

1139
ED

C₃H₄ClN

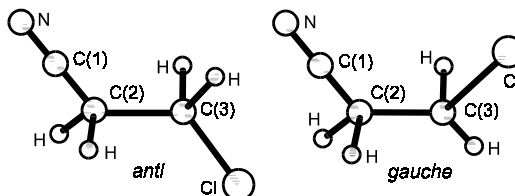
3-Chloropropionitrile

C_s (*anti*)
C₁ (*gauche*)
ClH₂C–CH₂–C≡N

r_a	Å ^{a)}	θ_α	deg ^{a)}
C–H (average)	1.097(17) ^{b)}	C–C–C	110.6 (10) ^{b)}
C≡N	1.160(4) ^{b)}	C–C–Cl	110.8 (8) ^{b)}
C(1)–C(2)	1.478(11) ^{b)}	C–C–H	109.47 ^{b) c)}
C(2)–C(3)	1.515(16) ^{b)}	C–C≡N	180.0 ^{b) c)}
C–Cl	1.784(5) ^{b)}	ϕ (<i>gauche</i>) ^{d)}	71(11)
		ϕ (<i>anti</i>) ^{d)}	180.0 ^{c)}

The molecule exists as a mixture of *anti* and *gauche* (36(23)%) conformers.
The nozzle temperatures was 74 °C.

- ^{a)} Twice the estimated standard errors including a systematic error.
^{b)} Conformational average.
^{c)} Assumed.
^{d)} Torsion angle Cl–C–C–C.



Stavnebrekk, P.J., Stølevik, R., Seip, R., Volden, H.V., Gundersen, S.: Acta Chem. Scand., Ser. A **42** (1988) 398.

MW

C_s (*anti*)

r_0	Å	θ_0	deg
C–H	1.097 ^{a)}	C–C–C	109.7(11)
C≡N	1.160 ^{a)}	C–C–Cl	108.4(11)
C(1)–C(2)	1.468(10)	C–C–H	108.7 ^{a)}
C(2)–C(3)	1.544(10)	C–C≡N	180 ^{a)}
C–Cl	1.789(12)		

- ^{a)} Assumed.

Xu, S.L., Harmony, M.D.: J. Mol. Struct. **274** (1992) 115.