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C₄H₇NS

Isopropyl isothiocyanate

C₁ (*skew*)
S=C=N-CH(CH₃)₂

r_a	Å ^{a)}	θ_a	deg ^{a)}
C-N	1.459(13)	N-C-C	110.4(10)
C-C	1.528(7)	C-C-C	115.7(13)
N=C	1.201(6)	C-N=C	135.9(17)
C=S	1.598(5)	N=C=S	166(3) ^{b)}
C(1,3)-H	1.116(5)	C(2)-C-H	107 ^{c)}
C(2)-H	1.09 ^{c)}	N-C-H	105 ^{c)}
		C(1)-C(2)-N=C ^{d)}	115(6)

The data are consistent with the presence of a single *skew* conformer. The structure was consistent with the limited information available from microwave studies.

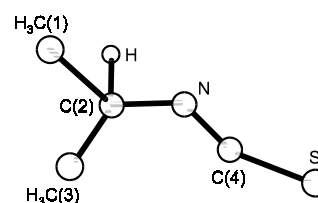
It was assumed that the two CH₃ groups were identical with local C_{3v} symmetry about the C-C bonds, and that the N and unique H atoms were in the plane bisecting the C-C-C angle. The measurements were made at room temperature.

^{a)} Unidentified, possibly estimated standard errors.

^{b)} The C=S bond was assumed to be coplanar with the C(3)-C-N=C atoms and *trans* to the C(2)-N bond.

^{c)} Assumed.

^{d)} Zero position for the *syn* conformation.



Cradock, S., Sullivan, J.F., Durig, J.R.: J. Mol. Struct. **140** (1986) 199.