

1551
ED

C₄H₄N₂

Ethylene diisocyanide
1,2-Diisocyanoethane

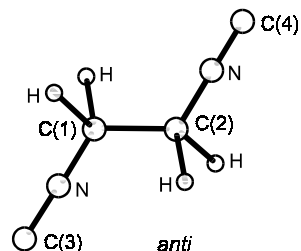
C_{2h} (*anti*)
C₂ (*gauche*)
C=N-CH₂-CH₂-N=C

r_a	Å ^{a)}	θ_α	deg ^{a)}
C(3,4)=N	1.172(3)	C-C-N (<i>anti</i>)	110.1(7)
N-C(1,2)	1.424(4)	C-C-N (<i>gauche</i>)	111.9(10)
C-C	1.529(6)	H-C-H	105.5(43)
C-H	1.123(15)	τ^b	68(5)

The molecule exists as a mixture of the low-energy *anti* form (57(9) %) and the higher-energy *gauche* form. The nozzle temperature was 150 °C.

^{a)} Estimated standard errors.

^{b)} Dihedral angle N-C-C-N of the *gauche* conformer from the *syn* position.



Schrumpf, G., Trättelberg, M., Bakken, P., Seip, R.: J. Mol. Struct. **197** (1989) 339.