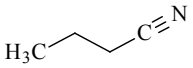
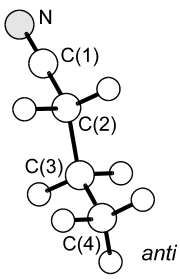
553 **C_4H_7N** **Butanenitrile** **C_1** (*gauche*)
ED, *ab initio* calculations Butyronitrile **C_s** (*anti*)

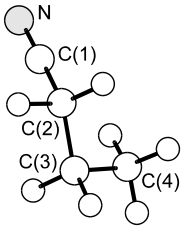


r_a	Å [a])	θ_α	deg [a])
C≡N	1.158(1)	N≡C(1)–C(2)	180.0 [b])
C(1)–C(2)	1.462(4)	C(1)–C(2)–C(3)	113.0(5)
C(2)–C(3)	1.534(2)	C(2)–C(3)–C(4)	112.3(6)
C(3)–C(4)	1.523 [c])	C(1)–C(2)–H [d])	109.7(9)
C–H [d])	1.105(2)	τ [e])	61.1(13)

The molecule was found to exist as a mixture of *gauche* (75.1(60)%) and *anti* (24.9%) conformers. Minor differences in the bond lengths and angles of the conformers were assumed at the values from MP2/6-31G* calculations. The parameters are listed for the *gauche* conformer.
The nozzle temperature was 295 K.



anti



gauche

[a]) Unidentified, possibly estimated standard errors.
[b]) Assumed at the value from MP2/6-31G* calculations.
[c]) Assumed.
[d]) Minor differences in the various C–H bond lengths and C–C–H bond angles were assumed at the values from MP2/6-31G* calculations.
[e]) Torsional angle C(1)–C(2)–C(3)–C(4), $\tau = 180°$ for the *anti* conformation.

Trætteberg, M., Bakken, P., Hopf, H.: J. Mol. Struct. **556** (2000) 189.