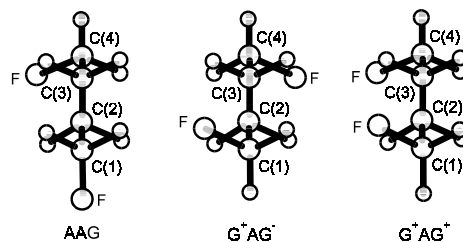


1725 **C₄H₈F₂**
ED, MM3 and *ab initio*
(HF/6-31G*) calculations

1,4-Difluorobutane

C₁ (AAG)
S₂ (G⁺AG⁻)
C₂ (G⁺AG⁺)
H₂FC-CH₂-CH₂-CFH₂

$r_g^a)$	Å ^{b)}	$\theta_\alpha^a)$	deg ^{b)}
C(1)-C(2) ^{c)}	1.513(2)	F-C-C	110.9(3)
C(2)-C(3) ^{c)}	1.537(2)	C-C-C	112.9(4)
C-H	1.105(3)	H-C-H	100(3)
C-F	1.398(2)		



The molecule exists as a mixture of ten conformers: AAA, AAG, G⁺AG⁻, G⁺AG⁺, AGA, AG⁺G⁺, AG⁺G⁻, G⁺G⁺G⁺, G⁺G⁺G⁻, and G⁺G⁻G⁺. The symbols A (*anti*), G⁺ and G⁻ (*gauche*) represent torsional angles of about 180, +60 and -60°, respectively, for torsion around a concerning C-C bond. The superscripts (+) and (-) indicate clockwise and anticlockwise rotation, respectively. According to the theoretical calculations the most abundant conformers were AAG, G⁺AG⁻ and G⁺AG⁺. All torsional angles and the differences between corresponding valence angles in different conformers were fixed at the calculated values. molecular mechanics-constrained results are listed. *Ab initio*-constrained results differed only slightly. The nozzle temperature was 23 °C.

^{a)} Mean values for all conformers.

^{b)} Twice the estimated standard errors.

^{c)} The difference between the C(1)-C(2) and C(2)-C(3) distances was fixed at the calculated value.

Krosley, K., Hagen, K., Hedberg, K.: J. Mol. Struct. **352/353** (1995) 87.