

1613 **C₄H₆**
 ED, *ab initio* calculations
 (MP2/6-31G* etc.)

1-Butyne



r_a	Å ^{a)}	θ_α	deg ^{a)}
C(1)≡C(2)	1.217(1)	C(2)–C(3)–C(4)	111.9(4)
C(2)–C(3)	1.457(3)	C(1)≡C(2)–C(3) ^{b)}	179.2(14)
C(3)–C(4)	1.544(4)	C(2)–C(3)–H	111.9(23)
C(1)–H	1.021(8)	C(3)–C(4)–H(1)	114.4(20)
C(3,4)–H	1.090(2)	C(1)–C(2)–C(3)–H	±61.9(24)
		C(2)–C(3)–C(4)–H(2,2')	±63.8(60)

The experiments were done at room temperature.

^{a)} Estimated standard errors.

^{b)} Bent away from the methyl group if $\theta < 180^\circ$.

Bastiansen, O., Bakken, P., Kloster-Jensen, E.,
 Samdal, S., Trætteberg, M.: J. Mol. Struct.
352/353 (1995) 77.

