

1624 **C₄H₆BrN**
ED, MM calculations

4-Bromobutanenitrile
4-Bromobutyronitrile

C_s (AA)
C₁ (other conformers)
BrH₂C–CH₂–CH₂–C≡N

r_a	Å ^{a)}	θ_α	deg ^{a)}			
C–H	1.136(22)	C(1)–C(2)–C(3)	111.8(19)			
C≡N	1.146(10)	C(2)–C(3)–C(4)	111.1(21)			
C(1)–C(2)	1.472(21)	C(3)–C(4)–Br	110.8(8)			
C(2)–C(3)	1.492(29) ^{b)}	C–C–H	109.5 ^{c)}			
C(3)–C(4)	1.546(17) ^{b)}	C–C≡N	180 ^{c)}			
C–Br	1.955(8)	GG		AG	GA	
		τ_1 (C–C–C)	129.9(15)	0.0 ^{c)}	118.1 ^{d)}	
		τ_2 (C–C–Br)	113.1(9)	115.1 ^{d)}	0.0 ^{d)}	

The molecule exists as a mixture of GG (59(3)%), AG (20(28)%) and GA (20(15)%) conformers. The conformer having all heavy atoms planar (AA) may be present in a small amount. The C–CH₂Br group was assumed to have C_s symmetry.

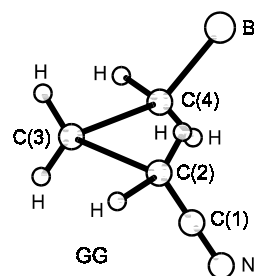
The nozzle temperature were 110 and 120 °C.

^{a)} Twice the estimated standard errors including the scale error.

^{b)} These distances seem to contain significant systematic errors due to strong correlation; the C(2)–C(3) and C(3)–C(4) distances are both likely to be 1.53(2) Å.

^{c)} Assumed.

^{d)} Value from molecular mechanics calculations.



Stavnebrekk, P.J., Stølevik, R.: J. Mol. Struct. **196** (1989) 269.