

1315
MW

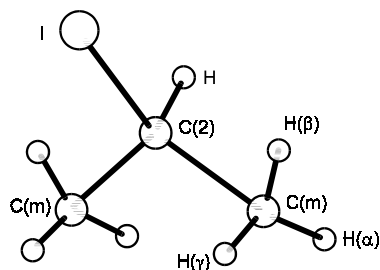
C₃H₇I

2-Iodopropane
Isopropyl iodide

C_s
H₃C–CHI–CH₃

r_s	Å	θ_s	deg
C(m)–C(2)	1.517(5)	C(m)–C(2)–C(m)	113.42(75)
C(2)–I	2.167(2)	C(m)–C(2)–I	109.73(28)
C(2)–H	1.090(4)	C(m)–C(2)–H	110.18(62)
C(m)–H(β)	1.086(7)	H–C(2)–I	103.02(32)
C(m)–H(γ)	1.109(8)	C(2)–C(m)–H(β)	112.17(118)
C(m)–H(α)	1.086 ^{a)}	C(2)–C(m)–H(γ)	109.70(98)
		C(2)–C(m)–H(α)	109.82(182)
		H(β)–C(m)–H(γ)	107.57(143)
		H(β)–C(m)–H(α)	109.92(213)
		H(γ)–C(m)–H(α)	107.50(342)
		I–C(2)–C(m)–H(γ) ^{b)}	62.93(70)
		I–C(2)–C(m)–H(β) ^{b)}	–59.55(68)
		I–C(2)–C(m)–H(α) ^{b)}	–179.08(223)

Atom	a_s [Å]	b_s [Å]	c_s [Å]
C(m)	–2.10030	±1.26812	–0.12746
H(α)	–3.16171	±1.27680	0.10020 ^{c)}
H(β)	–1.62958	±2.16229	0.26924
H(γ)	–1.99565	±1.29600	–1.23068
C(2)	–1.46838	0.0	0.41449
H	–1.49937	0.0	1.50405
I	0.65576	0.0	–0.01335



^{a)} Assumed.

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

^{c)} Assumption of [C–H(β)] = [C–H(α)].

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