

1712 **C₄H₈** **1-Butene**
ED, MW, *ab initio* calculations
(HF/4-31G (for C), HF/21G (for H))

C_s (*syn*)
C₁ (*skew*)
H₂C=CH-CH₂-CH₃

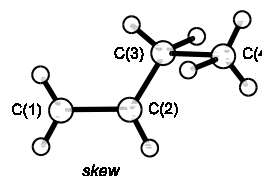
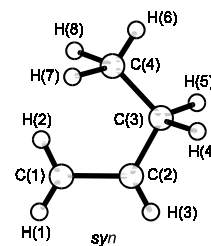
r_{av}	Å ^{a)}	θ_{av}	deg ^{a)}
C(1)=C(2)	1.336(4)	C(1)=C(2)-C(3)	126.4(3)
C(3)-C	1.511(2)	C(2)-C(3)-C(4)	113.3(3)
C-H	1.090(3)	C(1,2)=C-H	122.6(9)
		C-C-H	110.5(3)
		τ (<i>skew</i>) ^{b)}	119.9(3)

The molecule exists as a mixture of *syn* (17%) and *skew* (83%) conformer.

The measurements were made at room temperature.

^{a)} 2.5 times the estimated standard errors.

^{b)} Dihedral angle C(1)=C(2)-C(3)-C(4), $\tau = 0^\circ$ for the *syn* conformer.



Van Hemelrijk, D., Van den Enden, L., Geise, H.J., Sellers, H.L., Schäfer, L.: J. Am. Chem. Soc. **102** (1980) 2189.

MW

r_0	Å	
	<i>syn</i>	<i>skew</i>
C(1)=C(2)	1.336(10)	1.342(10)
C(2)-C(3)	1.507(15)	1.493(10)
C(3)-C(4)	1.536(10)	1.536(15)
C(1,2)-H	1.090 ^{b)}	
C(3,4)-H	1.095 ^{c)}	

θ_0	deg	
	<i>syn</i>	<i>skew</i>
C(1)=C(2)-C(3)	126.7(5)	125.4(3)
C(2)-C(3)-C(4)	114.8(7)	112.1(3)
C(3)=C(2)-H(3)	115.1(10)	117.1(15)
C(3)-C(4)-H(6)	110.4(10)	110.3(10)
C(3)-C(4)-H(7)	110.4(10)	110.3(10)
C(3)-C(4)-H(8)	110.4(10)	110.3(10)
H-C(3)-H	105.2(5)	105.7(10)
τ ^{d)}	0	119.9(5)

<i>syn</i>			
Atom	a_0 [Å]	b_0 [Å]	c_0 [Å]
H(1)	2.5751	0.6026	0.0
H(2)	0.9523	1.5598	0.0
H(3)	1.3820	-1.4871	0.0
H(4)	-0.9662	-1.3099	0.8713
H(5)	-0.9662	-1.3099	-0.8713
H(6)	-2.5341	0.4110	0.0
H(7)	-1.2164	1.2031	0.8812
H(8)	-1.2164	1.2031	-0.8812
C(1)	1.482	0.605	0.0
C(2)	0.818	-0.554	0.0
C(3)	-0.674	-0.718	0.0
C(4)	-1.456	0.597	0.0

In both forms the methyl group is staggered relative to CH₂. Assumptions: H(1) and H(2) are symmetrical to the C(1)=C(2) bond in the C(1)C(2)C(3) plane. The bisector of the angle

H(4)–C(3)–H(5) coincides with the bisector of the angle C(2)–C(3)–C(4). The H(6), H(7), and H(8) atoms are located symmetrically to the C(3)–C(4) bond.

^a) Dihedral angle C(1)=C(2)–C(3)–C(4).

Kondo, S., Hirota, E., Morino, Y.: J. Mol. Spectrosc. **28** (1968) 471.