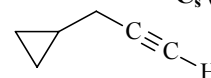


**730**      **C<sub>6</sub>H<sub>8</sub>**  
ED, MW, *ab initio*  
and DFT calculations

**2-Propynylcyclopropane**

**C<sub>1</sub>** (*gauche*)  
**C<sub>s</sub>** (*syn*)



$r_{av}$	$\text{\AA}^a)$		$\theta_{av}$	$\text{deg}^a)$	
	<i>syn</i>	<i>gauche</i>		<i>syn</i>	<i>gauche</i>
C(1')-C(2')	1.509(9)	1.509(9)	C(1')-C(2')-C(3') <sup>b)</sup>	59.8(1)	59.7(3)
C(1')-C(3')	1.509(9)	1.506(14)	C(2')-C(1')-C(3') <sup>b)</sup>	60.3(2)	60.4(3)
C(2')-C(3') <sup>b)</sup>	1.517(14)	1.516(14)	C(2')-C(1')-C(1) <sup>b)</sup>	121.0(7)	118.9(17)
C(1')-C(1)	1.518(28)	1.517(28)	H-C(2',3')-H <sup>b)</sup>	115.5(24)	117.2(24)
C(1)-C(2)	1.450(13) <sup>b)</sup>	1.450(13)	H-C(1)-H <sup>b)</sup>	106.9(33)	111.6(33)
C(2)≡C(3)	1.215(3)	1.215(3)	C(1')-C(1)-C(2) <sup>b)</sup>	114.1(8)	114.1(8)
C(3)-H <sup>b)</sup>	1.065(5)	1.065(5)	C(1)-C(2)≡C(3) <sup>b)</sup>	180	180
C-H (ring) <sup>c)</sup>	1.107(6) <sup>b)</sup>	1.107(6)	C(2)≡C(3)-H <sup>b)</sup>	180	180
C(1)-H <sup>b)</sup>	1.095(5)	1.095(5)	$\phi_1^b)^d)$	120.2(25)	121.7(33)
			$\phi_2^c)$	126.5(9)	123.5(26)
			C(1)-C(1')-C(2')-C(3')	110.4(19)	107.7(24)
			C(2')-C(1')-C(1)-C(2)	35.9(4)	149.6(16)
			C(2)-C(1)-C(1')-H <sup>b)</sup>	180.0	61.3(17)

According to the results of combined ED and MW analysis, the molecule exists as a mixture of *gauche* (58(11)%) and *syn* (42(11)%) conformers, the latter being estimated to be more stable by *ca.* 0.92 kJ mol<sup>-1</sup>, in fair agreement with quantum chemical calculations. The nozzle temperature was 0 °C.

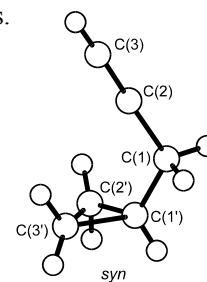
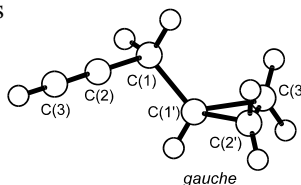
<sup>a)</sup> 2.5 times the estimated standard errors including errors propagated from assumed parameters for refined parameters, propagated errors for dependent parameters and estimated errors for assumed parameters.

<sup>b)</sup> Assumed or dependent parameter.

<sup>c)</sup> Average value.

<sup>d)</sup> Angle between the H-C(1') bond and the ring plane.

<sup>e)</sup> Angle between the C(1)-C(1') bond and the ring plane.



Dakkouri, M., Typke, V.: J. Mol. Struct. **550-551** (2000) 349.

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