

**1675**     **C<sub>4</sub>H<sub>7</sub>Br**  
ED, MM calculations

**3-Bromo-2-methyl-1-propene**

**C<sub>1</sub> (*gauche*)**  
**C<sub>s</sub> (*syn*)**  
**H<sub>2</sub>C=C(CH<sub>3</sub>)–CBrH<sub>2</sub>**

<i>r<sub>a</sub></i>	Å <sup>a)</sup>	<i>θ<sub>α</sub></i>	deg <sup>a)</sup>
C(1)=C(2)	1.331(9)	C(1)=C(2)–C(3)	121.5(7)
C(2)–C(3)	1.484(6)	Δ(C=C–C) <sup>b)</sup>	–0.6 <sup>c)</sup>
Δ(C–C) <sup>b)</sup>	0.017 <sup>d)</sup>	C–C–Br	112.2(5)
C–Br	1.965(6)	C–C(3)–H	107.7(62)
C–H (average)	1.103(14)	C–C(4)–H	111.0 <sup>d)</sup>
		C=C–H	120.4 <sup>c)</sup>
		φ <sup>e)</sup>	120.5 <sup>c)</sup>
		τ <sup>f)</sup>	112.5(22)

The molecule exists as a mixture of *gauche* (96(8)%) and *syn* conformers.

The nozzle temperatures were 20 and 180 °C. The parameters for the *gauche* conformer at 20 °C are listed.

<sup>a)</sup> Twice the estimated standard errors.

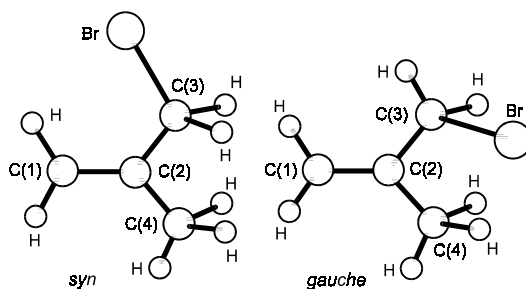
<sup>b)</sup> Δ(C–C) = [C(2)–C(4)] – [C(2)–C(3)],  
Δ(C=C–C) = [C(1)=C(2)–C(3)] –  
[C(1)=C(2)–C(4)].

<sup>c)</sup> Fixed at the values from molecular  
mechanics calculations.

<sup>d)</sup> Assumed.

<sup>e)</sup> Angle between the CC(3)Br and  
CC(3)H planes.

<sup>f)</sup> Torsional angle C(1)=C(2)–C(3)–Br, τ = 0° for *syn* conformer.



Schei, S.H.: J. Mol. Struct. **102** (1983) 305.