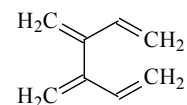


842 C₈H₁₀ED, *ab initio*
calculations**3,4-Bis(methylene)-1,5-hexadiene**2,3-Divinyl-1,3-butadiene
[4]DendraleneC₂ (main conformer)

r_{α}^0	Å ^{a)}	θ_{α}^0	deg ^{a)}
C(2)–C(3)	1.474(2)	C(1)=C(2)–C(3)	124.4(3)
C(3)–C(4)	1.496(3)	C(2)–C(3)–C(4)	119.2(5)
C(1)=C(2)	1.334(1)	C(4)–C(3)=C(7)	117.6(7)
C(3)=C(7)	1.340(1)	C(2)=C(1)–H(1)	119.4(4)
C–H ^{b)}	1.091(1)	C(1)=C(2)–H	121.4(7)
		τ_1^c	–174.8(28)
		τ_2^d	71.7(19)

MP2/6-311G* calculations predicted that the vapor consists of *ca.* 90% of the main conformer with C₂ symmetry, the other *ca.* 10% comprising four other conformers. The structural parameters of the main conformer were determined by ED employing flexible restraints derived from the calculations. This conformer was found to have two almost planar *anti* butadiene groups. The torsional angles of other minor conformers and their structural differences relative to the parameters of the main conformer were assumed at the values from MP2/6-31G* calculations.

The nozzle temperature was *ca.* 293 K.

^{a)} Estimated standard errors.

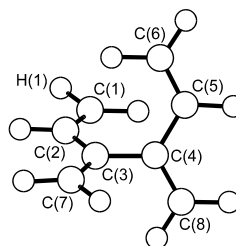
^{b)} Mean value.

^{c)} Torsional angle C(7)=C(3)–C(2)=C(1),

$\tau_1 = 0^\circ$ for the *syn* position.

^{d)} Torsional angle C(2)–C(3)–C(4)–C(5),

$\tau_2 = 0^\circ$ for the *syn* position.



Brain, P.T., Smart, B.A., Robertson, H.E., Davis, M.J., Rankin, D.W.H., Henry, W.J., Gosney, I.: J. Org. Chem. **62** (1997) 2767.