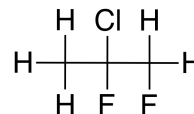


HCFC-262ba

Molecular Formula: CH₃CClFCH₂F
 Name: 2-Chloro-1,2-difluoropropane
 CAS number: 362631-59-2
 Molecular Weight: 114.52



Global Atmospheric Lifetime (years): 3.41
 Tropospheric Atmospheric Lifetime (years): 3.59
 Stratospheric Atmospheric Lifetime (years): 68.6
 Ozone Depletion Potential (ODP): 0.020

	<i>Well-mixed</i>	<i>Lifetime adjusted</i>
Radiative Efficiency (RE):	0.140	0.125
Global Warming Potential (GWP _H):		
GWP ₂₀	935	837
GWP ₁₀₀	254	227
Global Temperature Potentials (GTP _H):		
GTP ₂₀		378
GTP ₅₀		43
GTP ₁₀₀		32

* RE units: W m² ppb⁻¹
 * GWP and GTP: Relative to CO₂

Atmospheric Loss Processes *****

OH Reactivity

$k_{\text{Rec}}(T)$, *No recommendation*

$$k_{\text{SAR}}(298 \text{ K}) = 1.64 \times 10^{-14}; k_{\text{SAR}}(272 \text{ K}) \approx 1.04 \times 10^{-14} \quad \text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$\tau_{\text{Global}}^{\text{OH}} = 3.47 \text{ years}$$

$$\tau_{\text{Trop}}^{\text{OH}} = 3.59 \text{ years}$$

$$\tau_{\text{Strat}}^{\text{OH}} = 106.6 \text{ years}$$

Fractional Atmospheric Loss: 0.982

O(¹D) Reactivity

$k_{\text{Rec}}(T)$, *No recommendation*

$$k_{\text{Est}}(T) = 1.1 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$\tau_{\text{O}(\text{1D})} = 335 \text{ years}$$

Fractional Atmospheric Loss: 0.010

UV Photolysis

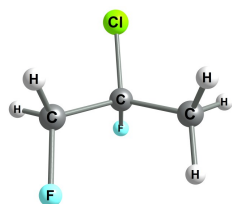
UV Spectrum: *No Recommendation*

$$\tau_{\text{hv}} = 450 \text{ years}$$

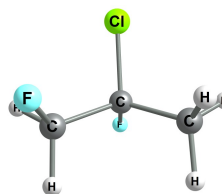
Fractional Atmospheric Loss: 0.008



Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.761



$\Delta E = 0.78 \text{ kcal mol}^{-1}$
Population = 0.205

Optimized Coordinates (Angstroms)

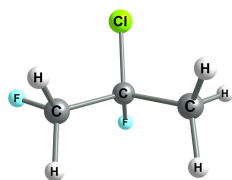
Atom	X	Y	Z
C	0.101996197100	1.519034819300	0.679936900000
C	-0.051573482500	0.212392324200	-0.070318636200
C	0.938546280600	-0.876015153700	0.333919471900
F	0.081398534900	0.441863590600	-1.404019818000
Cl	-1.717171565700	-0.486191373700	0.202476481200
H	-0.612500678900	2.250238422400	0.298736159100
H	1.119410502200	1.886696666800	0.524081397600
H	-0.067683644700	1.372999119800	1.748162470400
H	0.770230176900	-1.171766537900	1.373761872300
H	0.816601299500	-1.741412302900	-0.324496574300
F	2.214300380700	-0.377469575000	0.199996275900

Atom	X	Y	Z
C	0.000514208300	1.105692844900	1.282435669800
C	-0.117807053200	0.427100189100	-0.066102379100
C	1.216940689800	-0.006619169100	-0.670242217900
F	-0.692991515600	1.269906343900	-0.970486406100
Cl	-1.194347000300	-1.035061141500	0.080751116200
H	-0.988468076000	1.358930535100	1.666778310000
H	0.586629887200	2.023281514000	1.167209487700
H	0.507698926800	0.443970799000	1.985554262700
H	1.044416842900	-0.525867305100	-1.617564615000
H	1.819139850700	0.893680193400	-0.848372716200
F	1.882619239400	-0.830202803800	0.198649487900

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
119.7002	0.767
207.0847	0.771
241.5977	0.0521
293.4455	0.282
329.5408	0.178
372.9376	0.410
410.3209	0.416
475.2020	2.89
706.3344	9.62
843.1358	8.69
958.5636	2.27
994.2572	5.90
1088.3137	22.6
1102.6304	4.21
1203.5941	3.49
1249.3356	6.67
1304.0704	3.70
1402.3501	1.88
1422.2533	1.54
1477.8632	0.295
1485.7008	0.524
1495.9377	0.632
3056.6568	2.38
3062.5378	0.280
3116.7729	2.56
3144.3378	0.832
3154.7364	0.962

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
107.0079	0.552
205.4344	0.656
234.9753	0.00925
313.2612	0.536
318.5031	0.213
388.4202	0.317
433.3709	1.55
528.3363	0.783
596.7733	10.6
861.9367	6.79
953.1639	0.275
998.2754	2.89
1119.3529	11.1
1147.4732	16.1
1197.3498	10.2
1240.7645	2.61
1277.2538	3.16
1401.5970	2.03
1424.2163	1.12
1479.9116	0.226
1483.8804	0.807
1504.3175	0.446
3032.1208	3.90
3053.7010	1.49
3102.4840	2.93
3134.7909	1.30
3163.2886	0.474



$$\Delta E = 1.85 \text{ kcal mol}^{-1}$$

$$\text{Population} = 0.034$$

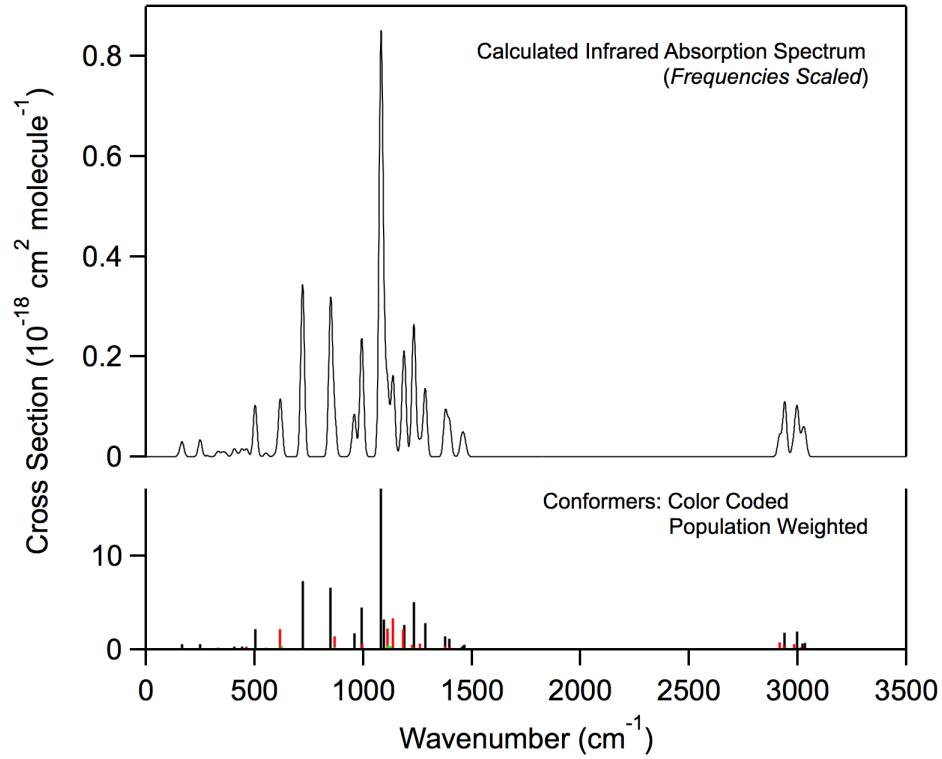
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.269146514400	1.303056969500	0.574320049500
C	-0.232009893800	0.386799262600	-0.046882518000
C	1.150509421600	0.528555026900	0.580743310200
F	-0.128006820700	0.654253976600	-1.377478977200
Cl	-0.773446473900	-1.346296243300	0.111375315400
H	-0.947989713300	2.343646941900	0.461403172900
H	-1.402566772800	1.079294827500	1.634201447900
H	-2.223384644000	1.171761051600	0.061644589800
H	1.486388130600	1.562812469000	0.427068589100
H	1.095142811900	0.316803408300	1.653737025800
F	2.039951468700	-0.319186690500	-0.013687005500

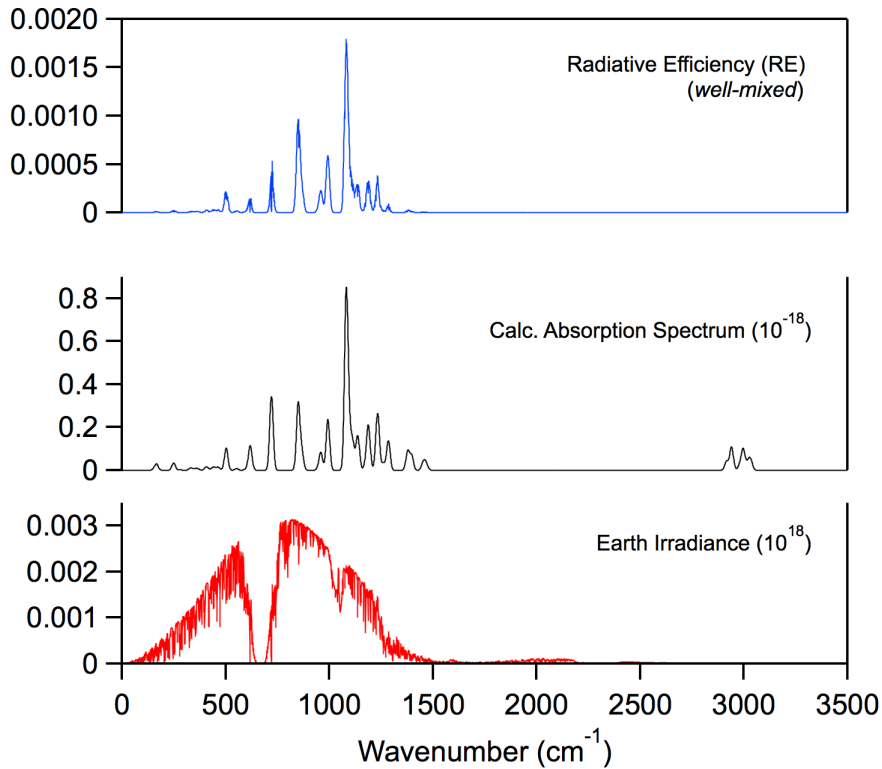
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
112.1627	0.290
199.4302	0.0420
224.2323	0.00282
296.0534	0.0595
335.2198	0.329
378.1265	0.391
398.4356	0.172
573.4546	3.04
604.0779	10.9
863.2189	7.57
944.1129	3.66
1004.4863	0.456
1122.3674	13.6
1134.2076	10.6
1182.0300	6.38
1246.7434	6.42
1294.1119	4.46
1409.4475	1.85
1431.3877	1.11
1477.9345	0.273
1485.5012	0.317
1495.1807	0.694
3024.9335	3.54
3052.3512	1.78
3088.4091	2.97
3131.4193	1.58
3154.2809	0.799

Infrared Spectrum

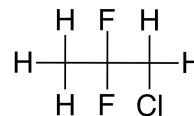


Radiative Efficiency



HCFC-262ca

Molecular Formula: CH₃CF₂CH₂Cl
 Name: 1-Chloro-2,2-difluoropropane
 CAS number: 420-99-5
 Molecular Weight: 114.52



Global Atmospheric Lifetime (years): 3.17
 Tropospheric Atmospheric Lifetime (years): 3.33
 Stratospheric Atmospheric Lifetime (years): 65.2
 Ozone Depletion Potential (ODP): 0.019

	<i>Well-mixed</i>	<i>Lifetime adjusted</i>
Radiative Efficiency (RE):	0.131	0.117
Global Warming Potential (GWP _H):		
GWP ₂₀	814	724
GWP ₁₀₀	221	196
Global Temperature Potentials (GTP _H):		
GTP ₂₀		316
GTP ₅₀		37
GTP ₁₀₀		27

* RE units: W m² ppb⁻¹
 * GWP and GTP: Relative to CO₂

Atmospheric Loss Processes *****

OH Reactivity

$k_{\text{Rec}}(T)$, *No recommendation*

$$k_{\text{SAR}}(298 \text{ K}) = 1.76 \times 10^{-14}; k_{\text{SAR}}(272 \text{ K}) \approx 1.13 \times 10^{-14} \quad \text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$\tau_{\text{Global}}^{\text{OH}} = 3.22 \text{ years}$$

$$\tau_{\text{Trop}}^{\text{OH}} = 3.33 \text{ years}$$

$$\tau_{\text{Strat}}^{\text{OH}} = 99.6 \text{ years}$$

Fractional Atmospheric Loss: 0.984

O(¹D) Reactivity

$k_{\text{Rec}}(T)$, *No recommendation*

$$k_{\text{Est}}(T) = 1.1 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$\tau_{\text{O}(\text{1D})} = 335 \text{ years}$$

Fractional Atmospheric Loss: 0.009

UV Photolysis

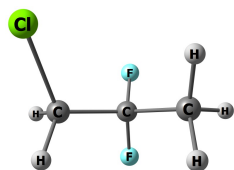
UV Spectrum: *No Recommendation*

$$\tau_{\text{hv}} = 450 \text{ years}$$

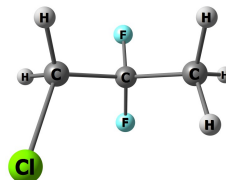
Fractional Atmospheric Loss: 0.007



Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.436



E = 0
Population = 0.436

Optimized Coordinates (Angstroms)

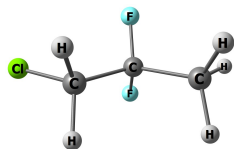
Atom	X	Y	Z
C	-1.027255792700	1.418261005500	-0.349674722100
C	-0.787406563600	-0.033505692900	0.003584091800
C	0.473894059200	-0.684881779600	-0.564990303600
F	-1.824017421400	-0.792479340400	-0.473858694300
F	-0.788298800100	-0.181707069600	1.354498049900
H	-1.973063926700	1.734271613000	0.095523205800
H	-1.084787334500	1.537458835000	-1.434078480800
H	-0.219314130900	2.040168717000	0.037925251700
H	0.508825485300	-1.723148946700	-0.235934567000
H	0.459746706500	-0.638786866200	-1.653406963000
Cl	1.978742718800	0.117011525000	-0.000702868600

Atom	X	Y	Z
C	-0.974741036600	1.425476216400	0.357583489300
C	-0.779005264900	-0.025967540400	-0.023122390500
C	0.471363688100	-0.720749218800	0.517533773900
F	-0.801408640700	-0.150956460600	-1.376182388100
F	-1.829607418700	-0.764783414000	0.455401065900
H	-1.917292270100	1.774417296100	-0.069564925100
H	-0.155281966500	2.031927444500	-0.030330554600
H	-1.014986008900	1.527614329100	1.444502771300
H	0.472520640900	-0.692938584000	1.606661136500
H	0.473804959100	-1.753785838300	0.170657183500
Cl	1.990052318200	0.049823769900	-0.053285162100

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
93.1968	0.568
189.1437	0.429
213.2915	0.0347
326.7358	0.527
337.6400	0.0608
416.5027	0.192
500.0941	2.25
554.0842	1.05
755.9228	3.11
813.0699	5.02
888.7603	1.40
958.8394	6.64
980.0993	3.00
1114.7613	5.72
1173.2080	19.9
1257.7242	12.2
1300.5185	8.06
1315.5179	2.24
1416.7951	6.41
1463.1983	1.26
1484.9827	0.725
1486.5338	0.0223
3064.4174	0.461
3100.9950	1.43
3143.7081	1.39
3157.6557	0.817
3168.8155	0.376

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
93.1898	0.568
189.1408	0.429
213.2950	0.0347
326.7312	0.527
337.6414	0.0608
416.5016	0.192
500.0945	2.25
554.0813	1.05
755.9205	3.11
813.0703	5.02
888.7597	1.40
958.8255	6.64
980.1110	3.00
1114.7694	5.72
1173.1837	19.9
1257.7340	12.2
1300.5297	8.06
1315.5115	2.24
1416.7952	6.41
1463.1925	1.26
1484.9800	0.725
1486.5344	0.0225
3064.4200	0.461
3101.0036	1.43
3143.7163	1.39
3157.6516	0.817
3168.8305	0.376



$\Delta E = 0.72 \text{ kcal mol}^{-1}$
 Population = 0.128

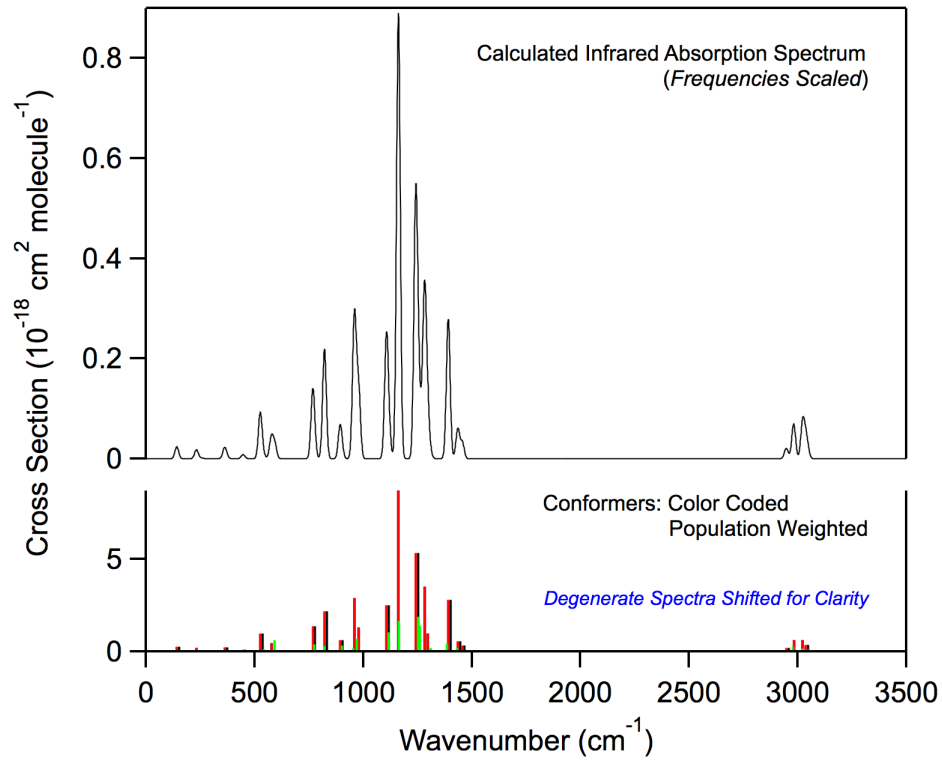
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-2.095513633600	0.710755921600	-0.020896479000
C	-0.769914360500	-0.032267737600	-0.011358909000
C	0.438083622500	0.899656372300	0.042125870400
F	-0.687094871400	-0.810073470600	-1.124614985900
F	-0.736902623300	-0.870913208500	1.059485088200
H	-2.163909822000	1.360877485400	-0.895943167500
H	-2.204542882000	1.311237786600	0.884963152100
H	-2.903247277100	-0.023308151700	-0.059780262700
H	0.441101713500	1.550396187600	-0.832379001000
H	0.400474173900	1.500773689500	0.950681253500
Cl	1.987557959900	-0.002830874700	0.052328440900

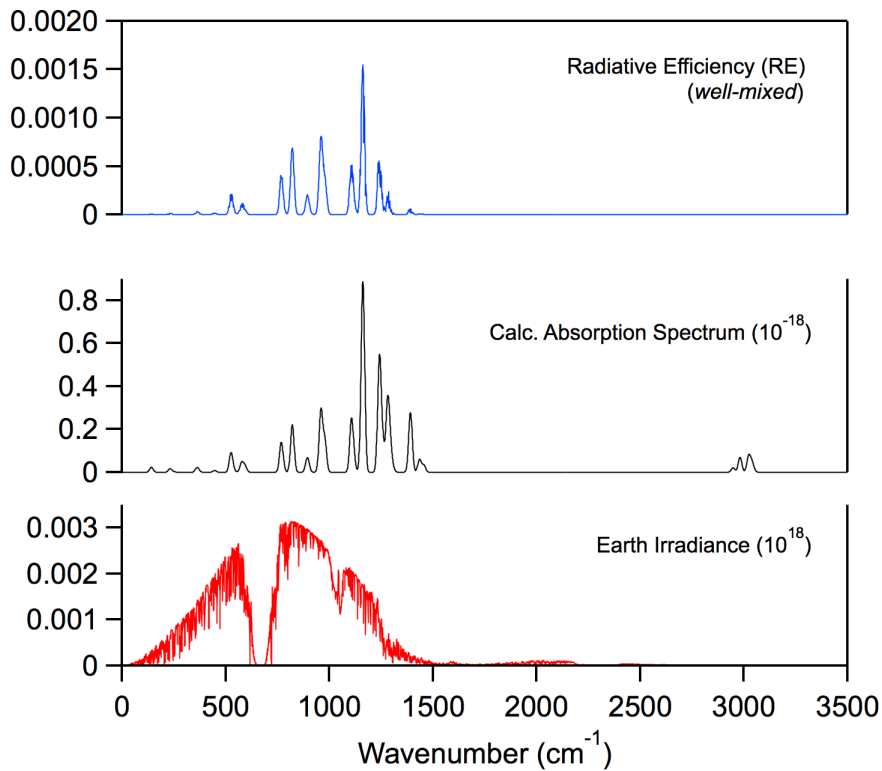
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
89.9347	0.117
179.8590	0.0622
206.7911	0.00913
313.1445	0.106
338.7149	0.0246
411.2104	0.0687
517.3525	1.04
571.0275	4.90
764.0979	3.16
813.0392	2.40
896.3641	2.55
952.7530	1.43
971.4030	5.29
1127.3463	8.01
1176.0425	13.0
1268.7726	14.8
1278.4636	10.9
1330.4629	1.45
1410.8697	3.23
1460.6046	1.42
1483.6883	0.0663
1485.0796	0.313
3059.6538	0.407
3095.8923	2.04
3141.8438	1.19
3145.3869	1.13
3160.8673	0.723

Infrared Spectrum

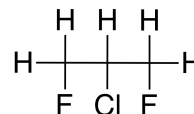


Radiative Efficiency



HCFC-262da

Molecular Formula: CH₂FCHClCH₂F
Name: 2-Chloro-1,3-difluoropropane
CAS number: 102738-79-4
Molecular Weight: 114.52



Global Atmospheric Lifetime (years): 0.924
Tropospheric Atmospheric Lifetime (years): 0.956
Stratospheric Atmospheric Lifetime (years): 27.7
Ozone Depletion Potential (ODP): 0.009

	<i>Well-mixed</i>	<i>Lifetime adjusted</i>
Radiative Efficiency (RE):	0.081	0.059
Global Warming Potential (GWP _H):		
GWP ₂₀	147	107
GWP ₁₀₀	40	29
Global Temperature Potentials (GTP _H):		
GTP ₂₀		34
GTP ₅₀		5
GTP ₁₀₀		4

* RE units: W m² ppb⁻¹

* GWP and GTP: Relative to CO₂

Atmospheric Loss Processes *****

OH Reactivity

$k_{\text{Rec}}(\text{T})$, *No recommendation*

$k_{\text{SAR}}(298 \text{ K}) = 6.13 \times 10^{-14}$; $k_{\text{SAR}}(272 \text{ K}) \approx 3.91 \times 10^{-14}$ cm³ molecule⁻¹ s⁻¹

$\tau_{\text{Global}}^{\text{OH}} = 0.930$ years

$\tau_{\text{Trop}}^{\text{OH}} = 0.956$ years

$\tau_{\text{Strat}}^{\text{OH}} = 32.4$ years

Fractional Atmospheric Loss: 0.995

O(¹D) Reactivity

$k_{\text{Rec}}(\text{T})$, *No recommendation*

$k_{\text{Est}}(\text{T}) = 1.1 \times 10^{-10}$ cm³ molecule⁻¹ s⁻¹

$\tau_{\text{O}(\text{1D})} = 335$ years

Fractional Atmospheric Loss: 0.003

UV Photolysis

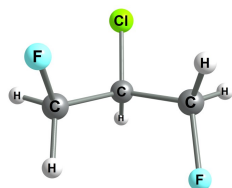
UV Spectrum: *No Recommendation*

$\tau_{\text{hv}} = 450$ years

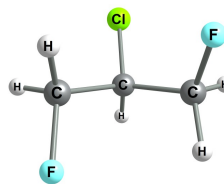
Fractional Atmospheric Loss: 0.002



Molecular Structure and Infrared Spectrum (7 conformers)



E = 0
Population = 0.368



E = 0
Population = 0.368

Optimized Coordinates (Angstroms)

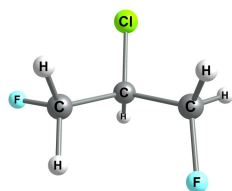
Atom	X	Y	Z
C	0.855676380300	-1.018646305100	-0.368106916800
C	-0.092292036200	-0.239978005300	0.539141182400
C	0.245595347100	1.239425822900	0.596262377700
H	-0.066296000000	-0.650029738900	1.551400532400
Cl	-1.777620545300	-0.492551917700	-0.073535443500
F	2.133345089600	-0.886012968100	0.140582960600
H	0.828544271400	-0.606264532600	-1.380772991200
H	0.587186493000	-2.078648765200	-0.392550740700
H	-0.476717611600	1.780960806000	1.215323849700
H	1.250457792600	1.344651742500	1.023724237200
F	0.245043819000	1.776690861500	-0.669404047800

Atom	X	Y	Z
C	-0.099401413800	1.267418734000	0.608391518500
C	-0.007694645100	-0.245542693500	0.515577603700
C	-1.020219244100	-0.830713846100	-0.464447219000
H	-0.156258333100	-0.672475385000	1.510136135500
Cl	1.643708389700	-0.758995774800	-0.021704299600
F	0.058946214200	1.830793385400	-0.635851819900
H	0.667481574900	1.664208680500	1.281206511500
H	-1.094945014500	1.527167881000	0.989125319400
H	-0.870098564300	-0.401631231500	-1.459251110500
H	-0.929414161800	-1.919598310900	-0.513179787800
F	-2.284319802100	-0.500648438900	-0.015131851800

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
91.1339	0.380
143.8924	0.738
209.5418	0.427
244.9205	2.19
317.7409	0.426
405.2176	0.877
610.6645	2.42
713.9934	5.06
887.2164	0.469
987.3364	1.17
1018.3011	5.10
1073.8898	15.5
1131.4863	7.74
1146.6967	1.06
1229.6287	0.965
1256.9145	0.961
1288.7368	1.60
1361.5438	0.172
1404.5055	0.869
1433.9007	1.55
1496.5821	0.786
1510.5273	0.761
3037.1461	3.36
3060.7466	2.75
3093.7927	2.23
3095.3810	1.99
3121.9576	3.03

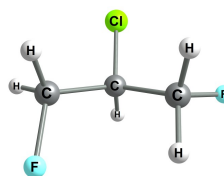
Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
91.1491	0.380
143.8969	0.738
209.5390	0.427
244.9219	2.19
317.7418	0.426
405.2222	0.877
610.6621	2.42
714.0036	5.06
887.2175	0.469
987.3317	1.17
1018.2912	5.10
1073.9057	15.5
1131.4596	7.74
1146.6908	1.05
1229.6308	0.965
1256.9200	0.961
1288.7309	1.60
1361.5420	0.172
1404.4991	0.869
1433.8940	1.55
1496.5727	0.785
1510.5202	0.761
3037.1736	3.36
3060.7494	2.75
3093.7993	2.22
3095.3888	2.00
3121.9696	3.03



$\Delta E = 0.82 \text{ kcal mol}^{-1}$
Population = 0.092

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.447897269900	-0.615151371300	-0.120745896300
C	0.094467171700	-0.081763314600	0.337358355500
C	-0.247015890000	1.251096432400	-0.304450789900
H	0.076315622500	0.021892506100	1.424065341100
Cl	-1.156501088200	-1.326590743500	-0.066354884400
F	2.422675709000	0.295360578300	0.237067863100
H	1.464925963800	-0.745816696800	-1.209111643500
H	1.660549131400	-1.576004247400	0.357105715900
H	0.578970473300	1.946011719300	-0.110336022100
H	-0.376598931300	1.135620982000	-1.387198042300
F	-1.400327431900	1.759886155400	0.235534003000



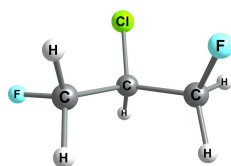
$\Delta E = 0.82 \text{ kcal mol}^{-1}$
Population = 0.092

Atom	X	Y	Z
C	0.290180055300	1.244169309300	-0.360962978700
C	-0.092897779200	-0.071558282500	0.292645646600
C	-1.441907602200	-0.589351646300	-0.195422156500
H	-0.103954508500	0.050277946900	1.377563176200
Cl	1.146900813000	-1.344307991800	-0.054248872700
F	1.436399806400	1.742222212700	0.203578098500
H	-0.528637597700	1.956332846100	-0.202232633700
H	0.448548745700	1.108107122200	-1.437477458700
H	-1.430141912100	-0.738189360000	-1.281521657400
H	-1.685038029100	-1.538140490500	0.291904841300
F	-2.410282991600	0.343717333900	0.119025995100

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
104.4177	0.815
123.7502	1.00
208.5983	0.764
217.2815	0.191
365.9498	0.218
384.9192	0.614
510.4210	3.20
704.7593	6.13
899.3161	0.358
1008.8585	4.06
1071.1914	12.1
1097.4587	2.82
1121.7604	12.8
1139.6702	0.430
1235.2758	0.588
1250.1759	0.0753
1302.4282	2.11
1338.9596	1.35
1416.7036	1.68
1433.0624	1.22
1505.7065	0.486
1512.9932	0.508
3030.5558	3.24
3043.1966	3.17
3080.5571	1.93
3097.1358	2.13
3113.7382	3.51

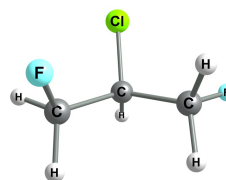
Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
104.4173	0.815
123.7471	1.00
208.5969	0.764
217.2852	0.192
365.9599	0.218
384.9272	0.613
510.4247	3.20
704.8034	6.13
899.3137	0.358
1008.8687	4.06
1071.2021	12.1
1097.4531	2.83
1121.7515	12.8
1139.6622	0.430
1235.2907	0.587
1250.1808	0.0753
1302.4327	2.11
1338.9560	1.35
1416.7020	1.68
1433.0572	1.22
1505.7112	0.486
1512.9884	0.508
3030.5506	3.24
3043.1932	3.18
3080.5519	1.92
3097.1321	2.13
3113.7195	3.52



$\Delta E = 1.50 \text{ kcal mol}^{-1}$
Population = 0.029

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.447180507900	0.586541039700	0.598301656300
C	-0.000093525700	0.125175574400	0.608691490700
C	-0.906986707100	1.063723879700	-0.173293755400
H	-0.346068650600	0.056026176100	1.643007861600
Cl	-0.132718360800	-1.554404943400	-0.062934935200
F	1.874477689000	0.795043278900	-0.692728753300
H	2.092421480300	-0.158467660100	1.073819110700
H	1.526683711000	1.534600063000	1.148991044600
H	-0.781633981200	2.084108354200	0.216233438300
H	-0.642926369200	1.051421011500	-1.234451267200
F	-2.218183793600	0.692897225900	-0.022907891200



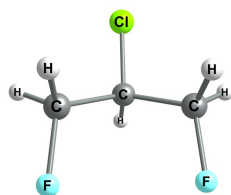
$\Delta E = 1.50 \text{ kcal mol}^{-1}$
Population = 0.029

Atom	X	Y	Z
C	-0.828933569500	-1.091987056700	-0.174718895700
C	0.007122276800	-0.073852748400	0.586343070200
C	1.481836085200	-0.438089093200	0.598585966400
H	-0.351399125700	0.000910956800	1.615986676000
Cl	-0.230800947500	1.573867137900	-0.133450455800
F	-2.163048032800	-0.805102887700	-0.043573713400
H	-0.639554179200	-2.090559150600	0.244350129100
H	-0.557278385600	-1.091684084100	-1.234031204000
H	2.072220536900	0.361134759800	1.057038486600
H	1.619341114400	-1.363055048700	1.176447715900
F	1.932935227000	-0.653592785200	-0.683160775200

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
96.2674	0.642
116.2141	0.603
174.1693	0.336
275.6337	0.196
327.2135	0.162
437.9153	1.91
596.7443	5.84
687.6943	2.99
918.9982	0.566
925.5326	0.938
1049.4696	1.95
1107.4436	7.68
1125.6161	14.5
1143.0663	1.97
1243.0503	0.714
1271.5627	0.652
1289.0880	1.08
1325.3642	3.54
1417.2529	2.92
1437.9714	0.966
1500.2208	1.02
1504.5157	0.291
3012.0849	1.62
3019.2983	8.43
3087.9000	1.16
3091.4995	2.26
3106.3689	3.68

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
96.2613	0.642
116.2126	0.603
174.1675	0.336
275.6331	0.196
327.2122	0.162
437.9150	1.91
596.7379	5.84
687.6877	2.99
919.0031	0.567
925.5246	0.937
1049.4659	1.95
1107.4480	7.68
1125.6195	14.5
1143.0711	1.97
1243.0508	0.715
1271.5634	0.652
1289.0871	1.08
1325.3647	3.54
1417.2538	2.92
1437.9786	0.966
1500.2204	1.02
1504.5178	0.291
3012.0871	1.62
3019.3002	8.43
3087.8899	1.15
3091.4951	2.26
3106.3510	3.68



$\Delta E = 1.90 \text{ kcal mol}^{-1}$
Population = 0.015

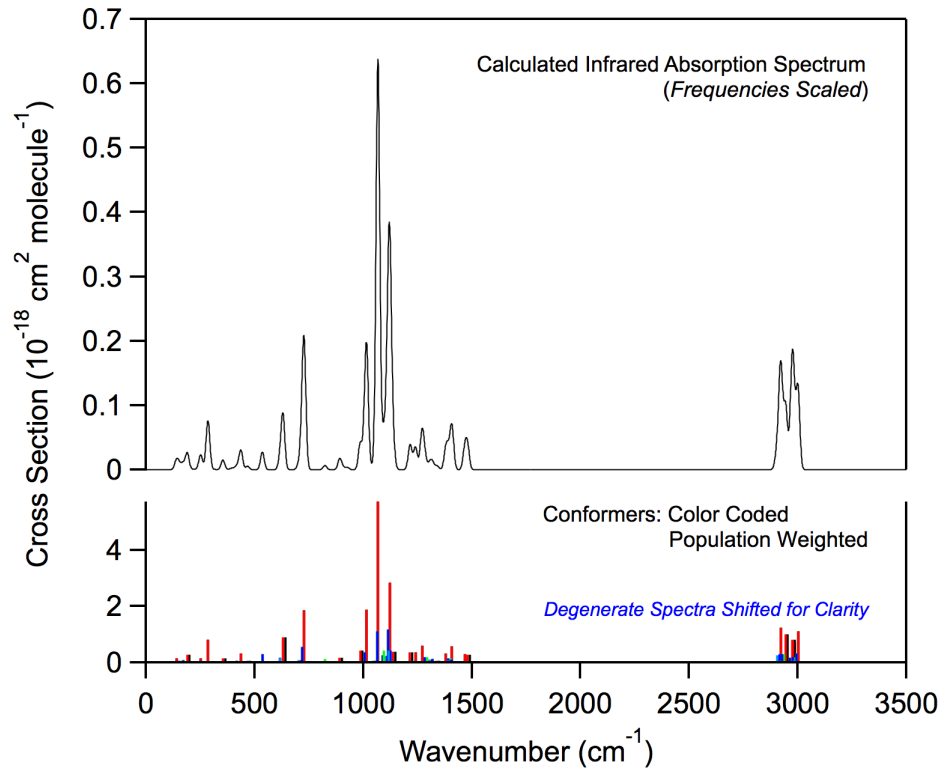
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-0.345025827300	1.311459334600	-0.159576899500
C	0.210177234400	-0.009072099800	0.368640834400
C	-0.382920821300	-1.254061684800	-0.286566730700
H	0.080216122200	-0.060750239700	1.451482541000
Cl	1.993396144200	-0.019831352300	0.053865019900
F	-1.675933185600	1.407532101800	0.169611445400
H	-0.238081771800	1.358958556700	-1.250366100400
H	0.196862041000	2.151895545600	0.287050206100
H	-0.275840508100	-1.196755095700	-1.376871703100
H	0.133324641600	-2.150087532300	0.074098773800
F	-1.716557069400	-1.342919534000	0.033479613100

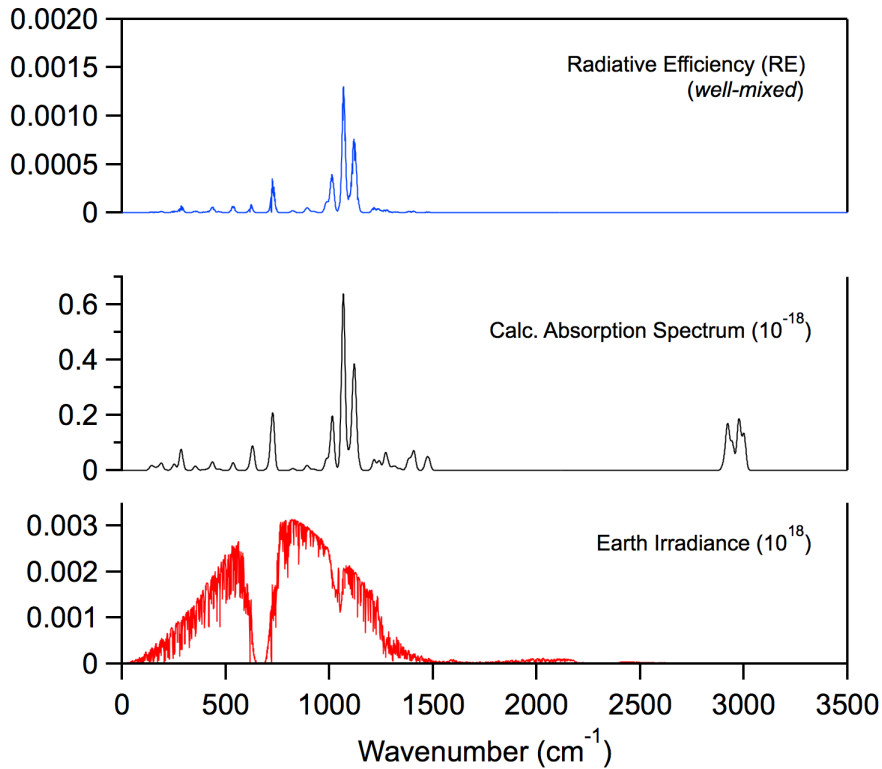
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
63.3553	0.224
145.4042	0.839
199.7514	1.09
254.3499	1.58
354.4068	1.49
386.1727	0.0731
418.4010	0.105
815.4858	9.25
903.9762	1.20
931.0391	0.0178
1082.3142	0.792
1101.4100	28.1
1132.8933	0.867
1158.9674	1.71
1213.0062	0.647
1249.0864	0.107
1296.6333	0.0112
1365.3691	0.211
1416.9668	0.934
1440.5090	2.21
1504.7752	0.358
1516.8481	0.204
3031.5651	2.38
3034.4329	4.62
3083.7221	3.15
3086.5628	3.01
3111.7026	3.31

Infrared Spectrum

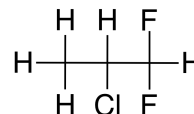


Radiative Efficiency



HCFC-262db

Molecular Formula: CH₃CHClCHF₂
 Name: 2-Chloro-1,1-difluoropropane
 CAS number: 430-93-3
 Molecular Weight: 114.52



Global Atmospheric Lifetime (years): 0.642
 Tropospheric Atmospheric Lifetime (years): 0.662
 Stratospheric Atmospheric Lifetime (years): 20.8
 Ozone Depletion Potential (ODP): 0.007

	<i>Well-mixed</i>	<i>Lifetime adjusted</i>
Radiative Efficiency (RE):	0.124	0.081
Global Warming Potential (GWP _H):		
GWP ₂₀	156	103
GWP ₁₀₀	42	28
Global Temperature Potentials (GTP _H):		
GTP ₂₀		32
GTP ₅₀		5
GTP ₁₀₀		4

* RE units: W m² ppb⁻¹
 * GWP and GTP: Relative to CO₂

Atmospheric Loss Processes *****

OH Reactivity

$k_{\text{Rec}}(T)$, *No recommendation*

$$k_{\text{SAR}}(298 \text{ K}) = 8.86 \times 10^{-14}; k_{\text{SAR}}(272 \text{ K}) \approx 5.65 \times 10^{-14} \quad \text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$\tau_{\text{Global}}^{\text{OH}} = 0.644 \text{ years}$$

$$\tau_{\text{Trop}}^{\text{OH}} = 0.662 \text{ years}$$

$$\tau_{\text{Strat}}^{\text{OH}} = 23.3 \text{ years}$$

Fractional Atmospheric Loss: 0.997

O(¹D) Reactivity

$k_{\text{Rec}}(T)$, *No recommendation*

$$k_{\text{Est}}(T) = 1.1 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$\tau_{\text{O}(\text{1D})} = 335 \text{ years}$$

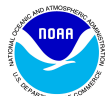
Fractional Atmospheric Loss: 0.002

UV Photolysis

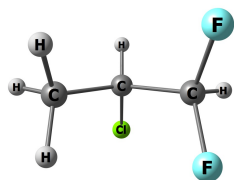
UV Spectrum: *No Recommendation*

$$\tau_{\text{hv}} = 450 \text{ years}$$

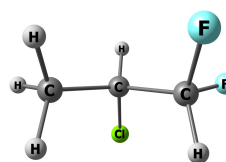
Fractional Atmospheric Loss: 0.001



Molecular Structure and Infrared Spectrum (3 conformers)



$E = 0$
Population = 0.568



$\Delta E = 0.29 \text{ kcal mol}^{-1}$
Population = 0.347

Optimized Coordinates (Angstroms)

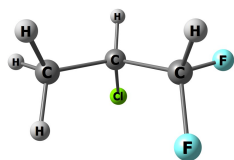
Atom	X	Y	Z
C	-0.112988308100	1.652325720300	-0.536795773800
C	-0.243923617500	0.491914846200	-0.436430726000
C	0.897888226100	-0.515103261400	-0.312860321300
H	-0.268575203100	0.837542312300	-1.471376755400
Cl	-1.805027412800	-0.398876753100	-0.187423707000
H	-0.927454953400	2.364561020800	0.395760418900
H	0.838863221700	2.161126744700	0.356394359200
H	-0.128011846100	1.292107691500	1.566915473300
F	1.037189913000	-0.926256818800	0.966854934500
H	0.759520056800	-1.393546305400	-0.952837477000
F	2.050089923300	0.112869802800	-0.673998973000

Atom	X	Y	Z
C	-0.438926065700	1.858664149400	0.023924497100
C	-0.259537243700	0.400055327500	-0.364770894400
C	0.943784956700	-0.247830357800	0.315755855000
H	-0.135489798500	0.282172537700	-1.443236630000
Cl	-1.731568714100	-0.564460453900	0.071632032900
H	0.452013609700	2.422262742400	-0.266147338600
H	-0.584368791700	1.962231479800	1.103049417800
H	-1.307778902700	2.282819881200	-0.482429852100
F	2.047742027800	0.490581869900	0.019651699400
H	0.833756558100	-0.297262693000	1.406087713400
F	1.144636364000	-1.493293483300	-0.162832500500

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
84.5692	0.364
204.9202	0.388
239.2096	0.00845
256.4564	0.827
311.5174	0.418
386.4804	0.684
533.2575	1.32
666.4844	1.12
722.1083	5.07
886.4858	1.94
1002.5409	4.88
1057.5795	6.83
1104.6180	25.5
1129.0860	0.773
1187.3121	11.5
1256.3140	2.22
1348.5387	0.800
1381.4806	2.52
1404.6967	1.95
1424.0766	3.35
1487.0172	0.831
1495.8276	1.34
3056.5871	1.34
3070.0992	5.03
3103.9188	1.15
3133.0046	1.35
3152.9604	1.24

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
80.8058	0.244
192.1979	0.269
234.8593	0.100
297.0704	0.121
349.3910	1.07
397.1358	0.987
464.8153	1.40
579.9417	1.02
729.3765	5.31
907.3210	1.87
1023.7855	4.62
1102.2563	10.1
1108.5518	15.6
1149.0689	17.9
1163.0538	1.20
1252.4092	3.45
1317.5300	0.644
1387.7532	1.69
1410.1032	0.110
1425.5944	5.84
1488.9017	1.73
1494.7832	0.816
3051.4295	1.09
3055.7996	4.78
3101.5203	0.808
3128.7605	2.38
3141.4593	1.23



$\Delta E = 1.12 \text{ kcal mol}^{-1}$
Population = 0.085

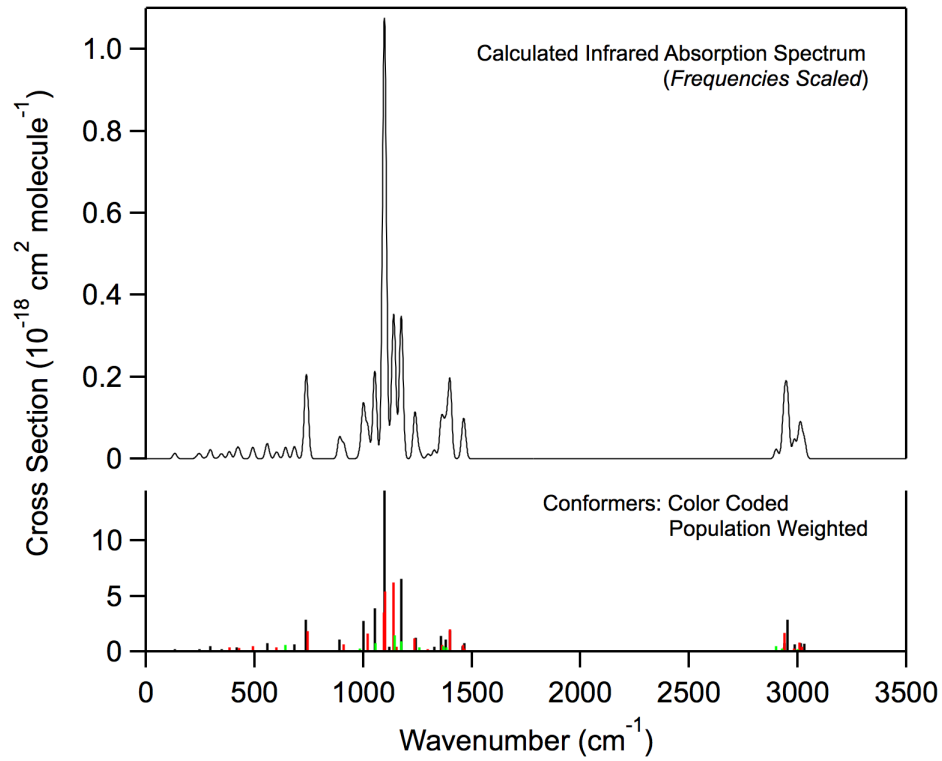
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.048595218200	1.674871483100	-0.156374975300
C	-0.401746592700	0.361690861300	-0.572017840400
C	1.079356395700	0.314907860500	-0.211749032300
H	-0.483928053400	0.198895913800	-1.648728840500
Cl	-1.253723935800	-1.038938317400	0.196395611700
H	-2.103082210600	1.686210173000	-0.436344093100
H	-0.549033997000	2.512087334500	-0.657673860100
H	-0.965882399500	1.815199682100	0.923256354300
F	1.633009751800	-0.855245260100	-0.595670618000
H	1.616434697900	1.133508658100	-0.714064694900
F	1.253684561800	0.449059611100	1.123132988700

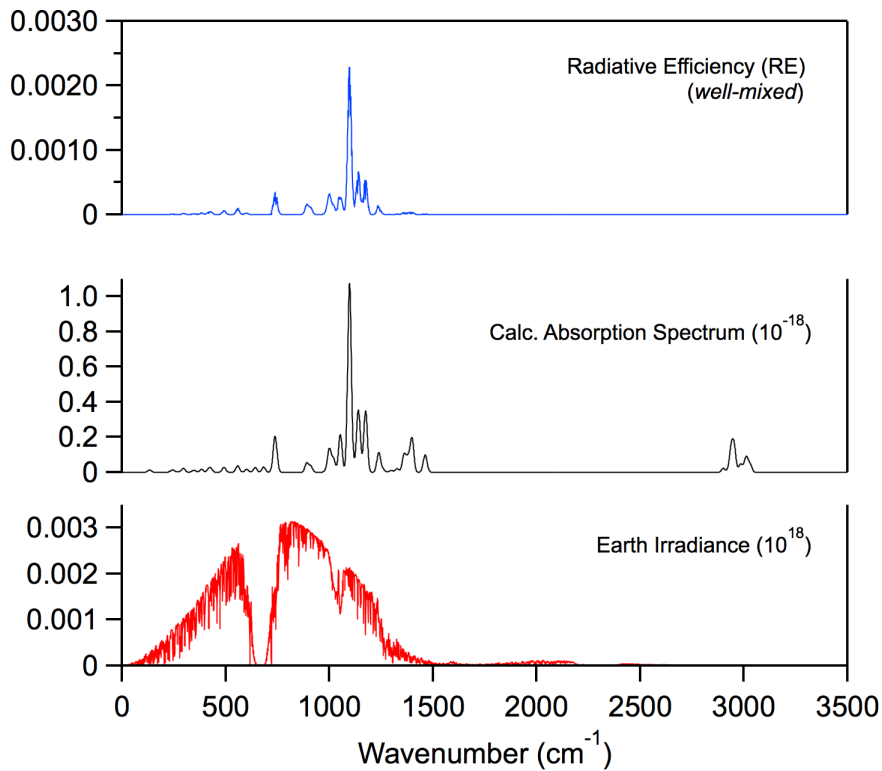
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
85.8809	0.0188
197.1301	0.156
232.5507	0.0772
246.5251	0.0281
314.9067	0.0804
459.9588	1.49
541.3861	0.805
623.5104	6.88
710.4587	0.614
904.9073	1.13
986.8412	3.26
1061.3064	8.75
1104.4107	1.22
1155.8989	17.0
1187.8298	10.7
1275.3572	4.46
1328.7826	0.365
1393.3924	5.46
1408.5054	4.64
1416.3526	1.78
1486.9401	1.44
1495.8488	0.670
3014.7651	5.75
3042.8956	3.21
3097.0674	0.945
3120.9879	2.25
3151.5941	1.13

Infrared Spectrum

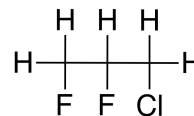


Radiative Efficiency



HCFC-262ea

Molecular Formula: CH₂FCHFCH₂Cl
 Name: 1-Chloro-2,3-difluoropropane
 CAS number: 37161-81-2
 Molecular Weight: 114.52



Global Atmospheric Lifetime (years): 0.828
 Tropospheric Atmospheric Lifetime (years): 0.856
 Stratospheric Atmospheric Lifetime (years): 25.4
 Ozone Depletion Potential (ODP): 0.009

	<i>Well-mixed</i>	<i>Lifetime adjusted</i>
Radiative Efficiency (RE):	0.093	0.066
Global Warming Potential (GWP _H):		
GWP ₂₀	151	107
GWP ₁₀₀	41	29
Global Temperature Potentials (GTP _H):		
GTP ₂₀		34
GTP ₅₀		5
GTP ₁₀₀		4

* RE units: W m² ppb⁻¹
 * GWP and GTP: Relative to CO₂

Atmospheric Loss Processes *****

OH Reactivity

$k_{\text{Rec}}(T)$, *No recommendation*

$$k_{\text{SAR}}(298 \text{ K}) = 6.86 \times 10^{-14}; k_{\text{SAR}}(272 \text{ K}) \approx 4.38 \times 10^{-14} \quad \text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$\tau_{\text{Global}}^{\text{OH}} = 0.831 \text{ years}$$

$$\tau_{\text{Trop}}^{\text{OH}} = 0.856 \text{ years}$$

$$\tau_{\text{Strat}}^{\text{OH}} = 29.3 \text{ years}$$

Fractional Atmospheric Loss: 0.996

O(¹D) Reactivity

$k_{\text{Rec}}(T)$, *No recommendation*

$$k_{\text{Est}}(T) = 1.1 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$\tau_{\text{O}(\text{1D})} = 335 \text{ years}$$

Fractional Atmospheric Loss: 0.002

UV Photolysis

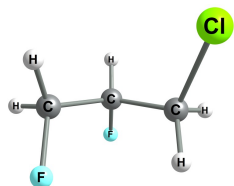
UV Spectrum: *No Recommendation*

$$\tau_{\text{hv}} = 450 \text{ years}$$

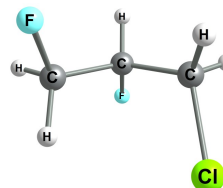
Fractional Atmospheric Loss: 0.002



Molecular Structure and Infrared Spectrum (7 conformers)



$E = 0$
Population = 0.444



$\Delta E = 0.59 \text{ kcal mol}^{-1}$
Population = 0.165

Optimized Coordinates (Angstroms)

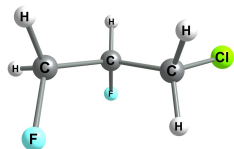
Atom	X	Y	Z
C	-0.586930114700	0.793402813000	0.446028193500
C	0.586891974100	0.575485133300	-0.503979488300
C	1.068073406000	-0.862062179400	-0.567293028000
F	1.619346196600	1.368400788300	-0.031107895400
H	0.325310468300	0.910777413800	-1.515455840100
Cl	-2.093964470000	0.053568249800	-0.212905435400
H	-0.773440705800	1.859239487400	0.568955296700
H	-0.387456623800	0.330056436700	1.410901719900
H	0.318154202700	-1.489804162800	-1.060552007300
H	2.008812327500	-0.905558554100	-1.127709347400
F	1.288536339100	-1.336671425800	0.707376831700

Atom	X	Y	Z
C	-0.583430195600	-0.144779332900	-0.957684182300
C	0.586095240900	0.655254462800	-0.411459743900
C	1.443359556700	-0.097764288400	0.600329054800
F	0.142881195000	1.812665028000	0.187118882600
H	1.215165354500	0.927903132100	-1.272054525600
Cl	-1.767252918900	-0.607650640900	0.324522024900
H	-0.213979355200	-1.065881984200	-1.408907673400
H	-1.135579957700	0.438296663800	-1.694402824900
H	2.259393117600	0.546658706500	0.944455203300
H	0.842561256400	-0.414993484900	1.458157742600
F	1.969964706400	-1.208889262000	-0.025292958100

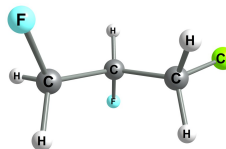
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
71.2904	0.377
145.6807	0.918
209.5276	1.07
246.6218	1.05
369.1505	1.19
398.1042	0.405
637.8786	1.66
765.3057	6.75
834.6218	2.03
946.9507	5.18
959.0085	4.58
1072.3167	3.19
1111.9659	6.76
1143.3932	7.86
1181.6353	0.671
1275.8818	2.79
1284.8011	0.137
1377.0609	0.745
1392.3454	0.602
1424.5612	1.13
1479.3427	1.18
1496.0140	1.50
3037.8256	1.00
3050.9077	5.97
3096.8692	3.55
3108.5482	1.45
3177.7261	0.178

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
69.6006	0.320
144.9595	0.822
201.4120	0.339
234.9440	1.93
374.5212	1.57
467.3817	0.0948
570.4891	2.79
714.2652	2.98
848.3764	1.27
902.8450	0.825
1050.4859	1.12
1093.0285	17.6
1096.9330	0.126
1149.9292	6.61
1220.1325	1.17
1250.8071	0.414
1312.5312	3.03
1347.8530	1.83
1386.0382	3.20
1433.0400	0.0851
1458.2241	1.80
1515.7725	0.811
3010.1016	3.52
3050.5184	4.10
3098.5591	1.60
3108.5860	3.97
3163.2699	0.251



$\Delta E = 0.74 \text{ kcal mol}^{-1}$
Population = 0.126



$\Delta E = 0.75 \text{ kcal mol}^{-1}$
Population = 0.124

Optimized Coordinates (Angstroms)

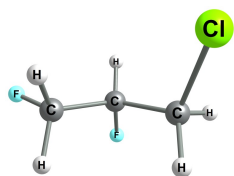
Atom	X	Y	Z
C	-0.530255640300	-0.685559495100	0.098342319900
C	0.404889298400	0.352098308200	-0.501022275200
C	1.832191299000	-0.165968916300	-0.598770181400
F	0.391822617100	1.481868321600	0.288267846000
H	0.066652382900	0.633180014900	-1.507203507300
Cl	-2.238094855400	-0.113961518300	0.092799757200
H	-0.254560405800	-0.886057470800	1.132419096200
H	-0.498308671400	-1.612140361300	-0.476529202100
H	1.903773124300	-0.930168932200	-1.383044187900
H	2.501353698600	0.666310804600	-0.844398106300
F	2.226987152700	-0.717382755200	0.600424441000

Atom	X	Y	Z
C	-0.505591731400	-0.471046192200	0.500157956400
C	0.455577912400	0.417866709500	-0.264711327800
C	1.905537538100	0.148807097600	0.139077819600
F	0.200984332300	1.743716680600	0.012744077500
H	0.337537575700	0.257849705300	-1.342808625700
Cl	-2.195394297800	-0.303230253500	-0.100495017300
H	-0.513868555100	-0.203392734800	1.558205176600
H	-0.213945044700	-1.514649286800	0.383307634200
H	2.569016004700	0.835093115100	-0.397964754700
H	2.038083215900	0.296474869800	1.217978768900
F	2.229913050000	-1.150543710700	-0.184512707700

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
87.3874	0.681
108.3233	0.622
175.6008	0.270
255.5258	0.0274
340.5055	0.152
445.2973	2.46
626.1369	6.46
791.9422	1.71
851.1059	1.91
894.7709	1.84
957.9934	5.43
1059.6749	2.52
1120.6753	9.63
1149.6381	4.78
1217.6598	1.15
1261.2815	1.48
1290.7664	2.15
1366.1558	0.891
1396.9259	2.16
1424.5739	1.63
1466.3298	1.01
1496.7707	0.774
3025.5951	1.19
3040.5392	6.89
3084.9189	3.74
3096.5870	2.02
3167.2474	0.333

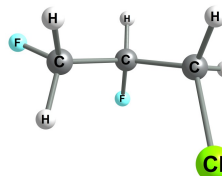
Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
83.4393	0.405
113.4729	1.40
202.3006	0.0599
214.4689	0.674
406.7724	0.727
428.9142	2.82
497.3759	1.51
750.1189	4.23
853.1109	1.46
915.9242	0.469
1072.8331	5.90
1093.5647	9.86
1108.0718	3.87
1143.8546	6.28
1214.6493	1.16
1247.6401	0.722
1290.9113	3.52
1351.2283	0.578
1395.2263	1.71
1429.9498	0.792
1464.2634	1.24
1516.2423	0.460
3033.5543	3.76
3054.7651	2.46
3088.2717	1.71
3093.6214	5.55
3158.8578	0.380



$\Delta E = 1.07 \text{ kcal mol}^{-1}$
Population = 0.073

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-0.914329600800	0.825579125600	0.152200748600
C	0.482030077500	0.441362022500	-0.329543899600
C	1.045741043700	-0.792698550400	0.348041579900
F	1.302763050700	1.517940198700	-0.039477693700
H	0.482150598100	0.294609074500	-1.415885082000
Cl	-2.158615382800	-0.344936866800	-0.423667578600
H	-1.178657111300	1.804315518500	-0.246717643700
H	-0.970043185100	0.852039397900	1.241710090800
H	1.217998208100	-0.581201348800	1.411266873600
H	0.347910022600	-1.631339222800	0.251994508900
F	2.242077279300	-1.127461348900	-0.239546904300



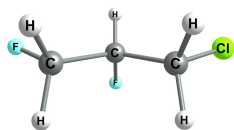
$\Delta E = 1.32 \text{ kcal mol}^{-1}$
Population = 0.048

Atom	X	Y	Z
C	-0.908563890100	0.234127049700	-0.987439088100
C	0.509645993700	0.475562243000	-0.499632929900
C	1.259988508600	-0.777501520700	-0.081627860400
F	0.492518663100	1.361874334100	0.554337005600
H	1.062844792800	0.947654487300	-1.325837597800
Cl	-1.930956972700	-0.642112932500	0.218461140800
H	-0.906656724500	-0.362875302000	-1.900530317200
H	-1.400553020800	1.188197400200	-1.175581980800
H	0.867193200100	-1.153605331300	0.867639734100
H	1.156457232400	-1.554674570100	-0.849496674800
F	2.591858217400	-0.470220857700	0.071242568600

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
92.1556	0.762
102.9034	0.984
205.7358	0.574
239.2269	0.406
356.5104	0.305
442.2402	0.543
507.5319	2.83
767.4549	7.12
839.3662	1.30
918.1876	4.62
1058.3929	1.26
1101.0405	11.9
1114.8314	12.1
1122.4785	2.33
1191.4282	0.723
1277.0073	1.03
1284.5833	0.969
1349.3499	0.631
1387.7485	0.641
1443.4825	0.649
1486.1887	1.21
1500.4419	0.706
3029.1930	2.94
3058.3340	2.23
3089.9814	0.290
3093.6493	5.84
3157.5316	0.551

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
85.0956	0.677
110.1971	0.575
165.7613	0.148
274.2849	0.242
348.6242	0.174
461.2633	2.37
614.8707	4.74
697.4973	2.47
875.5702	0.281
896.0844	4.10
989.2692	1.08
1086.4193	4.76
1106.5356	16.7
1154.2523	2.82
1223.1960	1.59
1278.4830	1.05
1292.9471	1.04
1334.7267	4.16
1394.8584	2.36
1440.1936	0.427
1463.5293	1.82
1498.1598	0.332
3008.9453	2.80
3033.5645	4.13
3092.3459	1.30
3103.5880	3.83
3155.8940	0.499



$\Delta E = 1.85 \text{ kcal mol}^{-1}$
 Population = 0.020

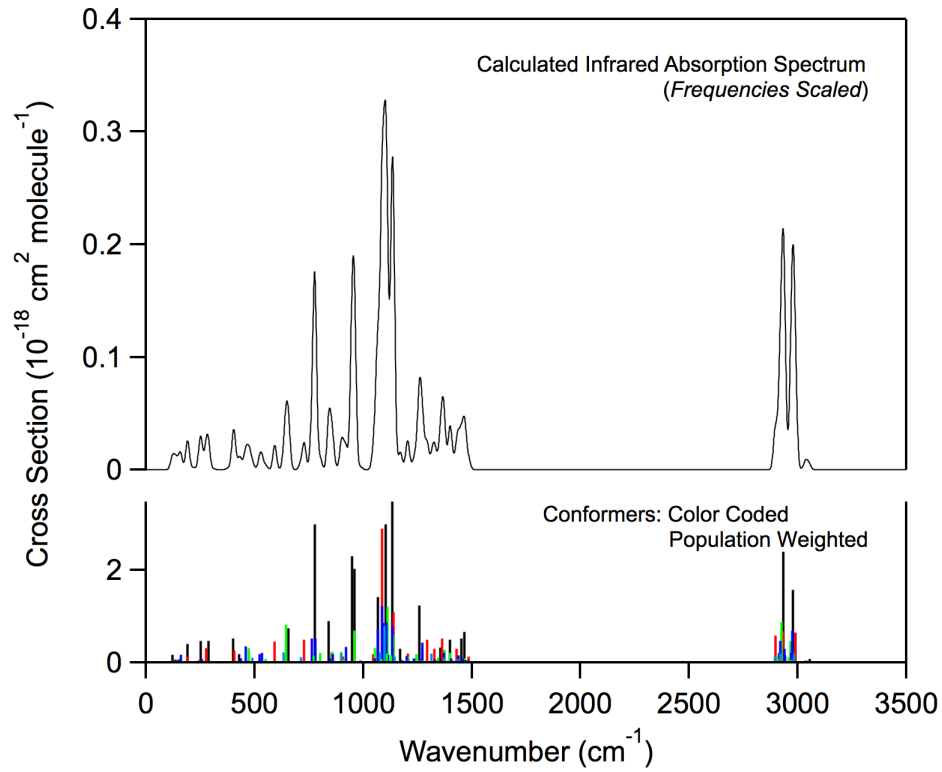
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-0.787867790800	-0.704884029300	0.360724110600
C	0.418943712400	0.047877450700	-0.175821606100
C	1.720919842900	-0.659419710800	0.173730070400
F	0.450149611800	1.311794630700	0.369222459500
H	0.348959292800	0.150454140600	-1.265750451100
Cl	-2.328538079400	0.088158545800	-0.128272958200
H	-0.777100312700	-0.727744443000	1.451667063400
H	-0.815391767000	-1.723982056800	-0.027516087200
H	1.887283082700	-0.623261688500	1.257463794400
H	1.688319684400	-1.706867882500	-0.152100508700
F	2.762823723000	-0.026665956800	-0.457460887100

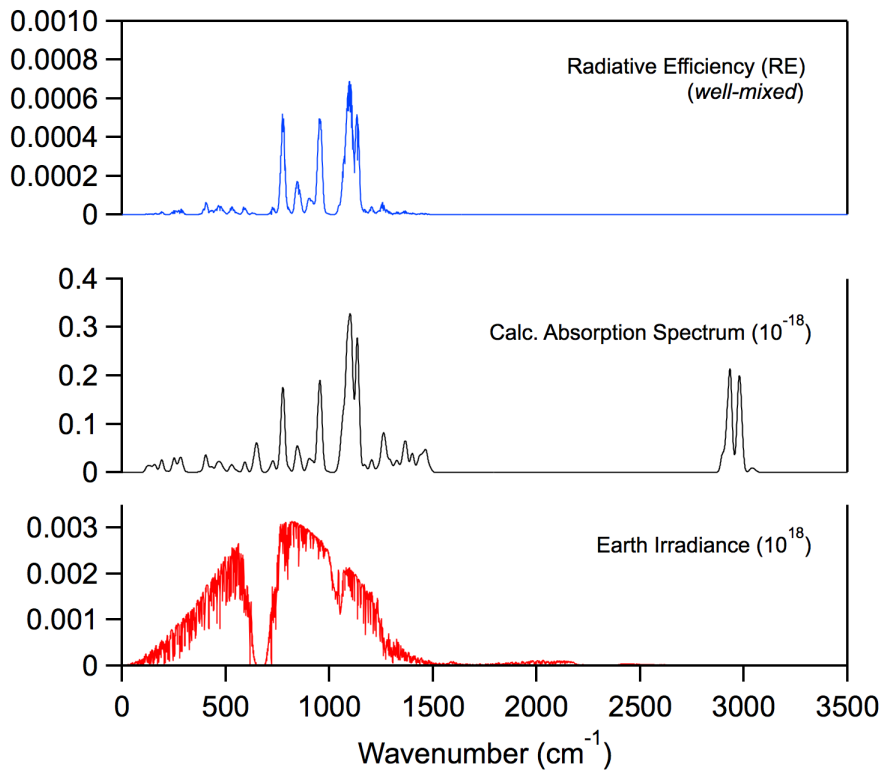
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength ($10^{-18} \text{ cm}^2 \text{ molecule}^{-1} \text{ cm}^{-1}$)
80.3884	0.525
107.0859	0.209
156.9076	0.647
268.9759	0.114
336.9820	0.124
452.4227	1.03
526.8930	3.97
759.2778	7.13
862.3350	1.36
905.8759	3.54
1049.9613	1.30
1090.8997	3.83
1117.6762	10.1
1138.5237	8.15
1216.1411	0.698
1262.8319	1.71
1288.7368	0.340
1346.9488	1.37
1408.9442	1.93
1438.6480	1.86
1464.0430	0.844
1500.6938	0.281
3022.4669	3.93
3048.2395	1.10
3076.7725	5.86
3084.7586	2.44
3147.8599	1.03

Infrared Spectrum

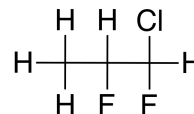


Radiative Efficiency



HCFC-262eb

Molecular Formula: CH₃CHFCHFCI
Name: 1-Chloro-1,2-difluoropropane
CAS number: 430-96-6
Molecular Weight: 114.52



Global Atmospheric Lifetime (years): 0.663
Tropospheric Atmospheric Lifetime (years): 0.685
Stratospheric Atmospheric Lifetime (years): 21.3
Ozone Depletion Potential (ODP): 0.007

	<i>Well-mixed</i>	<i>Lifetime adjusted</i>
Radiative Efficiency (RE):	0.148	0.098
Global Warming Potential (GWP _H):		
GWP ₂₀	193	128
GWP ₁₀₀	52	35
Global Temperature Potentials (GTP _H):		
GTP ₂₀		40
GTP ₅₀		6
GTP ₁₀₀		5

* RE units: W m² ppb⁻¹

* GWP and GTP: Relative to CO₂

Atmospheric Loss Processes *****

OH Reactivity

$k_{\text{Rec}}(T)$, *No recommendation*

$k_{\text{SAR}}(298 \text{ K}) = 8.57 \times 10^{-14}$; $k_{\text{SAR}}(272 \text{ K}) \approx 5.47 \times 10^{-14}$ cm³ molecule⁻¹ s⁻¹

$\tau_{\text{Global}}^{\text{OH}} = 0.670$ years

$\tau_{\text{Trop}}^{\text{OH}} = 0.685$ years

$\tau_{\text{Strat}}^{\text{OH}} = 24.0$ years

Fractional Atmospheric Loss: 0.997

O(¹D) Reactivity

$k_{\text{Rec}}(T)$, *No recommendation*

$k_{\text{Est}}(T) = 1.1 \times 10^{-10}$ cm³ molecule⁻¹ s⁻¹

$\tau_{\text{O}(\text{1D})} = 335$ years

Fractional Atmospheric Loss: 0.002

UV Photolysis

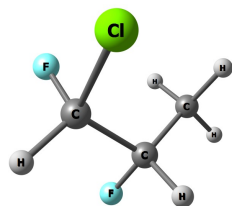
UV Spectrum: *No Recommendation*

$\tau_{\text{hv}} = 450$ years

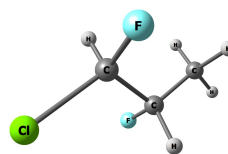
Fractional Atmospheric Loss: 0.001



Molecular Structure and Infrared Spectrum (6 conformers)



E = 0
Population = 0.365



$\Delta E = 0.30 \text{ kcal mol}^{-1}$
Population = 0.219

Optimized Coordinates (Angstroms)

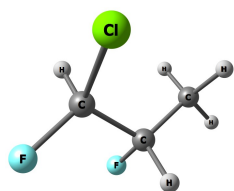
Atom	X	Y	Z
C	1.157422322064	-1.307898688713	0.671739953983
C	0.887704655210	-0.345304385954	-0.469518361654
C	-0.290851462333	0.597989501599	-0.230251111635
H	2.056119472224	-1.887793554675	0.450528164903
H	1.310083514565	-0.754267886822	1.600359293960
H	0.318069487158	-1.994798251072	0.801583713066
H	0.712694700352	-0.874797517327	-1.412857784489
F	1.989242605252	0.479936520871	-0.642169716243
F	-0.200660642420	1.172676322154	0.990152980819
H	-0.329880895246	1.379948943938	-0.991381817046
Cl	-1.853602556825	-0.304128003998	-0.346291315664

Atom	X	Y	Z
C	2.232071398356	-0.396491716019	0.004876080817
C	0.908858792792	0.278039489352	-0.320648338850
C	-0.266918405497	-0.425158640527	0.356733317950
H	2.230382297430	-1.427512952019	-0.355167603753
H	3.047776301164	0.146720666556	-0.478036288393
H	2.408038128124	-0.398488934994	1.085058929363
H	0.727871319161	0.292778440484	-1.402111538343
F	0.929230871200	1.578678551475	0.135346010647
F	-0.291463487570	-1.724733390508	-0.031227733830
H	-0.200514151186	-0.368260642445	1.446192201062
Cl	-1.829065063972	0.349853128645	-0.091280036669

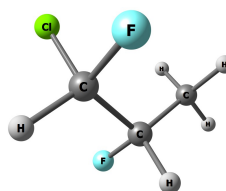
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
83.2849	0.393
199.3764	0.499
225.5135	0.196
257.9011	0.390
326.0160	0.383
387.8964	0.926
436.5348	1.05
652.5322	1.34
782.8835	15.4
850.7728	5.85
942.0826	2.86
1026.4117	8.92
1112.9814	13.5
1139.8745	3.18
1178.8125	10.7
1259.7808	1.64
1359.4025	0.837
1375.4188	0.625
1390.0938	0.874
1420.6351	4.28
1487.1214	0.739
1497.3341	0.271
3057.3795	3.06
3062.0982	0.866
3105.3778	2.21
3140.6361	1.71
3147.7785	1.49

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
75.1680	0.252
181.8905	0.177
217.6310	0.0664
305.2886	0.362
364.0622	2.22
379.1806	0.0620
442.3595	2.35
512.4099	0.676
767.1457	13.3
885.0899	2.36
959.8348	6.34
1109.9475	8.30
1112.5902	5.84
1143.5655	17.2
1164.4299	1.56
1268.5794	4.84
1332.1374	2.75
1368.7207	0.663
1398.7654	0.397
1407.8929	1.12
1486.9188	0.963
1496.1840	0.335
3049.1151	0.667
3051.5448	2.39
3094.5258	2.87
3126.8716	2.89
3142.6306	1.35



$\Delta E = 0.46 \text{ kcal mol}^{-1}$
Population = 0.167



$\Delta E = 0.54 \text{ kcal mol}^{-1}$
Population = 0.146

Optimized Coordinates (Angstroms)

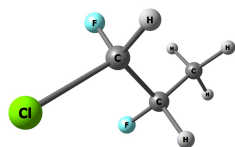
Atom	X	Y	Z
C	-1.298571431301	1.545242874741	0.073751235371
C	-0.938973699953	0.131451318887	-0.343901481068
C	0.287824795401	-0.448344253740	0.357554327002
H	-2.252357928450	1.817995002565	-0.384281220091
H	-1.407145476410	1.611907861505	1.160728900065
H	-0.536667490986	2.256238825846	-0.249874793158
H	-0.778564865739	0.056670272861	-1.426252178503
F	-1.981895832518	-0.716680500083	-0.007840852369
H	0.186266977302	-0.427161698622	1.445615782439
F	0.478001841381	-1.721917202300	-0.048552042481
Cl	1.765038111273	0.513609498339	-0.041891677208

Atom	X	Y	Z
C	-1.499838136759	0.373809177842	1.119442693987
C	-1.081834036769	0.137505335887	-0.318444756960
C	0.401414953010	0.381875306115	-0.604140463205
H	-2.580815154627	0.246660723448	1.213481383166
H	-0.999962683100	-0.331326466762	1.786560111697
H	-1.237494815220	1.391842770716	1.418284427283
H	-1.625607568115	0.817443058989	-0.990475642674
F	-1.370203334342	-1.153850564692	-0.703460494246
H	0.647536584971	0.159497900741	-1.644461346383
F	0.688544500491	1.680245826447	-0.336630491474
Cl	1.474066690460	-0.679332068731	0.382541578808

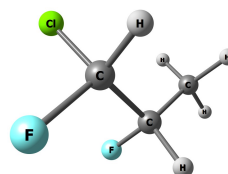
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
80.6631	0.256
190.8576	0.230
216.0726	0.164
312.7471	0.276
352.4337	0.951
393.7912	0.940
414.1060	0.772
524.1505	1.58
782.4764	16.3
881.8905	4.66
935.0101	1.07
1109.4323	16.1
1127.8349	8.95
1138.6173	9.27
1164.9270	4.20
1247.1181	3.17
1337.1454	1.18
1366.5240	0.352
1411.0894	0.618
1411.9073	3.57
1488.6809	0.935
1495.9580	0.389
3049.8883	0.702
3053.5044	2.23
3094.9436	2.93
3126.5527	2.70
3148.3944	1.43

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
84.0178	0.350
193.0467	0.105
213.8587	0.132
244.9084	0.852
354.8600	0.246
399.9321	1.23
510.7267	0.398
563.9793	5.19
730.1944	8.03
860.4098	3.39
969.6279	4.47
1074.8990	0.467
1110.7479	11.1
1146.7099	20.7
1177.7893	1.58
1296.2331	3.00
1334.7417	1.56
1379.2589	3.60
1385.6744	0.888
1415.4028	4.03
1485.0051	0.550
1496.7807	0.421
3013.4601	4.42
3059.2532	0.917
3103.0077	2.66
3136.1322	1.66
3146.1109	1.44



$\Delta E = 1.09 \text{ kcal mol}^{-1}$
Population = 0.058



$\Delta E = 1.24 \text{ kcal mol}^{-1}$
Population = 0.045

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-2.228590629324	0.249943549806	-0.460982773885
C	-0.882315187797	-0.452994061305	-0.357550918031
C	0.271495935126	0.545867762286	-0.319077590875
H	-2.299265487552	0.821771418954	-1.391221570493
H	-3.028276896382	-0.493946277093	-0.450310058538
H	-2.361953640326	0.929449826319	0.383454216674
H	-0.718214784941	-1.122270952353	-1.211090495037
F	-0.853280048296	-1.205415657804	0.794457354157
H	0.333914394167	1.113310142678	-1.251488591746
F	0.114800748185	1.403438485585	0.717842294090
Cl	1.854094597140	-0.298237237072	-0.141090866315

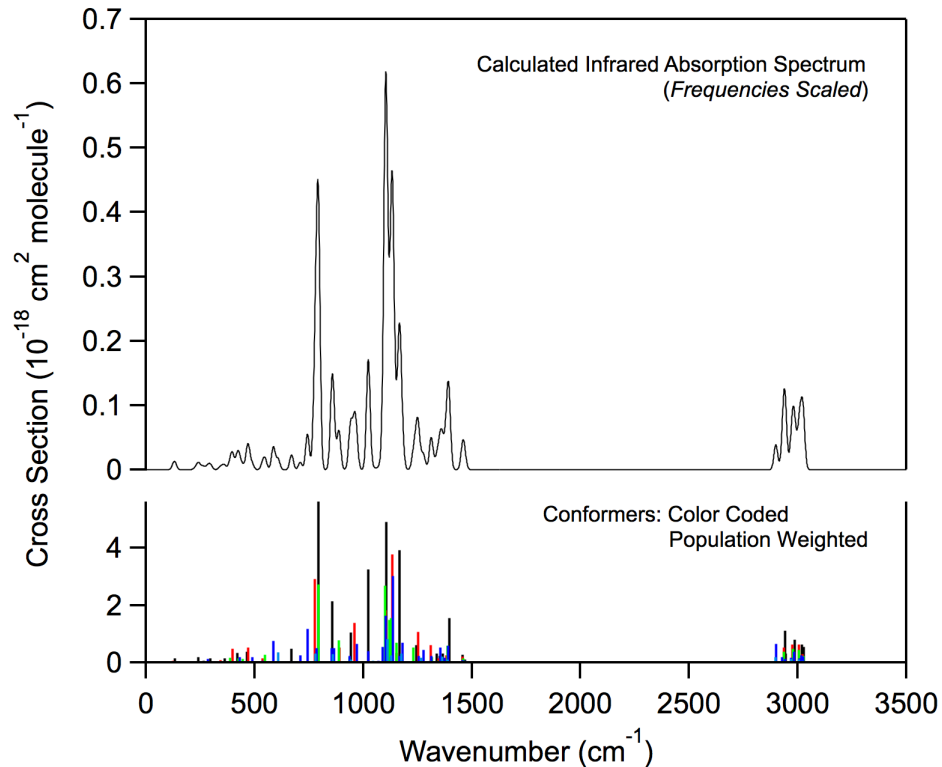
Atom	X	Y	Z
C	1.782637890212	-0.967507265452	-0.494551239631
C	1.056590574220	0.327901692160	-0.181178513487
C	-0.409295213995	0.345903615116	-0.606269989765
H	2.826100983691	-0.881896247739	-0.182415964488
H	1.323328357365	-1.804508731502	0.035727680690
H	1.760660680540	-1.173682266719	-1.569124973515
H	1.522827089643	1.171680810371	-0.711384413726
F	1.127200772764	0.594479027684	1.166524412703
F	-0.925859910790	1.577826477724	-0.387025196921
H	-0.519625595026	0.090141259777	-1.663408954280
Cl	-1.391964628623	-0.858766371421	0.308453152421

Infrared Absorption Spectrum (unscaled frequencies)

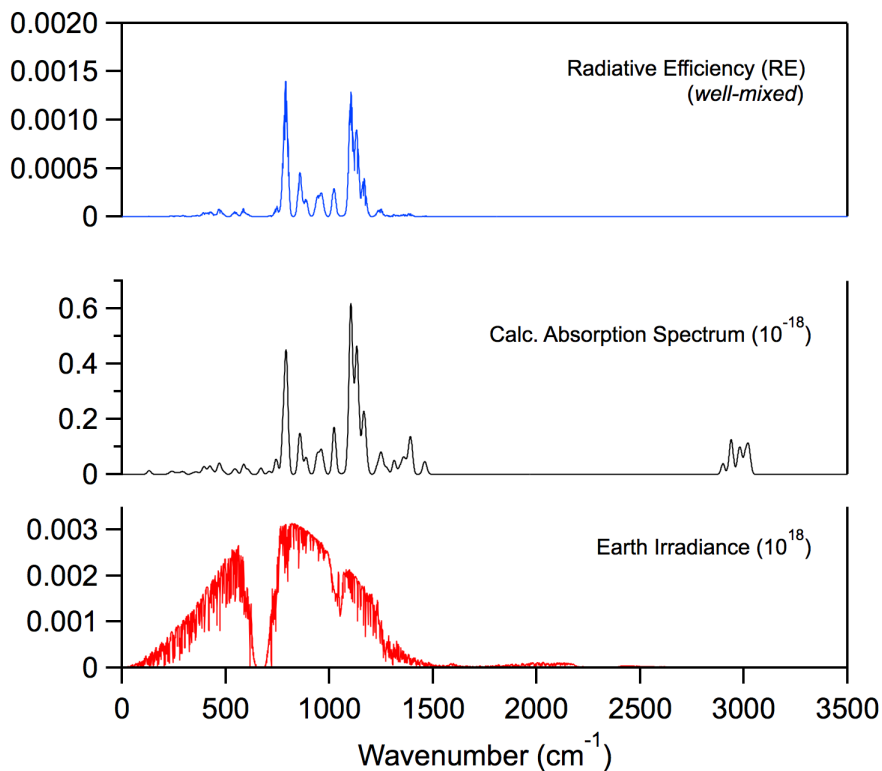
Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
77.1040	0.0412
196.2696	0.0828
224.9203	0.0112
252.4111	0.0860
319.9627	0.238
385.8012	0.336
460.4664	3.23
694.8717	4.17
775.0515	8.70
848.5022	8.55
936.4349	4.14
1027.6357	6.83
1095.9764	9.54
1136.8822	3.36
1192.5559	11.8
1272.8746	3.82
1360.9037	0.305
1372.0999	0.619
1398.8309	2.75
1406.6073	1.07
1484.9297	0.822
1498.0661	0.282
3044.4129	3.19
3052.4520	1.09
3086.5020	2.97
3127.5230	2.43
3145.3119	1.56

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
82.4080	0.0731
201.2260	0.0322
213.2012	0.0601
235.1570	0.0898
341.5511	0.0387
395.5979	0.581
522.8556	1.16
586.8763	7.81
768.8418	6.85
854.6832	6.62
942.7101	2.14
1051.1332	1.58
1119.6004	18.1
1138.8719	5.73
1187.9949	6.84
1284.8106	3.79
1329.5015	1.49
1385.8039	4.63
1397.1339	0.775
1412.1950	2.43
1484.2033	0.477
1498.7805	0.574
3011.4388	4.10
3051.7944	0.916
3087.0239	2.88
3125.6570	2.33
3142.9195	1.55

Infrared Spectrum

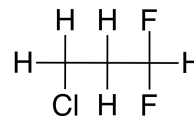


Radiative Efficiency



HCFC-262fa

Molecular Formula: CH₂ClCH₂CHF₂
 Name: 3-Chloro-1,1-difluoropropane
 CAS number: 83124-57-6
 Molecular Weight: 114.52



Global Atmospheric Lifetime (years): 0.801
 Tropospheric Atmospheric Lifetime (years): 0.828
 Stratospheric Atmospheric Lifetime (years): 24.8
 Ozone Depletion Potential (ODP): 0.008

	<i>Well-mixed</i>	<i>Lifetime adjusted</i>
Radiative Efficiency (RE):	0.122	0.086
Global Warming Potential (GWP _H):		
GWP ₂₀	193	135
GWP ₁₀₀	52	37
Global Temperature Potentials (GTP _H):		
GTP ₂₀		43
GTP ₅₀		6
GTP ₁₀₀		5

* RE units: W m² ppb⁻¹
 * GWP and GTP: Relative to CO₂

Atmospheric Loss Processes *****

OH Reactivity

$k_{\text{Rec}}(T)$, *No recommendation*

$$k_{\text{SAR}}(298 \text{ K}) = 7.09 \times 10^{-14}; k_{\text{SAR}}(272 \text{ K}) \approx 4.52 \times 10^{-14} \quad \text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$\tau_{\text{Global}}^{\text{OH}} = 0.804 \text{ years}$$

$$\tau_{\text{Trop}}^{\text{OH}} = 0.828 \text{ years}$$

$$\tau_{\text{Strat}}^{\text{OH}} = 28.4 \text{ years}$$

Fractional Atmospheric Loss: 0.996

O(¹D) Reactivity

$k_{\text{Rec}}(T)$, *No recommendation*

$$k_{\text{Est}}(T) = 1.1 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$\tau_{\text{O}(\text{1D})} = 335 \text{ years}$$

Fractional Atmospheric Loss: 0.002

UV Photolysis

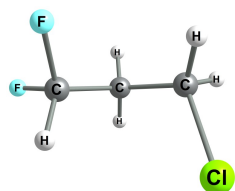
UV Spectrum: *No Recommendation*

$$\tau_{\text{hv}} = 450 \text{ years}$$

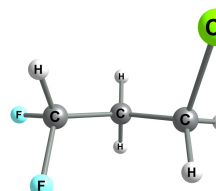
Fractional Atmospheric Loss: 0.002



Molecular Structure and Infrared Spectrum (7 conformers)



E = 0
Population = 0.309



E = 0
Population = 0.309

Optimized Coordinates (Angstroms)

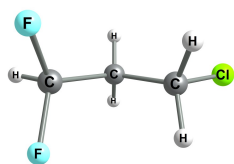
Atom	X	Y	Z
C	-1.038735861400	0.493213611800	-0.827855505400
C	0.284353201600	0.961365024600	-0.242911246300
C	1.160784145700	-0.173194418800	0.256994218200
H	0.118611741600	1.667351507500	0.575474098200
H	0.847013840900	1.481230816000	-1.028159101800
Cl	-2.131539931300	-0.209518278700	0.440478262500
H	-0.888989624200	-0.289495864800	-1.570993934400
H	-1.588871848900	1.320651046500	-1.274011555200
H	0.711966009500	-0.747001609200	1.075324634500
F	1.421400895800	-1.031753431400	-0.767583958000
F	2.346079430700	0.331545596500	0.684386087700

Atom	X	Y	Z
C	-1.046362878400	0.645885594300	0.724099274200
C	0.289318944100	1.002766781700	0.091268430200
C	1.155183863000	-0.205547706600	-0.217796049300
H	0.850711029100	1.630006554900	0.794736152200
H	0.142218502300	1.576908629400	-0.827625308800
Cl	-2.135152661300	-0.229701227300	-0.435471636300
H	-1.589691738900	1.538538448100	1.031219939200
H	-0.915516616000	-0.015394947200	1.580195700100
H	0.707247815000	-0.892518357300	-0.944279019400
F	2.351923794900	0.213338382800	-0.702297482200
F	1.392807946300	-0.900012152800	0.929386000100

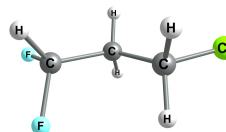
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
65.1716	0.480
113.4952	0.639
215.4903	0.266
310.3352	0.506
452.1772	2.21
494.8992	0.997
570.7124	0.581
666.6205	4.34
797.1521	0.294
951.4596	4.12
1002.8303	3.74
1087.8422	3.85
1117.4893	13.5
1138.0294	22.1
1190.1655	5.24
1248.2970	1.65
1318.4631	4.38
1350.0241	0.216
1415.9395	3.81
1430.3236	4.85
1463.9938	1.23
1481.2964	1.12
3045.6937	0.576
3070.6609	5.04
3099.7305	0.609
3111.1064	2.65
3164.3198	0.486

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
65.1732	0.480
113.4990	0.639
215.4866	0.266
310.3359	0.506
452.1751	2.21
494.9022	0.997
570.7088	0.581
666.6215	4.34
797.1501	0.294
951.4658	4.12
1002.8300	3.74
1087.8471	3.85
1117.4834	13.5
1138.0070	22.1
1190.1735	5.24
1248.2958	1.65
1318.4633	4.38
1350.0220	0.216
1415.9419	3.81
1430.3172	4.85
1463.9937	1.23
1481.2983	1.12
3045.7072	0.577
3070.6771	5.04
3099.7276	0.609
3111.1058	2.65
3164.3139	0.486



$\Delta E = 0.30 \text{ kcal mol}^{-1}$
Population = 0.185



$\Delta E = 0.85 \text{ kcal mol}^{-1}$
Population = 0.073

Optimized Coordinates (Angstroms)

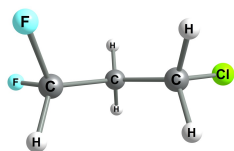
Atom	X	Y	Z
C	-0.726180010400	-0.021069873200	-0.465850422600
C	0.153797755000	-0.006763608600	0.778500848800
C	1.628915629100	0.000434143000	0.415598815800
H	-0.045664216700	-0.886860984600	1.396942715700
H	-0.057206998100	0.879059129800	1.384824820200
Cl	-2.476546018700	-0.029484905000	-0.016712048200
H	-0.551087901100	-0.912373556800	-1.066788970100
H	-0.562774895500	0.864134750600	-1.078967046500
H	2.283426238700	0.010754831300	1.296149133300
F	1.935178724100	-1.098813770500	-0.325799066600
F	1.920773693600	1.093343844000	-0.340816779800

Atom	X	Y	Z
C	-0.918357683600	-0.486212886100	-0.321822435200
C	0.165368335300	0.508467401700	0.071403503300
C	1.547177215700	0.011100495200	-0.317391811300
H	0.159424678300	0.671545114500	1.153234500200
H	-0.004748249800	1.473350545400	-0.414727943100
Cl	-2.556972792900	0.128216000400	0.127953623600
H	-0.787685688400	-1.438763542300	0.190156433900
H	-0.942507282700	-0.661074955800	-1.399074368300
H	1.675060414200	-0.123112682700	-1.400346690600
F	2.484456639900	0.890960669500	0.112497256900
F	1.794851414000	-1.186013159700	0.281631930600

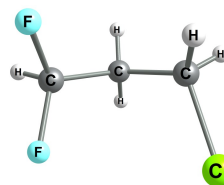
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
73.9112	0.644
107.3385	0.0636
173.3290	1.08
267.7143	0.364
380.9054	0.0281
512.8519	1.81
649.7343	6.79
774.5760	0.0130
801.7669	1.24
891.3580	0.581
974.5784	7.51
1077.2010	2.33
1091.1103	10.3
1158.5994	15.7
1188.6809	8.30
1273.2042	0.360
1307.2803	0.463
1372.6866	12.0
1406.6563	3.58
1411.9385	3.58
1475.9205	0.884
1493.2595	0.465
3046.0530	6.17
3067.6149	3.50
3106.2884	1.59
3110.5954	0.969
3169.2010	0.569

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
82.2940	0.759
108.9080	0.210
153.8324	0.643
271.6009	0.0810
411.5195	0.464
492.5960	3.44
574.8378	0.620
748.0211	7.18
782.9915	0.444
923.7126	3.14
1058.7057	0.481
1073.0962	0.965
1120.5032	22.0
1143.7005	18.1
1199.0583	3.77
1261.9033	2.29
1303.1412	0.212
1351.5286	2.22
1413.3196	4.11
1427.1945	10.4
1479.5061	0.785
1493.3357	0.298
3030.7753	7.53
3065.6304	0.686
3087.5563	2.63
3115.4284	1.11
3156.4837	1.04



$\Delta E = 0.85 \text{ kcal mol}^{-1}$
Population = 0.073



$\Delta E = 1.73 \text{ kcal mol}^{-1}$
Population = 0.017

Optimized Coordinates (Angstroms)

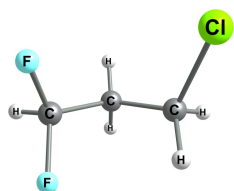
Atom	X	Y	Z
C	-0.918711728000	-0.467994050500	0.356813164700
C	0.168559507300	0.514875827400	-0.055854932400
C	1.550174767400	0.011385347700	0.325686755300
H	0.009673478100	1.485734969100	0.422107840200
H	0.154165044100	0.667259145800	-1.139164207900
Cl	-2.556829516800	0.153785072300	-0.084574627500
H	-0.934514082400	-0.632003038100	1.435925231400
H	-0.799410551900	-1.426491652500	-0.146776032300
H	1.686709962100	-0.112996776200	1.408759235300
F	1.783926806700	-1.193369618000	-0.263510274200
F	2.489877313400	0.880123773000	-0.121216152600

Atom	X	Y	Z
C	-0.836860702600	1.051868984500	-0.171072989700
C	0.372504302200	0.954028938200	0.752893588000
C	1.435350802400	-0.034445194100	0.298996493800
H	0.066260664200	0.705261292600	1.772873341300
H	0.850920984100	1.940902603400	0.785420128700
Cl	-1.987771264600	-0.331915449400	0.014406656100
H	-0.529786646500	1.066390848000	-1.216406782800
H	-1.414091821300	1.949546848400	0.047309821000
H	2.338496456200	0.017312085100	0.921483511500
F	0.978266788700	-1.308190582200	0.326999904300
F	1.797409437300	0.242436625500	-0.985515672300

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
82.2864	0.759
108.9105	0.210
153.8359	0.643
271.6018	0.0810
411.5183	0.464
492.5959	3.44
574.8363	0.620
748.0278	7.18
782.9922	0.444
923.7173	3.14
1058.6980	0.481
1073.0979	0.965
1120.5007	22.0
1143.7001	18.1
1199.0619	3.77
1261.9034	2.29
1303.1402	0.212
1351.5278	2.22
1413.3241	4.11
1427.1889	10.4
1479.5060	0.785
1493.3370	0.298
3030.7743	7.53
3065.6368	0.686
3087.5550	2.64
3115.4346	1.11
3156.4764	1.04

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
45.5162	0.167
122.9775	0.0166
226.2198	0.646
305.0676	1.59
391.4702	0.276
505.5046	0.766
661.5792	4.03
675.5510	0.505
858.5266	0.405
921.3187	2.56
942.1830	2.67
1059.9010	9.54
1094.1916	13.0
1167.3100	11.7
1191.8736	4.46
1257.4946	5.37
1326.5190	4.36
1391.6239	2.42
1410.5411	3.13
1420.5345	4.28
1456.7034	1.50
1481.4955	1.33
3032.3683	4.47
3047.9119	6.86
3097.2751	0.735
3106.6274	2.35
3160.5080	0.464



$$\Delta E = 1.73 \text{ kcal mol}^{-1}$$

$$\text{Population} = 0.017$$

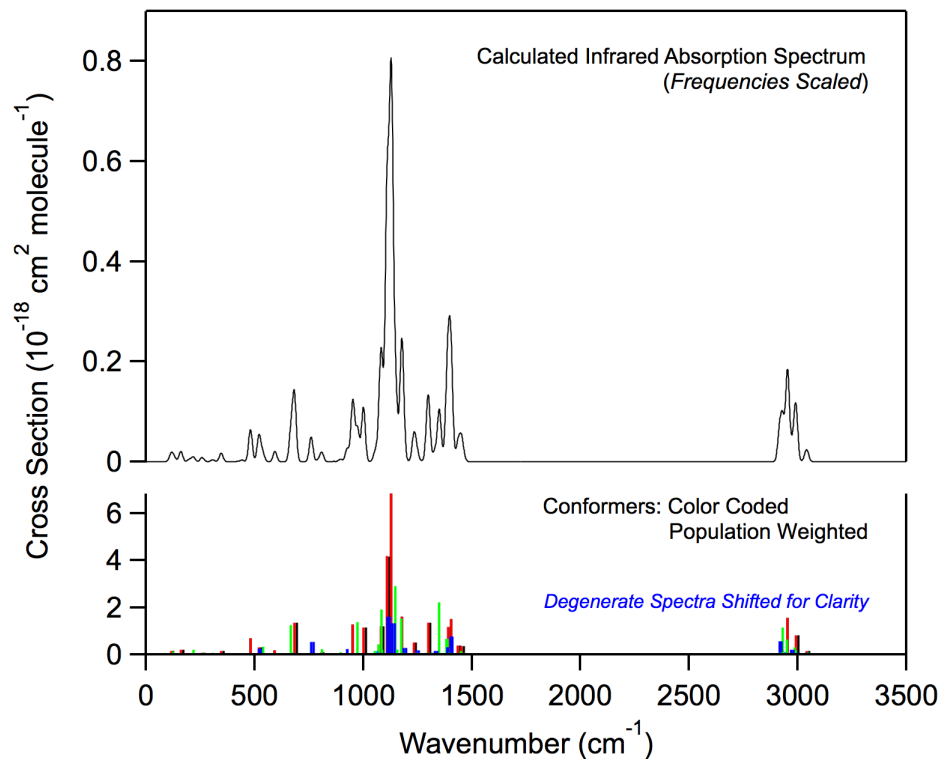
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-0.852807749400	-1.054453560600	-0.157276200500
C	0.376333122800	-0.977751416300	0.742272416600
C	1.435740727000	0.010817234900	0.280601565400
H	0.848978920800	-1.967906583500	0.750167503200
H	0.093218739100	-0.742277751500	1.772041192800
Cl	-1.990584616400	0.333488381900	0.072774467500
H	-1.431107094700	-1.951700448600	0.060049202800
H	-0.567880566700	-1.055379553900	-1.208961925700
H	2.351436188200	-0.055731142900	0.883022592200
F	1.768880532800	-0.249213145000	-1.015218814600
F	0.987587796400	1.286787985500	0.336999000200

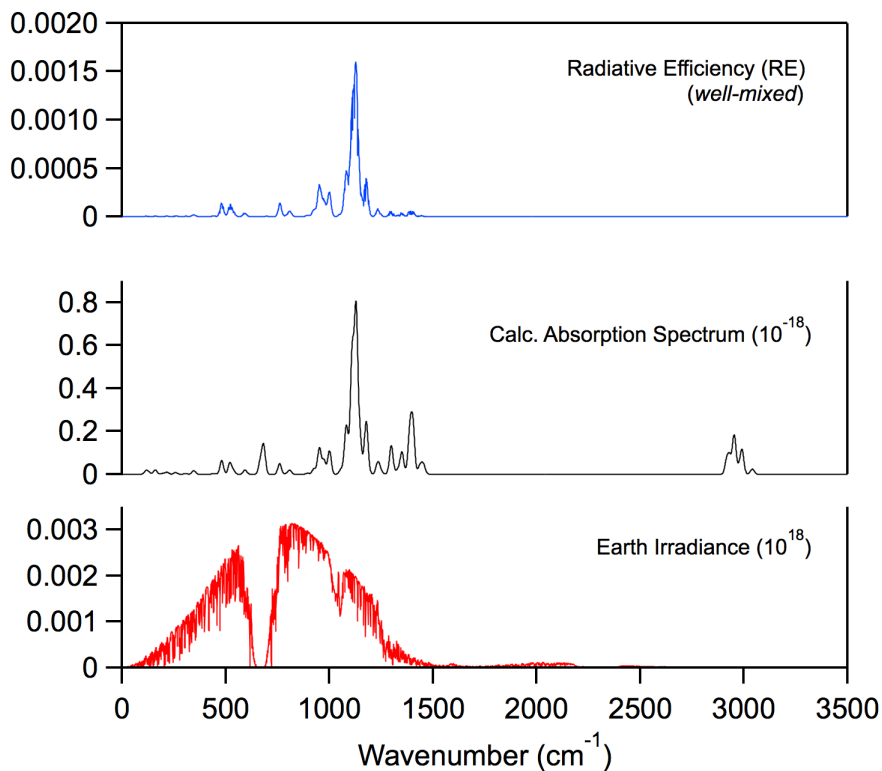
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength ($10^{-18} \text{ cm}^2 \text{ molecule}^{-1} \text{ cm}^{-1}$)
45.5254	0.167
122.9835	0.0166
226.2277	0.646
305.0692	1.59
391.4737	0.276
505.4981	0.766
661.5849	4.03
675.5483	0.506
858.5244	0.405
921.3196	2.56
942.1813	2.67
1059.8961	9.54
1094.1819	13.0
1167.3054	11.7
1191.8705	4.46
1257.4970	5.37
1326.5192	4.36
1391.6200	2.42
1410.5316	3.13
1420.5387	4.28
1456.7038	1.50
1481.4949	1.33
3032.3742	4.46
3047.9094	6.87
3097.2805	0.736
3106.6342	2.35
3160.5105	0.464

Infrared Spectrum

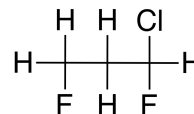


Radiative Efficiency



HCFC-262fb

Molecular Formula: CH₂FCH₂CHFCI
 Name: 1-Chloro-1,3-difluoropropane
 CAS number: 151771-13-0
 Molecular Weight: 114.52



Global Atmospheric Lifetime (years): 0.873
 Tropospheric Atmospheric Lifetime (years): 0.902
 Stratospheric Atmospheric Lifetime (years): 26.5
 Ozone Depletion Potential (ODP): 0.009

	<i>Well-mixed</i>	<i>Lifetime adjusted</i>
Radiative Efficiency (RE):	0.138	0.099
Global Warming Potential (GWP _H):		
GWP ₂₀	237	170
GWP ₁₀₀	64	46
Global Temperature Potentials (GTP _H):		
GTP ₂₀		54
GTP ₅₀		8
GTP ₁₀₀		6

* RE units: W m² ppb⁻¹
 * GWP and GTP: Relative to CO₂

Atmospheric Loss Processes *****

OH Reactivity

$k_{\text{Rec}}(T)$, *No recommendation*

$$k_{\text{SAR}}(298 \text{ K}) = 6.50 \times 10^{-14}; k_{\text{SAR}}(272 \text{ K}) \approx 4.15 \times 10^{-14} \quad \text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$\tau_{\text{Global}}^{\text{OH}} = 0.877 \text{ years}$$

$$\tau_{\text{Trop}}^{\text{OH}} = 0.902 \text{ years}$$

$$\tau_{\text{Strat}}^{\text{OH}} = 30.7 \text{ years}$$

Fractional Atmospheric Loss: 0.995

O(¹D) Reactivity

$k_{\text{Rec}}(T)$, *No recommendation*

$$k_{\text{Est}}(T) = 1.1 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$\tau_{\text{O}(\text{1D})} = 335 \text{ years}$$

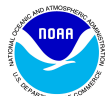
Fractional Atmospheric Loss: 0.003

UV Photolysis

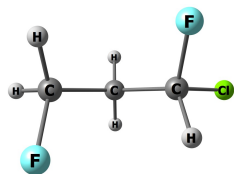
UV Spectrum: *No Recommendation*

$$\tau_{\text{hv}} = 450 \text{ years}$$

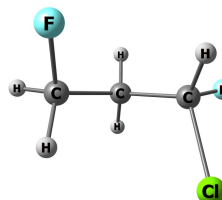
Fractional Atmospheric Loss: 0.002



Molecular Structure and Infrared Spectrum (7 conformers)



E = 0
Population = 0.544



$\Delta E = 0.36 \text{ kcal mol}^{-1}$
Population = 0.296

Optimized Coordinates (Angstroms)

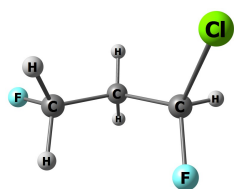
Atom	X	Y	Z
C	-1.946893273700	0.128436575200	0.503008691200
C	-0.518881487700	0.655927819100	0.558835352100
C	0.416003675000	-0.211893419600	-0.263769896100
H	-0.171520183100	0.669774784000	1.596960531500
H	-0.483296166400	1.679168261900	0.175148578300
F	-2.389205495300	0.140135136100	-0.807598872500
H	-2.613519030400	0.758212787400	1.102905521500
H	-1.997160993600	-0.900561846400	0.875216361200
F	0.426011420500	-1.479049576400	0.228179918300
H	0.138166788500	-0.247415245800	-1.317943184000
Cl	2.105438746200	0.436453724600	-0.216489001700

Atom	X	Y	Z
C	-1.771047929600	-0.226619768900	-0.516365894600
C	-0.615525346400	0.749764977100	-0.660246254500
C	0.530663061400	0.472025975500	0.295915419600
H	-0.967922303100	1.764171486100	-0.438636029100
H	-0.240994166300	0.740273908200	-1.688538643400
F	-2.246516997600	-0.183058175200	0.782545152000
H	-1.455437440700	1.102905521500	-0.734035657000
H	-2.586918494000	0.045792965000	-1.195514449100
F	1.443627250900	1.470697690000	0.223409516100
H	0.197118409600	0.361319214900	1.328465828200
Cl	1.367083955800	-1.089113381000	-0.109598988200

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
68.3515	0.517
123.0153	0.790
213.2307	0.106
286.9891	0.725
374.4140	0.292
457.4142	2.37
509.2336	3.13
736.4189	7.70
848.6636	8.00
912.0226	2.64
1011.6004	5.62
1091.7251	13.2
1107.8322	4.18
1142.6796	14.6
1222.9047	1.57
1262.0605	0.266
1299.7236	3.09
1372.0669	2.34
1396.4831	1.99
1428.0521	2.84
1459.7558	0.787
1515.0695	0.472
3039.3651	5.57
3063.6073	0.443
3089.0090	3.76
3111.2447	1.06
3125.7751	2.56

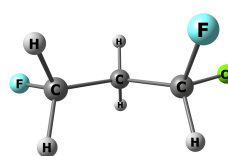
Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
67.5590	0.469
133.0092	0.882
205.3487	0.345
344.1945	0.233
374.1698	0.650
426.3160	1.36
545.1126	2.04
650.8468	9.49
859.0465	7.48
912.8685	1.65
1068.1063	6.81
1088.2677	5.27
1109.0450	6.30
1133.1667	20.3
1217.1356	1.77
1269.4743	0.562
1318.6842	6.10
1341.7243	0.321
1408.0078	3.00
1429.3209	1.61
1463.2957	0.778
1515.1733	0.707
3039.9327	5.11
3046.6532	0.883
3089.7563	3.70
3102.0067	1.52
3122.2785	2.28



$\Delta E = 1.59 \text{ kcal mol}^{-1}$
Population = 0.037

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.480003693300	-0.152001853100	-0.460610212700
C	-0.678038193400	0.362180610500	0.731042026800
C	0.788850669000	0.599042457500	0.432088507700
H	-0.764422627100	-0.332535522500	1.571085991000
H	-1.101219466100	1.322709563800	1.049431675400
F	-2.806725225000	-0.231574880200	-0.091951557800
H	-1.140511128800	-1.145856532600	-0.769297023900
H	-1.389980530800	0.532060005800	-1.310995771300
F	0.925807646800	1.443732663600	-0.623096446400
H	1.330238072200	1.011855168500	1.285249885900
Cl	1.657296476500	-0.948869681100	0.034072925300



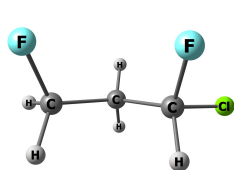
$\Delta E = 1.63 \text{ kcal mol}^{-1}$
Population = 0.035

Atom	X	Y	Z
C	-1.890358277800	-0.247412025700	-0.247203072200
C	-0.588296823800	0.500674544100	0.033141626100
C	0.619500839200	-0.311456338400	-0.387096710100
H	-0.514606995700	0.724762403100	1.101339905100
H	-0.586625444900	1.449475731900	-0.510557371900
F	-2.951422073900	0.554997104300	0.108269984800
H	-1.938218261100	-1.175717746500	0.331767457900
H	-1.982784683400	-0.495909783000	-1.313041471500
F	0.634742579200	-1.502324983700	0.269746934100
H	0.655132071200	-0.510086153200	-1.461464053800
Cl	2.154964071000	0.570828247000	-0.013564228400

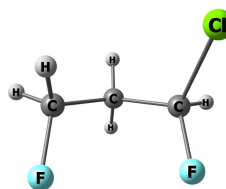
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
80.2425	0.769
104.4576	0.0118
182.5796	0.906
304.7366	0.708
359.9434	0.343
391.2122	0.287
620.2991	8.51
698.5123	6.03
802.5528	0.815
926.0843	7.72
1046.0583	3.51
1085.8274	18.6
1105.7127	0.941
1150.5793	15.6
1241.6612	0.257
1280.5705	6.57
1315.1640	1.33
1338.3592	1.88
1384.2061	2.18
1440.5543	1.71
1474.4959	0.626
1527.3067	0.269
3043.5185	0.243
3050.1177	4.60
3091.8010	1.07
3103.0970	3.32
3113.9037	3.79

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
93.2803	0.784
105.3660	0.274
151.0812	0.658
298.3644	0.528
370.7227	1.50
395.5105	0.135
514.4098	1.84
765.3487	18.8
802.2813	0.446
945.1722	5.83
1051.1520	2.90
1094.7697	13.6
1129.2694	9.32
1141.6687	10.1
1238.3130	1.75
1267.9833	1.04
1311.0207	0.135
1336.3275	4.52
1395.3062	2.43
1437.6923	4.36
1479.7834	0.482
1525.5351	0.139
3020.0519	5.64
3067.6012	0.542
3078.6732	3.75
3084.6235	2.28
3123.9583	3.06



$\Delta E = 1.78 \text{ kcal mol}^{-1}$
Population = 0.027



$\Delta E = 1.89 \text{ kcal mol}^{-1}$
Population = 0.022

Optimized Coordinates (Angstroms)

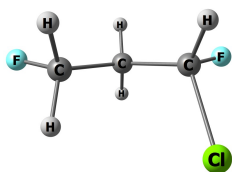
Atom	X	Y	Z
C	-1.936217162900	0.706225074000	-0.192025491600
C	-0.474351475500	0.910251418500	0.192594596800
C	0.448328222900	-0.121170893800	-0.431803634900
H	-0.366355155700	0.867399162000	1.280682156200
H	-0.159146296200	1.904831589800	-0.137693886600
F	-2.421228829000	-0.468195685200	0.335588781000
H	-2.056264472900	0.672912597500	-1.283687434900
H	-2.538388568800	1.538227320900	0.193162246200
F	0.171197110300	-1.360841079500	0.030308004400
H	0.397513356100	-0.132173111100	-1.524251874600
Cl	2.181897271800	0.262263606800	-0.042283461900

Atom	X	Y	Z
C	-1.523847049800	-0.784948272500	0.103764045100
C	-0.630516223100	-0.072311443600	1.111099826200
C	0.616409074200	0.573551515400	0.528216175300
H	-0.320573864500	-0.777225875300	1.888658807000
H	-1.211430554600	0.722432898400	1.595101852800
F	-2.124574149600	0.130404435800	-0.732270809600
H	-2.308562084000	-1.336673945000	0.635601538600
H	-0.948934425400	-1.492411626100	-0.503957153700
F	0.301966594400	1.437883955800	-0.462159842200
H	1.202247006800	1.098811452900	1.285897768400
Cl	1.757374675500	-0.677259095900	-0.145955207900

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
47.9149	0.484
138.5957	0.215
220.8657	0.0326
280.1999	0.0571
361.2156	0.584
452.6618	3.59
476.3256	1.78
750.5672	13.0
847.6707	3.87
936.3794	2.81
979.4774	1.26
1099.1808	2.22
1122.0351	9.66
1156.3129	22.3
1235.6782	3.53
1278.4339	0.398
1290.9734	3.96
1367.0218	2.80
1407.7199	2.02
1433.1775	4.03
1454.3673	0.921
1513.7540	0.380
3014.0624	6.31
3055.5162	2.56
3068.6515	3.18
3078.6354	3.25
3116.8343	2.16

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
49.4545	0.265
147.8037	0.207
211.9760	0.653
327.9634	0.785
358.8995	0.277
411.8172	1.37
567.9550	4.31
723.6907	9.27
835.9562	2.86
943.8888	3.63
981.4520	1.71
1066.7769	1.52
1109.6584	11.6
1153.8124	21.7
1245.4837	0.992
1281.8691	6.32
1296.7554	2.41
1383.7079	2.57
1397.0537	0.333
1436.8456	2.45
1449.7271	1.22
1514.5437	0.736
3031.7647	5.60
3042.9511	0.537
3083.4557	4.19
3093.4745	3.96
3101.6044	1.64



$\Delta E = 1.95 \text{ kcal mol}^{-1}$
Population = 0.020

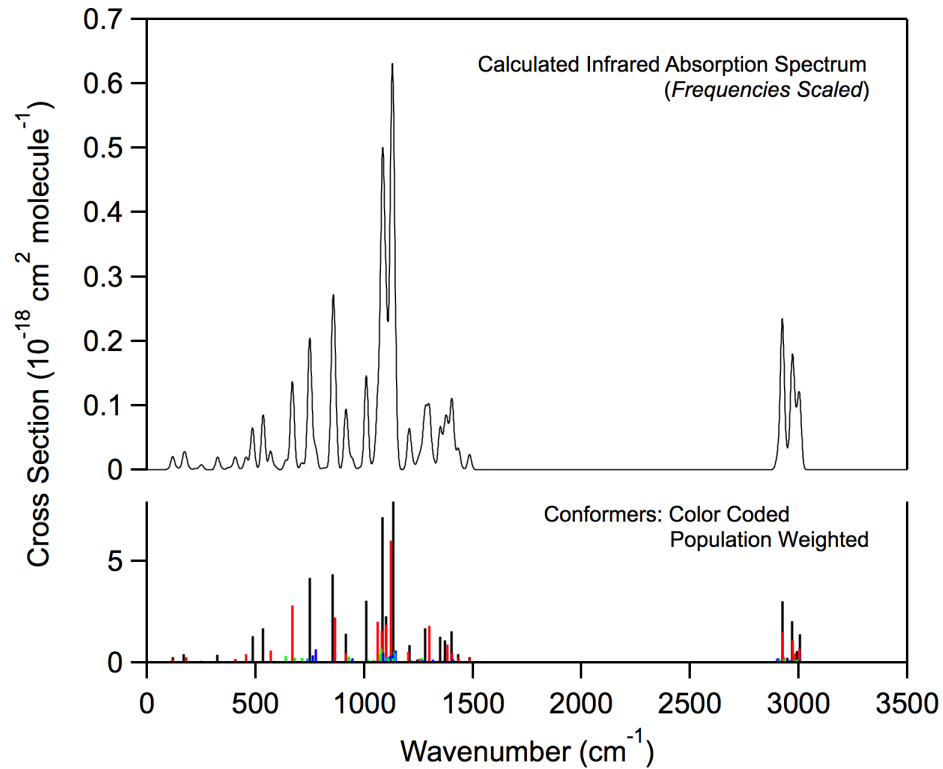
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.651169548600	-0.399755951700	0.302688070200
C	-0.657326938700	0.625592433000	-0.229496513300
C	0.732192648900	0.505562316800	0.361898654600
H	-1.021351056800	1.629803320500	0.018394645000
H	-0.587853726900	0.555105856900	-1.318908929400
F	-2.903071122600	-0.092895392900	-0.185605400100
H	-1.691324144300	-0.379395858000	1.400129803800
H	-1.387754448400	-1.413253213600	-0.016201410400
F	1.520586405000	1.499461637000	-0.112795766700
H	0.742943904900	0.538191912000	1.454455465000
Cl	1.504981027500	-1.082592060000	-0.066941618800

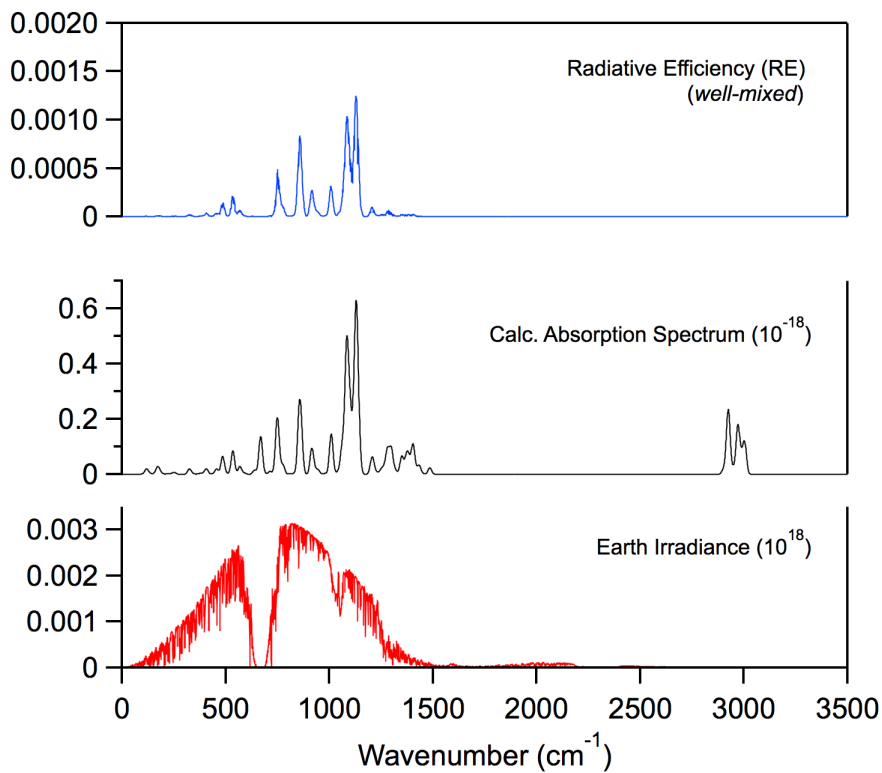
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
87.7067	0.798
111.5731	0.279
171.9550	0.641
296.6993	0.450
367.7685	0.717
441.0311	0.0864
507.9618	2.90
662.1121	11.6
817.7161	1.96
1022.1444	5.66
1064.8426	0.581
1077.9031	20.1
1118.9866	9.98
1139.7013	10.2
1229.9787	1.49
1290.6108	2.83
1300.9132	0.971
1322.3283	3.56
1401.2509	1.78
1442.3073	3.80
1482.0166	0.414
1523.9586	0.186
3020.9441	5.23
3047.9883	1.26
3081.0057	3.15
3085.6249	1.19
3113.0299	4.13

Infrared Spectrum

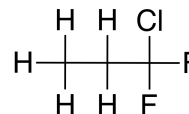


Radiative Efficiency



HCFC-262fc

Molecular Formula: CH₃CH₂CF₂Cl
Name: 1-Chloro-1,1-difluoropropane
CAS number: 421-02-3
Molecular Weight: 114.52



Global Atmospheric Lifetime (years): 1.19
Tropospheric Atmospheric Lifetime (years): 1.24
Stratospheric Atmospheric Lifetime (years): 33.7
Ozone Depletion Potential (ODP): 0.011

	<i>Well-mixed</i>	<i>Lifetime adjusted</i>
Radiative Efficiency (RE):	0.218	0.168
Global Warming Potential (GWP _H):		
GWP ₂₀	511	394
GWP ₁₀₀	138	107
Global Temperature Potentials (GTP _H):		
GTP ₂₀		131
GTP ₅₀		18
GTP ₁₀₀		15

* RE units: W m² ppb⁻¹

* GWP and GTP: Relative to CO₂

Atmospheric Loss Processes *****

OH Reactivity

$k_{\text{Rec}}(T)$, *No recommendation*

$k_{\text{SAR}}(298 \text{ K}) = 4.74 \times 10^{-14}$; $k_{\text{SAR}}(272 \text{ K}) \approx 3.02 \times 10^{-14}$ cm³ molecule⁻¹ s⁻¹

$\tau_{\text{Global}}^{\text{OH}} = 1.20$ years

$\tau_{\text{Trop}}^{\text{OH}} = 1.24$ years

$\tau_{\text{Strat}}^{\text{OH}} = 40.9$ years

Fractional Atmospheric Loss: 0.994

O(¹D) Reactivity

$k_{\text{Rec}}(T)$, *No recommendation*

$k_{\text{Est}}(T) = 1.1 \times 10^{-10}$ cm³ molecule⁻¹ s⁻¹

$\tau_{\text{O}(\text{1D})} = 335$ years

Fractional Atmospheric Loss: 0.004

UV Photolysis

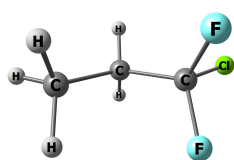
UV Spectrum: *No Recommendation*

$\tau_{\text{hv}} = 450$ years

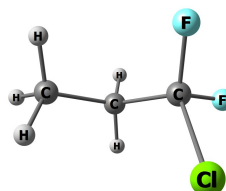
Fractional Atmospheric Loss: 0.002



Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.432



$\Delta E = 0.25 \text{ kcal mol}^{-1}$
Population = 0.284

Optimized Coordinates (Angstroms)

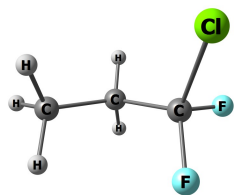
Atom	X	Y	Z
C	-2.382475757200	0.342123188400	-0.008075856800
C	-0.956595448300	0.902693260000	0.036804873400
C	0.080290410200	-0.204945541300	0.010107227200
H	-0.789407525200	1.487932229400	0.944771981900
H	-0.761076719000	1.556907958000	-0.816796890700
H	-3.105969251400	1.160730666500	0.012338503800
H	-2.575201871100	-0.306599684500	0.850037495900
H	-2.546731331200	-0.237296427400	-0.920016333100
F	-0.024426623200	-0.947643472300	-1.101809141300
Cl	1.768078184700	0.463086129100	0.063412797000
F	-0.059141068300	-1.032163305700	1.056620342700

Atom	X	Y	Z
C	-2.146364130000	-0.545778739500	0.080384093900
C	-1.167835123700	0.394292741100	-0.622351235000
C	0.210349666500	0.442266493700	0.011593496400
H	-1.533700624000	1.427669793200	-0.590823791400
H	-1.037081562300	0.126127151800	-1.673924053900
H	-2.252591145600	-0.279942870900	1.135123615000
H	-1.811745426100	-1.584173902200	0.020023978200
H	-3.130426875800	-0.476646255900	-0.390006422500
F	0.140439990100	0.760552169100	1.312060337400
Cl	1.085359213800	-1.147032217700	-0.112867051500
F	0.975578017200	1.364235637400	-0.588287966800

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
102.8150	0.0150
200.2704	0.0378
213.6954	0.00830
326.8934	0.0743
339.5317	1.44
416.4275	1.43
425.4851	0.00
547.8058	1.15
736.0126	4.46
795.5928	0.00322
926.6706	38.4
985.1759	4.71
1043.2848	11.9
1092.2289	8.92
1201.7592	11.4
1239.1296	18.4
1318.6584	5.66
1370.9195	1.62
1409.6328	0.241
1473.5163	0.346
1495.8392	0.651
1509.8855	1.59
3054.5570	2.53
3073.3132	1.13
3113.8543	0.0105
3129.5622	2.53
3137.3916	3.22

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
104.7739	0.00626
205.2314	0.0371
220.6623	0.0815
320.1269	0.107
344.7425	0.191
414.7708	0.759
467.6331	1.03
563.4345	2.49
648.6905	6.58
799.0534	0.00679
905.3304	25.8
1003.0237	7.18
1078.0126	4.81
1140.0375	12.3
1184.0044	23.8
1228.2100	15.2
1304.0577	6.24
1378.7283	2.58
1414.9335	0.605
1473.0272	0.270
1496.9880	0.709
1509.4013	1.47
3047.8442	1.71
3055.3421	2.41
3104.8590	0.403
3128.1083	2.75
3136.1185	2.82



$\Delta E = 0.25 \text{ kcal mol}^{-1}$
 Population = 0.284

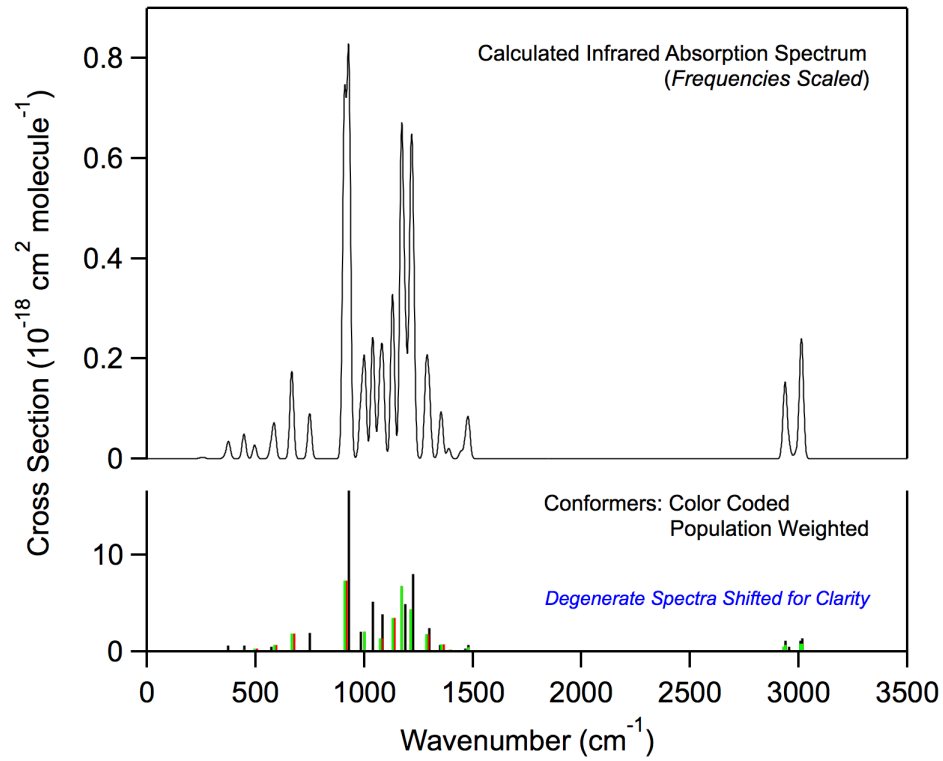
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-2.137180557500	0.597336224900	0.070671651800
C	-1.168873962300	-0.340792288100	-0.648611892500
C	0.200822524900	-0.433969355600	-0.001440637800
H	-1.021030631500	-0.044805679300	-1.690413626600
H	-1.554777529500	-1.367336611500	-0.651303845100
H	-3.116945940800	0.561105479900	-0.412206978800
H	-1.782061082000	1.630333294900	0.044395139500
H	-2.260531768400	0.303080753200	1.115960002400
F	0.955053308500	-1.352866633100	-0.619692678800
Cl	1.107452277000	1.140930003900	-0.069904913400
F	0.110010361500	-0.788423189200	1.288337793000

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
104.7755	0.00626
205.2338	0.0371
220.6658	0.0816
320.1284	0.107
344.7452	0.191
414.7755	0.759
467.6328	1.03
563.4348	2.49
648.6913	6.58
799.0549	0.00679
905.3311	25.8
1003.0270	7.18
1078.0176	4.81
1140.0392	12.3
1183.9936	23.8
1228.2072	15.2
1304.0581	6.24
1378.7335	2.58
1414.9410	0.605
1473.0313	0.270
1496.9873	0.709
1509.4053	1.47
3047.8359	1.71
3055.3376	2.41
3104.8479	0.402
3128.1072	2.75
3136.1008	2.82

Infrared Spectrum



Radiative Efficiency

