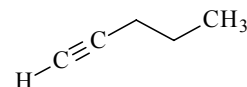


**646**      **C<sub>5</sub>H<sub>8</sub>**ED, *ab initio*  
calculations**1-Pentyne****C<sub>1</sub>** (*gauche*)**C<sub>s</sub>** (*anti*)

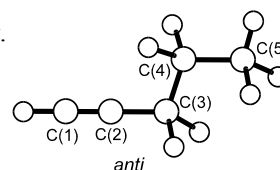
$r_a$	Å <sup>a)</sup>	$\theta_a$	deg <sup>a)</sup>
C≡C	1.2220(7)	C(1)≡C(2)–C(3)	180.0 <sup>b)</sup>
C(2)–C(3)	1.4604(30)	C(2)–C(3)–C(4)	113.5(4)
C(3)–C(4)	1.5372(15)	C(3)–C(4)–C(5)	111.7(5)
C(4)–C(5)	1.5262 <sup>c)</sup>	C(2)–C(3)–H	110.0(5) <sup>c)</sup>
C(3)–H	1.1072(9) <sup>c)</sup>	$\tau^d$	64.9(11)



The molecule was found to exist as a mixture of *gauche* (68.6(45)%) and *anti* (31.4%) conformers. Differences between the parameters of two conformers were assumed at the values from MP2/6-31G\* calculations.

The parameters are listed here for the *gauche* conformer.

The nozzle was at 297 K.



<sup>a)</sup> Uncertainties were not identified, possibly estimated standard errors.

<sup>b)</sup> Assumed.

<sup>c)</sup> Difference between the C(3)–C(4) and C(4)–C(5) bond lengths and those between the various C–H bond lengths and C–C–H angles were assumed at the values from MP2/6-31G\* calculations.

<sup>d)</sup> Torsional angle C(2)–C(3)–C(4)–C(5), zero degree for the *syn* position.

Trætteberg, M., Bakken, P., Hopf, H.: J. Mol. Struct. **509** (1999) 213.

[II/25D \(3, 1988\)](#)