

1715
MW

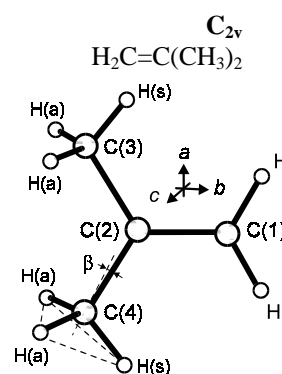
C₄H₈

2-Methyl-1-propene
Isobutene

r_0	Å	θ_0	deg
C(2)–C(3,4)	1.509(3)	C(3)–C(2)–C(4)	115.6(1)
C(1)=C(2)	1.336(6)	H–C(1)–H	118.6(3)
C(3,4)–H(a)	1.094(2)	H(a)–C(3,4)–C(2)	110.5(1)
C(3,4)–H(s)	1.098(4)	H(s)–C(3,4)–C(2)	110.7(4)
C(1)–H	1.088(2)	H(a)–C(3,4)–H(a)	106.0(2)
		β^a	0.8(2)

^{a)} Tilt angle of the CH₃ group toward the double bond.

Gutowsky, H.S., Germann, T.C.: J. Mol. Spectrosc. **147** (1991) 91.



ED, MW

r_g	Å ^{a)}	θ_α	deg ^{a)}
C(2)–C(3,4)	1.508(2)	C(3)–C(2)–C(4)	115.6(2) ^{b)}
C(1)=C(2)	1.342(3)	H–C(3,4)–H	107.9(8) ^{b)}
C(3,4)–H	1.119(7)	C(1)=C(2)–C(3)	122.2(2)
C(1)–H	1.095(20)	H(s)–C(3,4)–C(2)	111.5(8)
		C(2)=C(1)–H	121.3(15)
		tilt (CH ₃) ^{c)}	–0.4(14)

^{a)} Estimated limits of error.

^{b)} Dependent parameter.

^{c)} Tilt angle of the methyl group. The negative sign implies that the angle between the methyl axes is smaller than the angle C(3)–C(2)–C(4).

Tokue, I., Fukuyama, T., Kuchitsu, K.: J. Mol. Struct. **23** (1974) 33.