

1305
MW

C₃H₇F

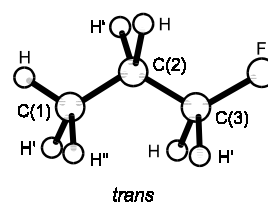
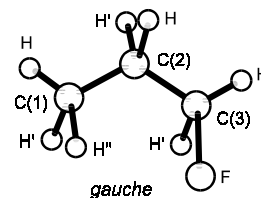
1-Fluoropropane
Propyl fluoride

C_s (*trans*)
C₁ (*gauche*)
H₃C–CH₂–CH₂F

<i>trans</i>	<i>r_s</i>	Å	<i>θ_s</i>	deg
C(1)–C(2)	1.534(1)		C(1)–C(2)–C(3)	110.6(3)
C(2)–C(3)	1.501(2)		C(2)–C(3)–F	110.0(4)
C(3)–F	1.401(3)		F–C(3)–H,H'	107.2(2)
C(3)–H,H'	1.095(1)		C(2)–C(3)–H,H'	111.6(1)
C(2)–H,H'	1.094(1)		H–C(3)–H'	109.0(2)
C(1)–H	1.084(2)		C(3)–C(2)–H,H'	109.0(1)
C(1)–H',H''	1.093(2)		C(1)–C(2)–H,H'	110.4(2)
			H–C(2)–H'	107.3(2)
			C(2)–C(1)–H	111.4(4)
			C(2)–C(1)–H',H''	111.0(2)
			H–C(1)–H',H''	107.7(3)
			H'–C(1)–H''	108.5(5)
			γ ^{a)}	111.1(3)
			δ ^{b)}	180
			tilt(CH ₃) ^{c)}	–0.2(4)

<i>gauche</i>	<i>r_s</i>	Å	<i>θ_s</i>	deg
C(1)–C(2)	1.526(3)		C(1)–C(2)–C(3)	113.0(3)
C(2)–C(3)	1.506(2)		C(2)–C(3)–F	110.1(6)
C(3)–F	1.390(5)		F–C(3)–H	106.8(9)
C(3)–H	1.097(4) ^{d)}		F–C(3)–H'	107.7(5)
C(3)–H'	1.097(1)		C(2)–C(3)–H	112.4(7)
C(2)–H	1.099(2)		C(2)–C(3)–H'	110.3(3)
C(2)–H'	1.099(6) ^{d)}		H–C(3)–H'	109.4(8)
C(1)–H	1.086(3)		C(3)–C(2)–H	107.4(3)
C(1)–H'	1.102(4)		C(3)–C(2)–H'	107.9(7)
C(1)–H''	1.102(9) ^{d)}		C(1)–C(2)–H	111.2(4)
			C(1)–C(2)–H'	110.2(9)
			H–C(2)–H'	107.0(12)
			C(2)–C(1)–H	111.6(6)
			C(2)–C(1)–H'	110.0(5)
			C(2)–C(1)–H''	110.3(11)
			H–C(1)–H'	107.7(7)
			H–C(1)–H''	110.9(16)
			H'–C(1)–H''	106.2(23)
			γ ^{a)}	110.6(7)
			δ ^{b)}	62.6(5)
			tilt(CH ₃) ^{c)}	–1.0(9)

Atom	<i>a_s</i> [Å]	<i>b_s</i> [Å]	<i>c_s</i> [Å]
<i>trans</i>			
H (C(1))	–2.79107	0.59283	0.0
C(1)	–1.99447	–0.14278	0.0
H',H'' (C(1))	–2.12377	–0.77260	0.88439
C(2)	–0.61449	0.52791	0.0
H,H' (C(2))	–0.49963	1.16602	0.88120
C(3)	0.47569	–0.50418	0.0
H,H' (C(3))	0.43034	–1.13836	0.89187
F	1.72818	0.12279	0.0



Atom	a_s [Å]	b_s [Å]	c_s [Å]
<i>gauche</i>			
H (C(1))	2.57584	-0.50821	0.33578
C(1)	1.59117	-0.54952	-0.12122
H' (C(1))	1.72836	-0.54769	-1.21425
H'' (C(1))	1.08510	-1.49714	0.12258
C(2)	0.72664	0.63532	0.29870
H (C(2))	0.60268	0.66861	1.38973
H' (C(2))	1.20448	1.57878	0.00143
C(3)	-0.65083	0.60231	-0.30963
H (C(3))	-1.25596	1.47173	-0.02276
H' (C(3))	-0.58328	0.55080	-0.40377
F	-1.33710	-0.52571	0.12545

^{a)} $\gamma = [\theta(\text{C}(2)\text{C}(1)\text{H}) + \theta(\text{C}(2)\text{C}(1)\text{H}') + \theta(\text{C}(2)\text{C}(1)\text{H}'')]/3$; unperturbed $\theta(\text{C}(2)\text{C}(1)\text{H})$.

^{b)} Skeletal dihedral angle around the C(2)–C(3) bond.

^{c)} $\theta = (2/3) [(\theta(\text{C}(2)\text{C}(1)\text{H}') + \theta(\text{C}(2)\text{C}(1)\text{H}''))/2 - \theta(\text{C}(2)\text{C}(1)\text{H})]$;
tilt angle of the methyl group.

^{d)} Obtained under one of the assumptions of $r(\text{C}(3)\text{--H}) = r(\text{C}(3)\text{--H}')$, $r(\text{C}(2)\text{--H}') = r(\text{C}(2)\text{--H})$,
and $r(\text{C}(1)\text{--H}') = r(\text{C}(1)\text{--H}'')$.

Hayashi, M., Fujitake, M.: J. Mol. Struct. **146** (1986) 9.