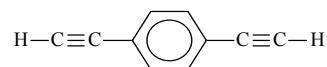


881 **C₁₀H₆**
ED, *ab initio*
calculations

1,4-Diethynylbenzene
p-Diethynylbenzene

D_{2h} (large-amplitude bending
motions of the ethynyl groups)



r_g	Å ^{a)}	θ^b	deg ^{a)}
C(1)–C(2)	1.408 ^{c)}	C(2)–C(1)–C(6)	119.2(2)
C(2)–C(3)	1.392 ^{c)}	C(3)–C(2)–H	120.3 ^{d)}
C(1)–C(7)	1.431(3)	φ^e	6.8(12)
C–C(ring) ^{f)}	1.402(3)		
C(7)≡C(9)	1.211(3)		
C–H(ring)	1.101 ^{c)} ^{g)}		
C(9)–H	1.081 ^{c)}		

Based on spectroscopic information on low-frequency mode, *ca.* 90 cm^{−1}, the ED data were approximated by a dynamical model consisting of a mixture of rigid conformers, differing only in the extent of the symmetric out-of-plane bending of the C≡C–H groups.

The nozzle was at *ca.* 405 K.

^{a)} Estimated total errors.

^{b)} Unidentified, probably θ_a .

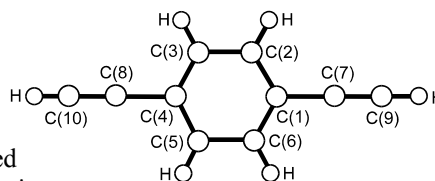
^{c)} Differences [C(2)–C(3)] – [C(1)–C(2)] and [C–H(ring)] – [C(9)–H] were assumed at the values from MP2(fc)/6-31G* calculations.

^{d)} Assumed at the value from MP2(fc)/6-31G* calculations.

^{e)} Average angle between the ring plane and the ethynyl group.

^{f)} Mean value.

^{g)} Assumed at the value for benzene from the literature.



Domenicano, A., Arcadi, A., Ramondo, F., Campanelli, A.R., Portalone, G., Schultz, G., Hargittai, I.: J. Phys. Chem. **100** (1996) 14625.