

1249
ED

C₃H₆F₂

1,3-Difluoropropane

C₂ (GG)
C_s (GG'')
C₁ (AG)
H₂FC-CH₂-CFH₂

r_a	Å ^{a)}	θ_α	deg ^{a)}			
C-H	1.094(5)	F-C-H ^{b)}	107.8(8)			
C-C	1.513(3)	H-C(1)-H ^{b)}	105.9(15)			
C-F	1.391(2)	C-C(2)-H ^{b)}	108.5(12)			
		C-C-C	112.9(8)			
		C-C-F	110.1(3)			
		C(2)-C-H	112.1(14)			
		H-C(2)-H	108.5 ^{c)}			
		$\phi^d)$	119.5 ^{c)}			
			GG	AG	GG''	
		$\Delta\tau_1$ ^{e)}	-4.0(20)	-2.0(20)	+4.0(20)	
		$\Delta\tau_2$ ^{e)}	-4.0(20)	-2.0(20)	-4.0(20)	

The molecule exists as a mixture of GG (63(4)%),
AG(27(2)%) and GG''(10(5)%) conformers.
The nozzle temperature was 20 °C.

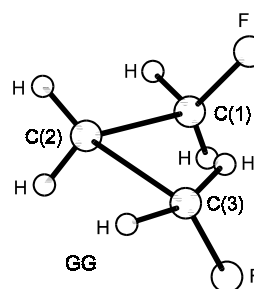
^{a)} Estimated standard errors including a systematic error.

^{b)} Dependent parameter.

^{c)} Assumed.

^{d)} Projected angle H-C(1)-H on a plane perpendicular to the
C(1)-C(2) axis.

^{e)} Torsional angle deviations from staggered forms (around
C(1)-C(2) and C(2)-C(3), respectively).



Klæboe, P., Powell, D.L., Stølevik, R., Vorren, Ø.: Acta Chem. Scand. Ser. A **36** (1982) 471.