

1296
MW

C₃H₇Br

1-Bromopropane
Propyl bromide

C₁ (*gauche*)
H₃C–CH₂–CH₂Br

r_0	Å ^{a)}	θ_0	deg ^{a)}
C–Br	1.970(10)	C–C–C	110.50 ^{b)}
C(1)–C(2)	1.534 ^{b)}	C–C–Br	111.0(10)
C(2)–C(3)	1.534 ^{b)}	H–C(3)–H	108.80 ^{b)}
C–H	1.094 ^{b)}	H–C(2)–H, H–C(1)–H	108.80 ^{b)}
		C(3)–C(2)–H, C(2)–C(1)–H, C(1)–C(2)–H	109.64 ^{b)}
		C(2)–C(3)–H	110.14 ^{b)}
		C–C–C–Br	110.0(30) ^{c)}

^{a)} Uncertainties were not estimated in the original paper.

^{b)} Assumed.

^{c)} From the *anti* position.

Niide, Y., Ohkoshi, I., Takano, M.: J. Mol. Spectrosc. **89** (1981) 387.

ED, MW, *ab initio*
calculations (HF/6-31G*)

r_g	Å ^{a)}	θ_α	deg ^{a)}
C(1)–C(2)	1.521(5)	C–C–C (<i>anti</i>) ^{b)}	110.0(11)
C(2)–C(3)	1.535(5)	C–C–C (<i>gauche</i>) ^{b)}	113.3(11)
C(1)–Br	1.962(6)	C–C–Br (<i>anti</i>) ^{c)}	111.1(6)
C–H (mean)	1.114(9)	C–C–Br (<i>gauche</i>) ^{c)}	112.1(6)
		C(2)–C(1)–H	112.1 ^{d)}
		C(2)–C(3)–H	111.4 ^{d)}
		H–C(2)–H	107.0 ^{d)}
		C–C–C–Br (<i>anti</i>)	180 ^{d)}
		C–C–C–Br (<i>gauche</i>)	66.0(17)

The molecule exists as a mixture of *anti* (36(14)%) and *gauche* (64(14)%) conformers.

Local C_{3v} symmetry was assumed for the methyl group.

The nozzle temperature was 24 °C.

^{a)} Twice the estimated standard errors including the scale error.

^{b)} Difference between the C–C–C angles for the *anti* and *gauche* conformers was fixed at the *ab initio* value.

^{c)} Difference between the C–C–Br angles for the *anti* and *gauche* conformers was fixed at the *ab initio* value.

^{d)} *Ab initio* value.

Hagen, K., Stølevik, R.: Struct. Chem. **6** (1995) 175.

C₁ (*gauche*)
C_s (*anti*)

