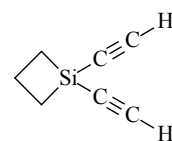


806 **C₇H₈Si**ED, *ab initio* and DFT
calculations**1,1-Diethynylsilacyclobutane****C_s**

r_a	Å ^{a)}	θ_a	deg ^{a)}
Si–C(ring)	1.874(2)	C(1')–Si–C(1'')	106.5(6)
Si–C(1')	1.817(1)	C(2)–Si–C(4)	79.2(6)
C(1')≡C(2')	1.209(1)	Si–C(2)–C(3)	86.8 ^{b)}
C–C	1.563(2)	C–C–C	99.6 ^{b)}
C(2')–H	1.058 ^{b)}	H–C–H	108.6 ^{b)}
C–H (ring)	1.091 ^{b)}	δ^c	3.1(15)
		φ^d	30.0(15)



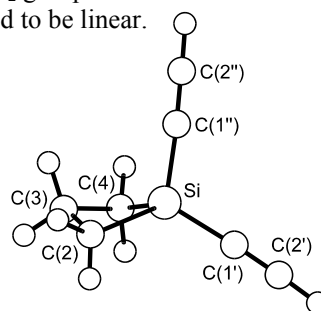
The Si–C≡C–H fragments were assumed to be equal. The CH₂ groups were assumed to have local C_{2v} symmetry and ethynyl fragments were assumed to be linear. The nozzle was at room temperature.

^{a)} Three times the estimated standard errors.

^{b)} Assumed at the values from theoretical calculations.

^{c)} Outward bending of the Si–C≡C chains.

^{d)} Puckering angle, *i.e.*, dihedral angle between the C(2)SiC(4) and C(2)C(3)C(4) planes.



Dakkouri, M., Grosser, M.: J. Mol. Struct. **610** (2002) 159.