

1802
MW

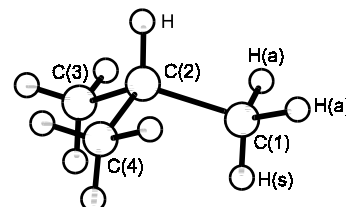
C₄H₁₀

Isobutane

C_{3v}
HC(CH₃)₂

r_s	Å	θ_s	deg
C(1)–C(2)	1.525(3)	C(1)–C(2)–C(3)	111.15(20)
C(2)–H	1.108(5)	C(2)–C(1)–H(s)	109.4(5)
C(1)–H(s)	1.100(5)	H(a)–C(1)–H(a)	108.5 ^a
C(1)–H(a)	1.092 ^a	H(a)–C(1)–H(s)	107.9 ^a

Atom	a_s [Å]	b_s [Å]	c_s [Å]
C(2)	0.0	0.0	0.3630
H	0.0	0.0	1.4706
C(1)	1.4529	0.0	–0.1018
H(s)	1.4850	0.0	–1.2015
H(a)	1.9853	±0.8863	0.2500



Each methyl group is staggered with respect to the C(2)–H and the adjacent C–C bonds.

^a) Based on the assumption that the H atoms form an equilateral triangle.

Lide, D.R.: J. Chem. Phys. **33** (1960) 1519.

See also: Lide, D.R., Mann, D.E.: J. Chem. Phys. **29** (1958) 914.

ED, MW

r_g	Å ^a)	θ_α	deg ^a)
C(1)–C(2)	1.535(1)	C(1)–C(2)–C(3)	110.8(2)
C(2)–H	1.122(6)	C(2)–C(1)–H ^b)	111.4(2)
C(1)–H ^b)	1.113(2)		

The temperature of the measurements was not given, possibly room temperature.

^a) Estimated limits of error.

^b) Average value.

Hilderbrandt, R.L., Wieser, J.D.: J. Mol. Struct. **15** (1973) 27.