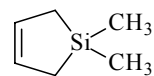


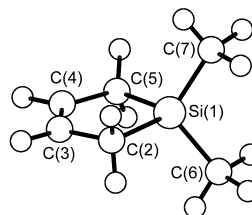
753 **C₆H₁₂Si**ED, *ab initio*
calculations**1,1-Dimethylsilacyclopent-3-ene**1,1-Dimethyl-2,5-dihydro-1*H*-silole**C_{2v}** assumed

r_g	Å ^{a)}	θ_α	deg ^{a)}
Si–C(2)	1.888(3)	Si–C(2)–C(3)	102.3(4)
Si–C(6)	1.867(3)	C(2)–C(3)=C(4)	119.6(4)
C(2)–C(3)	1.503(9)	C(2)–Si–C(5)	96.3(5)
C(3)=C(4)	1.335(14)	C(6)–Si–C(7)	110.6 ^{b)}
C–H (average)	1.109(7)	H–C(2)–H	106.1 ^{b)}
		C(4)=C(3)–H	120.7 ^{b)}
		Si–C(6)–H	111.4 ^{b)}

Local C_{3v} symmetry was assumed for methyl groups.
The nozzle temperature was 25 °C.

^{a)} Twice the estimated standard errors.

^{b)} Assumed at the value from MP2/6-311+G(d) calculations.



Aarset, K., Page, E.M., Rice, D.A.: J. Phys. Chem. A **103** (1999) 5574.