

1628 **C₄H₆ClN**
ED, MM calculations

4-Chlorobutanenitrile
4-Chlorobutyronitrile

C_s (AA)
C₁ (other conformers)
ClH₂C–CH₂–CH₂–C≡N

r_a	Å ^{a)}	θ_α	deg ^{a)}			
C–H	1.114(20)	C(1)–C(2)–C(3)	110.8(15)			
C≡N	1.145(10)	C(2)–C(3)–C(4)	113.7(20)			
C(1)–C(2)	1.475(15)	C(3)–C(4)–Cl	111.2(10)			
C(2)–C(3)	1.520(20)	C–C–H	109.5 ^{b)}			
C(3)–C(4)	1.530(15)	C–C≡N	180 ^{b)}			
C–Cl	1.790(8)	GG	AG	GA		
		τ_1 (C–C–C–C)	112.5(15)	0.0 ^{b)}	117.9 ^{c)}	
		τ_2 (C–C–C–Cl)	121.0(9)	116.4 ^{c)}	0.0 ^{b)}	

The molecule exists as a mixture of GG (63(24)%), AG (29(18)%) and GA (8(10)%) conformers. The conformer having all heavy atoms planar (AA) may be present in a small amount. The C–CH₂Cl group was assumed to have C_s symmetry. The nozzle temperature were 105 and 110 °C.

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

^{b)} Assumed.

^{c)} Value from molecular mechanics calculations.

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

