

1550
ED

C₄H₄N₂

Succinonitrile
Butanedinitrile
1,2-Dicyanoethane

C_{2h} (*anti*)
C₂ (*gauche*)
N≡C-CH₂-CH₂-C≡N

r_g	Å ^{a)}	θ_α	deg ^{a)}
C(1)-C(2)	1.561(6)	C-C-C	110.4(5)
C(1)-C(3)	1.465(2)	C-C-H	107.9(19)
C≡N	1.161(2)	τ (<i>gauche</i>) ^{b)}	75(8)
C-H	1.092(10)		

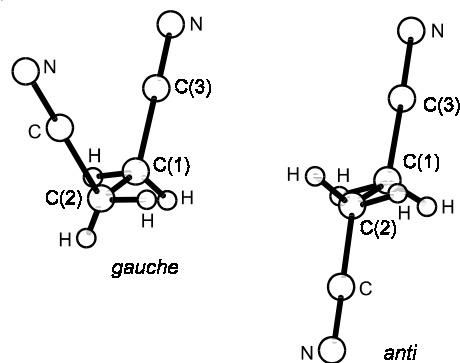
The more stable conformer (74(7)%) in the vapour is *anti*.

$\Delta E = E(\textit{gauche}) - E(\textit{anti}) = 1.5(3) \text{ kcal mol}^{-1}$
and $\Delta S = S(\textit{gauche}) - S(\textit{anti}) = 1.4 \text{ cal mol}^{-1} \text{ K}^{-1}$.

The C-C≡N fragment was found to be linear.
The nozzle temperature was 170 °C.

^{a)} Estimated standard errors.

^{b)} C-C-C-C torsional angle from the *syn* position.



Fernholt, L, Kveseth, K.: Acta Chem. Scand. Ser. A **33** (1979) 335.