rotation viewed from C to Si.

^{d)} A positive twist represents a clockwise rotation viewed from Si to N.

^{e)} Assumed.



Huntley, C.M., Rankin, D.W.H., Robertson, H.E.: J. Mol. Struct. **156** (1987) 103.