

1237
ED

$\text{C}_3\text{H}_6\text{Br}_2$

1,3-Dibromopropane

C_2 (GG)
 C_1 (AG)
 C_{2v} (AA)
 $\text{H}_2\text{BrC}-\text{CH}_2-\text{CBrH}_2$

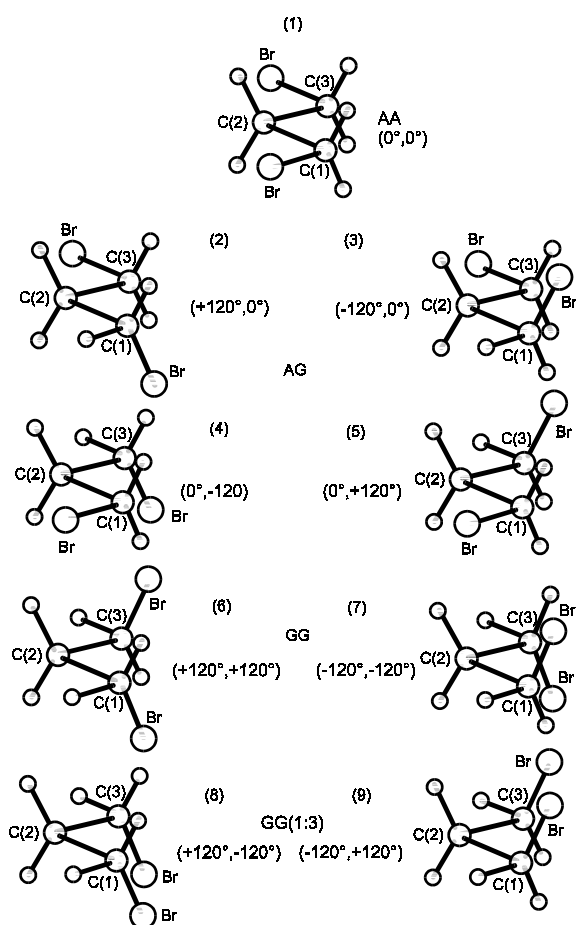
r_a	\AA^a	θ_a	deg^a
C–H	1.126(18)	C–C–C	111.4(32)
C–C	1.527(10)	C(2)–C–Br	112.0(6)
C–Br	1.959(4)	C(2)–C–H	115.4(72)
		C–C(2)–H	103.0(40)

The relative amounts of conformers at 65 °C (for numbering and definition see figure):

Conformer	%	$\theta_a[\text{Br}-\text{C}(1)-\text{C}(2)-\text{C}(3)]$ [deg]	$\theta_a[\text{Br}-\text{C}(3)-\text{C}(2)-\text{C}(1)]$ [deg]
GG	67(4)	113.4(4)	113.4(4)
AG	30(4)	119.2(12)	11.5(12)
AA	3(4)	0	0

Only four conformers (AA, AG, GG, and GG(1:3)) are spectroscopically distinguishable.

^a) Twice the estimated standard errors.



Farup, P.E., Stølevik, R.: Acta
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