

1609
ED

C₄H₅N₃

1-Azido-2-butyne

C₁ (*gauche*)
H₃C–C≡C–CH₂–N=N≡N

r_a	Å ^{a)}	θ_α	deg ^{a)}
N(2)≡N(3)	1.142(5)	N=N≡N	174(5) ^{b)}
N(1)=N(2)	1.240(6)	N=N–C	116.5(14)
N–C	1.474(15)	N–C–C	113.7(16)
C(1)–C(2)	1.468(5)	C(2)–C(1)–H	110 ^{c)}
C(2)≡C(3)	1.208(6)	N–C–H	110 ^{c)}
C(3)–C(4)	1.460 ^{c)}	C(3)–C(4)–H	111 ^{c)}
C–H	1.11(3)	C(1)–C(2)≡C(3)	180 ^{c)}
		$\tau^d)$	37(10)

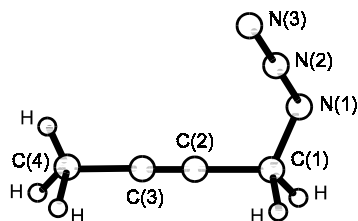
The molecule exists in only one conformation, *gauche* around the C–N bond.
The nozzle temperature was 293 K.

^{a)} Three times the estimated standard errors including a systematic error.

^{b)} The NNN linkage is bent *trans* to the C–N bond.

^{c)} Assumed.

^{d)} Dihedral angle C(2)–C(1)–N(1)=N(2) from the *syn* position.



Nielsen, C.J., Priebe, H., Salzer, R., Schei, S.H.: J. Mol. Struct. **162** (1987) 41.