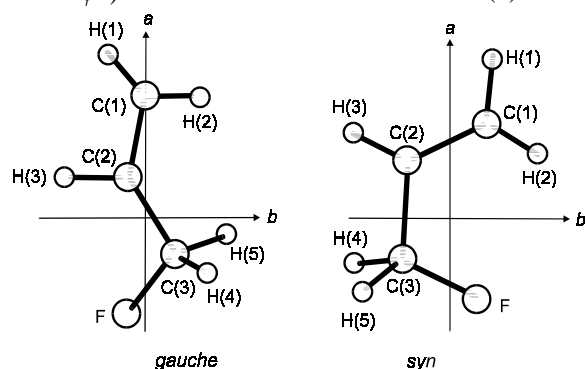


r_0	\AA	
	<i>syn</i>	<i>gauche</i>
C(1)=C(2)	1.333(3)	1.335(3)
C(2)-C(3)	1.495(4)	1.490(4)
C(3)-F	1.388(4)	1.394(4)
C(1)-H(1)	1.083(2)	1.086 ^a
C(1)-H(2)	1.084 ^a	1.084 ^a
C(2)-H(3)	1.089 ^a	1.088 ^a
C(3)-H(4,5)	1.098(2)	1.095 ^a

θ_0	deg	
	<i>syn</i>	<i>gauche</i>
C(1)=C(2)-C(3)	124.5(3)	123.3(5)
C(2)-C(3)-F	111.5(3)	110.4(5)
C(2)=C(1)-H(1)	121.1(2)	121.5 ^a
C(2)=C(1)-H(2)	121.3(2)	121.8 ^a
H(1)-C(1)-H(2)		116.7 ^a
C(1)=C(2)-H(3)	120.9(2)	120.7 ^a
C(2)-C(3)-H(4)	111.1(3)	111.5 ^a
C(2)-C(3)-H(5)	111.1(3)	111.2 ^a
H(4)-C(3)-H(5)	108.2(2)	108.9 ^a
H(4)-C(3)-F	107.9(2)	107.1 ^a
H(5)-C(3)-F		108.4 ^a
ϕ^b		124.6(5)

^a) Assumed.^b) Dihedral angle F-C(3)-C(2)=C(1).

Durig, D.T., Little, T.S., Costner,
T.G., Durig, J.R.: J. Mol. Struct.
266 (1992) 277.



r_s	\AA	
	<i>syn</i>	<i>gauche</i>
C(1)=C(2)	1.333(10)	1.354(15)
C(2)-C(3)	1.488(15)	1.486(15)
C(3)-F	1.382(15)	1.371(15)
C(1)-H(1)	1.080(10)	1.098(15)
C(1)-H(2)	1.105(10)	1.054(15)
C(2)-H(3)	1.090 ^a	1.090 ^a
C(3)-H(4)	1.098(10)	1.127(20)
C(3)-H(5)	1.098(10)	1.137(20)

θ_s	deg	
	<i>syn</i>	<i>gauche</i>
C(1)=C(2)-C(3)	124.6(10)	121.6(10)
C(2)-C(3)-F	111.7(10)	110.9(10)
C(2)=C(1)-H(1)	120.9(7)	119.2(10)
C(2)=C(1)-H(2)	119.2(7)	121.5(10)
H(1)-C(1)-H(2)	119.9(7)	119.3(10)
C(1)=C(2)-H(3)	119 ^a	119 ^a
C(2)-C(3)-H(4)	111.1(7)	107.4(15)
C(2)-C(3)-H(5)	111.1(7)	105.2(15)
H(4)-C(3)-H(5)	108.1(7)	111.4(15)
H(4)-C(3)-F	107.4(7)	107.1(15)
H(5)-C(3)-F	107.4(7)	114.7(15)
ϕ^b	0	127.1(50)

Atom	<i>syn</i>		
	$a_s [\text{\AA}]$	$b_s [\text{\AA}]$	$c_s [\text{\AA}]$
C(1)	1.5176	0.5651	0.00
C(2)	0.8433	-0.5849	0.00
C(3)	-0.6406	-0.6933	0.00
F	-1.2436	0.5507	0.00
H(1)	2.5980	0.5752	0.00
H(2)	0.9573	1.5179	0.00
H(3)	1.3984	-1.5230	0.00
H(4)	-0.9973	-1.2306	0.8891
H(5)	-0.9973	-1.2306	-0.8891

	<i>gauche</i>		
	$a_s [\text{\AA}]$	$b_s [\text{\AA}]$	$c_s [\text{\AA}]$
	1.8800	0.0520	0.2875
	0.7290	-0.2986	-0.3340
	-0.5047	0.5211	-0.2094
	-1.5645	-0.2483	0.1947
	2.7685	-0.5828	0.1684
	1.9426	0.9199	0.8828
	0.7102	-1.2046	-0.9397
	-0.7531	0.9143	-1.2357
	-0.2319	1.3644	0.5020

^a) Assumed.^b) Dihedral angle F-C(3)-C(2)=C(1).

Hirota, E.: J. Chem. Phys. **42** (1965) 2071.

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