

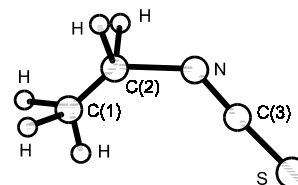
1223
ED, MW

C₃H₅NS

Ethyl isothiocyanate

C_s (*cis*)
H₃C–CH₂–N=C=S

r_{av}	\AA^a	θ_{av}	deg ^{a)}
C–N	1.438(7)	C–C–N	111.0(8)
C–H	1.105(8)	C–N=C	147.4(20)
C–C	1.520(8)	N=C=S ^{b)}	184.5(30)
N=C	1.187(5)	C(2)–C(1)–H	109.2(28)
C=S	1.580(4)		



A single *cis* conformation is compatible with the ED and MW data. Rotational constants were extrapolated to remove the zero-point effect of the torsion about the C(2)–N axis.

The temperature was not stated, probably room temperature.

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

^{b)} The direction of the bend was not defined in the original paper, possibly bent away from the CH₃ group.

Cradock, S., Durig, J.R., Sullivan, J.F.: J. Mol. Struct. **131** (1985) 121.