

1297
MW

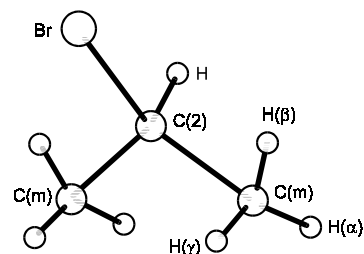
C₃H₇Br

2-Bromopropane
Isopropyl bromide

C_s
H₃C–CHBr–CH₃

r_s	Å	θ_s	deg
C(2)–C(m)	1.518(10)	C(m)–C(2)–C(m)	113.27(165)
C(2)–Br	1.962(6)	C(m)–C(2)–Br	109.25(72)
C(2)–H	1.089(6)	C(m)–C(2)–H	110.33(123)
C(m)–H(β)	1.087(13)	H–C(2)–Br	103.95(82)
C(m)–H(γ)	1.100(19)	C(2)–C(m)–H(β)	111.53(218)
C(m)–H(α)	1.087 ^{a)}	C(2)–C(m)–H(γ)	109.72(207)
		C(2)–C(m)–H(α)	109.70(347)
		H(β)–C(m)–H(γ)	108.02(283)
		H(β)–C(m)–H(α)	109.65(407)
		H(γ)–C(m)–H(α)	108.10(647)
		Br–C(2)–C(m)–H(γ) ^{b)}	62.67(162)
		Br–C(2)–C(m)–H(β) ^{b)}	–57.0(12)
		Br–C(2)–C(m)–H(α) ^{b)}	–178.68(435)

Atom	a_s [Å]	b_s [Å]	c_s [Å]
C(2)	–1.07237	0.0	0.41241
H	–1.09490	0.0	1.50108
Br	0.84151	0.0	–0.02150
C(m)	–1.70837	± 1.26810	–0.12850
H(α)	–2.76472	± 1.28662	0.12792
H(β)	–1.22132	± 2.15749	0.26361
H(γ)	–1.62228	± 1.28812	–1.22540



^{a)} Assumed.

^{b)} The dihedral angles of the H atoms in the CH₃ group against the BrCC plane.

Ikeda, C., Inagusa, T., Hayashi, M.: J. Mol. Spectrosc. **135** (1989) 334.