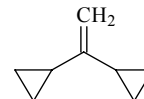


849 **C₈H₁₂**ED, *ab initio*
calculations**1,1'-Ethenyldenebiscyclopropane**

1,1-Dicyclopropylylene

C₂ (*gauche*⁺-*gauche*⁺)**C_s** (*gauche*⁺-*gauche*⁻)**C₁** (*gauche*-*anti*)

r_a	Å ^{a)}	θ_a	deg ^{a)}
C(1)=C(2)	1.327(3)	C(2)=C(1)-C(1')	123.0(3)
C(1)-C(1')	1.496(3)	C(1)-C(1')...D	127.2(3)
C(1')-C(2')	1.512(1)	C(1)=C(2)-H	121.57 ^{b)}
C(2')-C(3')	1.512(1)	H-C(ring)-H	114.53 ^{b)}
C(ring)-H	1.093(1)	C(1)-C(1')-H	114.11 ^{b)}
		τ^c	64.6(14)



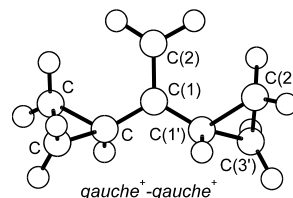
A mixture of 59(8)% *gauche*-*gauche* (47% *gauche*⁺-*gauche*⁺ and 12% *gauche*⁺-*gauche*⁻) and 41% *gauche*-*anti* conformers was observed. Differences between the corresponding parameters for the *gauche*-*gauche* and *gauche*-*anti* conformers were assumed at the values from MP2/6-31G* calculations. The structural parameters are listed for the *gauche*-*gauche* conformer.

The nozzle temperature was 294 K.

^{a)} Estimated standard errors.

^{b)} Assumed at the value from MP2/6-31G* calculations.

^{c)} Torsional angle C(2)=C(1)-C(1')...D, where D is a dummy atom on the bisector of the C(2')-C(1')-C(3'); $\tau = 0^\circ$ for the *syn* position.



Traetteberg, M., Bakken, P., Quesada, J.V., Mastryukov, V.S., Boggs, J.E.: J. Mol. Struct. **485-486** (1999) 73.