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MW

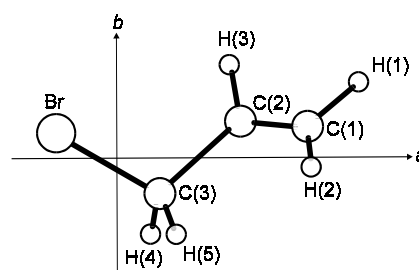
C₃H₅Br

3-Bromo-1-propene

C₁ (*skew*)
H₂C=CH-CH₂Br

r_s	Å ^{a)}	θ_s	deg ^{a)}
C=C	1.342 ^{b)}	C=C-C	122.77(20)
C-C	1.495(2)	C-C-Br	110.10(20)
C-Br	1.950 ^{b)}	H(1)-C=C	120.3 ^{b)}
C(1)-H(1)	1.094 ^{b)}	H(2)-C=C	120.3 ^{b)}
C(1)-H(2)	1.094 ^{b)}	H-C(3)-H	109.28(30)
C(2)-H	1.090 ^{b)}	H-C(1)-H	119.40(30)
C(3)-H(4)	1.089(3)	C=C-H(3)	120.40(30)
C(3)-H(5)	1.104(3)	C(3)-C(2)-H(3)	116.80(30)
		C(2)-C(3)-H(4)	107.83 ^{b)}
		C(2)-C(3)-H(5)	109.45 ^{b)}
		Br-C-H(4)	110.78(30)
		Br-C-H(5)	109.37(30)
		τ (C=C-C-Br) ^{c)}	117.67(50)

Atom	a_s [Å]	b_s [Å]	c_s [Å]
Br	-0.9599	0.0976	0.0140
C(3)	0.7323	-0.8691	0.0785
H(5)	0.9610	-1.1391	1.1242
H(4)	0.6833	-1.7746	-0.5244
C(2)	1.8329	-0.0158	-0.4652
H(3)	1.7585	0.2733	-1.5136
C(1)	2.8825	0.3746	0.2743
H(2)	2.9571	0.0804	1.3253
H(1)	3.6712	0.9900	-0.1686



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

^{b)} Assumed.

^{c)} Dihedral angle.

Niide, Y.: J. Sci. Hiroshima Univ., Ser. A **48** (1984) 23.

ED

C₁ (*skew*)
C_s (*syn*)

r_g	Å ^{a)}	θ_α	deg ^{a)}
C=C	1.335(7)	C=C-C	126.0(26)
C-C	1.485(8)	C-C-Br	111.5(8)
C-Br	1.961(6)	H-C=C	122 ^{b)}
C-H	1.078(15)	H-C(3)-C(2)	109.5 ^{b)}
		α ^{c)}	124(8)
		τ (<i>skew</i>) ^{d)}	117(5)
		τ (<i>syn</i>) ^{d)}	51(38)

Amount of *skew* form was 86(14)%.

A non-zero value of τ (*syn*) may be due to the large-amplitude torsional motion around the C_s form.

The measurements were made at 50 °C and 150 °C. The results at 50 °C are listed.

^{a)} Three times the estimated standard errors.

^{b)} Fixed.

^{c)} Projection of the angle Br-C-H onto the plane perpendicular to the C(2)-C(3) axis.

^{d)} Dihedral angle C=C-C-Br.

Schei, S.H., Shen, Q.: J. Mol. Struct. **81** (1982) 269.