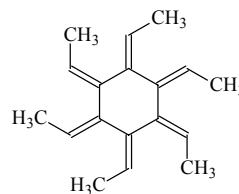
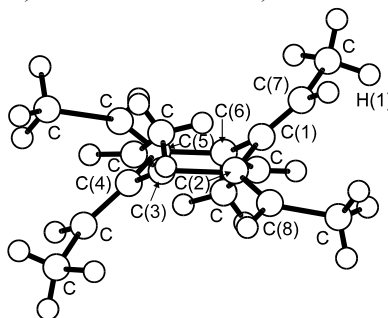


939 **C₁₈H₂₄**ED, *ab initio*
calculations**(*all-E*)-Hexaethylenecyclohexane****(*all-E*)-Hexamethyl-[6]radialene****S₆**

r_a	Å ^{a)}	θ_α	deg ^{a)}
C=C	1.349(1)	C–C–C (ring)	112.2(1)
C–C (ring)	1.494(1)	C(1)–C(2)=C(8)	122.3(4)
C–C(methyl)	1.508(1)	C(1)=C(7)–C(methyl)	126.8(4)
C–H(methyl) ^{b)}	1.108(2)	C(1)=C(7)–H	117.0 ^{c)}
		C(7)–C(methyl)–H(1) ^{b)}	111.3(18)
		C–C–C–C (ring) ^{d)}	±52.8 ^{c)}
		C=C–C=C ^{d)}	±55.4(17)
		C=C–C–H ^{d)}	12.5 ^{c)}



The nozzle was at 125 °C.

^{a)} Unidentified, possibly estimated
standard errors.^{b)} Differences in these parameters were
assumed at the MP2/6-31G* values.^{c)} Assumed at the MP2/6-31G* value.^{d)} Zero degree for the *syn* position.^{e)} Dependent parameter.Trætteberg, M., Bakken, P., Hopf, H., Höpfner, T.: J. Mol. Struct. **445** (1998) 99.