

**1135** **C<sub>3</sub>H<sub>4</sub>Br<sub>2</sub>**  
ED, MM calculations

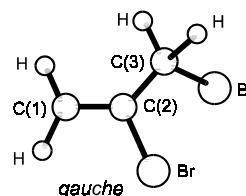
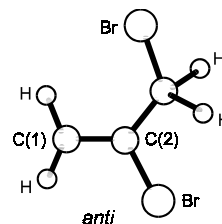
**2,3-Dibromo-1-propene**

**C<sub>s</sub> (*anti*)**  
**C<sub>1</sub> (*gauche*)**  
**H<sub>2</sub>C=CH-CHBr<sub>2</sub>**

$r_a$	Å <sup>a)</sup>	$\theta_\alpha$	deg <sup>a)</sup>
C=C	1.333(13)	C=C-Br ( <i>gauche</i> ) <sup>b)</sup>	120.1(44)
C-C	1.480(14)	C-C-Br ( <i>gauche</i> ) <sup>b)</sup>	113.4(35)
C(2)-Br	1.904(17)	C=C-C ( <i>gauche</i> ) <sup>b)</sup>	124.2(17)
$\Delta(\text{C-Br})$ <sup>c)</sup>	0.036(34)	C-C-H	106.2(70)
C-H	1.114(37)	C=C-H	120.5 <sup>d)</sup>
		$\phi$ <sup>e)</sup>	119.5 <sup>d)</sup>
		$\tau$ ( <i>gauche</i> ) <sup>f)</sup>	112.0(43)

Local C<sub>s</sub> symmetry for CH<sub>2</sub>Br group and local C<sub>2v</sub> symmetry for the C=CH<sub>2</sub> group were assumed.

Nozzle was at different temperatures: 20, 90, 180 °C. Results at 90 °C are listed; amount of *anti* form at this temperature is 39(5)%. The energy and entropy differences with standard deviation are  $\Delta E = E(\text{gauche}) - E(\text{anti}) = 4(1) \text{ kJ mol}^{-1}$ ,  $\Delta S = 8(4) \text{ J mol}^{-1} \text{ K}^{-1}$ .



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

<sup>b)</sup> In the *anti* conformer C=C-Br, C-C-Br and C=C-C are changed by  $-0.6^\circ$ ,  $+1.9^\circ$ , and  $+2.4^\circ$ , respectively, compared to the *gauche* values.

<sup>c)</sup>  $\Delta(\text{C-Br}) = (\text{C}(3)\text{-Br}) - (\text{C}(2)\text{-Br})$ .

<sup>d)</sup> Value kept constant at the result from molecular mechanics calculation.

<sup>e)</sup> Angle between projections of C-Br and C-H on plane perpendicular to the C-C bond.

<sup>f)</sup> Torsional angle Br-C-C-Br of *gauche* form;  $\tau = 0^\circ$  for the planar *anti* form.

Søvik, O.I., Trongmo, Ø., Hagen, K., Schei, S.H., Stølevik, R., Shen, Q.: J. Mol. Struct. **118** (1984) 1.