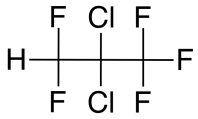
HCFC-225aa

Molecular Formula:	$CHF_2CCl_2CF_3$
Name:	2,2-Dichloro-1,1,1,3,3-pentafluoropropane
CAS number:	128903-21-9
Molecular Weight:	202.94



Global Atmospheric Lifetime (years):	11.8
Tropospheric Atmospheric Lifetime (years):	15.1
Stratospheric Atmospheric Lifetime (years):	53.8
Ozone Depletion Potential (ODP):	0.094

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.275	0.264
Global Warming Potential (GWP_H):		
GWP_{20}	2937	2818
GWP_{100}	974	934
Global Temperature Potentials (GTP_H)		
GTP_{20}		2237
GTP_{50}		438
GTP_{100}		139

* RE units: W m^2 ppb^{-1}
* GWP and GTP: Relative to CO_2

Atmospheric Loss Processes **********

OH Reactivity

k_{Rec}(T), *No recommendation*

$k_{SAR}(298\ K) = 3.89 \times 10^{-15}$; $k_{SAR}(272\ K) \approx 2.48 \times 10^{-15}$ cm^3 $molecule^{-1}$ s^{-1}

τ^{OH}_{Global} = 14.5 years
τ^{OH}_{Trop} = 15.1 years
τ^{OH}_{Strat} = 389.0 years

Fractional Atmospheric Loss: 0.812

$O(^1D)$ Reactivity

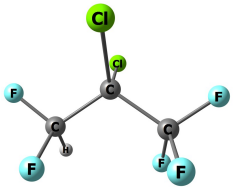
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 1.3 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)}$ = 285 years
Fractional Atmospheric Loss: 0.041

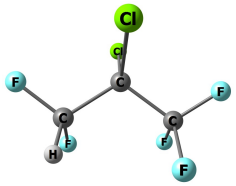
UV Photolysis

UV Spectrum: *No Recommendation*
τ_{hv} = 80 years
Fractional Atmospheric Loss: 0.147

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.389



E = 0
Population = 0.389

Optimized Coordinates (Angstroms)

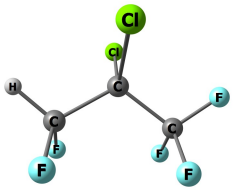
Atom	X	Y	Z
C	1.181052676200	-0.538385495000	0.803229054700
C	0.154081433400	0.222155637200	-0.076638912400
C	-1.286406727900	-0.324287471500	0.142471397500
Cl	0.181539610400	1.936612565200	0.432925469500
Cl	0.583001673000	0.054904202000	-1.794532727400
H	0.925692526300	-0.423566439200	1.862041982100
F	1.169165480700	-1.844896864000	0.477255881000
F	2.411285246000	-0.053228027800	0.579601078200
F	-2.184258907700	0.424936212400	-0.481880565900
F	-1.392312432700	-1.572495718400	-0.299449951400
F	-1.559967577700	-0.319830600900	1.453574294100

Atom	X	Y	Z
C	1.181466275600	-0.537207398200	-0.803418102700
C	0.153969885600	0.222187871400	0.076826589500
C	-1.286209530600	-0.324813327600	-0.142919072600
Cl	0.582685764100	0.053907986800	1.794671380600
Cl	0.180660606800	1.937025448000	-0.431493754900
H	0.926225254600	-0.421751503500	-1.862190559600
F	2.411419937000	-0.051599766700	-0.579234187400
F	1.170174634200	-1.843959221800	-0.478389134700
F	-2.184539260300	0.423513326000	0.481821561700
F	-1.559551625200	-0.319547656600	-1.454064640900
F	-1.391567941800	-1.573392757800	0.298082921000

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
61.6865	0.0683
89.8112	0.0915
155.1400	0.0751
173.1412	0.0500
214.3439	0.304
225.1578	0.0874
255.0432	0.0926
318.2705	0.0417
341.0939	0.0858
362.5363	0.0672
412.5428	0.222
539.0482	1.54
556.1570	1.06
582.4834	0.858
677.6932	9.25
725.6841	5.02
881.3471	19.4
945.0104	8.18
1052.8160	1.39
1150.8609	9.70
1179.3959	15.7
1215.3844	29.3
1251.8441	39.5
1267.6763	28.2
1380.4800	7.77
1396.4468	3.06
3081.6630	2.22

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
61.6863	0.0683
89.8113	0.0915
155.1401	0.0751
173.1411	0.0500
214.3440	0.304
225.1578	0.0874
255.0433	0.0926
318.2706	0.0417
341.0940	0.0858
362.5364	0.0672
412.5431	0.222
539.0484	1.54
556.1568	1.06
582.4836	0.858
677.6930	9.25
725.6841	5.02
881.3478	19.4
945.0106	8.17
1052.8158	1.39
1150.8610	9.70
1179.3959	15.7
1215.3843	29.3
1251.8448	39.5
1267.6765	28.2
1380.4800	7.77
1396.4468	3.06
3081.6626	2.22



$\Delta E = 0.33$ kcal mol^{-1}
Population = 0.222

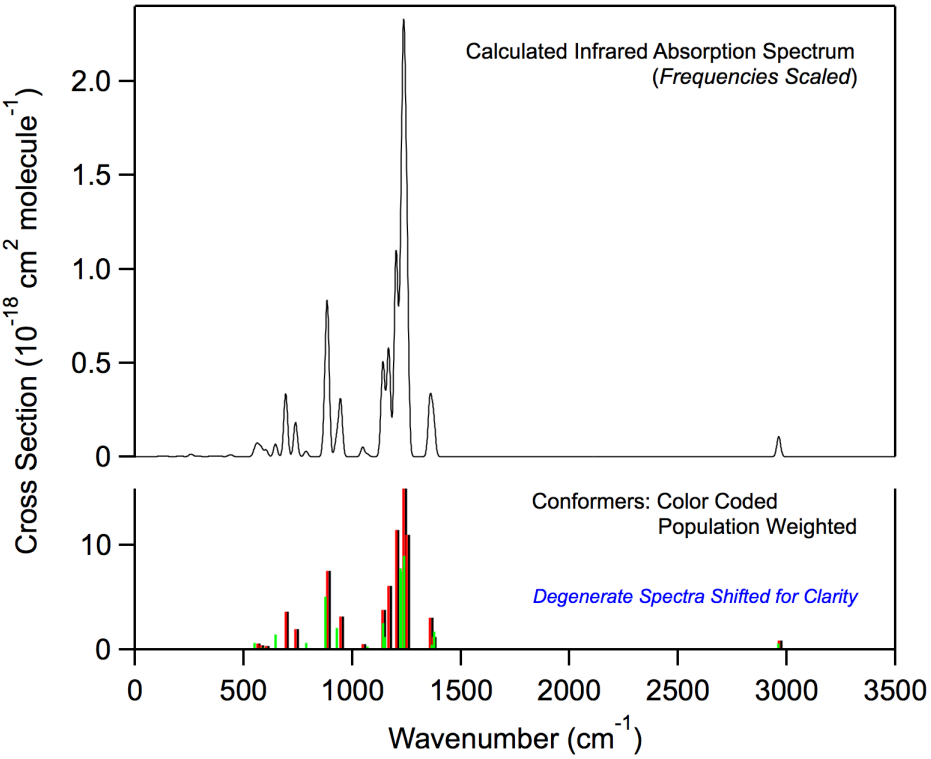
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.568526695200	0.120591790400	-0.000152252100
C	0.040892957300	0.405583322100	-0.000007860700
C	-0.837958263700	-0.881150101500	0.000122845300
Cl	-0.332857655200	1.349372492000	1.469227508300
Cl	-0.333150795300	1.349270746000	-1.469236468900
H	2.115163009100	1.069760193500	-0.000227489100
F	1.900501202100	-0.594111812500	1.090149401300
F	1.900285109900	-0.594160034200	-1.090488096300
F	-2.128181309400	-0.562723386300	0.000256130200
F	-0.581956880700	-1.614596888900	-1.080039239400
F	-0.581710069300	-1.614550320400	1.080261521600

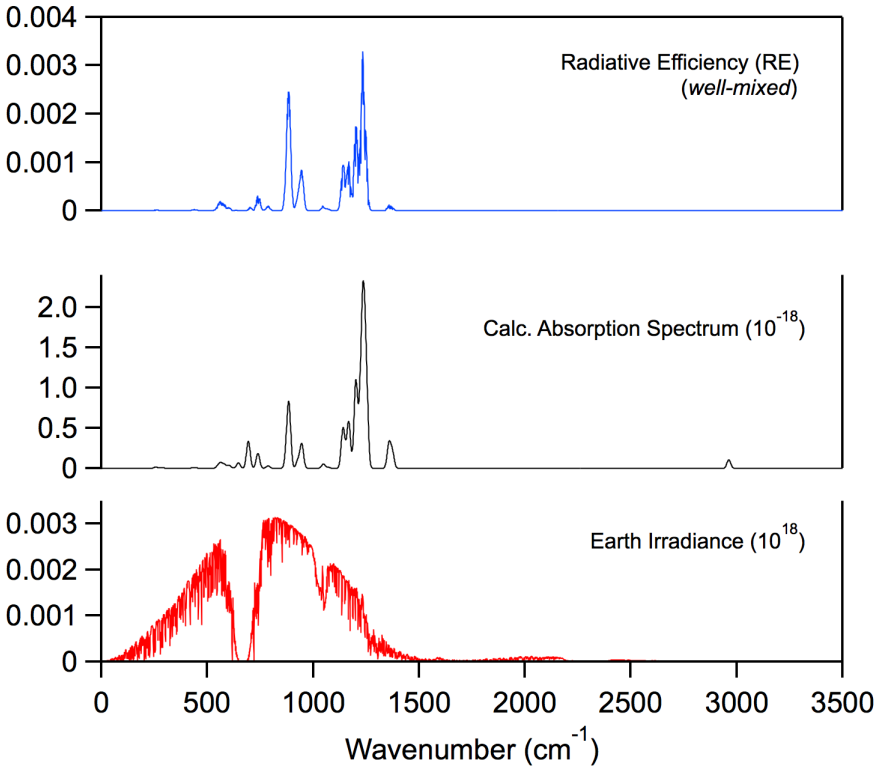
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
45.3890	0.0314
108.6223	0.110
165.7588	0.00540
167.5475	0.0267
214.5066	0.151
242.4283	0.185
252.1076	0.00948
306.0562	0.157
337.0659	0.001
399.5357	0.355
402.1901	0.0788
525.9244	2.76
559.2982	0.869
573.4677	0.710
628.0088	6.46
776.5432	2.88
870.4327	22.8
926.1424	9.25
1075.9044	1.29
1151.3794	11.3
1161.1289	5.33
1236.9098	34.7
1240.7305	33.4
1254.0284	40.3
1390.5752	2.09
1399.9428	7.85
3078.3742	2.66

Infrared Spectrum

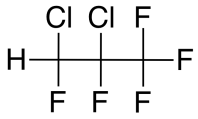


Radiative Efficiency



HCFC-225ba

Molecular Formula:	$CHClFCClFCF_3$
Name:	1,2-Dichloro-1,2,3,3,3-pentafluoropropane
CAS number:	422-48-0
Molecular Weight:	202.94



Global Atmospheric Lifetime (years):	4.20
Tropospheric Atmospheric Lifetime (years):	4.45
Stratospheric Atmospheric Lifetime (years):	74.3
Ozone Depletion Potential (ODP):	0.025

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.279	0.254
Global Warming Potential (GWP_H):		
GWP_{20}	1287	1172
GWP_{100}	352	320
Global Temperature Potentials (GTP_H)		
GTP_{20}		588
GTP_{50}		64
GTP_{100}		45

* RE units: W m^2 ppb^{-1}
* GWP and GTP: Relative to CO_2

Atmospheric Loss Processes **********

OH Reactivity

k_{Rec}(T), *No recommendation*

$k_{SAR}(298\ K) = 1.32 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 0.841 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 4.30$ years

$\tau^{OH}_{Trop} = 4.45$ years

$\tau^{OH}_{Strat} = 129.5$ years

Fractional Atmospheric Loss: 0.976

$O(^1D)$ Reactivity

k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 1.3 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 285$ years

Fractional Atmospheric Loss: 0.015

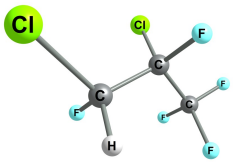
UV Photolysis

UV Spectrum: *No Recommendation*

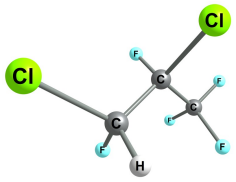
$\tau_{hv} = 450$ years

Fractional Atmospheric Loss: 0.009

Molecular Structure and Infrared Spectrum (6 conformers)



E = 0
Population = 0.511



$\Delta E = 0.59$ kcal mol^{-1}
Population = 0.189

Optimized Coordinates (Angstroms)

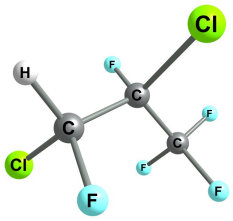
Atom	X	Y	Z
C	-0.992495970000	-0.809790744800	-0.023835407300
C	0.080794065900	0.253647311900	0.299151487300
C	1.513899999000	-0.312685331700	0.079208703900
F	-0.008147897400	0.559925023300	1.610320059400
Cl	-0.124083682200	1.718335847000	-0.690549595200
H	-0.789745903400	-1.707213953300	0.564379691700
F	-0.954702199400	-1.105013933900	-1.336996545900
Cl	-2.620868364600	-0.245222266100	0.438040473700
F	2.420958504100	0.555459289600	0.505075551200
F	1.639844837300	-1.441019804700	0.792027196600
F	1.740084610800	-0.593314437300	-1.197255615400

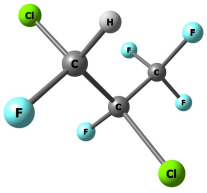
Atom	X	Y	Z
C	1.011955060400	0.582498572700	0.493363900500
C	-0.081277016400	-0.204682822400	-0.265836009600
C	-1.510883442600	0.314382412600	0.080882647100
Cl	0.022593637900	-1.931482995500	0.189130156700
F	0.076578489300	-0.065851811500	-1.593425528300
H	0.966887852900	0.365120067700	1.560583200700
F	0.816959891600	1.903826468900	0.283781286400
Cl	2.639737459000	0.135166251800	-0.088331232500
F	-2.437753942900	-0.499426163700	-0.408566050600
F	-1.654921899000	0.390009986500	1.406798192800
F	-1.696861090100	1.521158033000	-0.442521563300

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
51.3365	0.0669
76.2982	0.0379
141.1471	0.126
180.9565	0.0156
203.2714	0.329
230.0520	0.105
285.5811	0.165
321.0853	0.157
342.6870	0.0138
382.1683	0.0557
424.3014	0.366
522.2698	0.188
549.2161	1.83
601.6169	1.17
642.0668	6.76
720.5079	13.6
804.4088	12.4
950.2745	13.8
1087.7133	3.92
1149.2969	17.1
1169.9959	9.48
1220.1601	30.4
1264.6795	34.7
1282.7212	13.4
1302.0196	20.6
1363.5620	3.75
3109.1498	0.659

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
53.6197	0.0599
66.2300	0.0203
145.7228	0.0506
194.9131	0.0698
212.4286	0.414
232.6771	0.0397
297.6308	0.108
308.6103	0.133
325.0565	0.114
384.0299	0.0103
426.5261	0.499
457.7812	0.601
546.6508	1.00
582.8359	0.359
700.9282	15.7
791.9063	4.51
798.7487	10.7
938.7578	23.5
1024.8439	3.75
1113.1518	10.7
1202.5631	18.2
1233.3376	26.8
1255.1777	32.3
1271.9727	11.9
1301.6258	24.3
1369.5510	1.33
3130.0251	0.609





$\Delta E = 0.82$ kcal mol^{-1}
Population = 0.128

$\Delta E = 1.17$ kcal mol^{-1}
Population = 0.071

Optimized Coordinates (Angstroms)

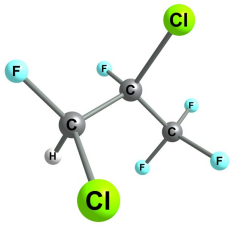
Atom	X	Y	Z
C	1.098872296400	-0.828502943500	0.193164760800
C	-0.247955395200	-0.351516075600	-0.400699146200
C	-0.828664925000	0.974331433400	0.172354585100
Cl	-1.440913946800	-1.660917641900	-0.095028971000
F	-0.101260651600	-0.189570552100	-1.728757847600
H	1.329973208700	-1.810777248000	-0.222909537800
F	1.006938992500	-0.900352628900	1.533775848600
Cl	2.457416055700	0.247259771300	-0.264113883300
F	-1.987851941400	1.240214604300	-0.423470818600
F	-1.024265322200	0.885104043000	1.482453848600
F	0.005162628900	1.982754237800	-0.071510838700

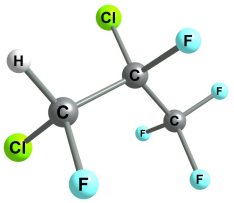
Atom	X	Y	Z
C	-1.132030123700	0.465408417800	-0.532762860500
C	0.168097828000	0.343814105700	0.296333773400
C	1.058934001100	-0.873386746400	-0.088005915600
F	-0.119413994800	0.250996496200	1.605172386600
Cl	1.118224176600	1.840949236900	-0.001818337000
H	-0.903469031700	0.475711776700	-1.598567732300
F	-1.762295892100	1.600445350600	-0.175826568200
Cl	-2.236248554000	-0.914169989000	-0.233035503400
F	2.260070236100	-0.770622030800	0.466072165300
F	0.505571671800	-2.005692038400	0.333178770800
F	1.194820682600	-0.927511579200	-1.416323179200

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
30.9915	0.0270
93.9702	0.0784
155.5246	0.0416
179.2452	0.0148
200.4375	0.134
253.6566	0.0372
270.5568	0.449
315.9970	0.217
343.9380	0.00467
390.6643	0.00224
414.1018	0.224
517.5487	1.61
531.3678	1.95
578.6736	2.54
641.0664	3.27
766.4317	2.96
771.7944	28.4
915.2704	10.0
1097.7868	6.50
1149.3141	17.7
1185.5496	10.7
1229.7724	19.3
1251.7919	33.6
1263.6506	27.1
1317.4473	11.6
1383.4442	2.08
3110.5661	0.770

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
40.7936	0.0356
73.8235	0.0301
148.3045	0.0673
197.9518	0.0724
205.4242	0.406
254.4107	0.0447
269.0984	0.110
311.2699	0.0863
340.2784	0.148
384.9938	0.001
421.2044	0.440
441.5483	0.809
549.2729	1.13
583.9889	0.0605
727.9694	7.97
766.8497	27.4
787.4437	2.49
929.0835	13.0
1014.6837	11.6
1133.3760	10.0
1207.9529	23.0
1231.1737	26.6
1254.8299	28.2
1282.3437	5.84
1299.0547	17.3
1378.4898	3.01
3129.7907	0.587





ΔE = 1.20 kcal mol^{-1}
Population = 0.067

ΔE = 1.61 kcal mol^{-1}
Population = 0.034

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.179887927000	0.073165262600	-0.730322527800
C	-0.164355393500	-0.510773034300	-0.237203522900
C	-1.285172572300	0.547461023200	-0.039248303300
Cl	0.032940741500	-1.475645445800	1.243496544100
F	-0.592730712700	-1.317933627600	-1.240862058500
H	1.002036653300	0.609741277900	-1.664458622700
F	2.023421648800	-0.952455092200	-0.948792505800
Cl	1.916179448300	1.228211695700	0.412531360700
F	-2.459916606300	-0.061614467500	0.060509035600
F	-1.093561301300	1.294334635000	1.038203407600
F	-1.310879832700	1.346492773200	-1.115415807100

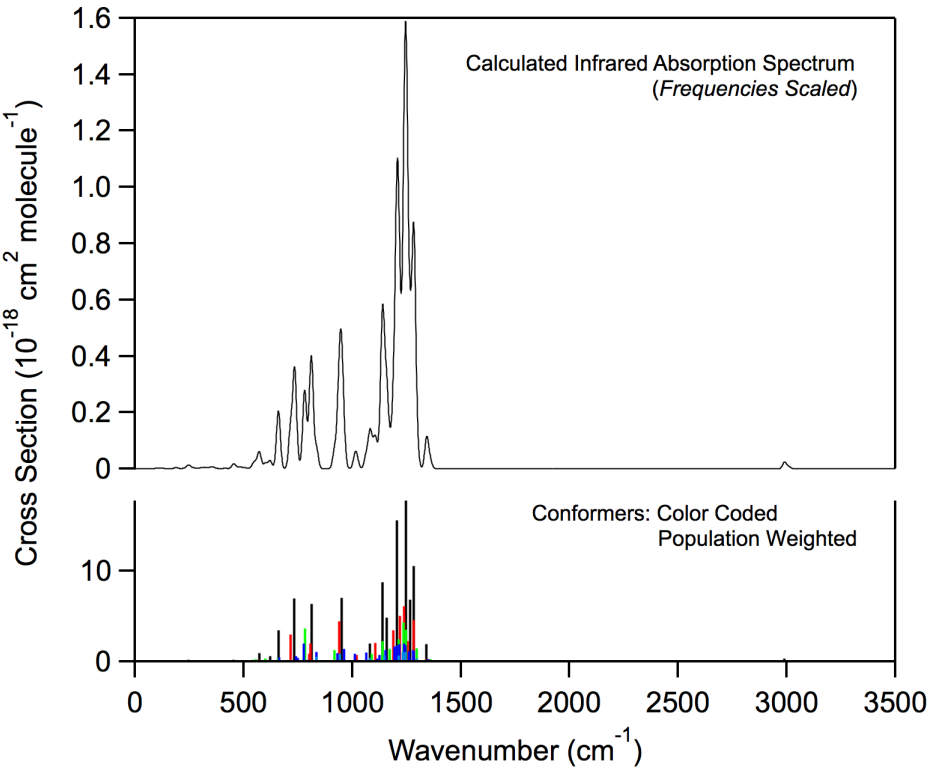
Atom	X	Y	Z
C	-1.247383618300	0.072374424600	0.687949609300
C	0.266519876300	0.338359703400	0.497622164900
C	1.045164607000	-0.666259889600	-0.400302760300
F	0.809836987400	0.235020443900	1.734263290400
Cl	0.514174110900	1.998318564800	-0.110356515000
H	-1.653820299500	0.870958483800	1.312194454200
F	-1.395588488000	-1.113243543700	1.313384783800
Cl	-2.176082902700	0.065072201200	-0.837094936800
F	2.349293761800	-0.431421839700	-0.284774197600
F	0.801903561200	-1.910826394300	0.007155781200
F	0.701530403900	-0.557078154400	-1.677485674100

Infrared Absorption Spectrum (unscaled frequencies)

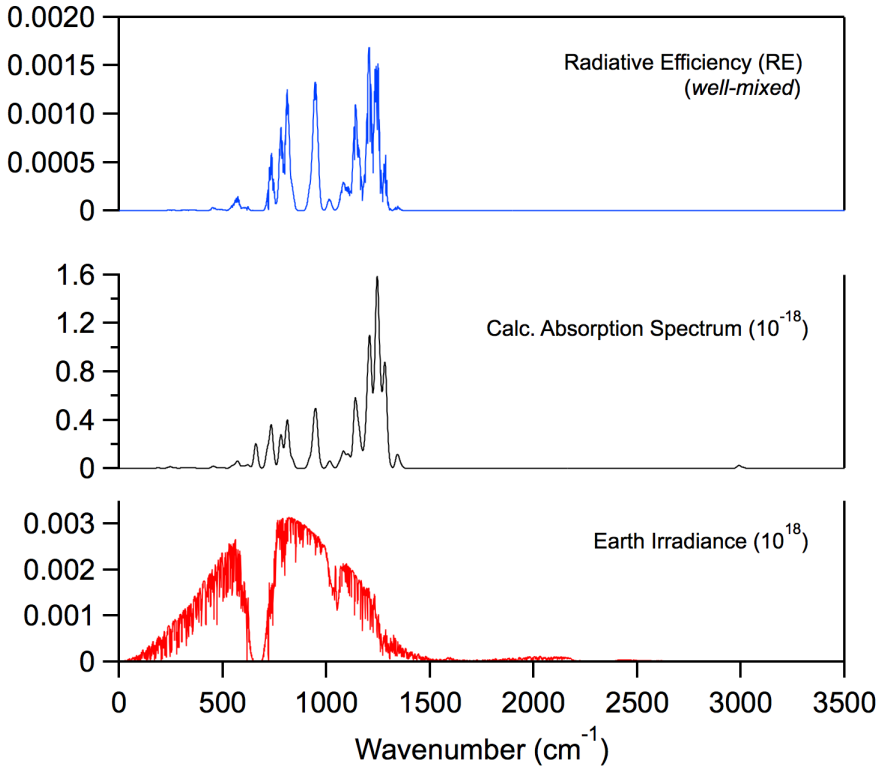
Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
50.7656	0.0509
82.0678	0.0401
142.6974	0.0688
176.2224	0.151
194.6056	0.225
253.6595	0.222
302.7810	0.205
317.5268	0.0573
340.3952	0.0872
384.1258	0.0684
423.7884	0.503
478.1082	0.791
556.3903	1.22
590.2711	0.212
645.9973	7.00
735.5842	6.03
828.4083	15.2
962.8387	20.6
1069.5270	14.8
1124.3323	4.85
1162.9069	18.9
1219.7384	27.0
1260.9945	26.9
1279.5153	17.0
1301.4388	16.4
1370.8003	3.95
3110.4938	0.718

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
36.1193	0.0155
92.7385	0.0538
153.3225	0.0341
176.2955	0.0142
196.2957	0.117
262.1733	0.442
301.9368	0.0560
321.2651	0.242
334.5413	0.0406
387.2863	0.0277
430.4401	0.330
482.1018	0.710
530.2308	2.99
574.1169	1.25
631.6881	4.70
766.5866	2.42
826.6826	15.3
940.4157	24.7
1088.3105	11.1
1119.4590	2.91
1159.0539	19.9
1227.2338	19.3
1249.0913	31.4
1260.3054	31.8
1316.3633	10.6
1383.6708	3.09
3105.6149	0.860

Infrared Spectrum

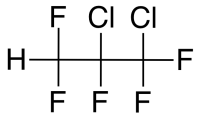


Radiative Efficiency



HCFC-225bb

Molecular Formula:	$CHF_2CClFCClF_2$
Name:	1,2-Dichloro-1,1,2,3,3-pentafluoropropane
CAS number:	422-44-6
Molecular Weight:	202.94



Global Atmospheric Lifetime (years):	15.9
Tropospheric Atmospheric Lifetime (years):	19.0
Stratospheric Atmospheric Lifetime (years):	99.5
Ozone Depletion Potential (ODP):	0.069

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.330	0.319
Global Warming Potential (GWP_H):		
GWP_{20}	4169	4033
GWP_{100}	1577	1526
Global Temperature Potentials (GTP_H)		
GTP_{20}		3475
GTP_{50}		992
GTP_{100}		260

* RE units: W m^2 ppb^{-1}
* GWP and GTP: Relative to CO_2

Atmospheric Loss Processes **********

OH Reactivity

k_{Rec}(T), *No recommendation*

$k_{SAR}(298\ K) = 3.09 \times 10^{-15}$; $k_{SAR}(272\ K) \approx 1.97 \times 10^{-15}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 18.3$ years

$\tau^{OH}_{Trop} = 19.0$ years

$\tau^{OH}_{Strat} = 478.6$ years

Fractional Atmospheric Loss: 0.873

$O(^1D)$ Reactivity

k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 1.3 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 285$ years

Fractional Atmospheric Loss: 0.056

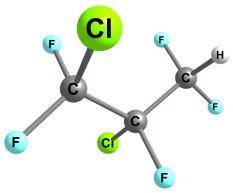
UV Photolysis

UV Spectrum: *No Recommendation*

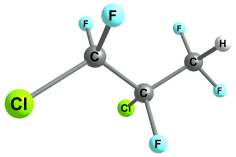
$\tau_{hv} = 225$ years

Fractional Atmospheric Loss: 0.071

Molecular Structure and Infrared Spectrum (9 conformers)



E = 0
Population = 0.318



$\Delta E = 0.01$ kcal mol^{-1}
Population = 0.312

Optimized Coordinates (Angstroms)

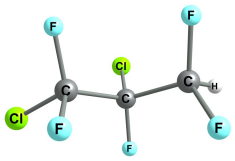
Atom	X	Y	Z
C	1.028556190200	-1.178735075800	-0.037806502000
C	0.381528678700	0.182726069000	-0.384719548400
C	-1.052644136700	0.375042738500	0.186890026200
Cl	1.404731167400	1.513096106900	0.228906873200
F	0.296831250800	0.260438067800	-1.728990006400
H	0.442716111600	-1.996845010200	-0.470531585700
F	2.269274542000	-1.203382572600	-0.552374825900
F	1.099334753600	-1.326807946700	1.296309035400
Cl	-2.145403033400	-0.930252534300	-0.408575777700
F	-1.041428238700	0.350923424600	1.513299197400
F	-1.538615285700	1.540782732800	-0.224209886300

Atom	X	Y	Z
C	1.582777809600	-0.670869567000	-0.323653588800
C	0.331839022900	0.245450692600	-0.315240050700
C	-0.944328777200	-0.544226349000	0.100368770400
Cl	0.587526617700	1.629728264100	0.769816232800
F	0.159052940700	0.673065545500	-1.584074535600
H	1.440428327500	-1.483306019800	-1.044653255300
F	2.650431223900	0.059337636700	-0.682387215800
F	1.788271653000	-1.181832054000	0.902800967100
Cl	-2.433713536300	0.386243255800	-0.213281429700
F	-0.980563752400	-1.669936031300	-0.632517608400
F	-0.891513529400	-0.883960373600	1.381915713900

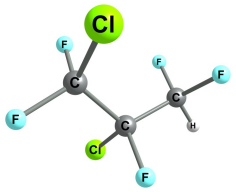
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
47.4128	0.105
84.3535	0.0902
147.9876	0.121
187.3204	0.0761
198.0534	0.195
258.0275	0.207
260.0140	0.115
314.8044	0.0409
348.3885	0.0720
377.3537	0.307
405.4523	0.295
421.4789	0.168
560.3539	0.558
580.9466	2.21
658.7072	7.96
666.6780	6.66
819.4202	40.0
1030.5849	10.7
1078.8415	6.54
1164.7462	7.73
1171.5899	27.3
1199.3433	14.9
1237.4915	31.5
1249.9075	10.0
1387.3586	5.50
1398.7445	3.03
3080.8928	2.71

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
54.4091	0.0903
78.2044	0.110
143.9424	0.102
187.1165	0.0687
209.0605	0.380
220.3575	0.0673
300.9013	0.383
308.8730	0.0666
328.8032	0.0371
378.1354	0.141
425.6331	0.001
449.9183	0.239
528.9745	2.14
587.3695	2.18
655.5488	5.10
679.9659	8.25
832.7908	32.3
1033.4830	17.8
1100.2471	10.8
1147.8913	4.11
1171.3138	15.4
1193.8747	20.8
1199.4709	36.0
1243.8009	13.3
1383.0862	8.66
1399.4711	3.28
3078.6305	2.75



$\Delta E = 0.54$ kcal mol^{-1}
Population = 0.127



$\Delta E = 0.89$ kcal mol^{-1}
Population = 0.070

Optimized Coordinates (Angstroms)

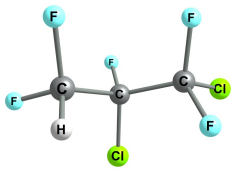
Atom	X	Y	Z
C	1.794008026400	-0.071950859000	-0.164561344000
C	0.318140649000	0.351484868600	-0.399775150700
C	-0.724321060400	-0.563213222800	0.313084426000
Cl	0.138858280600	2.037220246200	0.163833056300
F	0.100045420200	0.286697817500	-1.727537988300
H	2.457178209100	0.669529543000	-0.624940965200
F	2.048509262000	-0.158392505400	1.152342599500
F	2.008833935400	-1.273140903600	-0.730841781100
Cl	-2.394244921800	-0.160571668200	-0.192065052100
F	-0.477966732500	-1.832175314500	-0.017604452400
F	-0.620173068100	-0.440716001800	1.631775652000

Atom	X	Y	Z
C	0.792622949300	-1.446176519400	0.002843982200
C	0.535923198000	0.017324969600	-0.437983895300
C	-0.681683236000	0.747176695900	0.206009845200
Cl	2.012497256000	0.955951978300	-0.028665483500
F	0.367274729400	0.017472021000	-1.773900013100
H	1.733562250700	-1.788249268700	-0.443606564200
F	0.866228092400	-1.524134933600	1.341830013000
F	-0.210225470600	-2.234589842200	-0.425160705100
Cl	-2.231742911300	-0.030897453400	-0.240033756200
F	-0.563027615300	0.757553966000	1.529801132900
F	-0.710196242700	2.004140386500	-0.234261555800

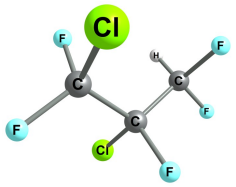
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
40.9207	0.0227
93.8010	0.159
154.1535	0.0113
188.2990	0.0259
206.5948	0.171
220.1771	0.130
299.9005	0.00580
318.4688	0.146
329.2781	0.0108
404.9397	0.119
423.5274	0.0187
443.0590	0.204
528.6745	1.08
560.0699	12.5
611.5829	6.60
664.1930	1.94
924.1540	21.1
958.5370	22.0
1103.5982	6.58
1151.8361	7.52
1168.1044	25.5
1198.8166	10.1
1218.1369	46.9
1236.7556	9.35
1391.3107	2.78
1400.9621	8.60
3069.7251	3.15

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
30.3944	0.0463
99.3873	0.140
158.8184	0.0538
185.7656	0.0287
202.5828	0.0834
246.7106	0.0960
276.8247	0.446
314.5312	0.0764
335.7205	0.146
403.0977	0.375
404.1626	0.139
428.6606	0.0431
525.0712	2.17
572.2642	3.24
636.5886	3.63
698.3432	7.94
840.0384	43.6
975.6535	2.78
1119.9787	13.2
1150.2602	5.36
1166.0188	13.1
1201.6655	34.3
1226.2657	20.4
1246.1422	18.6
1393.7713	2.32
1408.1413	3.33
3069.0451	3.30



ΔE = 1.05 kcal mol^{-1}
Population = 0.053



ΔE = 1.19 kcal mol^{-1}
Population = 0.043

Optimized Coordinates (Angstroms)

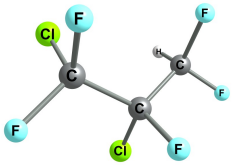
Atom	X	Y	Z
C	1.643554335200	-0.431678833300	0.373557590500
C	0.360158036800	0.206208358800	-0.226729011500
C	-0.932056562500	-0.489228051300	0.294410125900
Cl	0.347723201600	1.933815347500	0.229893615900
F	0.396441241100	0.076813153800	-1.563475802400
H	1.638025404100	-0.376270018600	1.466767151500
F	1.718591628800	-1.717717710500	-0.019514047500
F	2.712285170300	0.219293788400	-0.114348877400
Cl	-2.413505302000	0.238857054900	-0.382538958100
F	-0.902490430700	-1.776317081200	-0.050076300300
F	-0.958258722700	-0.411347008600	1.628862513300

Atom	X	Y	Z
C	1.098192915400	-0.987615893100	0.545128674500
C	0.447415193700	0.144079267500	-0.290296799300
C	-1.025606423000	0.460159819800	0.112430710600
Cl	1.417362411000	1.631363352700	-0.015039609800
F	0.485200969600	-0.181738590600	-1.591885836700
H	1.102423317200	-0.738966169500	1.610590237000
F	0.421741113700	-2.135797755000	0.347560247100
F	2.356252896100	-1.163090101400	0.107198941900
Cl	-2.154696845800	-0.822919817100	-0.409912496100
F	-1.084409896500	0.582291218200	1.444010032500
F	-1.417944651400	1.603409668400	-0.439712101900

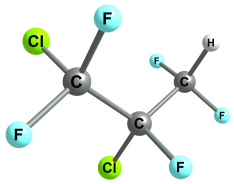
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
42.5895	0.0786
71.9590	0.0696
149.9615	0.114
187.7338	0.0193
209.4915	0.307
243.8829	0.242
283.3313	0.0476
309.4635	0.134
331.0675	0.239
359.9650	0.144
426.2434	0.0556
434.2682	0.526
497.7540	0.993
566.2898	3.48
648.1869	1.58
795.7372	28.4
864.3152	11.6
950.7483	21.8
1083.5111	20.5
1147.6923	10.6
1161.2568	7.21
1195.9483	16.3
1208.3875	29.1
1254.7109	24.0
1393.4018	4.79
1403.0836	3.18
3086.9569	2.86

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
40.0770	0.0947
73.1884	0.0561
156.0737	0.0426
181.9567	0.0962
218.2729	0.342
250.7457	0.241
263.7145	0.0901
311.5331	0.0252
335.7275	0.316
373.8835	0.363
402.0681	0.179
429.3220	0.0140
504.5895	0.443
573.1241	2.39
649.5386	1.21
805.5254	34.5
830.1627	23.1
972.8821	3.72
1054.7493	15.8
1148.9677	9.65
1155.9867	20.4
1201.3577	29.2
1233.9327	23.1
1253.0354	5.36
1396.7045	2.60
1403.7220	3.63
3092.9951	2.58



$\Delta E = 1.41$ kcal mol^{-1}
Population = 0.029



$\Delta E = 1.43$ kcal mol^{-1}
Population = 0.028

Optimized Coordinates (Angstroms)

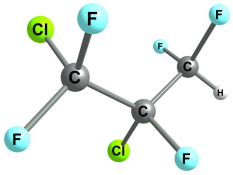
Atom	X	Y	Z
C	1.337720564300	-0.496954560300	0.714514750800
C	0.424404719900	0.187637758400	-0.331264700400
C	-1.038277368200	-0.351730360000	-0.370043066700
Cl	0.417905234500	1.946288058000	-0.017281718300
F	0.936258397600	-0.048784258000	-1.557506301300
H	1.030525898700	-0.264297001800	1.737613615800
F	1.296865369900	-1.830117813600	0.517073260300
F	2.595743109800	-0.073766119100	0.505188729300
Cl	-1.816213766100	-0.309363066200	1.246964895200
F	-1.757828109400	0.374276445900	-1.218902382400
F	-1.020600051000	-1.608427083300	-0.806817082400

Atom	X	Y	Z
C	1.309491237700	-0.827476830900	-0.513121340600
C	0.436645290500	0.415652903800	-0.217120939800
C	-1.090201949200	0.179244735500	-0.423013983200
Cl	0.772855272000	1.059788302600	1.403818761300
F	0.773902106600	1.341687508000	-1.148946071200
H	1.063330429400	-1.225101839000	-1.504658981400
F	2.597774908900	-0.446653418700	-0.492067722100
F	1.120726895800	-1.777870453600	0.416509366000
Cl	-1.815103860800	-0.978405628700	0.719923450800
F	-1.723854295200	1.343295863300	-0.332167761200
F	-1.250615035800	-0.290562142300	-1.670818778400

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
50.0789	0.0800
80.7119	0.0572
147.7168	0.0746
179.6329	0.0640
206.7803	0.174
265.4783	0.0962
294.3660	0.0510
308.1053	0.311
346.4384	0.312
358.2412	0.149
406.0233	0.388
432.2816	0.791
463.5042	0.803
567.1609	2.06
644.1048	2.21
800.1254	10.5
897.2880	32.0
978.9779	31.1
1041.5682	14.8
1139.8123	6.81
1157.3850	10.4
1199.9883	12.1
1231.5043	26.0
1246.9941	28.3
1396.2117	3.43
1401.9154	2.81
3101.9344	2.51

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
47.5950	0.104
82.9631	0.0897
152.5038	0.0982
166.6924	0.0227
194.8450	0.234
249.2551	0.343
306.1080	0.325
315.0483	0.0591
323.0383	0.0354
380.7307	0.313
424.4829	0.0874
437.5597	0.258
528.3039	0.698
584.7682	2.31
636.0878	1.97
679.4404	11.3
894.0030	29.9
1034.6724	29.9
1074.8229	4.64
1126.7870	5.69
1172.0879	32.0
1194.6199	20.0
1199.3630	5.13
1238.7203	24.0
1388.7014	5.77
1399.8703	3.58
3070.8281	2.77



$\Delta E = 1.65$ kcal mol^{-1}
Population = 0.020

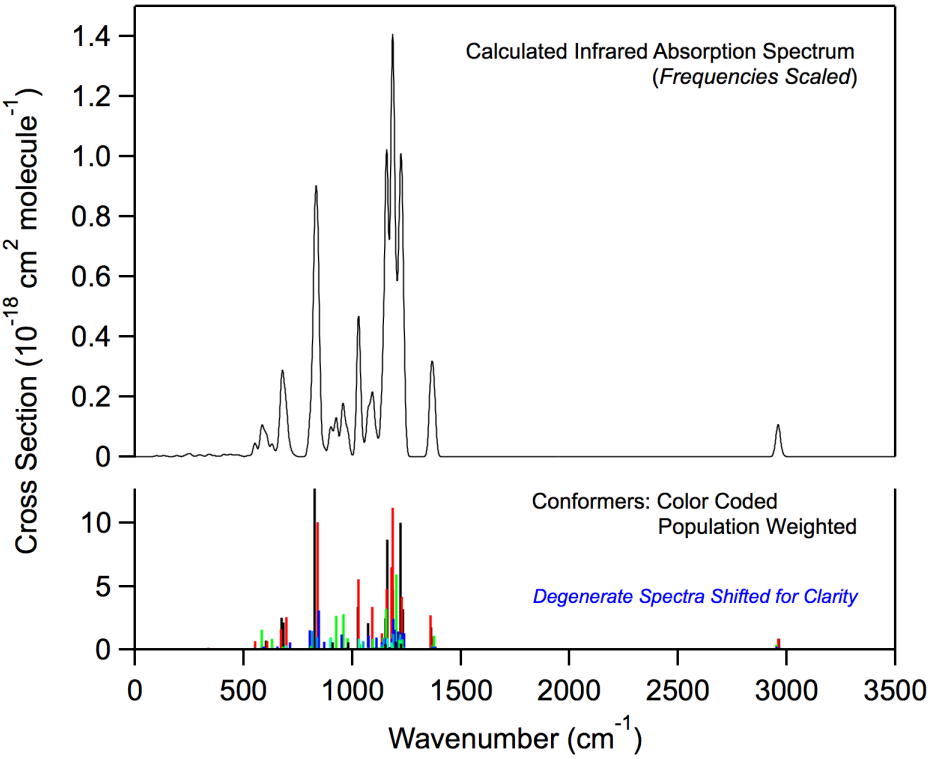
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.592332242200	-0.373007820000	0.410004002700
C	0.485414710700	0.431522718400	-0.315005347400
C	-0.885287058700	-0.284414497500	-0.528279119300
Cl	0.254095804300	1.984057540100	0.531441813400
F	0.960331382300	0.673468696700	-1.561944514900
H	2.534112817500	0.180458714800	0.312482993400
F	1.303876494600	-0.553546838600	1.707474530700
F	1.718542761100	-1.578357870500	-0.178523654700
Cl	-1.658809067700	-0.803005464000	0.993752604800
F	-1.702429615800	0.547464389600	-1.172037127700
F	-0.686805470600	-1.351071569000	-1.302473180900

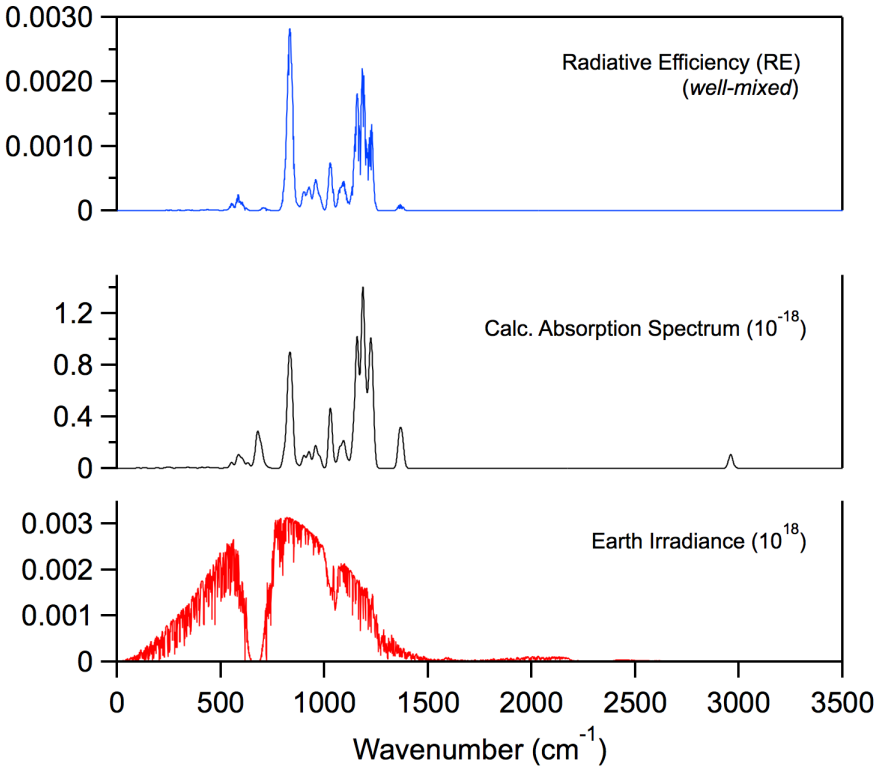
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
38.2586	0.0544
99.7797	0.123
157.6135	0.0437
173.4792	0.0128
199.0080	0.0545
267.6289	0.470
298.4237	0.00314
312.6548	0.336
321.2566	0.0883
396.4899	0.235
427.4594	0.130
433.5754	0.664
493.2071	1.57
569.5265	4.69
608.9707	2.05
718.4297	5.78
906.0127	29.7
981.4514	28.7
1112.1386	6.94
1125.1739	6.72
1163.1546	21.6
1185.8177	8.70
1212.5689	30.6
1241.3983	24.2
1390.6136	1.90
1405.5514	5.08
3064.7725	3.54

Infrared Spectrum

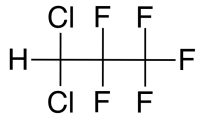


Radiative Efficiency



HCFC-225ca

Molecular Formula:	$CHCl_2CF_2CF_3$
Name:	3,3-Dichloro-1,1,1,2,2-pentafluoropropane
CAS number:	422-56-0
Molecular Weight:	202.94



Global Atmospheric Lifetime (years):	1.81		1.9 #
Tropospheric Atmospheric Lifetime (years):	1.92		2.0 #
Stratospheric Atmospheric Lifetime (years):	30.8		44 #
Ozone Depletion Potential (ODP):	0.020		
	Well-mixed	*Lifetime adjusted*	
Radiative Efficiency (RE):	0.271	0.225	0.22 #
Global Warming Potential (GWP_H):			
GWP_{20}	544	451	469 #
GWP_{100}	147	122	127 #
Global Temperature Potentials (GTP_H)			
GTP_{20}		162	170 #
GTP_{50}		22	22 #
GTP_{100}		17	18 #

* RE units: W m^2 ppb^{-1}
* GWP and GTP: Relative to CO_2
# Value taken from WMO (2014)

Atmospheric Loss Processes **********

OH Reactivity

$k_{Rec}(T) = 6.3 \times 10^{-13} \exp(-960/T)$; $k_{Rec}(272\ K) = 1.85 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$k_{SAR}(298\ K) = 3.05 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 1.95 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 1.86$ years

$\tau^{OH}_{Trop} = 1.92$ years

$\tau^{OH}_{Strat} = 60.7$ years

Fractional Atmospheric Loss: 0.971

$O(^1D)$ Reactivity

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

$k_{Est}(T) = 1.3 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 285$ years

Fractional Atmospheric Loss: 0.006

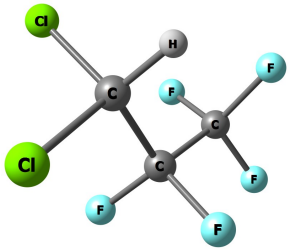
UV Photolysis

UV Spectrum: *Recommendation available*

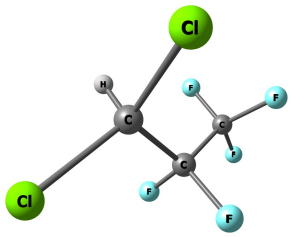
$\tau_{hv} = 80$ years

Fractional Atmospheric Loss: 0.023

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.467



E = 0
Population = 0.467

Optimized Coordinates (Angstroms)

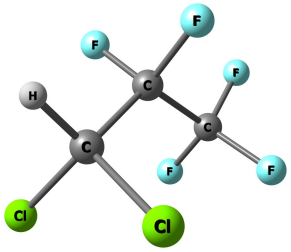
Atom	X	Y	Z
C	-1.601694827961	-0.052216397713	0.164107922771
C	-0.221141393964	0.620436259697	-0.100391233715
C	0.993923404722	-0.209687825453	0.366227484745
F	-1.631852666729	-0.532887397450	1.412244169877
F	-2.561384806563	0.856770290988	0.032831253865
F	-1.836210797772	-1.043026429760	-0.685871118413
F	-0.225491373104	1.770881126950	0.603965186890
F	-0.141581318460	0.910276125748	-1.405235747788
H	0.877057394346	-0.452769511656	1.419236036975
Cl	1.126274800734	-1.742439683444	-0.531904660828
Cl	2.475524584749	0.769819442093	0.200309705620

Atom	Z	Z	Z
C	-1.612914048055	0.240646558296	0.293907499745
C	-0.313529511533	-0.138168406419	-0.478388029991
C	0.959037611465	-0.181055957688	0.394511380844
F	-1.675092263248	-0.459015841686	1.432505335898
F	-1.654658818139	1.535126265808	0.579818362408
F	-2.668141300281	-0.064058176210	-0.453184300662
F	-0.173899904462	0.713050755213	-1.502539291059
F	-0.517457433987	-1.379390895496	-0.965667719085
H	0.795448917299	-0.855339898688	1.231262865165
Cl	2.311810203452	-0.834133004582	-0.567571324725
Cl	1.352872547488	1.423383601453	1.060959221463

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
36.7592	0.0262
69.7733	0.0211
138.5096	0.0889
197.5098	0.338
213.9493	0.0662
236.3127	0.160
262.8119	0.175
323.0302	0.0626
354.6306	0.178
364.5536	0.00420
437.9556	0.494
529.6048	1.26
583.4366	0.0751
611.1929	1.71
712.2595	14.4
754.8112	2.40
788.5652	9.52
828.2589	8.24
1042.3404	15.3
1159.7179	15.9
1219.9556	46.1
1227.3349	2.25
1244.2583	10.3
1259.9352	31.3
1295.5136	7.38
1346.9804	12.5
3159.1109	0.381

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
36.7585	0.0262
69.7727	0.0211
138.5088	0.0889
197.5089	0.338
213.9497	0.0662
236.3125	0.160
262.8121	0.175
323.0310	0.0626
354.6312	0.178
364.5541	0.00420
437.9557	0.494
529.6043	1.26
583.4371	0.0751
611.1932	1.71
712.2590	14.4
754.8112	2.40
788.5649	9.52
828.2601	8.24
1042.3420	15.3
1159.7166	15.9
1219.9561	46.1
1227.3351	2.25
1244.2581	10.3
1259.9355	31.3
1295.5145	7.38
1346.9836	12.5
3159.1118	0.381



$\Delta E = 1.16$ kcal mol^{-1}
Population = 0.066

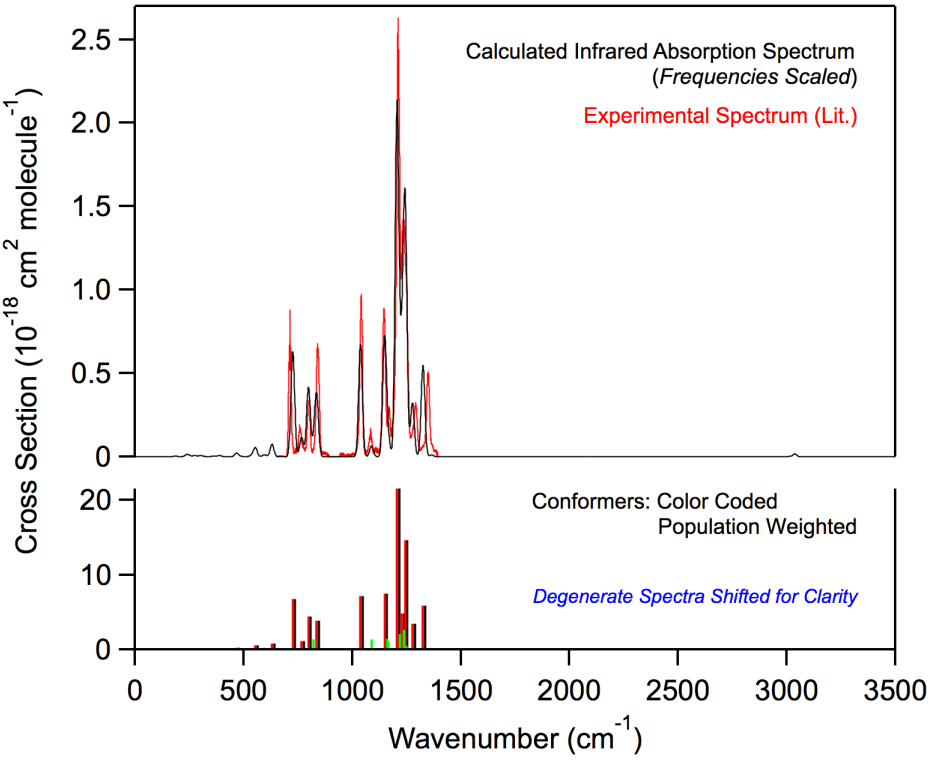
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.204872244208	0.729492898358	0.047946156205
C	0.347866632238	0.740823480699	0.130089625442
C	1.135233583854	-0.564020260671	-0.132305320500
F	-1.727439844729	-0.105417583947	0.939962253694
F	-1.639208166361	1.960853017609	0.311386542260
F	-1.619588399799	0.383204360132	-1.166113104124
F	0.672676743120	1.164805337343	1.367756320893
F	0.781515551896	1.657879830442	-0.757625301756
H	2.186186392442	-0.302516437700	-0.017827095517
Cl	0.777981083182	-1.823423698431	1.075830132642
Cl	0.925186668365	-1.156467943834	-1.799100209240

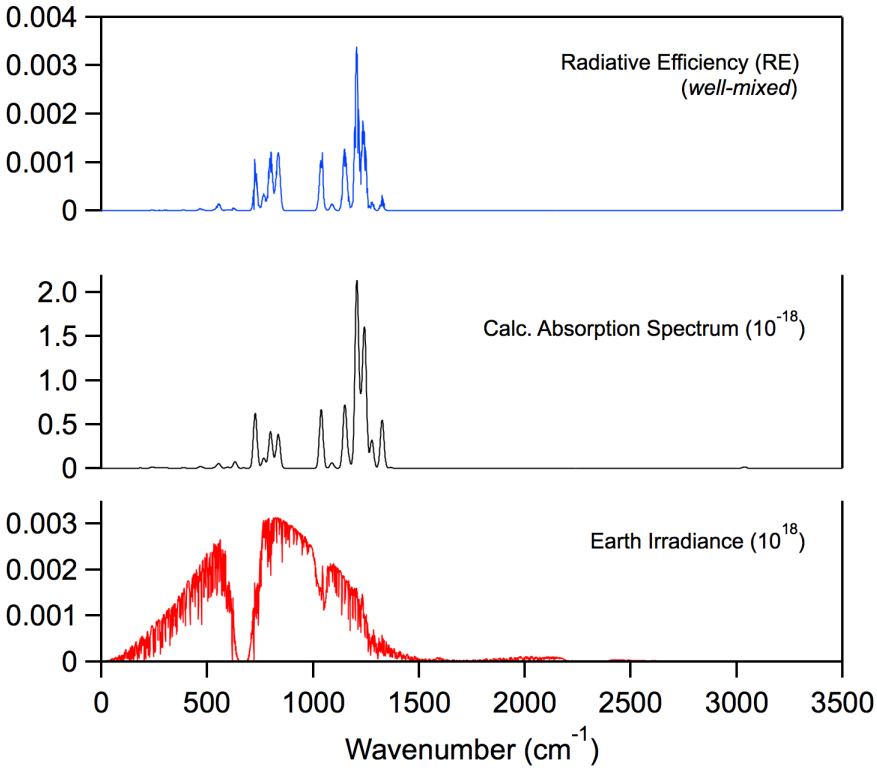
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
19.3291	0.0110
88.4948	0.0428
146.3628	0.0103
181.4033	0.138
218.0803	0.127
227.2114	0.151
285.3860	0.405
328.5844	0.0579
344.9822	0.00915
378.0982	0.133
459.5309	0.650
510.7183	2.78
572.4053	3.05
593.4618	0.00535
655.2364	1.50
756.7939	3.77
812.8101	20.1
822.3614	3.93
1096.0599	20.7
1173.3643	22.1
1179.9602	16.0
1226.6609	0.635
1234.1962	32.1
1254.1006	39.7
1265.6531	7.51
1388.8442	3.38
3133.0587	0.539

Infrared Spectrum

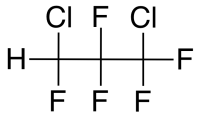


Radiative Efficiency



HCFC-225cb

Molecular Formula:	$CHClFCF_2CClF_2$
Name:	1,3-Dichloro-1,1,2,2,3-pentafluoropropane
CAS number:	507-55-1
Molecular Weight:	202.94



Global Atmospheric Lifetime (years):	5.36		5.9 #
Tropospheric Atmospheric Lifetime (years):	5.80		6.3 #
Stratospheric Atmospheric Lifetime (years):	71.2		101 #
Ozone Depletion Potential (ODP):	0.034		
	Well-mixed	*Lifetime adjusted*	
Radiative Efficiency (RE):	0.314	0.290	0.29 #
Global Warming Potential (GWP_H):			
GWP_{20}	1820	1685	1860 #
GWP_{100}	505	468	525 #
Global Temperature Potentials (GTP_H)			
GTP_{20}		959	1110 #
GTP_{50}		102	120 #
GTP_{100}		66	73 #

* RE units: W m^2 ppb^{-1}
* GWP and GTP: Relative to CO_2
# Value taken from WMO (2014)

Atmospheric Loss Processes **********

OH Reactivity

$k_{Rec}(T) = 5.5 \times 10^{-13} \exp(-1230/T)$; $k_{Rec}(272\ K) = 6.0 \times 10^{-15}$ cm^3 $molecule^{-1}$ s^{-1}

$k_{SAR}(298\ K) = 1.01 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 0.646 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 5.60$ years

$\tau^{OH}_{Trop} = 5.80$ years

$\tau^{OH}_{Strat} = 164.3$ years

Fractional Atmospheric Loss: 0.957

O(^{1}D) Reactivity

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

$k_{Est}(T) = 1.3 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 285$ years

Fractional Atmospheric Loss: 0.019

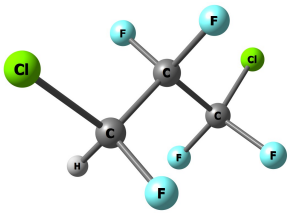
UV Photolysis

UV Spectrum: *Recommendation available*

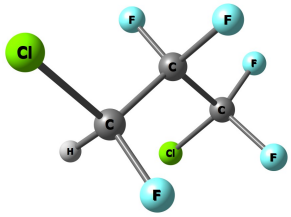
$\tau_{hv} = 225$ years

Fractional Atmospheric Loss: 0.024

Molecular Structure and Infrared Spectrum (5 conformers)



E = 0
Population = 0.571



$\Delta E = 0.72$ kcal mol^{-1}
Population = 0.169

Optimized Coordinates (Angstroms)

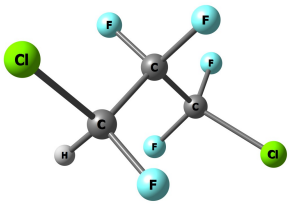
Atom	X	Y	Z
C	-1.206136152272	-0.395933398385	0.166966074684
C	0.134580816686	0.360325123021	-0.075944818554
C	1.357996084452	-0.477248141966	0.359139791375
Cl	-2.602538949609	0.674980752790	-0.129543122528
F	-1.285934682185	-1.453112899441	-0.634028001881
F	-1.232864852150	-0.817279734706	1.438228376511
F	0.117129769599	1.487834285953	0.654121133268
F	0.213191837023	0.666198264045	-1.376442166301
H	1.309615719113	-0.688276388261	1.428203319479
F	1.379834601989	-1.629070069984	-0.342151045163
Cl	2.857867807352	0.445460206935	0.060517459110

Atom	Z	Z	Z
C	-1.320191349569	0.206086596400	-0.247479559302
C	0.162414081588	0.515545755561	0.128700875987
C	1.133565116352	-0.665936013676	-0.059192146313
Cl	-1.958567350597	-1.178831520230	0.700915644509
F	-2.048883474483	1.285387057624	0.022022474560
F	-1.419853364706	-0.065182372936	-1.543538780547
F	0.185207892258	0.898955501847	1.415409615282
F	0.534707415079	1.548037630060	-0.646515016238
H	0.888334312461	-1.479402956019	0.623982129429
F	1.065634220816	-1.093073493463	-1.336795984630
Cl	2.797917500800	-0.136396185166	0.320072747261

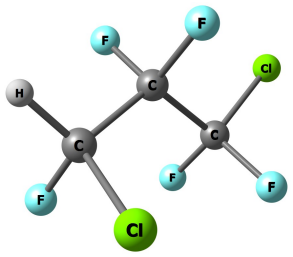
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
40.7077	0.0792
65.9495	0.0311
125.9957	0.0991
210.4220	0.533
220.4006	0.152
231.3543	0.0568
245.5012	0.0956
323.5553	0.0222
351.2802	0.0439
378.3401	0.143
427.0332	0.0402
447.3353	0.328
525.8876	0.788
600.6867	1.47
676.4534	4.97
720.8745	41.0
799.3985	3.04
927.5875	10.9
1100.2404	18.1
1134.0558	17.7
1182.9728	9.87
1212.4635	44.6
1238.8257	13.2
1276.8636	3.18
1310.1256	4.94
1372.8254	1.03
3122.4016	0.780

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
37.2198	0.0789
73.5158	0.0227
132.9885	0.106
182.0631	0.178
227.7003	0.160
237.9334	0.167
290.9598	0.118
316.2270	0.314
345.5864	0.140
368.5415	0.388
422.9897	0.218
446.5909	0.130
477.7581	1.39
616.6275	3.52
658.1696	3.50
765.6483	16.4
796.7979	14.0
940.3414	36.7
1074.7151	10.8
1131.0640	9.52
1197.3155	24.5
1218.8336	26.7
1242.0971	14.3
1278.5260	14.2
1307.0659	5.97
1374.9743	0.588
3128.9593	0.884



$\Delta E = 1.11$ kcal mol^{-1}
Population = 0.087



$\Delta E = 1.14$ kcal mol^{-1}
Population = 0.083

Optimized Coordinates (Angstroms)

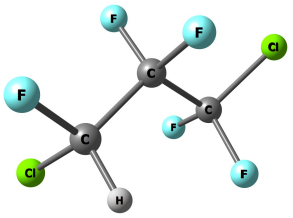
Atom	X	Y	Z
C	-1.308560925129	0.319456877180	0.187151594490
C	0.187950713919	0.496642854137	-0.228318148026
C	1.160772285963	-0.424797124521	0.534939294616
Cl	-2.036565456397	-1.181578862341	-0.436154406018
F	-1.376739940702	0.326307780822	1.525408506700
F	-1.997472817187	1.358695952609	-0.276179453179
F	0.503231998251	1.772268500376	0.074144904648
F	0.295644712584	0.320301793569	-1.549539167948
H	1.084660298457	-0.245235114281	1.608112642547
F	0.877448591360	-1.713044208965	0.257744575338
Cl	2.840298538881	-0.057577448586	0.046488656832

Atom	Z	Z	Z
C	-0.899099204105	0.332620337643	-0.406178169418
C	0.021137090463	-0.549665895976	0.486088345152
C	1.513834785585	-0.631055663459	0.081843072345
Cl	-2.586359537851	0.253076482252	0.192107439061
F	-0.489467874048	1.597731491418	-0.379071060508
F	-0.860629535625	-0.107361827511	-1.661201336402
F	-0.447132805289	-1.813624530788	0.426738160855
F	-0.054542932214	-0.117393726302	1.753175975277
H	1.982538238452	-1.371593908680	0.735173424081
F	1.612585892871	-1.025491929907	-1.202428703500
Cl	2.387647881763	0.906749171312	0.323397853057

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
34.5189	0.0904
68.1456	0.0313
135.6899	0.0764
185.9903	0.142
221.4390	0.393
233.6594	0.129
290.4434	0.187
315.3821	0.247
340.1913	0.165
394.4321	0.260
430.1284	0.161
433.1062	0.470
495.9957	0.285
616.3257	3.29
640.0515	4.05
779.4241	30.1
796.7867	4.31
941.3637	21.7
1079.6318	20.4
1140.8936	23.3
1167.1581	10.1
1197.1275	26.6
1247.9241	23.8
1279.3477	7.27
1306.6984	2.98
1377.3279	0.941
3122.7996	0.746

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
21.5304	0.0189
86.5753	0.0920
148.0672	0.0459
181.4263	0.136
217.7239	0.262
219.6416	0.0427
305.0401	0.0900
322.6676	0.0150
357.8614	0.0514
391.2233	0.168
421.3041	0.0771
447.5387	0.124
547.6725	4.13
556.5958	10.9
611.3000	4.14
695.3044	0.869
829.5206	21.9
938.8346	22.6
1122.6776	13.8
1150.4289	30.3
1179.3295	11.9
1213.9723	2.08
1223.6474	49.1
1251.2033	1.70
1313.6224	3.76
1389.5834	2.13
3094.3195	1.19



$\Delta E = 1.30$ kcal mol^{-1}
Population = 0.064

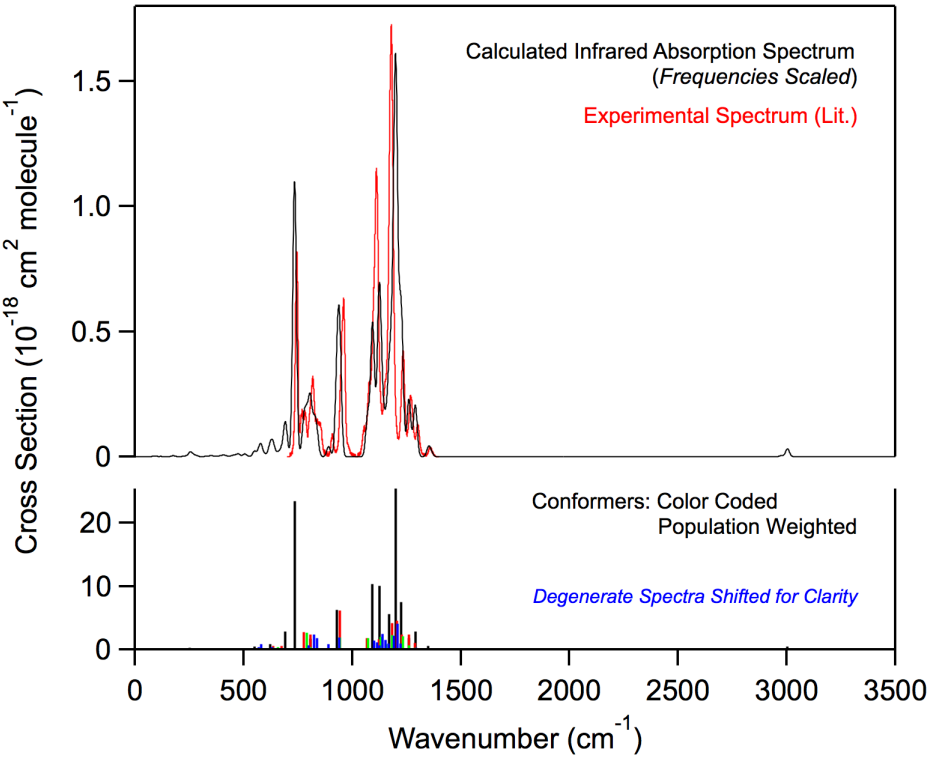
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.010303592312	0.448688478161	0.248452256849
C	0.071199270850	-0.607691456871	-0.116657071783
C	1.467388838547	-0.334009806598	0.496496825161
Cl	-2.635582233550	-0.122482450084	-0.219903262013
F	-0.975165576185	0.650765054331	1.572413609397
F	-0.762975793292	1.601116946207	-0.364357366735
F	0.152593360655	-0.705339430875	-1.448312966499
F	-0.326774839529	-1.793751063394	0.386426185063
H	1.384894556189	-0.193329029366	1.574929420872
F	2.233091426198	-1.410537534003	0.227788665684
Cl	2.235060582431	1.126012292492	-0.185789295996

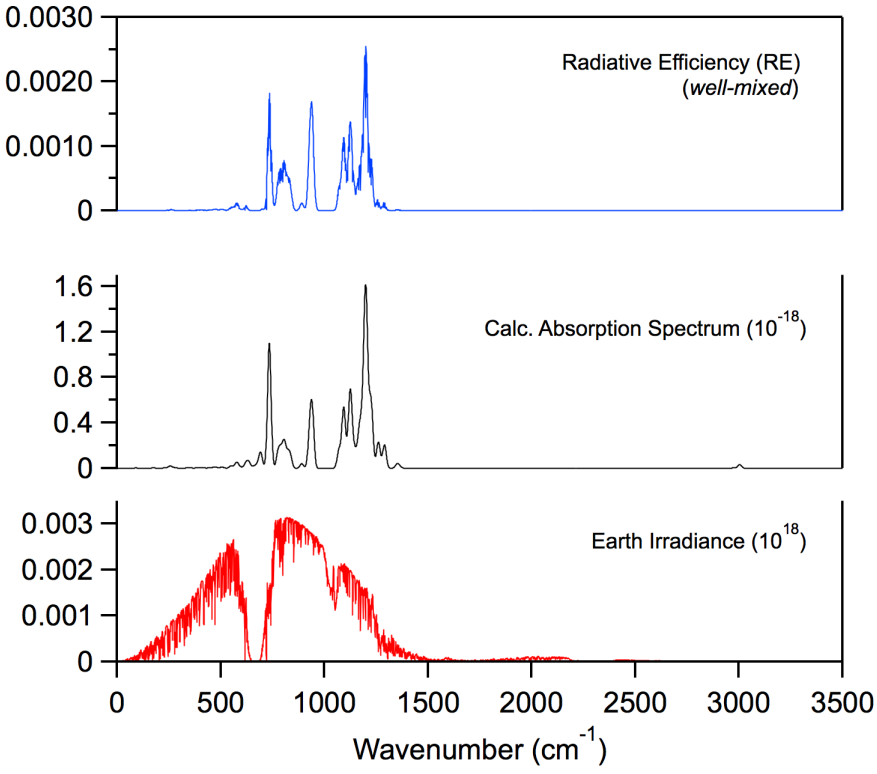
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
33.3073	0.0423
74.0610	0.0410
133.6127	0.160
188.6229	0.267
217.1155	0.238
235.9844	0.0658
300.3325	0.331
317.1565	0.0443
352.9893	0.120
375.5420	0.213
413.3101	0.756
429.4851	0.247
522.5795	0.286
576.2154	3.01
668.7773	1.78
788.0208	10.1
816.7440	37.7
886.6288	13.5
1108.6219	21.7
1134.3333	10.5
1164.2274	23.2
1205.3576	34.3
1237.1959	15.5
1290.0669	2.69
1297.4644	1.89
1383.1804	3.04
3122.6486	0.774

Infrared Spectrum

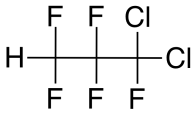


Radiative Efficiency



HCFC-225cc

Molecular Formula:	$CHF_2CF_2CCl_2F$
Name:	1,1-Dichloro-1,2,2,3,3-pentafluoropropane
CAS number:	13474-88-9
Molecular Weight:	202.94



Global Atmospheric Lifetime (years):	14.1
Tropospheric Atmospheric Lifetime (years):	19.0
Stratospheric Atmospheric Lifetime (years):	55.2
Ozone Depletion Potential (ODP):	0.110

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.356	0.344
Global Warming Potential (GWP_H):		
GWP_{20}	4231	4081
GWP_{100}	1512	1458
Global Temperature Potentials (GTP_H)		
GTP_{20}		3412
GTP_{50}		840
GTP_{100}		232

* RE units: W m^2 ppb^{-1}
* GWP and GTP: Relative to CO_2

Atmospheric Loss Processes **********

OH Reactivity

k_{Rec}(T), *No recommendation*

$k_{SAR}(298\ K) = 3.09 \times 10^{-15}$; $k_{SAR}(272\ K) \approx 1.97 \times 10^{-15}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 18.3$ years

$\tau^{OH}_{Trop} = 19.0$ years

$\tau^{OH}_{Strat} = 478.6$ years

Fractional Atmospheric Loss: 0.774

$O(^1D)$ Reactivity

k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 1.3 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 285$ years

Fractional Atmospheric Loss: 0.050

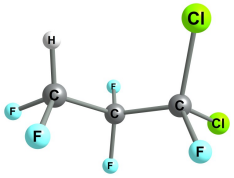
UV Photolysis

UV Spectrum: *No Recommendation*

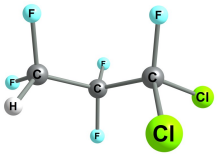
$\tau_{hv} = 80$ years

Fractional Atmospheric Loss: 0.176

Molecular Structure and Infrared Spectrum (9 conformers)



E = 0
Population = 0.231



E = 0
Population = 0.231

Optimized Coordinates (Angstroms)

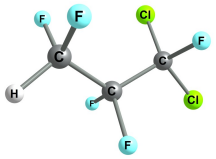
Atom	X	Y	Z
C	-1.755384461300	0.436385675700	-0.162220045300
C	-0.515207793900	-0.489434101700	-0.220751791600
C	0.815490249700	0.157637448700	0.266715191400
F	-0.747801683500	-1.561855420000	0.553636594400
F	-0.366037160100	-0.889096231000	-1.494691450400
H	-1.662768589700	1.278517611200	-0.854260405400
F	-2.820813781800	-0.311780917500	-0.502556728600
F	-1.922840668100	0.890135277500	1.093421093700
Cl	2.146821953300	-1.016112232300	0.093536651400
Cl	1.165543320000	1.637518576300	-0.682226286500
F	0.692605615300	0.487248313300	1.552429176800

Atom	X	Y	Z
C	-1.741006443400	0.468217147600	0.062788049600
C	-0.502639746200	-0.440966901700	0.258843683700
C	0.827943554600	0.120535882400	-0.325409178500
F	-0.350433689200	-0.641543196500	1.578504330800
F	-0.739892545200	-1.618570734600	-0.341840325900
H	-1.644469669400	1.406013458000	0.617679944800
F	-1.911330290100	0.725089352300	-1.247010760300
F	-2.806986383300	-0.216366886900	0.516382970500
Cl	1.184060708900	1.727192296400	0.385188439900
Cl	2.157288133200	-1.016364322900	0.021591593100
F	0.701832370000	0.250038905800	-1.646060747700

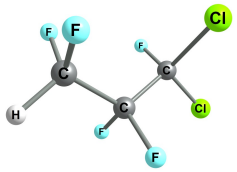
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
36.9336	0.114
80.3472	0.0595
139.2201	0.134
191.1008	0.140
209.3542	0.118
255.6200	0.137
271.8040	0.248
297.2157	0.118
329.9615	0.413
364.3913	0.114
390.7306	0.268
450.8677	0.734
513.5688	0.651
562.4508	3.85
649.6231	1.74
779.1509	24.4
827.0023	21.3
904.4456	22.4
1120.3784	2.92
1157.0368	13.1
1165.9685	12.8
1198.3637	41.5
1217.8062	5.38
1268.9515	16.4
1398.3985	2.58
1410.6823	3.15
3094.8569	3.07

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
36.9330	0.114
80.3461	0.0595
139.2200	0.134
191.1004	0.140
209.3533	0.118
255.6191	0.137
271.8038	0.248
297.2151	0.118
329.9605	0.413
364.3908	0.114
390.7281	0.268
450.8662	0.734
513.5688	0.651
562.4517	3.85
649.6237	1.74
779.1521	24.4
826.9995	21.3
904.4411	22.4
1120.3829	2.92
1157.0423	13.1
1165.9686	12.8
1198.3684	41.5
1217.8080	5.38
1268.9551	16.4
1398.4005	2.58
1410.6851	3.15
3094.8465	3.07



$\Delta E = 0.38$ kcal mol^{-1}
Population = 0.123



$\Delta E = 0.38$ kcal mol^{-1}
Population = 0.123

Optimized Coordinates (Angstroms)

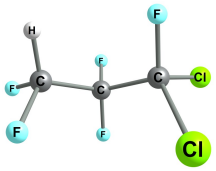
Atom	X	Y	Z
C	-1.876435595900	-0.296391661100	-0.065410203300
C	-0.404940997400	-0.696259660100	-0.341119284500
C	0.710092075300	0.164592341500	0.326574068400
F	-0.267442092500	-1.955159234000	0.126393347700
F	-0.227484180200	-0.705075016600	-1.670863537600
H	-2.515213695300	-1.107405925200	-0.438646195200
F	-2.075842344000	-0.137808564800	1.255065595200
F	-2.188030810800	0.845306785200	-0.699920232100
Cl	2.305397602600	-0.531391129300	-0.091754008400
Cl	0.625294347500	1.863281574900	-0.203787475500
F	0.553832690700	0.108725489500	1.651020925200

Atom	X	Y	Z
C	-1.884168401600	-0.143396767700	0.201254931600
C	-0.427473746500	-0.616253254500	0.437158553900
C	0.698504981700	0.096102585800	-0.372099866400
F	-0.171742433200	-0.508620002300	1.749715909500
F	-0.399139712400	-1.921011422400	0.092041665900
H	-2.550135698700	-0.867964941800	0.687644752000
F	-2.083453602600	1.073302518500	0.733323365600
F	-2.151626814500	-0.099919219300	-1.115994978400
Cl	0.754620569800	1.839918867900	-0.011581144400
Cl	2.268083175600	-0.665585453200	0.028691807000
F	0.460047682600	-0.076696911000	-1.674014996400

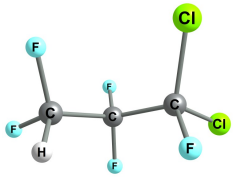
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
24.2648	0.0555
94.6789	0.189
151.0856	0.0253
195.8529	0.0478
210.9167	0.162
219.1927	0.186
273.9741	0.104
308.1460	0.100
356.7955	0.0202
378.6885	0.155
387.2475	0.0871
486.3341	0.199
530.1507	3.17
567.2188	5.95
596.5862	11.1
673.5783	4.07
860.9839	31.1
922.6837	7.34
1136.1350	2.86
1156.0180	24.9
1171.7964	9.58
1200.1995	44.9
1225.2448	4.73
1247.4898	8.01
1392.3505	2.31
1415.8192	7.12
3053.7043	4.41

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
24.2644	0.0555
94.6789	0.189
151.0847	0.0253
195.8524	0.0478
210.9161	0.162
219.1930	0.186
273.9744	0.104
308.1461	0.100
356.7957	0.0202
378.6892	0.155
387.2480	0.0871
486.3349	0.199
530.1514	3.17
567.2191	5.95
596.5859	11.1
673.5790	4.07
860.9869	31.1
922.6846	7.34
1136.1287	2.86
1156.0161	24.9
1171.7964	9.58
1200.1973	44.9
1225.2428	4.73
1247.4914	8.00
1392.3507	2.31
1415.8202	7.12
3053.7049	4.41



$\Delta E = 0.43$ kcal mol^{-1}
Population = 0.112



$\Delta E = 0.43$ kcal mol^{-1}
Population = 0.112

Optimized Coordinates (Angstroms)

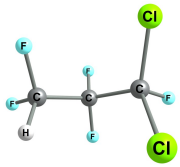
Atom	X	Y	Z
C	-1.782354833900	0.118533416000	-0.430473445700
C	-0.508254675500	-0.548641883300	0.147486106400
C	0.829128970700	0.101146863000	-0.321549719100
F	-0.564193961500	-0.556347053600	1.483543282700
F	-0.514376203900	-1.820212142400	-0.302045322800
H	-1.745717160400	0.152742241100	-1.524132370900
F	-2.831178822200	-0.625764378000	-0.034546916200
F	-1.925476286400	1.360678628200	0.063058243300
Cl	1.053287983700	1.726891838600	0.364160184600
Cl	2.198651422200	-0.948998893400	0.128122247100
F	0.774040567200	0.195387363800	-1.662097289400

Atom	X	Y	Z
C	-1.763301492100	0.165779413200	0.429164580000
C	-0.504462291100	-0.517476077400	-0.163269972600
C	0.846747837200	0.105429691600	0.302599966300
F	-0.529113391600	-1.792789000100	0.274873354200
F	-0.569270692000	-0.512108809000	-1.498940120800
H	-1.718931513300	0.189456565900	1.522815684400
F	-1.888657104600	1.414575052900	-0.052263926600
F	-2.827116011000	-0.557148917400	0.033632282900
Cl	2.195364828600	-0.963487062600	-0.165639428000
Cl	1.093837781800	1.733331611000	-0.369976945000
F	0.802039048200	0.188401532100	1.644281525200

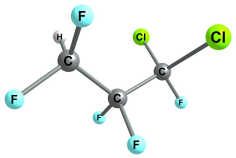
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
31.1055	0.125
74.8875	0.0726
144.8140	0.0858
189.6615	0.144
220.0834	0.138
239.3863	0.426
266.2598	0.179
297.0566	0.162
323.9831	0.208
379.2412	0.0333
396.3520	0.0798
450.9253	0.537
529.2139	0.475
569.7692	4.11
625.1908	1.88
791.4541	31.1
846.9296	15.7
895.2811	17.3
1111.7063	19.9
1139.9658	6.99
1167.7409	18.5
1180.3620	12.3
1208.9251	20.6
1285.6987	15.6
1399.5862	2.37
1413.5720	3.38
3085.3847	3.16

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
31.1036	0.125
74.8877	0.0726
144.8137	0.0858
189.6609	0.144
220.0835	0.138
239.3870	0.426
266.2599	0.179
297.0569	0.162
323.9833	0.208
379.2424	0.0333
396.3521	0.0798
450.9266	0.537
529.2145	0.475
569.7689	4.11
625.1902	1.88
791.4548	31.1
846.9310	15.7
895.2844	17.4
1111.6975	19.9
1139.9649	6.99
1167.7437	18.5
1180.3622	12.3
1208.9261	20.6
1285.6921	15.6
1399.5869	2.37
1413.5708	3.38
3085.3863	3.16



$\Delta E = 1.28$ kcal mol^{-1}
Population = 0.027



$\Delta E = 1.28$ kcal mol^{-1}
Population = 0.027

Optimized Coordinates (Angstroms)

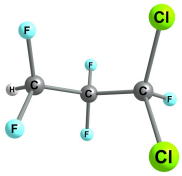
Atom	X	Y	Z
C	-1.533347214200	-0.035808537300	-0.708547417000
C	-0.580684372300	0.321005429700	0.454383962800
C	0.944568295400	0.060597477000	0.241802807000
F	-0.716688875600	1.642366884100	0.686366453400
F	-0.958104140700	-0.346682145700	1.556060074600
H	-1.303899549700	0.543800595300	-1.607751098000
F	-1.461743395100	-1.351017858000	-0.981379546400
F	-2.780299637100	0.252947093500	-0.290771863400
Cl	1.324666003800	-1.674459099300	0.173843510400
Cl	1.506271239500	0.890885528300	-1.245288137400
F	1.577795645900	0.595755632500	1.289342253900

Atom	X	Y	Z
C	-1.551820654700	0.061390919100	-0.710872752500
C	-0.603418897900	-0.381688468600	0.425568419600
C	0.924871962200	-0.126722734000	0.228879419100
F	-0.972434367200	0.217738387300	1.568574516900
F	-0.755589253600	-1.713557251900	0.571516374800
H	-1.329647237300	-0.461480122600	-1.645971880600
F	-2.802149232300	-0.238558338000	-0.311486257500
F	-1.464127902700	1.390543041500	-0.897968674900
Cl	1.476121745600	-0.865645412500	-1.309411110500
Cl	1.326179196800	1.604337086800	0.273153428000
F	1.551631641100	-0.736334107200	1.238957517500

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
31.4476	0.129
80.5094	0.0591
146.7662	0.0666
176.2886	0.124
220.7753	0.168
247.5805	0.185
285.2247	0.302
298.9979	0.184
329.2855	0.266
366.6126	0.155
390.7554	0.288
450.1012	0.986
490.1190	1.30
575.9743	1.31
619.9520	2.01
797.9285	11.3
860.9410	40.5
918.5712	15.3
1080.3530	20.2
1160.2787	8.05
1168.4951	19.4
1176.8484	11.3
1213.2763	23.6
1274.8593	14.4
1398.6801	1.70
1416.2106	1.74
3092.7350	2.99

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
31.4511	0.129
80.5130	0.0591
146.7683	0.0666
176.2939	0.124
220.7786	0.168
247.5842	0.185
285.2278	0.302
299.0031	0.184
329.2862	0.266
366.6148	0.155
390.7617	0.287
450.0976	0.986
490.1217	1.30
575.9741	1.31
619.9457	2.00
797.9372	11.3
860.9456	40.5
918.5748	15.3
1080.3619	20.2
1160.2779	8.05
1168.4970	19.4
1176.8322	11.4
1213.2824	23.6
1274.8583	14.4
1398.6845	1.70
1416.2156	1.74
3092.7120	2.99



$\Delta E = 1.61$ kcal mol^{-1}
Population = 0.015

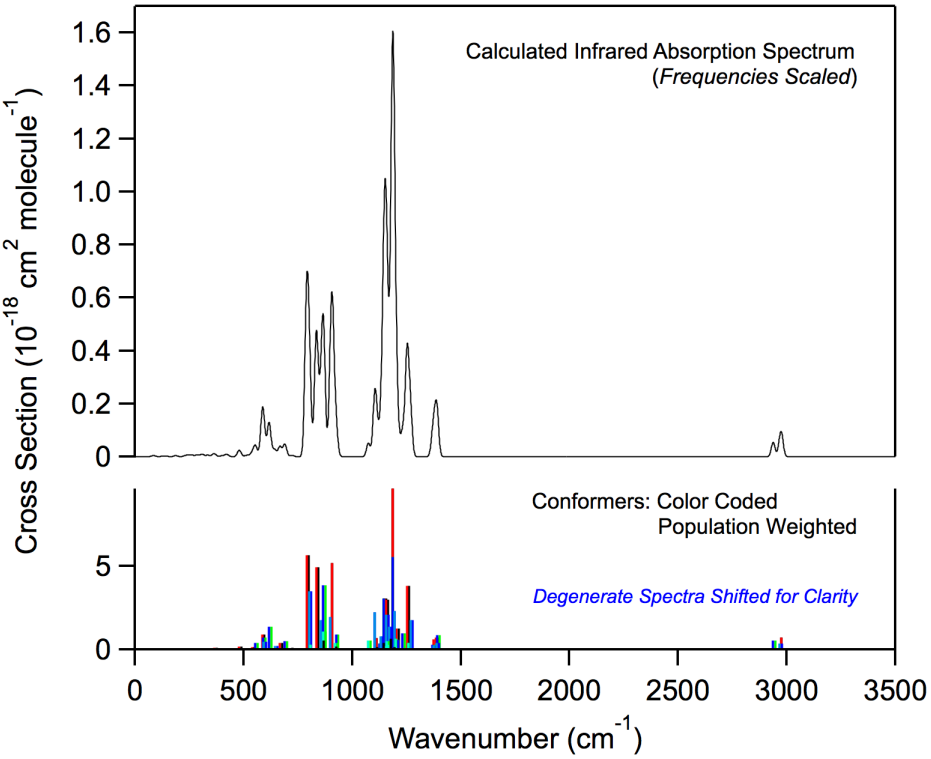
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.771001251100	0.226303152900	-0.230236471500
C	-0.580768615200	0.088287918700	0.745206744200
C	0.869757534400	-0.108446671900	0.199216478000
F	-0.569264340400	1.200639860700	1.506928052900
F	-0.849597022100	-0.965107849800	1.542552292200
H	-2.675888438500	0.353451400700	0.378517221100
F	-1.614253227900	1.296943648900	-1.026845868700
F	-1.895285312500	-0.874175911200	-0.991111507300
Cl	1.019337741900	-1.622426538400	-0.728414737100
Cl	1.395895205600	1.286778375100	-0.776255500300
F	1.661188726000	-0.193173385700	1.276420296600

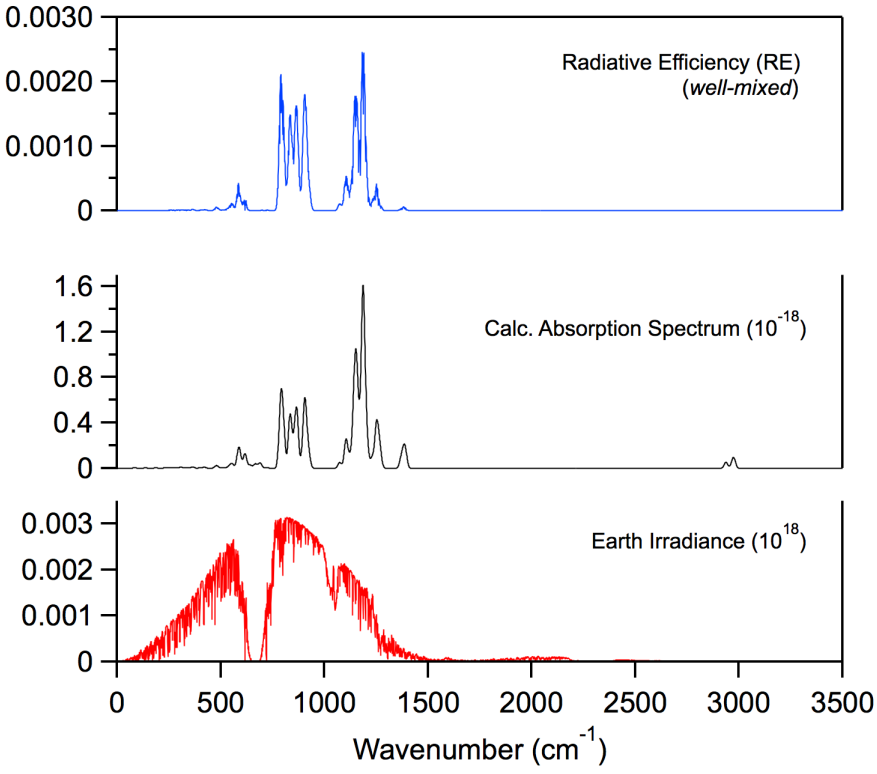
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
20.2012	0.0682
101.6554	0.153
154.6496	0.0990
177.5995	0.0232
213.7323	0.114
228.6021	0.129
296.9270	0.397
324.7791	0.360
325.6067	0.247
366.2521	0.165
389.8782	0.0961
465.6930	1.96
518.0931	0.549
559.9762	1.83
618.1377	5.91
709.8014	7.51
862.8324	36.1
922.7305	12.2
1123.5472	9.03
1155.9557	26.1
1167.8976	2.56
1188.9863	42.2
1208.0298	10.2
1260.5265	5.67
1392.8885	2.16
1424.1947	2.94
3051.8039	4.65

Infrared Spectrum

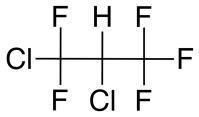


Radiative Efficiency



HCFC-225da

Molecular Formula:	$CClF_2CHClCF_3$
Name:	1,2-Dichloro-1,1,3,3,3-Pentafluoropropane
CAS number:	431-86-7
Molecular Weight:	202.94



Global Atmospheric Lifetime (years):	16.3
Tropospheric Atmospheric Lifetime (years):	19.5
Stratospheric Atmospheric Lifetime (years):	100.0
Ozone Depletion Potential (ODP):	0.071

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.312	0.302
Global Warming Potential (GWP_H):		
GWP_{20}	3986	3858
GWP_{100}	1525	1476
Global Temperature Potentials (GTP_H)		
GTP_{20}		3342
GTP_{50}		980
GTP_{100}		256

* RE units: W m^2 ppb^{-1}
* GWP and GTP: Relative to CO_2

Atmospheric Loss Processes **********

OH Reactivity

k_{Rec}(T), *No recommendation*

$k_{SAR}(298\ K) = 3.01 \times 10^{-15}$; $k_{SAR}(272\ K) \approx 1.92 \times 10^{-15}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 18.8$ years

$\tau^{OH}_{Trop} = 19.5$ years

$\tau^{OH}_{Strat} = 490.1$ years

Fractional Atmospheric Loss: 0.870

$O(^1D)$ Reactivity

k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 1.3 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 285$ years

Fractional Atmospheric Loss: 0.057

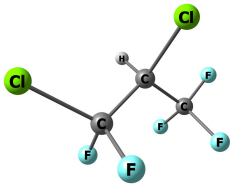
UV Photolysis

UV Spectrum: *No Recommendation*

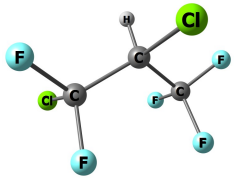
$\tau_{hv} = 225$ years

Fractional Atmospheric Loss: 0.073

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.469



$\Delta E = 0.17$ kcal mol^{-1}
Population = 0.353

Optimized Coordinates (Angstroms)

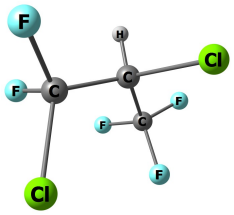
Atom	X	Y	Z
C	-0.986628830400	-0.497960440100	0.157676586800
C	0.179608729800	0.304952763200	-0.460779524900
C	1.563360469500	-0.297121470800	-0.125274017900
H	0.069846390700	0.289872862600	-1.544872609800
Cl	0.122649767000	2.002008500400	0.081477891900
Cl	-2.570196740100	0.085623647100	-0.464130330000
F	-0.865380978000	-1.787361510200	-0.175984101100
F	-0.986550912500	-0.409043678700	1.484108805600
F	2.527582219800	0.478058366100	-0.620328806900
F	1.748783107100	-0.419769164200	1.186754551200
F	1.683640777000	-1.504508875400	-0.685338445000

Atom	X	Y	Z
C	-1.130395433300	0.396525424500	0.025150901100
C	0.305735274100	0.332520795200	-0.538828918800
C	1.192811731000	-0.792584648200	0.036234061300
H	0.245366952200	0.197459388700	-1.618287685800
Cl	1.114200677700	1.902434335200	-0.231445590900
Cl	-2.112539953700	-1.014075364700	-0.514881083700
F	-1.127695876100	0.433120460400	1.355501891100
F	-1.734934243300	1.495886709000	-0.426460667100
F	2.395844176400	-0.740567238500	-0.538015223900
F	1.346679486100	-0.681973644800	1.352100565200
F	0.669312209000	-1.992416216900	-0.227277248400

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
36.0118	0.00159
75.1099	0.00327
157.1949	0.115
192.5648	0.0890
207.1897	0.232
246.9505	0.0460
299.4139	0.00817
308.7977	0.101
366.2220	0.0441
421.9157	0.150
427.8970	0.195
531.8925	0.614
548.4743	1.01
613.0599	1.27
668.7260	12.9
821.3550	2.83
826.4628	13.0
894.5435	7.24
972.9483	22.0
1146.5918	2.01
1172.4198	31.1
1209.4894	11.0
1241.7650	28.9
1271.5715	43.8
1282.4694	26.2
1352.3905	15.0
3134.6565	0.507

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
27.7428	0.00179
82.7224	0.00096
161.6584	0.0783
195.1769	0.185
206.7552	0.133
251.3091	0.235
296.1516	0.0100
323.5308	0.0466
359.4589	0.106
402.4200	0.226
424.2862	0.196
529.3991	0.746
550.0929	0.730
610.5838	2.37
707.9693	4.39
793.7562	28.1
820.0775	1.90
894.8701	3.18
962.5385	15.5
1134.6565	24.9
1180.3268	17.6
1221.2966	15.1
1239.0270	27.4
1268.1730	9.15
1288.7352	41.3
1356.7789	15.3
3137.5234	0.509



$\Delta E = 0.57$ kcal mol^{-1}
Population = 0.178

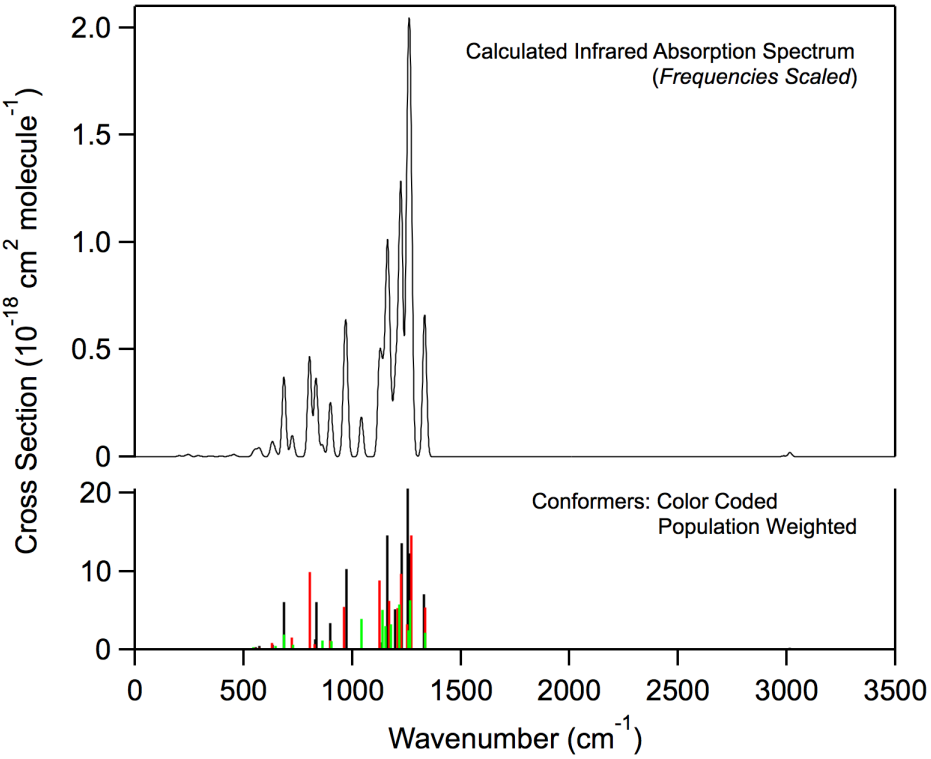
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.114932008300	-0.290099237800	-0.491422912800
C	0.282913630200	0.360282107400	-0.586663860900
C	1.430806011900	-0.411352269400	0.093581414800
H	0.514756614900	0.391597423700	-1.653772759900
Cl	0.249415332900	2.040871655100	0.002720779800
Cl	-1.720114957100	-0.505659010600	1.177617825300
F	-1.983567688400	0.469929949000	-1.162529766800
F	-1.073288244700	-1.486193687100	-1.089649001600
F	2.593603181700	0.147726919500	-0.249912162700
F	1.341063544300	-0.406530137000	1.418802431500
F	1.443904582600	-1.680084712900	-0.325470986700

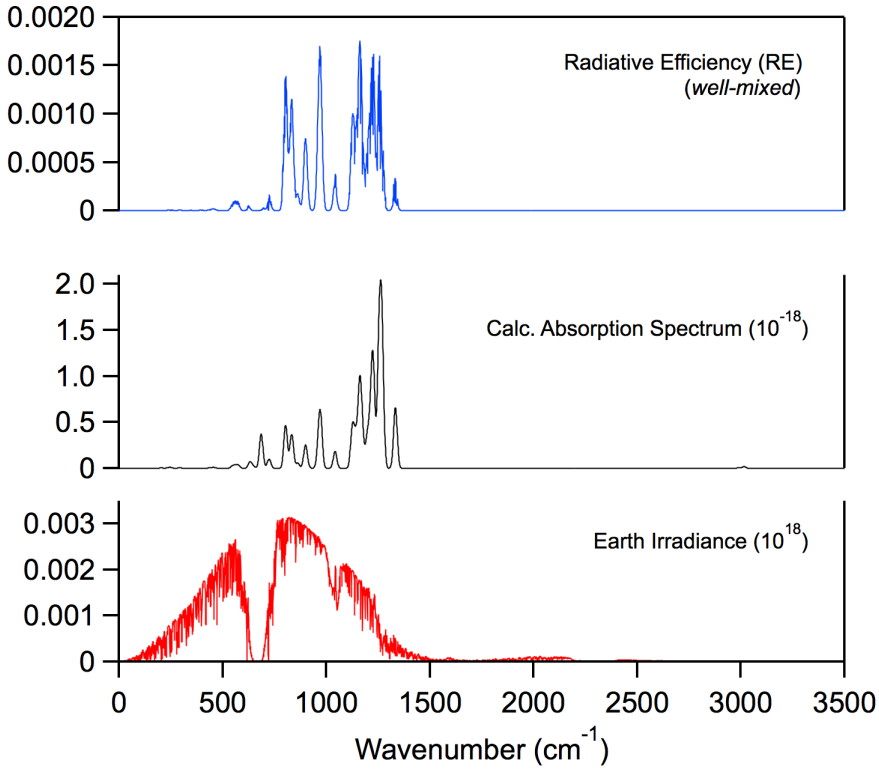
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
34.6160	0.000
84.2923	0.00794
156.8889	0.136
181.9332	0.0953
198.6582	0.0780
266.0759	0.162
297.3439	0.0229
321.3888	0.0697
363.7274	0.0678
424.1383	0.00814
443.3792	0.120
519.4693	1.66
554.1145	0.645
627.4254	2.67
670.7096	10.6
713.2053	3.57
855.8258	6.57
901.4809	6.14
1046.5747	22.1
1150.6832	28.3
1162.6609	16.9
1188.9934	17.9
1231.2042	32.2
1275.2661	13.8
1283.3268	35.5
1357.8857	12.2
3105.2643	0.505

Infrared Spectrum

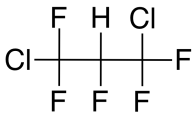


Radiative Efficiency



HCFC-225ea

Molecular Formula:	$CClF_2CHFCClF_2$
Name:	1,3-Dichloro-1,1,2,3,3-pentafluoropropane
CAS number:	136013-79-1
Molecular Weight:	202.94



Global Atmospheric Lifetime (years):	15.3
Tropospheric Atmospheric Lifetime (years):	18.1
Stratospheric Atmospheric Lifetime (years):	98.7
Ozone Depletion Potential (ODP):	0.068

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.352	0.340
Global Warming Potential (GWP_H):		
GWP_{20}	4357	4211
GWP_{100}	1616	1562
Global Temperature Potentials (GTP_H)		
GTP_{20}		3594
GTP_{50}		977
GTP_{100}		260

* RE units: W m^2 ppb^{-1}
* GWP and GTP: Relative to CO_2

Atmospheric Loss Processes **********

OH Reactivity

k_{Rec}(T), *No recommendation*

$k_{SAR}(298\ K) = 3.23 \times 10^{-15}$; $k_{SAR}(272\ K) \approx 2.06 \times 10^{-15}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 17.4$ years

$\tau^{OH}_{Trop} = 18.1$ years

$\tau^{OH}_{Strat} = 459.1$ years

Fractional Atmospheric Loss: 0.878

O(^{1}D) Reactivity

k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 1.3 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 285$ years

Fractional Atmospheric Loss: 0.054

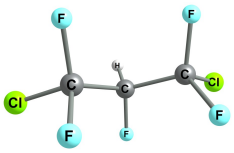
UV Photolysis

UV Spectrum: *No Recommendation*

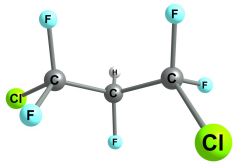
$\tau_{hv} = 225$ years

Fractional Atmospheric Loss: 0.068

Molecular Structure and Infrared Spectrum (7 conformers)



E = 0
Population = 0.475



$\Delta E = 0.72$ kcal mol^{-1}
Population = 0.140

Optimized Coordinates (Angstroms)

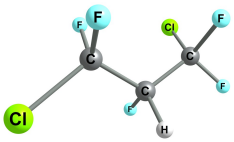
Atom	X	Y	Z
C	1.288032697700	0.344958161400	-0.006463522600
C	0.005559211300	-0.456567891300	-0.322674099800
C	-1.288342271300	0.340446202700	-0.043813063700
F	-0.003848947200	-1.566896799000	0.459694922600
H	0.021384253400	-0.729841378000	-1.381277054300
F	1.323988027500	0.713407603800	1.271663311100
F	1.342628259100	1.438356508000	-0.769883999600
Cl	2.731109447400	-0.670650630600	-0.352462863100
F	-1.362645287600	0.708675084900	1.232717299200
F	-1.324573309700	1.433710046800	-0.808531580400
Cl	-2.717209080800	-0.680160908700	-0.431512349400

Atom	X	Y	Z
C	1.387337159300	-0.089507641400	-0.461535987100
C	-0.058781286800	-0.636957892400	-0.417311689800
C	-1.153801454300	0.403322588800	-0.108736325000
F	-0.110546404600	-1.630030840100	0.506133599300
H	-0.260470462000	-1.041743060900	-1.415803458200
F	1.458532555500	0.947406827300	-1.299349869100
F	2.169961790700	-1.064611894900	-0.937754127000
Cl	2.012107113500	0.397192548200	1.140166255300
F	-0.970479103400	0.986281605100	1.072391578000
F	-1.159009745700	1.344682998900	-1.054753372600
Cl	-2.759224162300	-0.409601238500	-0.099689603800

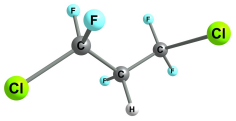
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
22.8954	0.000
81.6438	0.0109
133.2059	0.130
212.9746	0.161
218.5641	0.363
231.4767	0.146
263.7867	0.0466
316.1998	0.0566
363.8985	0.140
410.4575	0.000
423.7303	0.146
433.6170	0.117
501.8891	1.36
615.6005	5.10
645.7697	1.99
708.5147	41.0
859.0261	3.71
975.4119	20.9
986.0292	19.6
1160.3088	11.7
1162.2946	0.0940
1213.1475	50.8
1239.7788	3.73
1261.1038	43.8
1357.6191	4.30
1366.4281	0.945
3098.1126	0.656

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
21.4510	0.00269
85.1503	0.0275
147.7147	0.187
185.1948	0.0942
219.2868	0.132
237.3323	0.256
287.3382	0.154
317.5908	0.118
369.9628	0.162
412.4913	0.178
419.1329	0.0247
428.8812	0.233
521.6145	1.44
619.0759	3.99
647.3714	13.7
671.6841	8.83
831.8977	20.1
948.7161	13.9
1082.2643	37.8
1155.9799	6.21
1176.9156	8.66
1189.7643	28.8
1216.5198	37.9
1263.3527	19.2
1356.3240	5.09
1372.0613	1.35
3069.4697	0.839



$\Delta E = 0.72$ kcal mol^{-1}
Population = 0.140



$\Delta E = 0.95$ kcal mol^{-1}
Population = 0.096

Optimized Coordinates (Angstroms)

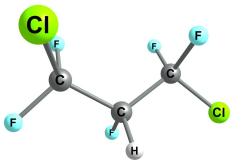
Atom	X	Y	Z
C	1.134455345300	0.360591842200	-0.220606909500
C	0.083371272400	-0.759515368400	-0.090043345300
C	-1.386181817900	-0.321816402300	-0.294367783500
F	0.190512576300	-1.334609670100	1.134464646200
H	0.290947190700	-1.499270476500	-0.871830212900
F	0.939460812300	1.334250590500	0.663977072900
F	1.086267528300	0.881454220900	-1.448410589700
Cl	2.774575227400	-0.330513117300	0.045272345200
F	-1.513652237600	0.325095882100	-1.455164952400
F	-2.130123302700	-1.432363857200	-0.352261239200
Cl	-2.012837594400	0.702892356100	1.028478968200

Atom	X	Y	Z
C	1.133437306800	0.384147058700	0.183288382700
C	0.064208514000	-0.507686430400	-0.481195896300
C	-1.370714328200	-0.351485525900	0.077164345800
F	0.419746477200	-1.805487511800	-0.258610780800
H	0.042861114600	-0.299753961600	-1.554231041900
F	1.203020510400	0.149677729900	1.491224748000
F	0.860510120500	1.674965695600	-0.006846510100
Cl	2.738678256500	0.027286987600	-0.548472312400
F	-2.119955547500	-1.319416594200	-0.456066956900
F	-1.395490544400	-0.487527150900	1.401073545900
Cl	-2.095804879900	1.229150703100	-0.368610524000

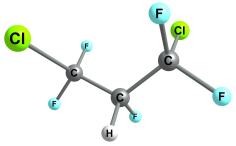
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
21.4500	0.00269
85.1503	0.0275
147.7143	0.187
185.1937	0.0942
219.2873	0.132
237.3339	0.256
287.3389	0.154
317.5912	0.118
369.9631	0.162
412.4916	0.178
419.1332	0.0247
428.8832	0.233
521.6145	1.44
619.0755	3.99
647.3721	13.7
671.6861	8.83
831.8988	20.1
948.7140	13.9
1082.2674	37.8
1155.9729	6.21
1176.9241	8.65
1189.7600	28.8
1216.5223	37.9
1263.3438	19.2
1356.3262	5.09
1372.0612	1.35
3069.4669	0.839

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
21.6904	0.00149
88.0552	0.0105
142.9386	0.115
186.1630	0.146
227.3209	0.393
256.9346	0.110
288.4744	0.0676
311.8610	0.247
366.2444	0.252
390.7237	0.360
420.4405	0.0991
424.7170	0.292
492.6616	0.914
595.7972	6.62
632.5415	1.45
796.9972	35.8
855.8683	4.55
949.0561	19.3
984.3619	29.2
1133.5420	2.33
1179.2236	36.5
1198.5742	15.9
1239.5025	11.6
1262.9333	40.5
1361.2059	5.32
1364.1796	0.512
3100.4997	0.502



$\Delta E = 0.95$ kcal mol^{-1}
Population = 0.096



$\Delta E = 1.73$ kcal mol^{-1}
Population = 0.026

Optimized Coordinates (Angstroms)

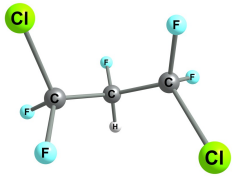
Atom	X	Y	Z
C	1.383943980100	-0.351743172700	0.007213399400
C	-0.067234519900	-0.551722964200	-0.492036198000
C	-1.113241314600	0.407207955100	0.113336850100
F	-0.421052114100	-1.819550900100	-0.134719506900
H	-0.076407898100	-0.448659209700	-1.580332809100
F	2.113631115300	-1.371626719200	-0.451024420600
F	1.446804929400	-0.359295655900	1.336823313000
Cl	2.101718773400	1.173557766600	-0.610135304700
F	-1.145553959700	0.300747041900	1.439282186200
F	-0.841070437400	1.671770521100	-0.208629334800
Cl	-2.740475554300	-0.008115662800	-0.534145174700

Atom	X	Y	Z
C	1.301797074500	-0.228815446300	0.108514239800
C	0.001252738100	-0.782532744300	-0.512835410600
C	-1.280563613100	0.070542690700	-0.394658985700
F	-0.248105060100	-1.983984897700	0.079702114600
H	0.180918642000	-0.931450490000	-1.583529303500
F	2.221856503900	-1.194638857200	0.030442621000
F	1.148910449900	0.093319369800	1.389954573700
Cl	1.912857683400	1.200639911500	-0.790003440500
F	-1.090031210800	1.287437046600	-0.905079890300
F	-2.225753310900	-0.540369436100	-1.119600752500
Cl	-1.876363897000	0.219863853100	1.284289234000

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
21.6928	0.00149
88.0560	0.0105
142.9380	0.115
186.1635	0.146
227.3217	0.393
256.9348	0.110
288.4755	0.0676
311.8625	0.247
366.2442	0.252
390.7245	0.360
420.4411	0.0991
424.7194	0.292
492.6637	0.914
595.7971	6.62
632.5413	1.45
796.9986	35.8
855.8686	4.55
949.0602	19.3
984.3620	29.2
1133.5311	2.33
1179.2215	36.5
1198.5696	15.9
1239.4988	11.6
1262.9327	40.5
1361.2068	5.32
1364.1751	0.512
3100.5012	0.502

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
15.6175	0.00178
93.0376	0.0303
148.5743	0.0825
188.4974	0.173
205.9177	0.209
267.7637	0.285
304.7860	0.220
314.7827	0.0552
362.2422	0.265
385.2864	0.547
423.0734	0.220
426.7343	0.127
508.3354	0.963
608.1424	3.65
658.0521	0.361
683.4869	16.8
858.0943	18.4
960.0242	20.0
1067.9916	32.7
1138.3171	9.09
1156.3922	28.9
1204.6542	19.1
1212.5655	26.4
1259.2833	21.1
1359.8941	4.36
1369.3301	2.21
3072.8696	0.655



$\Delta E = 1.73$ kcal mol^{-1}
Population = 0.026

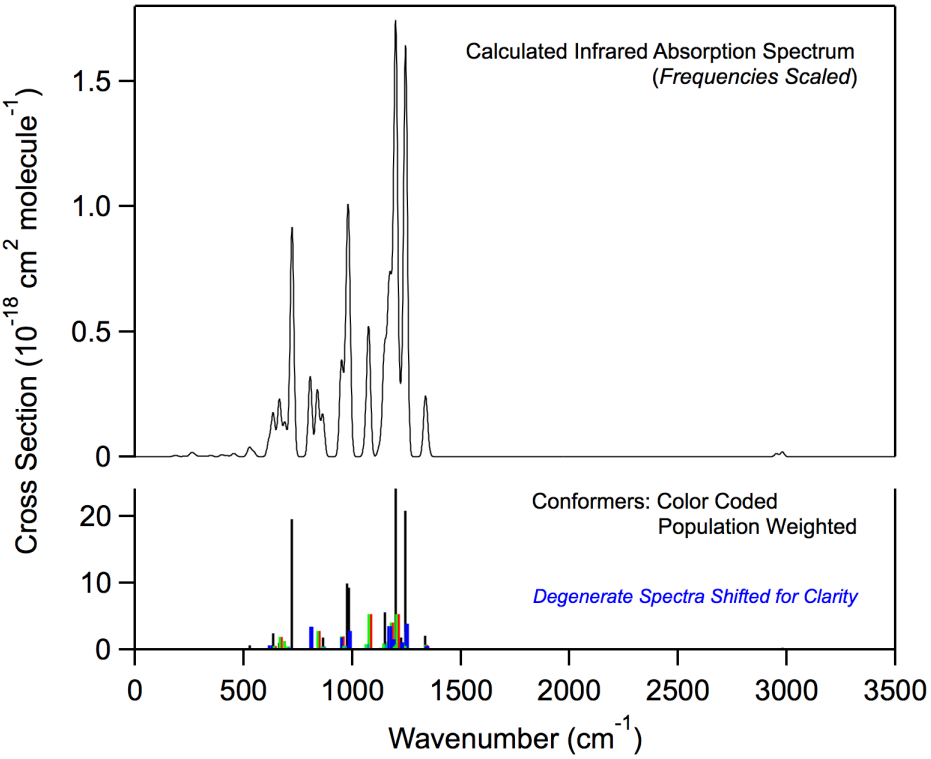
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.222485705100	0.453562692900	-0.345479265500
C	-0.001798102900	-0.381271553700	-0.780158911100
C	-1.252530479900	-0.361445818100	0.125032413900
F	0.400562110900	-1.679132714600	-0.882280248800
H	-0.299415531500	-0.010369805100	-1.767425492600
F	0.887254800600	1.731875840600	-0.168823578100
F	2.112750929000	0.391954616100	-1.343362075900
Cl	2.006012393700	-0.163074531800	1.138424917000
F	-2.105912828100	-1.269797684600	-0.356688755500
F	-0.967847336300	-0.688288376500	1.382557443900
Cl	-2.066056660500	1.239080334900	0.101478552700

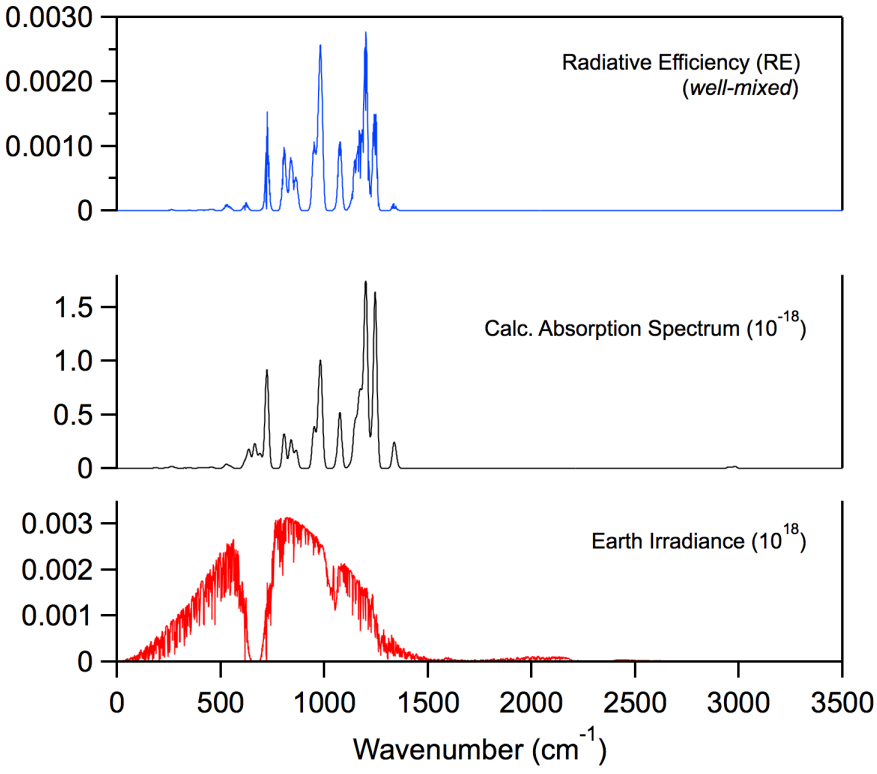
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
15.6151	0.00178
93.0391	0.0303
148.5793	0.0825
188.4988	0.173
205.9166	0.209
267.7649	0.285
304.7845	0.220
314.7802	0.0552
362.2437	0.265
385.2878	0.547
423.0744	0.220
426.7354	0.127
508.3349	0.963
608.1418	3.65
658.0516	0.361
683.4878	16.8
858.0957	18.4
960.0203	20.0
1067.9913	32.7
1138.3180	9.09
1156.3890	28.9
1204.6542	19.1
1212.5569	26.4
1259.2793	21.1
1359.8892	4.36
1369.3307	2.21
3072.8787	0.655

Infrared Spectrum

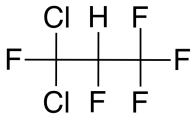


Radiative Efficiency



HCFC-225eb

Molecular Formula:	$CCl_2FCHFCF_3$
Name:	1,1-Dichloro-1,2,3,3,3-pentafluoropropane
CAS number:	111512-56-2
Molecular Weight:	202.94



Global Atmospheric Lifetime (years):	13.4
Tropospheric Atmospheric Lifetime (years):	17.7
Stratospheric Atmospheric Lifetime (years):	54.8
Ozone Depletion Potential (ODP):	0.105

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.298	0.287
Global Warming Potential (GWP_H):		
GWP_{20}	3433	3306
GWP_{100}	1198	1154
Global Temperature Potentials (GTP_H)		
GTP_{20}		2725
GTP_{50}		627
GTP_{100}		179

* RE units: W m^2 ppb^{-1}
* GWP and GTP: Relative to CO_2

Atmospheric Loss Processes **********

OH Reactivity

k_{Rec}(T), *No recommendation*

$k_{SAR}(298\ K) = 3.31 \times 10^{-15}$; $k_{SAR}(272\ K) \approx 2.11 \times 10^{-15}$ cm^3 $molecule^{-1}$ s^{-1}

τ^{OH}_{Global} = 17.0 years
τ^{OH}_{Trop} = 17.7 years
τ^{OH}_{Strat} = 449.8.1 years

Fractional Atmospheric Loss: 0.786

O(^{1}D) Reactivity

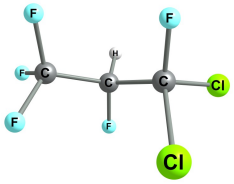
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 1.3 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)}$ = 285 years
Fractional Atmospheric Loss: 0.047

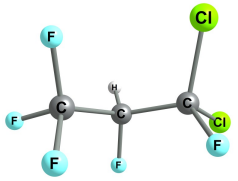
UV Photolysis

UV Spectrum: *No Recommendation*
τ_{hv} = 80 years
Fractional Atmospheric Loss: 0.167

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.525



$\Delta E = 0.23$ kcal mol^{-1}
Population = 0.353

Optimized Coordinates (Angstroms)

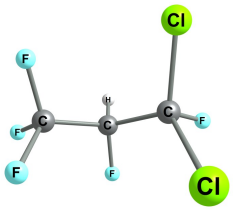
Atom	X	Y	Z
C	0.917475988900	0.106153030900	-0.317456260500
C	-0.319436857200	-0.771697713900	-0.026573865000
C	-1.689307655300	-0.070587881200	-0.145583662200
H	-0.313731954300	-1.582489763200	-0.763952882500
F	-0.225245202200	-1.283420960100	1.227725492100
Cl	1.119942597100	1.421423687900	0.868328533900
Cl	2.371069894100	-0.950891614300	-0.293694570100
F	0.799727300600	0.632305121400	-1.542063092400
F	-2.639650643600	-0.992010904900	0.040843880200
F	-1.858216702500	0.885918264000	0.760929442400
F	-1.847702765700	0.454112733400	-1.361909016000

Atom	X	Y	Z
C	0.917867575900	0.049691600800	0.195904808500
C	-0.326055295400	-0.524990379800	-0.518190187500
C	-1.683659604300	0.056126275400	-0.062036491300
H	-0.222060373700	-0.361709424200	-1.594352609000
F	-0.387921756400	-1.861108784600	-0.248694138500
Cl	2.349004781100	-0.930619771300	-0.262347629100
Cl	1.190429385300	1.755494562200	-0.272222341200
F	0.769321761300	-0.018758349100	1.521239110800
F	-2.647915296600	-0.572054300200	-0.740604521600
F	-1.890974722500	-0.140929298700	1.236627483700
F	-1.778255454500	1.360380869300	-0.319555484900

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
21.0740	0.00251
92.1526	0.0321
148.1110	0.164
191.5219	0.111
208.4564	0.0985
245.4509	0.178
270.3045	0.338
296.0078	0.0705
353.2381	0.0184
378.3851	0.0148
442.5658	0.372
522.2905	1.49
537.2615	0.0951
585.5958	1.91
669.1739	11.1
697.3509	17.7
813.5484	19.2
889.5339	2.25
1085.5912	7.46
1156.2073	12.0
1174.0958	8.76
1190.5645	32.3
1232.7256	46.1
1297.4436	29.4
1354.6443	0.738
1386.1492	8.41
3070.2774	0.830

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
20.0936	0.000
89.6920	0.00653
147.1863	0.0729
207.1061	0.285
221.1732	0.0521
232.9851	0.317
290.3328	0.0521
303.7706	0.230
334.2686	0.0742
375.9926	0.0305
438.8867	0.718
467.2089	0.823
534.0485	0.355
572.5749	1.64
680.8462	14.7
806.1088	13.7
841.9712	22.7
873.1133	9.67
982.7895	6.47
1131.4671	6.47
1181.3876	12.7
1214.2571	28.9
1232.6561	34.6
1288.8758	37.7
1358.6977	1.21
1376.3245	9.56
3098.1895	0.563



$\Delta E = 0.86$ kcal mol^{-1}
Population = 0.122

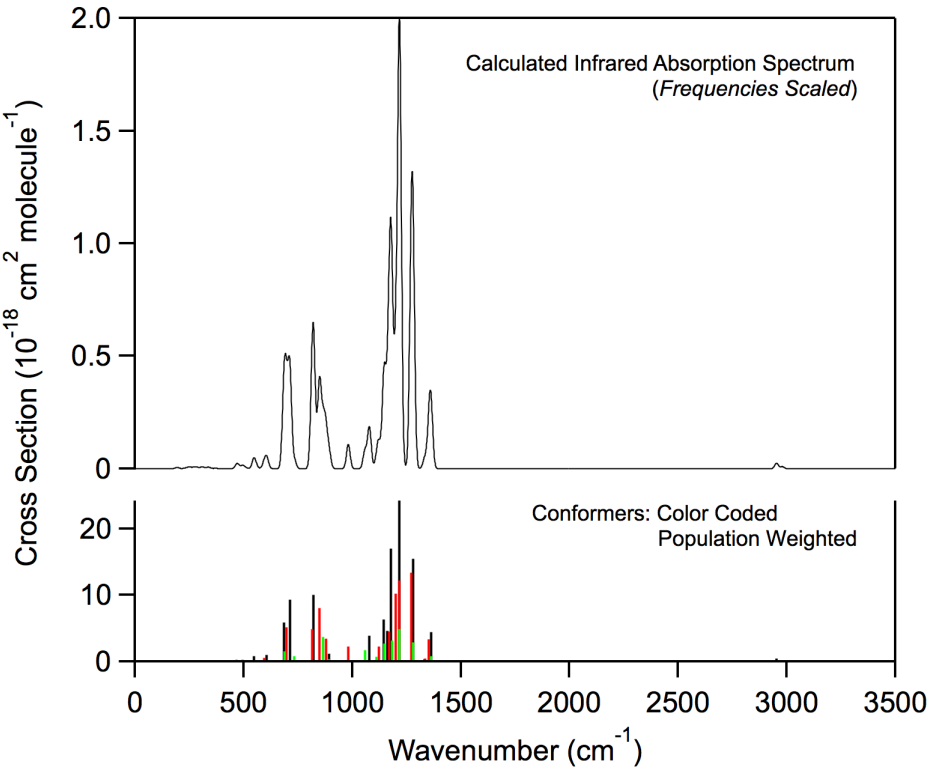
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.033764653000	-0.111533688000	-0.295380351000
C	-0.421221128900	-0.208859454800	-0.806538312200
C	-1.567908507700	0.253966470700	0.113580697800
H	-0.470601044000	0.391249622700	-1.722426274600
F	-0.658546381900	-1.517991899400	-1.104637846200
Cl	1.505070629200	1.590181763300	-0.008219699400
Cl	1.321659727100	-1.101198917000	1.159675129200
F	1.807650360200	-0.593197081700	-1.281001794600
F	-2.713942097000	0.079976902400	-0.552798105800
F	-1.633271998600	-0.450919525000	1.238404887700
F	-1.460093211500	1.546170807000	0.422175669200

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
20.1435	0.00123
96.7965	0.0224
152.1511	0.115
181.6173	0.148
222.2468	0.171
240.9038	0.196
290.3630	0.212
308.7386	0.205
340.0627	0.0855
384.5918	0.0146
447.5634	0.690
481.0833	0.821
525.4061	1.59
585.1198	0.0718
673.4905	12.6
720.1555	6.49
859.2901	30.4
888.3376	3.02
1063.6975	13.9
1120.3127	6.15
1158.5710	22.0
1194.9047	25.9
1230.7814	39.7
1299.1543	23.5
1352.8853	1.79
1387.3744	6.64
3069.9939	0.686

Infrared Spectrum



Radiative Efficiency