

1341
MW

C₃H₈

Propane

C_{2v}
H₃C–CH₂–CH₃

r_m^ρ ^{a)}	Å	θ_m^ρ	deg
C–C	1.5209(9)	C–C–C	112.35(11)
C–H ^{b)}	1.0929(20)	H–C–H ^{b)}	106.13(32)
C–H(s)	1.0877(35)	H(a)–C–H(s)	107.04(28)
C–H(a)	1.0907(19)	C–C–H(s)	111.60(31)
		C–C–H(a)	110.62(10)

^{a)} Multiple isotope substitution structure.

^{b)} Unlabelled hydrogens occupy the methylene group.

Tam, H.S., Choe, J.I., Harmony, M.D.: J. Phys. Chem. **95** (1991) 9267.

r_s	Å	θ_s	deg
C–C	1.526 (2)	C–C–C	112.4(2)
C–H (CH ₂)	1.096(2)	H–C–H (CH ₂)	106.1(2)
C–H(s)	1.089(9)	H(a)–C–H(s)	108.1
C–H(a)	1.094	H(a)–C–H(a)	107.3
C–H (CH ₃)	1.091(10) ^{a)}	C–C–H(s)	111.8(10)
		C–C–H(a)	110.6
		H–C–H (CH ₃)	107.7(10) ^{a)}

Atom	$ a_s $ [Å]	$ b_s $ [Å]	$ c_s $ [Å]
C (CH ₃)	±1.2682	0.2698	0.0
H(s)	±2.1664	–0.3412	0.0
H(a)	±1.2976	0.9172	±0.8809
C (CH ₂)	0.0	–0.5819	0.0
H (CH ₂)	0.0	–1.2381	±0.8757

The conformation of the methyl groups is staggered with respect to the CH₂ group.

^{a)} Average value.

Lide, D.R.: J. Chem. Phys. **33** (1960) 1514.

ED, MW

r_g	Å ^{a)}	θ_α	deg ^{a)}
C–C	1.532(3)	C–C–C	112(1)
C–H	1.107(5)	H–C–H	107(3)

By combining the ED results with the MW data, the zero-point average structure has also been determined. Local C_{3v} symmetry was assumed for the methyl groups.

The nozzle was at room temperature.

^{a)} Estimated limits of error.

Iijima, T.: Bull. Chem. Soc. Jpn. **45** (1972) 1291.