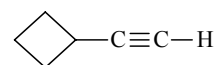


732 **C₆H₈**
ED, MW, *ab initio*
and DFT calculations

Ethynylcyclobutane

C_s (equatorial)
C_s (axial)



r_{av}	$\text{\AA}^a)$		θ_{av}	$\text{deg}^a)$	
	equatorial	axial		equatorial	axial
C(1)–C(2)	1.555(16)	1.560(24)	C(2)–C(1)–C(4)	88.0(16) ^{b)}	88.0(16)
C(2)–C(3)	1.549(16) ^{b)}	1.549(16)	C(1)–C(2)–C(3) ^{b)}	88.2(11)	87.8(29)
C(1')–C(1)	1.452(8)	1.455(13)	C(2)–C(3)–C(4) ^{b)}	88.4(10)	88.8(16)
C(1')≡C(2')	1.211(2) ^{b)}	1.211(2)	C(1')–C(1)–H ^{b)}	107.7(17)	107.7(17)
C(2')–H ^{b)}	1.066(7)	1.066(7)	C(2)–C(1)–C(1') ^{b)}	118.9(7)	114.1(31)
C–H (ring) ^{c)}	1.095(2) ^{b)}	1.095(2)	C(1')≡C(2')–H ^{b)}	180.0	180.0
			C(1)–C(1')≡C(2') ^{b)}	178.0(17)	178.0(17)
			H–C–H ^{b)} ^{c)}	110.0(17)	110.0(17)
			C(2)–C(1)–H ^{b)}	111.1(25)	116.1(44)
			C(1)–C(2)–H(1) ^{b)}	116.9(16)	117.0(19)
			C(1)–C(2)–H(2) ^{b)}	113.2(17)	113.3(20)
			C(3)–C(2)–H(1) ^{b)}	113.7(24)	113.8(27)
			C(3)–C(2)–H(2) ^{b)}	113.4(23)	113.5(27)
			C(2)–C(3)–H(3) ^{b)}	115.5(14)	115.4(14)
			C(2)–C(3)–H(4) ^{b)}	113.0(14)	112.9(14)
			$\phi^d)$	29.2(99)	28.5(42)
			$\phi^e)$	132.3(17)	124.6(50)

According to the results of combined ED and MW analysis, the molecule exists as a mixture of axial (16(13)%) and equatorial (84(13)%) conformers, the latter being more stable by *ca.* 4.0 kJ mol^{−1}.

The nozzle temperature was 0 °C.

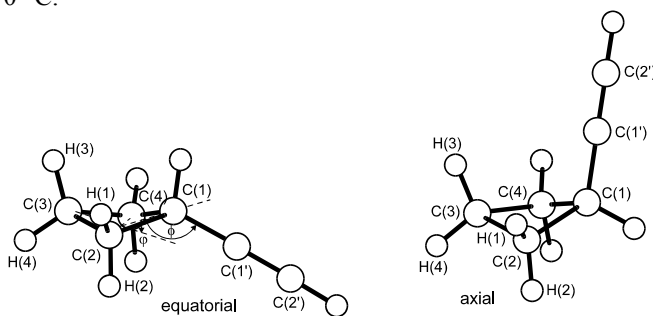
^{a)} 2.5 times the estimated standard errors including errors propagated from assumed parameters for refined parameters, propagated errors for dependent parameters, and estimated errors for assumed parameters.

^{b)} Assumed or dependent parameter.

^{c)} Average value.

^{d)} Puckering angle, see figure.

^{e)} Angle between the C(1)–C(1') bond and the C(2)–C(1)–C(4) plane, see figure.



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

[II/25D \(3, 2267\)](#)