

1230
MW

C₃H₆

Propene
Propylene

C_s
H₂C=CH-CH₃

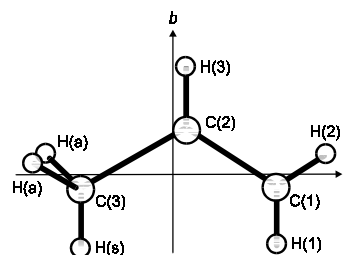
r_m^p ^{a)}	Å	θ_m^p ^{a)}	deg
C(1)=C(2)	1.3330(17)	H(2)-C(1)=C(2)	121.57(48)
C(2)-C(3)	1.4957(18)	C(1)=C(2)-C(3)	124.28(12)
C(1)-H(1)	1.0942(28)	H(1)-C(1)=C(2)	120.37(20)
C(1)-H(2)	1.0817(36)	H(3)-C(2)-C(3)	117.43(60)
C(2)-H(3)	1.0910(20)	H(s)-C-C	111.27(25)
C-H(s)	1.0840(73)	H(a)-C-C	109.90(156)
C-H(a)	1.1078(169)	H(a)-C-H(a)	106.73(109)

^{a)} Multiple isotope substitution structure.

Tam, H.S., Choe, J.I., Harmony, M.D.: J. Phys. Chem. **95** (1991) 9267.

r_s	Å	θ_s	deg
C(1)=C(2)	1.336(4)	H(2)-C(1)=C(2)	121.5(5)
C(2)-C(3)	1.501(4)	C(1)=C(2)-C(3)	124.3(3)
C(1)-H(1)	1.091(5)	H(1)-C(1)=C(2)	120.5(5)
C(1)-H(2)	1.081(5)	H(3)-C(2)-C(3)	116.7(5)
C(2)-H(3)	1.090(5)	H(s)-C(3)-C(2)	111.2(7)
C(3)-H(s)	1.085(7)	H(s)-C(3)-H(a)	109.0(20)
C(3)-H(a)	1.098(20)	H(a)-C(3)-H(a)	106.2(20)
		H(1)-C(1)-H(2)	118.0(5)
		H(3)-C(2)=C(1)	119.0(5)

Atom	a_s [Å]	b_s [Å]	c_s [Å]
C(1)	1.2538	-0.2312	0.00
C(2)	0.1060	0.4525	0.00
C(3)	-1.2550	-0.1810	0.00
H(1)	1.2486	-1.3226	0.00
H(2)	2.2110	0.2708	0.00
H(3)	0.1391	1.5416	0.00
H(a)	-1.8315	0.14	±0.8775
H(s)	-1.1838	-1.2633	0.00



One of the methyl C-H bonds is eclipsed with respect to the C=C bond.

Lide, D.R., Christensen, D.: J. Chem. Phys. **35** (1961) 1374.

ED, MW

r_g	Å ^{a)}	θ_α	deg ^{a)}
C(1)=C(2)	1.3417(20)	C=C-H ^{b)}	121.3(14)
C(2)-C(3)	1.5063(30)	C(1)=C(2)-C(3)	124.3(4)
C(1,2)-H	1.104(10)	C(2)-C(3)-H	110.7(9)
C(3)-H	1.117(8)		

The measurements were made at room temperature.

^{a)} Estimated limits of error.

^{b)} C(1)=C(2)-H and C(2)=C(1)-H angles were assumed to be equal.

Tokue, I., Fukuyama, T., Kuchitsu, K.: J. Mol. Struct. **17** (1973) 207.

See also: (MW) Hirota, E., Morino, Y.: J. Chem. Phys. **45** (1966) 2326.

(MW): Lide, D.R., Mann, D.E.: J. Chem. Phys. **27** (1957) 868.