

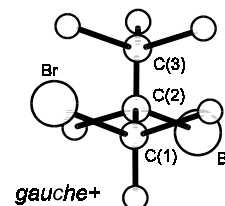
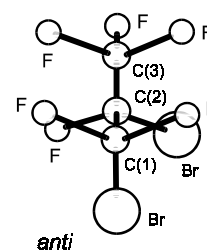
995 $\text{C}_3\text{Br}_2\text{F}_6$
ED, *ab initio*
calculations (HF/STO-3G)

1,2-Dibromo-1,1,2,3,3,3-hexafluoropropane

C_1 (*gauche+*)
 C_1 (*anti*)
 $\text{F}_2\text{BrC}-\text{CFBr}-\text{CF}_3$

r_g	\AA^a		θ_α	deg^a	
	<i>anti</i>	<i>gauche+</i>		<i>anti</i>	<i>gauche+</i>
C–F	1.336(3)	1.336(3)	C(1)–C(2)–F	109.7(9)	110.2(9)
C(1)–C(2)	1.570(19)	1.572(19)	C(2)–C(1)–F	109.9(9)	110.1(9)
C(2)–C(3)	1.577(19)	1.576(19)	C(2)–C(3)–F	110.3(9)	110.4(9)
C(1)–Br	1.927(13)	1.936(13)	C–C–C	111.7(33)	112.8(33)
C(2)–Br	1.940(13)	1.945(13)	C(1)–C(2)–Br	110.4(10)	110.1(10)
			C(2)–C(1)–Br	110.5(10)	110.6(10)
			Br–C–F	111.9(27)	111.9(27)
			ϕ_1^b	6.4(40)	122.0(302)
			ϕ_2^c	–13.3 ^d	–9.5 ^d

The molecule exists as a mixture of a more stable *anti* form (with the C(1)–Br bond *anti* to the C(2)–C(3) bond) and a less stable *gauche+* form ($\Delta E = 1.0(5)$ kcal/mol). The mole fraction of the *anti* conformer was found to be 0.82(11). Local C_{3v} symmetry was assumed for the CF_3 group. The differences between corresponding parameters (r_α , θ_α) and conformational variations within these parameters were fixed at the *ab initio* values. The nozzle temperature was 25...26 °C.



- ^a) Twice the estimated standard errors including a systematic error.
^b) Dihedral angle Br–C(1)–C(2)–C(3), positive values for clockwise rotation from the exact *anti* position looking from C(1) to C(2).
^c) Dihedral angle F–C(3)–C(2)–C(1), positive values for clockwise rotation from the exact *anti* position looking from C(2) to C(3).
^d) Fixed at the *ab initio* value.

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