

1134 **C₃H₄BrN**
ED, MM calculations

3-Bromopropionitrile

C_s (*anti*)
C₁ (*gauche*)
BrH₂C–CH₂–C≡N

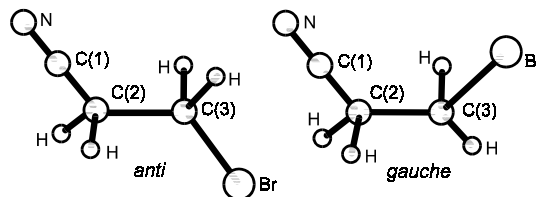
r_a	\AA^a		θ_α	deg^a	
	<i>gauche</i>	<i>anti</i>		<i>gauche</i>	<i>anti</i>
C–H (average)	1.119(31)	1.120(31)	C–C–C	112.6(13)	111.3(13)
C≡N	1.156(11)	1.148(11)	C–C–Br	112.6(11)	111.2(11)
C(1)–C(2)	1.490(22)	1.488(22)	C–C–H	109.47 ^b	109.47 ^b
C(2)–C(3)	1.517(27)	1.509(27)	C–C≡N	180.0 ^b	180.0 ^b
C–Br	1.944(5)	1.941(8)	ϕ^c	65(8)	180 ^b

The molecule exists as a mixture of *anti* and *gauche* (37(17)%) conformers.
The nozzle temperatures were 85 and 98 °C.

^a) Twice the estimated standard errors
including a systematic error.

^b) Assumed.

^c) Torsion angle Br–C–C–C.



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

MW

r_0	\AA	θ_0	deg
C–H	1.097 ^a	C–C–C	110.7(11)
C≡N	1.160 ^a	C–C–Br	106.1(11)
C(1)–C(2)	1.469(10)	C–C–H	108.7 ^a
C(2)–C(3)	1.544(10)	C–C≡N	180 ^a
C–Br	1.969(14)		

C_s (*anti*)

^a) Assumed.

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