Supporting Information

Infrared Spectra of CF_2=CHD and CF_2=CD_2; Scaled Quantum-Chemical Force Fields and an Equilibrium Structure for 1,1-Difluoroethylene

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Figure S1a. Gas-phase infrared spectrum from 4000 – 2000 cm^{-1} of F_2C=CDH at 9 torr. Many lines from uncompensated H_2O and CO_2.

Figure S1b. Gas-phase infrared spectrum from 2000 – 400 cm^{-1} of F_2C=CDH at 9 torr. Many lines from uncompensated H_2O and CO_2.

Figure S2. Gas-phase infrared spectrum from 650 – 200 cm^{-1} of F_2C=CDH at 259 torr. Sharp features at 629.8, 594.0, and 588.1 are from an impurity. Weak broad features below 500 cm^{-1} are also regarded as impurity bands from F_2BrC-CFDH.

Figure S3a. Gas-phase infrared spectrum from 3000 – 2000 cm^{-1} of F_2C=CD_2 at 4 torr. Many lines from uncompensated H_2O and CO_2.

Figure S3b. Gas-phase infrared spectrum from 2000 – 400 cm^{-1} of F_2C=CD_2 at 4 torr. Many lines from uncompensated H_2O and CO_2.

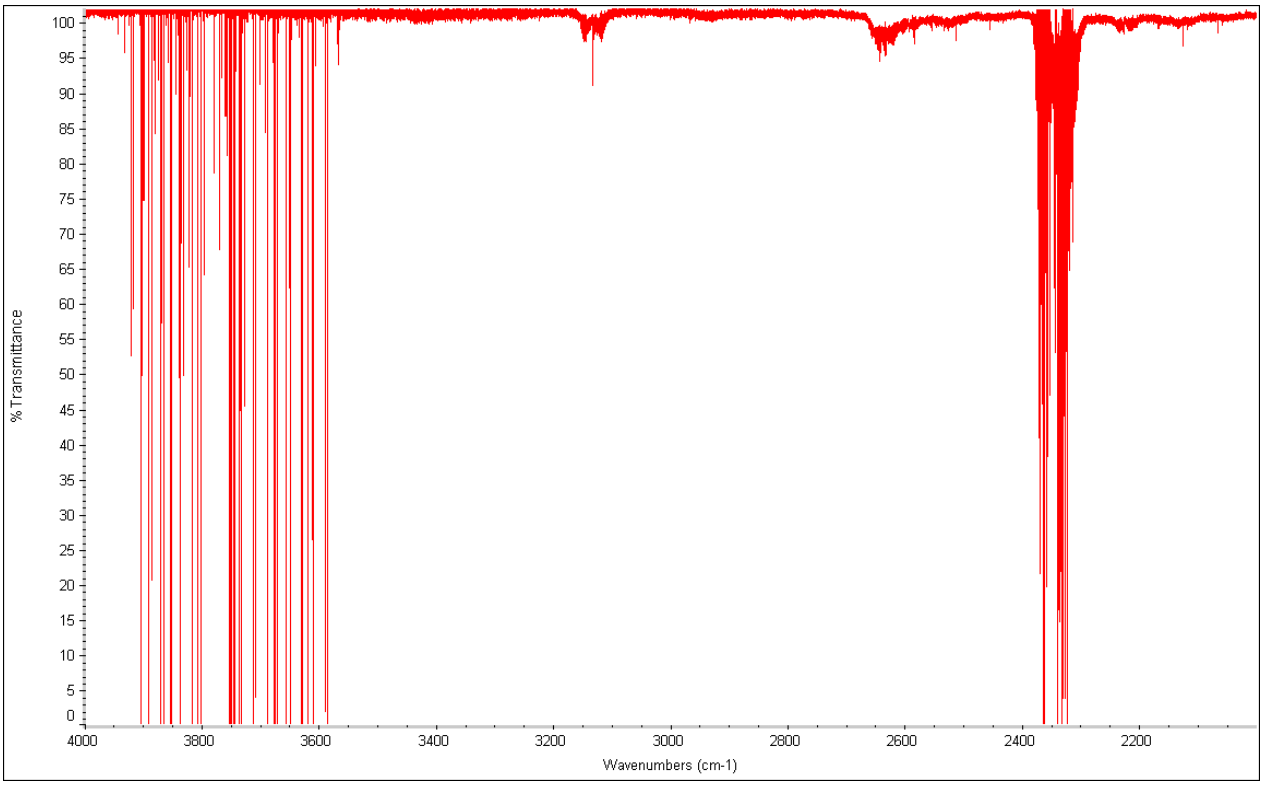
Figure S4. Gas-phase infrared spectrum from 700 – 200 cm^{-1} of F_2C=CD2 at 252 torr. Weak sharp features from uncompensated H_2O.

TABLE S1. Equilibrium Geometry and Symmetry Coordinates for 1,1-Difluoroethylene.

TABLE S2. Scaled Harmonic Force Field for 11DFE; units aJ $Å^{-2}$, aJ rad^{-2}, aJ $Å^{-1}rad^{-1}$.

TABLE S3. Microwave Lines for the Isotopomers of 1,1-Difluoroethylene (in MHz).

TABLE S4. Equilibrium Rotational Constants for the Isotopomers of 1,1-Difluoroethylene (in MHz).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85
80
75
70
65
60
55
50
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40
35
30
25
20
15
10
5
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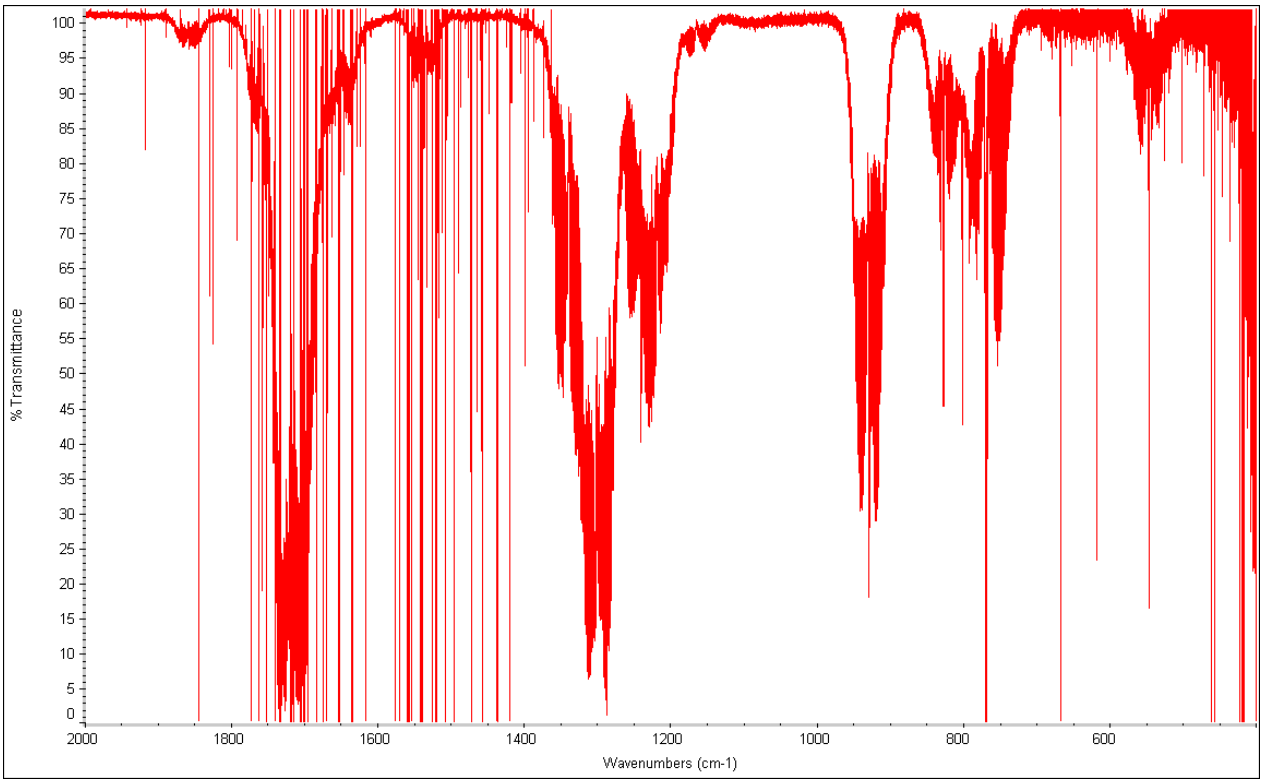
3600
3400
3200
3000
2800
2600
2400
2200
Wavenumbers (cm-1)

Figure S1a.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35
30
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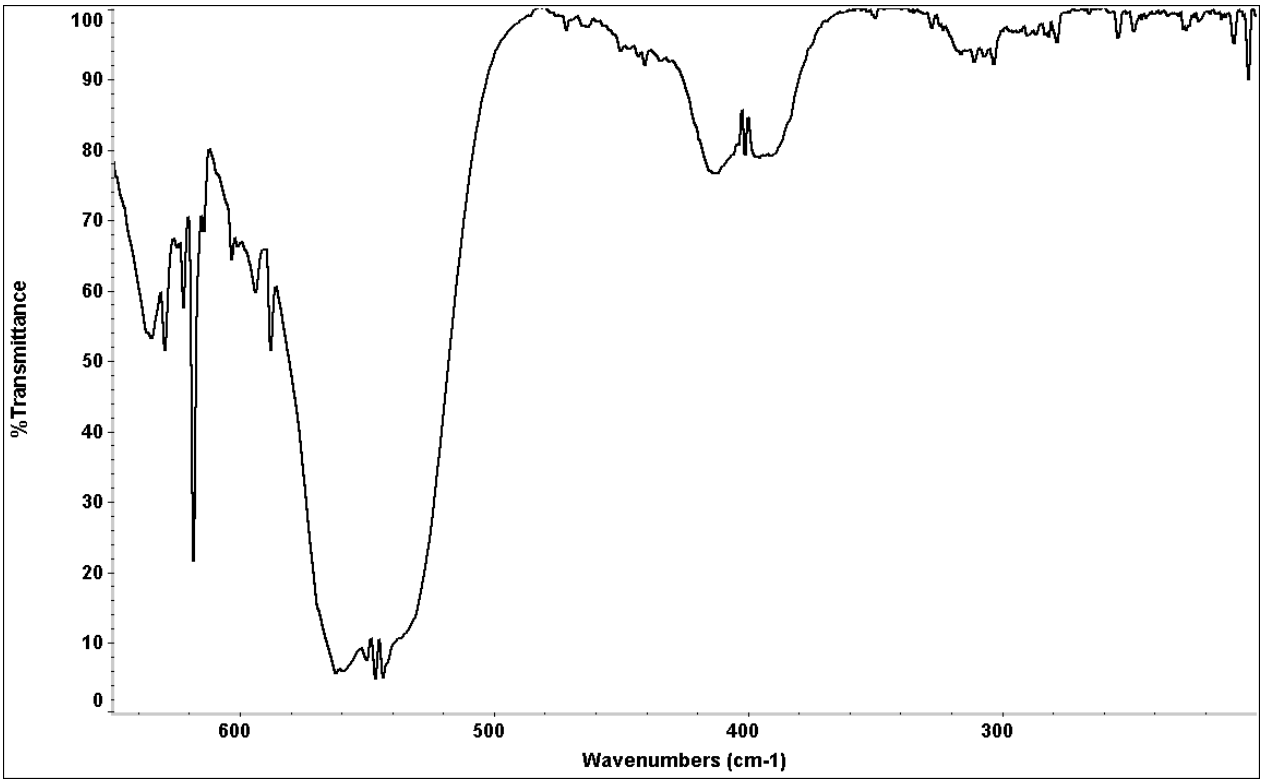
2000
1800
1600
1400
1200
1000
800
600
Wavenumbers (cm-1)

Figure S1b.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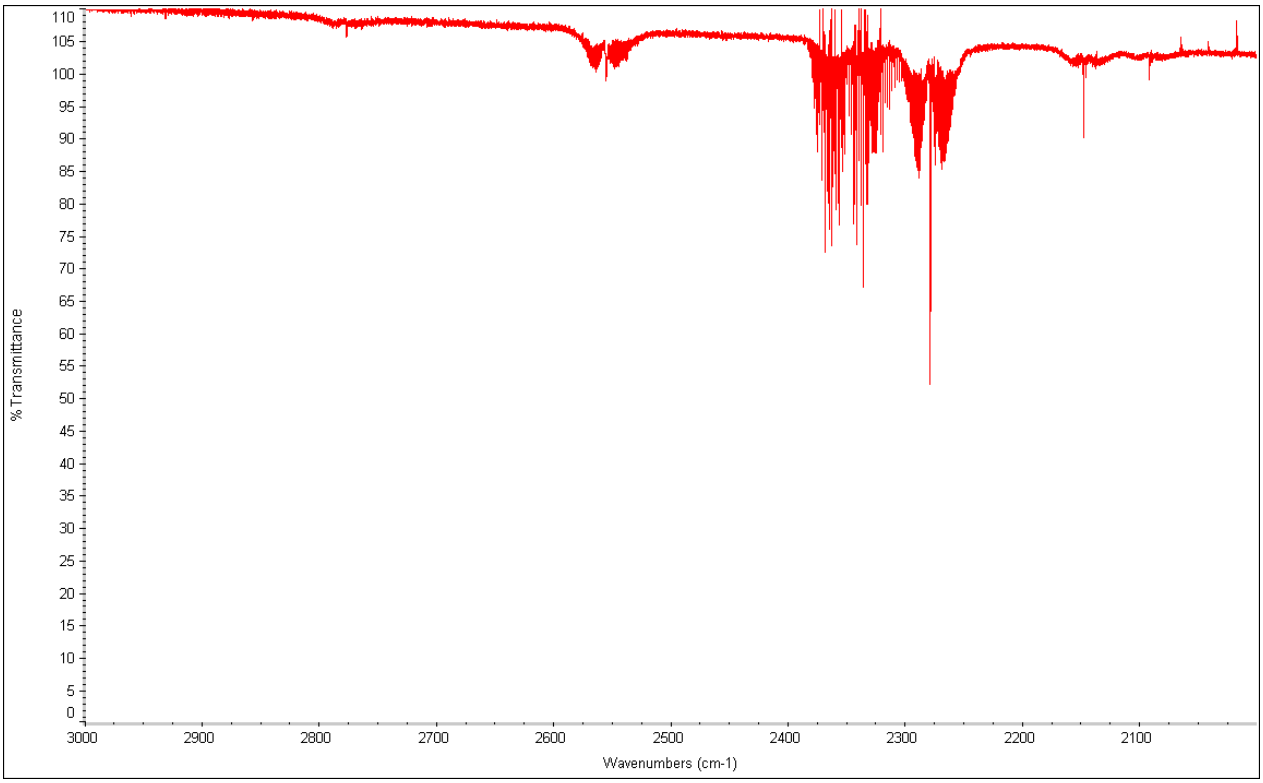
50
40
30
20
10
0
%Transmittance
600
500
400
300
Wavenumbers (cm-1)

Figure S2.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40
35
30
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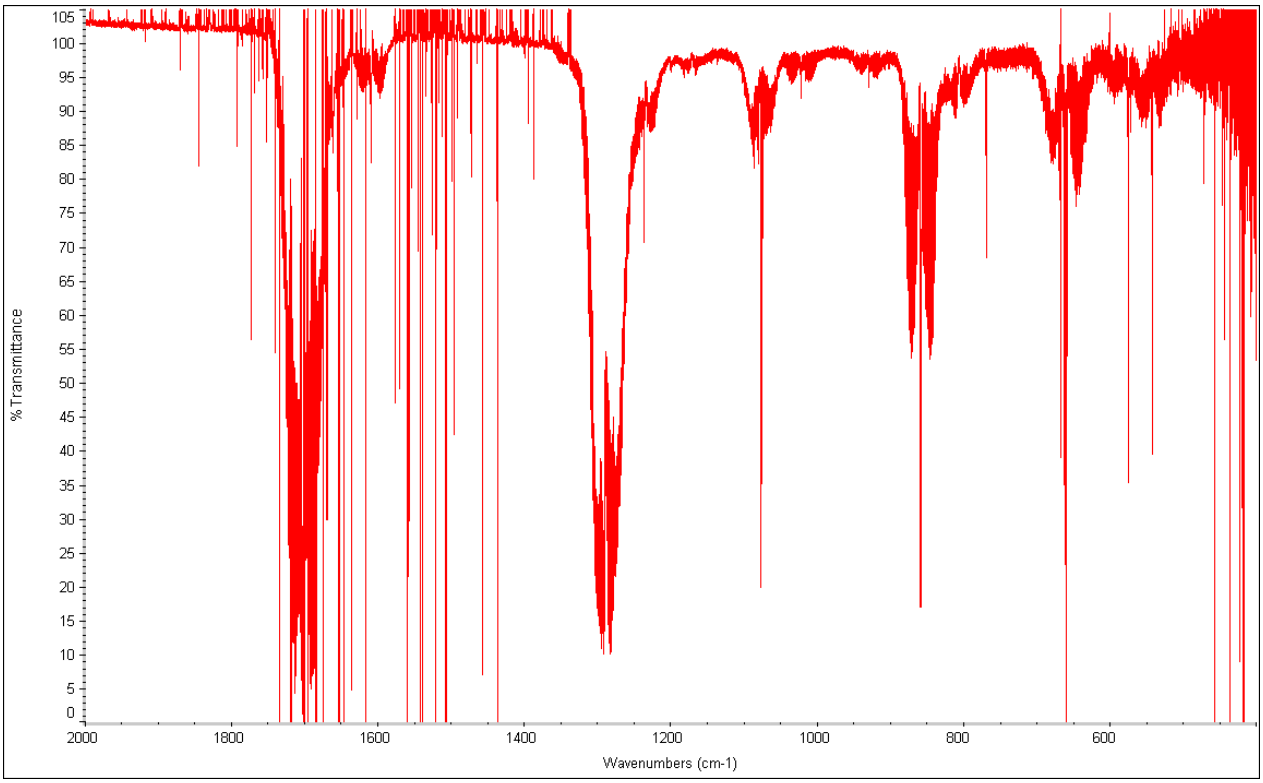
15
10
5
0
3000
2900
2800
2700
2600
2500
2400
2300
2200
2100
Wavenumbers (cm-1)

Figure S3a.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100
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50
45
40
35
30
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15
10
5
0
2000
1800
1600
1400
1200
1000
800
600
Wavenumbers (cm-1)

Figure S3b.

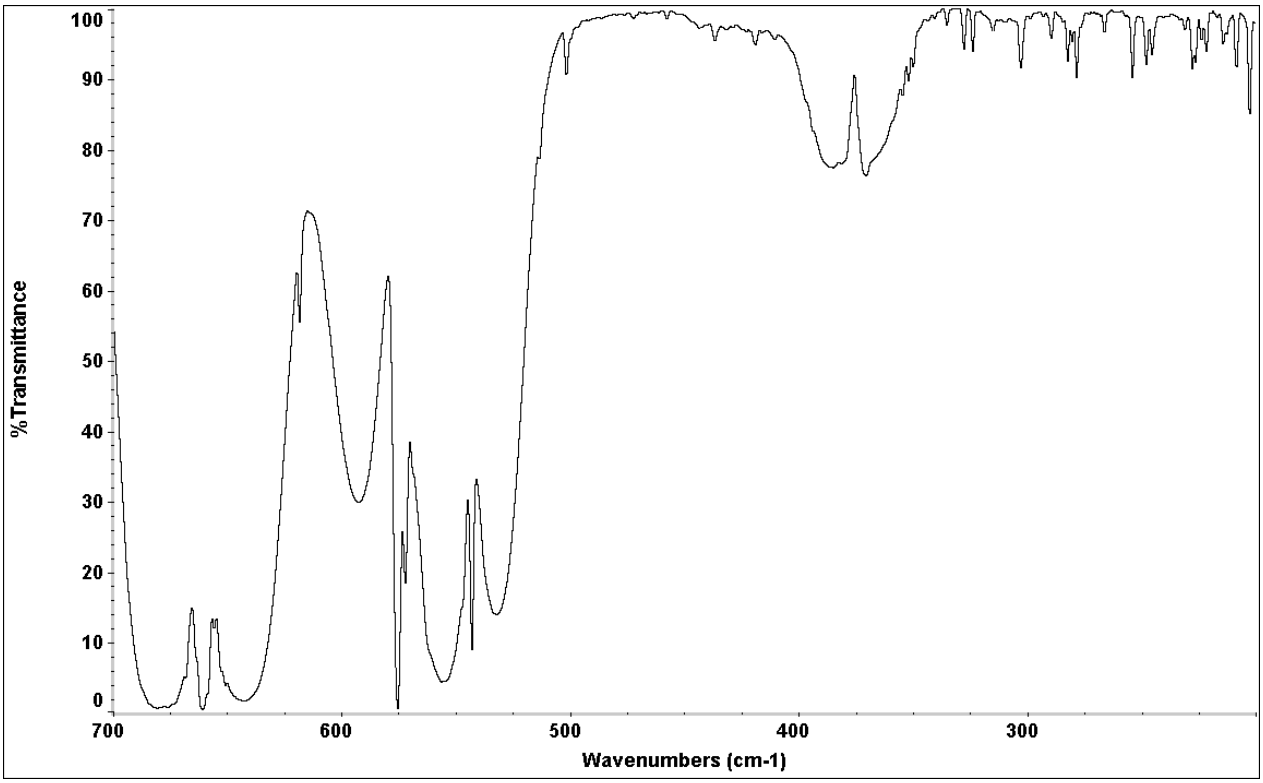
100
90
80
70
60
50
40
30
20
10
0
%Transmittance
700
600
500
400
300
Wavenumbers (cm-1)

Figure S4.

Table S1: Equilibrium Geometry and Symmetry Coordinates for 1,1-Difluoroethylene

Geometry (macct model)

rC$_1$=C$_2$ = 1.321311 Å; rC$_2$-H$_3$ = 1.075012 Å; rC$_1$-F$_5$ = 1.319682 Å; ∠H$_3$C$_2$H$_4$ = 121.6127°; ∠F$_5$C$_1$F$_6$ = 109.6403°; Dihedral ∠F$_5$C$_1$C$_2$H$_3$ = 0.0°.

Symmetry Coordinates

S[a]		type	Coordinate
A$_1$	1	ν_sCH$_2$	rC$_2$H$_3$ + rC$_2$H$_4$
	2	ν_sCF$_2$	rC$_1$F$_5$ + rC$_1$F$_6$
	3	νCC	rC$_1$C$_2$
	4	δHCH	2∠H$_3$C$_2$H$_4$ − ∠H$_3$C$_2$C$_1$ − ∠H$_4$C$_2$C$_1$
	5	δFCF	2∠F$_5$C$_1$F$_6$ − ∠F$_5$C$_1$C$_2$ − ∠F$_6$C$_1$C$_2$
A$_2$	6	Twist	Di ∠F$_5$C$_1$C$_2$H$_3$ + Di ∠F$_5$C$_1$C$_2$H$_4$ + Di ∠F$_6$C$_1$C$_2$H$_3$ + Di ∠F$_6$C$_1$C$_2$H$_4$ [b]
B$_1$	7	ν_{as}CH$_2$	rC$_2$H$_3$ - rC$_2$H$_4$
	8	ν_{as}CF$_2$	rC$_1$F$_5$ - rC$_1$F$_6$
	9	ρCH$_2$	∠H$_3$C$_2$C$_1$ − ∠H$_4$C$_2$C$_1$
	10	ρCF$_2$	∠F$_5$C$_1$C$_2$ − ∠F$_6$C$_1$C$_2$
B$_2$	11	wCH$_2$	⊥C$_2$C$_1$H$_3$H$_4$ [c]
	12	wCF$_2$	⊥C$_1$C$_2$F$_6$F$_5$ [c]

[a] For the purposes of the scale factor refinement, coordinates S$_1$-S$_5$ and S$_7$- S$_{10}$ were grouped together in an A′ block; similarly S$_6$,S$_{11}$ and S$_{12}$ constituted an A″ block.

[b] Di∠ = Dihedral angle.

[c] Out-of-plane bending angle.

TABLE S2: Scaled Harmonic Force Field for 11DFE; units aJ Å^{-2}; aJ rad^{-2}

	i	j	F_{ij}				F_{ij}
A_1	1	1	5.8191	A_2	6	6	0.1312
	1	2	-0.0285	B_1	7	7	5.8193
	2	2	7.7243		7	8	0.0089
	1	3	-0.0071		8	8	6.3427
	2	3	0.6502		7	9	0.1563
	3	3	9.9317		8	9	-0.1054
	1	4	0.0376		9	9	0.4671
	2	4	-0.0399		7	10	-0.0698
	3	4	-0.2100		8	10	0.6722
	4	4	0.4300		9	10	-0.1256
	1	5	-0.0027		10	10	0.8759
	2	5	0.3546	B_2	11	11	0.1743
	3	5	-0.2759		11	12	0.0706
	4	5	0.0223		12	12	0.5455
	5	5	1.2537				

TABLE S3: Microwave Lines for the Isotopomers of 1,1-Difluoroethylene (in MHz)

Transition	$F_2C=CH_2$		$F_2{}^{13}C=CH_2$		$F_2C={}^{13}CH_2$	
$J'K_a'K_c'$-$J''K_a''K_c''$		obs–calc		obs–calc		obs–calc
6 5 1 – 6 5 2	10532.465	-0.0022				
5 4 1 – 5 4 2	12025.643	0.0023	11993.052	-0.0036		
4 3 1 – 4 3 2	13335.799	0.0011	13312.590	0.0043	11067.234	0.0067
3 2 1 – 3 2 2	14419.908	-0.0005	14404.897	0.0074	12871.193	-0.0026
2 1 1 – 2 1 2	15250.619	-0.0014	15242.073	0.0040	14290.274	0.0019
1 0 1 – 0 0 0	15774.359	0.0073	15770.277	0.0066	15219.294	-0.0160
3 0 3 – 2 2 0	15885.545	0.0015			15318.257	0.0085
2 2 1 – 2 0 2	17017.135	-0.0027	17023.272	0.0001	17467.978	0.0142
6 1 5 – 5 3 2						
3 3 1 – 3 1 2	18086.032	0.0021	18102.508	0.0020	19628.258	-0.0061
4 4 1 – 4 2 2	19723.423	0.0032	19756.895	0.0051		
5 5 1 – 5 3 2	22071.019	-0.0020	22129.741	-0.0023		
7 5 2 – 7 5 3						
5 2 4 – 4 4 1					20107.537	-0.0017
6 4 2 – 6 4 3					20989.861	-0.0016
5 3 2 – 5 3 3						
4 2 2 – 4 2 3						
2 1 2 – 1 1 1	26465.00[a]	-0.0556	26459.71[a]	-0.0328		
3 1 2 – 3 1 3	26651.71[a]	0.0243	26645.70[a]	-0.1077		
3 2 2 – 3 0 3	26881.20[a]	-0.0183				
2 0 2 – 1 0 1	26992.80[a]	-0.0030			26541.64[a]	-0.0059

Transition[b]	$F_2C=CHD$		$F_2C=CD_2$	
$J'K_a'K_c'$-$J''K_a''K_c''$		obs–calc		obs–calc
3 2 1 – 3 2 2	11494.753	-0.0124	10289.345	-0.0093
2 1 1 – 2 1 2	13375.030	-0.0222	12411.172	-0.0144
1 0 1 – 0 0 0	14631.982	-0.0022	13849.316	0.0115
3 0 3 – 2 2 0	14606.565	-0.0338	13676.937	-0.0017
2 2 1 – 2 0 2	17793.877	0.1015	17581.312	-0.0038
6 1 5 – 5 3 2			20732.079	0.0049
3 3 1 – 3 1 2	21055.631	0.0057	21587.788	0.0174
7 5 2 – 7 5 3	13713.566	-0.0256	10565.425	0.0031
5 2 4 – 4 4 1			13930.190	0.0226
6 4 2 – 6 4 3	17332.850	-0.0068	14452.902	-0.0026
5 3 2 – 5 3 3	20525.821	-0.0012	18098.578	-0.0346
4 2 2 – 4 2 3			21085.556	0.0084

[a] From reference 8. Given weights of 0.1 in fitting rotational constants.
[b] In order of increasing frequency for $F_2C=CH_2$.

TABLE S4: Equilibrium Rotational Constants (in MHz)

	macct[a]	single ave. scale factor from ω_{obs}[b]	selective scaling on ω_{obs}[c]	single ave. scale factor from ν[d]	selective scaling on ν[e]
11DFE					
A_e	11050.481	11050.641	11050.681	11054.896	11055.220
B_e	10492.753	10492.933	10493.029	10498.122	10498.426
C_e	5382.2701	5382.3638	5382.3498	5384.9303	5384 .8841
Δ	-0.001245	-0.001390	-0.000541	-0.004737	-0.001198
11DFE-1-$^{13}C_1$					
A_e	11050.472	11050.629	11050.674	11054.802	11055.119
B_e	10488.277	10488.454	10488.550	10493.571	10493.874
C_e	5381.0910	5381.1830	5381.1629	5383.7109	5383.6583
Δ	-0.001260	-0.001402	-0.000427	-0.004744	-0.001126
11DFE-2-$^{13}C_1$					
A_e	11050.479	11050.636	11050.668	11054.890	11055.214
B_e	10051.997	10052.168	10052.253	10057.093	10057.383
C_e	5263.8820	5263.9726	5263.9571	5266.4742	5266.4255
Δ	-0.001351	-0.001497	-0.000656	-0.004882	-0.001206
11DFE-d_1					
A_e	10976.941	10977.218	10977.244	10981.587	10981.881
B_e	9598.5955	9598.6807	9598.7440	9603.0424	9603.2737
C_e	5120.8366	5120.9194	5120.9037	5123.2858	5123.2324
Δ	-0.000698	-0.000663	-0.000662	-0.004019	-0.004019
11DFE-d_2					
A_e	10639.590	10639.696	10639.696	10643.899	10644.122
B_e	9042.3129	9042.3832	9042.4371	9046.3829	9046.5916
C_e	4888.1220	4888.1718	4888.1504	4890.3854	4890.3314
Δ	-0.001120	-0.001262	-0.000478	-0.004592	-0.001168

[a] Alphas calculated with the macct model.
[b] Harmonic contributions to alphas computed with a single average scale factor obtained from the scale factors from fitting force constants to ω_{obs}.
[c] Harmonic contributions to alphas computed with the scale factors obtained from fitting force constants to ω_{obs}.
[d] Harmonic contributions to alphas computed with a single average scale factor obtained from the scale factors from fitting force constants to ν.
[e] Harmonic contributions to alphas computed with the scale factors obtained from fitting force constants to ν.