

1721 C₄H₈Br₂

 ED, *ab initio* calculations

(HF/6-31G* (for C, H),

HF/6-31G*/Binning (for Br))

1,4-Dibromobutane

 S₂ (G⁺AG⁻)

 C₁ (G⁻AA)

 C₂ (G⁻G⁻G⁻)

 H₂BrC-CH₂-CH₂-CBrH₂

r_g	Å ^{a)}	θ_α	deg ^{a)}
C(1)-C(2)	1.524(6)	C-C-C	113.3(19)
C(2)-C(3)	1.532(6)	C-C(1)-Br	112.8(7)
C-Br	1.966(8)	C-C(1)-H	110.2(47)
C(1)-H	1.099(15)	C-C(2)-H	109.0(50)
C(2)-H	1.103(15)	τ_1 ^{b)}	66(9)
		τ_2 ^{c)}	-66(9)
		τ_3 ^{d)}	180 ^{e)}

The molecule exists as a mixture of the conformers:

 G⁻AA (22(36)%), G⁻G⁻G⁻ (21(36)%), G⁺AG⁻ (31(18)%),

 G⁻AG⁻ (15(19)%), AG⁻G⁺ (9(24)%), G⁺G⁺G⁺ (>1(21)%),

 AAA(2(8)%). The symbols refer to *anti* (A) and *gauche*

 (G⁺ or G⁻) dihedral angles at C(1)-C(2), C(2)-C(3) and

C(3)-C(4) bonds. The differences between corresponding

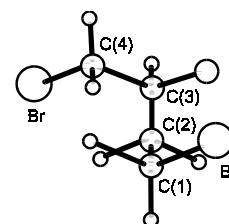
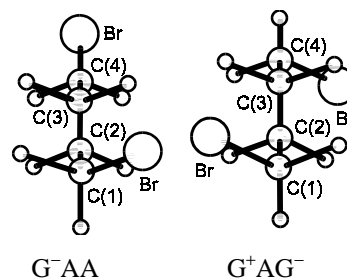
bond lengths and bond angles of the different conformers

 and the torsion angles for the G⁻AG⁻, AG⁻G⁺, G⁺G⁺G⁺

 and AAA conformers were fixed at the *ab initio* values.

 The parameters are given for the G⁺AG⁻ conformer.

The nozzle was at 80 °C.


 G⁻G⁻G⁻

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

^{b)} Torsional angle Br-C(1)-C(2)-C(3).

^{c)} Torsional angle C(2)-C(3)-C(4)-Br.

^{d)} Torsional angle C(1)-C(2)-C(3)-C(4).

^{e)} Fixed at the *ab initio* value.

 Aarset, K., Hagen, K., Stølevik, R.: J. Phys. Chem. **98** (1994) 5249.