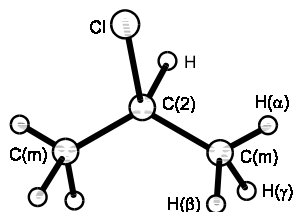


r_0	Å	θ_0	deg
C(2)–C(m)	1.5202(14)	C(m)–C(2)–C(m)	113.31(16)
C(2)–Cl	1.8039(23)	C(m)–C(2)–H	104.83(30)
C(2)–H	1.1050(21)	C(m)–C(2)–Cl	109.40(9)
C(m)–H(α)	1.0954(49)	C(2)–C(m)–H(α)	111.09(39)
C(m)–H(β)	1.0948(49)	C(2)–C(m)–H(β)	109.55(52)
C(m)–H(γ)	1.0999(36)	C(2)–C(m)–H(γ)	109.41(14)
		C(m)–C(2)–C(m)–H(α) ^{a)}	179.08(49)
		C(m)–C(2)–C(m)–H(β) ^{a)}	–59.93(90)
		C(m)–C(2)–C(m)–H(γ) ^{a)}	59.43(26)
$r_s(+)^b$	Å	$\theta_s(+)^b$	deg
C(2)–C(m)	1.5212(20)	C(m)–C(2)–C(m)	112.67(23)
C(2)–Cl	1.8026(15)	C(m)–C(2)–H	105.07(21)
C(2)–H	1.0974(31)	C(m)–C(2)–Cl	109.20(11)
C(m)–H(α)	1.0999(28)	C(2)–C(m)–H(α)	110.67(26)
C(m)–H(β)	1.0988(27)	C(2)–C(m)–H(β)	109.22(31)
C(m)–H(γ)	1.0967(23)	C(2)–C(m)–H(γ)	109.92(17)
		C(m)–C(2)–C(m)–H(α) ^{a)}	179.09(25)
		C(m)–C(2)–C(m)–H(β) ^{a)}	–61.14(60)
		C(m)–C(2)–C(m)–H(γ) ^{a)}	59.08(22)
r_s	Å	θ_s	deg
C(2)–C(m)	1.5231(21)	C(m)–C(2)–C(m)	112.62(26)
C(2)–Cl	1.7973(18)	C(m)–C(2)–H	105.37(21)
C(2)–H	1.0957(16)	C(m)–C(2)–Cl	109.33(12)
C(m)–H(α)	1.0972(24)	C(2)–C(m)–H(α)	110.75(28)
C(m)–H(β)	1.0998(21)	C(2)–C(m)–H(β)	109.43(25)
C(m)–H(γ)	1.1003(52)	C(2)–C(m)–H(γ)	109.82(22)
		C(m)–C(2)–C(m)–H(α) ^{a)}	179.17(14)
		C(m)–C(2)–C(m)–H(β) ^{a)}	–60.69(62)
		C(m)–C(2)–C(m)–H(γ) ^{a)}	59.22(26)
r_m^p ^{c)}	Å	θ_m^p ^{c)}	deg
C(2)–C(m)	1.5176(38)	C(m)–C(2)–C(m)	112.52(35)
C(2)–Cl	1.7964(40)	C(m)–C(2)–H	105.43(35)
C(2)–H	1.0933(42)	C(m)–C(2)–Cl	109.28(15)
C(m)–H(α)	1.0919(71)	C(2)–C(m)–H(α)	110.73(55)
C(m)–H(β)	1.0989(57)	C(2)–C(m)–H(β)	108.71(56)
C(m)–H(γ)	1.0908(41)	C(2)–C(m)–H(γ)	109.87(25)
		C(m)–C(2)–C(m)–H(α) ^{a)}	178.98(47)
		C(m)–C(2)–C(m)–H(β) ^{a)}	–61.78(106)
		C(m)–C(2)–C(m)–H(γ) ^{a)}	59.04(29)
r_s^d	Å	θ_s^d	deg
C(2)–C(m)	1.521(4)	C(m)–C(2)–C(m)	112.7(5)
C(2)–Cl	1.801(3)	Cl–C(2)–H	105.2(5)
C(2)–H	1.097(6)	C(m)–C(2)–H	109.3(2)
C(m)–H(α)	1.098(6)	C(m)–C(2)–Cl	110.0(4)
C(m)–H(β)	1.099(5)	C(2)–C(m)–H(α)	110.7(6)
C(m)–H(γ)	1.098(7)	C(2)–C(m)–H(β)	109.4(6)
		C(2)–C(m)–H(γ)	109.8(4)
		C(m)–C(2)–C(m)–H(α) ^{a)}	179.2(5)
		C(m)–C(2)–C(m)–H(β) ^{a)}	–60.8(13)
		C(m)–C(2)–C(m)–H(γ) ^{a)}	59.2(5)

Atom	a_s [Å]	b_s [Å]	c_s [Å]
C(2)	0.5154		-0.4003
Cl	-1.2249		0.0454
C(m)	1.1689	1.2619	0.1321
H	0.5356		-1.4933
H(α)	0.6656	2.1505	-0.2545
H(β)	2.2173	1.2817	-0.1969
H(γ)	1.1132	1.2771	1.2214



^a) Torsional angle.

^b) r_s fit plus three 1st and 2nd moment conditions (for a , c , and ac).

^c) Multiple isotope substitution structure.

^d) Weighted average of three r_s methods.

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ED, MW

r_g	Å ^a)	θ_{av}	deg ^a)
C(2)–Cl	1.812(1)	C(m)–C(2)–Cl	109.0(5)
C(m)–C(2)	1.527(1)	C(m)–C(2)–C(m)	112.7(4)
C–H	1.104(4)	H–C(m)–H	108.5(8)
		C(m)–C(2)–H	109.8 ^b)

One C–H bond of each methyl group lies on the CCC plane in the *anti* position to the C(m)–C(2) bond. The tilt angle of the methyl group was assumed to be zero.

The measurement was made at room temperature.

^a) Estimated total errors.

^b) Assumed.

Iijima, T., Seki, S., Kimura, M.: Bull. Chem. Soc. Jpn. **50** (1977) 2568.