

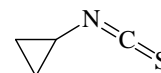
1607
MW, ED

C₄H₅NS

Cyclopropyl isothiocyanate

C_s (*cis*)
C_s (*trans*)

r_{av}	Å ^{a)}	θ_{av}	deg ^{a)}
C(1)–C(2)	1.520(3) ^{b)}	H–C–H	115.0 ^{b) c)}
C(2)–C(3)	1.515(3) ^{b)}	C(2)–C(1)–H	117.35 ^{b) c)}
C–H(<i>trans</i>)	1.072(5) ^{b)}	N=C=S	177.7(20) ^{b)}
C–H(<i>cis</i>)	1.072(5) ^{b)}		<i>cis</i> <i>trans</i>
C(1)–H(<i>sec</i>)	1.072(5) ^{b)}	C(1)–N=C	150.8(17)
N=C	1.193(3) ^{b)}	C(2)–C(1)–N	116.2(15)
C=S	1.574(3) ^{b)}		149.1(15)
	<i>cis</i> <i>trans</i>		118.9(6)
C(1)–N	1.413(5)		



The molecule exists as a mixture of *trans* (72(5)%) and *cis* conformers.

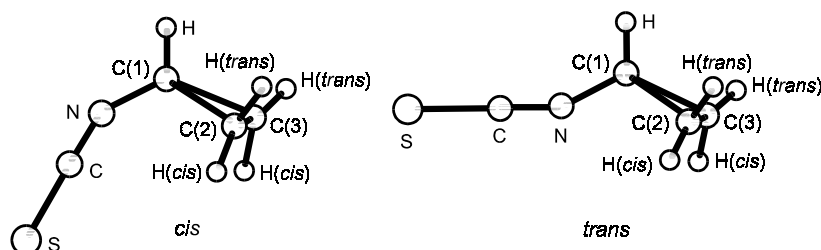
The effect of zero-point torsional motion was removed by extrapolation from the constants for the ground and first excited torsional states.

The nozzle temperature was 35 °C.

^{a)} Estimated uncertainties.

^{b)} Assumed to be the same in the two conformers.

^{c)} Assumed.



Durig, J.R., Sullivan, J.F., Berry, R.J., Craddock, S.: J. Chem. Phys. **86** (1987) 4313.

Durig, J.R., Nease, A.B., Berry, R.J., Sullivan, J.F., Li, Y.S., Wurrey, C.J.: J. Chem. Phys. **84** (1986) 3663.