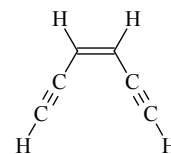


699
MW C_6H_4 *cis*-Hex-3-ene-1,5-diyne (1)
(*Z*)-3-Hexene-1,5-diyne C_{2v}

r_0	\AA^a	θ_0	deg a
C(3)=C(4)	1.346(3)	C(3)=C(4)–C(5)	123.9(2)
C(2)–C(3)	1.421(3)	C(3)–C(2)≡C(1)	179.0(2)
C(1)≡C(2)	1.213(3)	C(2)≡C(1)–H	179.6(5) ^{b)}
C(3,4)–H	1.097(5)	C(3)=C(4)–H	120.9(5)
C(1,6)–H	1.055(5)		

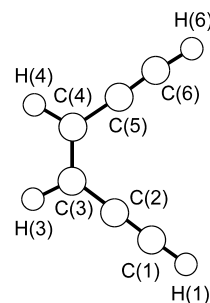


r_s	\AA^a	θ_s	deg a
C(3)=C(4)	1.345(3)	C(3)=C(4)–C(5)	123.5(2)
C(2)–C(3)	1.435(3)	C(3)–C(2)≡C(1)	178.0(2)
C(1)≡C(2)	1.198(3)	C(2)≡C(1)–H	178.9(5) ^{b)}
C(3,4)–H	1.099(5)	C(3)=C(4)–H	120.8(5)
C(1,6)–H	1.057(5)		

r_e	\AA^c	θ_e	deg c
C(3)=C(4)	1.347(3)	C(3)=C(4)–C(5)	123.9(2) ^{a)}
C(2)–C(3)	1.421(3)	C(3)–C(2)≡C(1)	178.8(2) ^{a)}
C(1)≡C(2)	1.208(3)	C(2)≡C(1)–H	179.4(5) ^{b)}
C(3,4)–H	1.080(5) ^{a)}	C(3)=C(4)–H	118.6(5)
C(1,6)–H	1.062(5) ^{a)}		

Atom	$ a_s [\text{\AA}]$	$ b_s [\text{\AA}]$
C(1,6)	0.6724	1.1122
C(2,5)	1.4643	0.0838
C(3,4)	2.1608	1.0582
H(1,6)	1.2354	2.0554
H(3,4)	2.7594	1.9290

The C(1)–C(6) distance (4.32 Å), which has been viewed as a critical parameter governing reactivity in the Bergman cyclization, is notably longer than an earlier, widely publicized value (4.12 Å).



^{a)} Uncertainties were not estimated in the original paper.

^{b)} Distorted away from each other.

^{c)} Vibration-rotation constants were calculated using the SDQ-MBPT(4)/TZ2P method.

McMahon, R.J., Halter, R.J., Fimmen, R.L., Wilson, R.J., Peebles, S.A., Kuczkowski, R.L., Stanton, J.F.: J. Am. Chem. Soc. **122** (2000) 939.