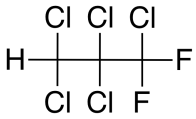
HCFC-222aa

Molecular Formula:	$CHCl_2CCl_2CClF_2$
Name:	1,2,2,3,3-Pentachloro-1,1-difluoropropane
CAS number:	422-30-0
Molecular Weight:	252.3



Global Atmospheric Lifetime (years):	1.11
Tropospheric Atmospheric Lifetime (years):	1.17
Stratospheric Atmospheric Lifetime (years):	20
Ozone Depletion Potential (ODP):	0.028

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.295	0.224
Global Warming Potential (GWP_H):		
GWP_{20}	291	221
GWP_{100}	79	60
Global Temperature Potentials (GTP_H)		
GTP_{20}		73
GTP_{50}		10
GTP_{100}		8

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 5.01 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 3.20 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 1.14$ years

$\tau^{OH}_{Trop} = 1.17$ years

$\tau^{OH}_{Strat} = 38.9$ years

Fractional Atmospheric Loss: 0.972

O(^{1}D) Reactivity

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

$k_{Est}(T) = 2.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 185$ years

Fractional Atmospheric Loss: 0.006

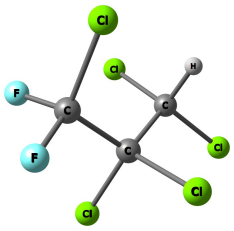
UV Photolysis

UV Spectrum: *No Recommendation*

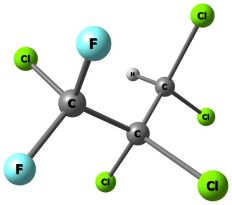
$\tau_{hv} = 50$ years

Fractional Atmospheric Loss: 0.022

Molecular Structure and Infrared Spectrum (5 conformers)



E = 0
Population = 0.384



E = 0
Population = 0.384

Optimized Coordinates (Angstroms)

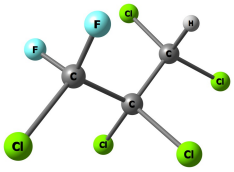
Atom	X	Y	Z
C	1.026460132029	0.392116919433	0.629579390043
C	-0.010384201390	-0.428846509939	-0.187512991222
C	-1.430594386123	0.247873170335	-0.291850561421
Cl	2.598512205682	-0.444884118609	0.734247146767
Cl	1.257219974189	2.044355008625	-0.008336843544
H	0.654583375523	0.494516687788	1.645423862225
Cl	-0.243081091190	-1.995456771931	0.656652117150
Cl	0.545790908621	-0.711590663069	-1.860011592280
F	-1.393447825018	1.312690794158	-1.083597343595
F	-2.291800607654	-0.619486340330	-0.811239854925
Cl	-2.045461484668	0.763651823540	1.320661670802

Atom	Z	Z	Z
C	1.027976214808	-0.363256903224	0.639660582302
C	-0.019023445339	0.414853975624	-0.205916532767
C	-1.434065031288	-0.276967116005	-0.275678348934
Cl	1.269542362407	-2.038582815421	0.069567970200
Cl	2.593550959816	0.489920232923	0.702411582470
H	0.661273998821	-0.426496278025	1.660566257693
Cl	0.527704787747	0.632594840045	-1.891207186782
Cl	-0.260971415272	2.013138117815	0.573811935393
F	-2.304553908310	0.561231562427	-0.826520039764
F	-1.391554344319	-1.373296403682	-1.022896098863
Cl	-2.037819179071	-0.730506212477	1.359579879052

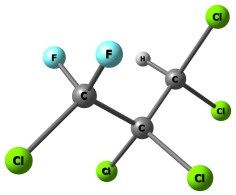
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
58.2626	0.0183
82.3720	0.0102
135.9145	0.0531
168.4957	0.0246
182.2589	0.0544
213.0452	0.0163
227.0717	0.0256
261.1110	0.0872
279.6241	0.103
308.5128	0.0445
335.3958	0.206
363.3552	0.0838
425.7657	0.142
440.1077	0.351
583.7297	4.46
635.4715	2.96
741.9089	13.4
759.2301	23.4
798.0953	20.3
852.1178	3.41
1000.0977	17.3
1040.0679	1.35
1191.4852	21.1
1214.5840	15.4
1232.0003	9.54
1280.0496	0.863
3162.8617	0.601

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
58.2647	0.0183
82.3729	0.0102
135.9153	0.0531
168.4958	0.0246
182.2598	0.0544
213.0448	0.0163
227.0719	0.0256
261.1117	0.0872
279.6252	0.103
308.5131	0.0445
335.3961	0.206
363.3557	0.0838
425.7653	0.142
440.1081	0.351
583.7290	4.46
635.4712	2.96
741.9095	13.4
759.2310	23.4
798.0959	20.3
852.1185	3.41
1000.0998	17.3
1040.0699	1.35
1191.4866	21.1
1214.5841	15.4
1232.0005	9.54
1280.0492	0.863
3162.8613	0.601



$\Delta E = 0.76$ kcal mol^{-1}
Population = 0.106



$\Delta E = 0.76$ kcal mol^{-1}
Population = 0.106

Optimized Coordinates (Angstroms)

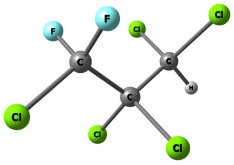
Atom	X	Y	Z
C	1.281890579853	0.192767215635	0.567243700951
C	-0.040869919450	-0.330685389552	-0.079646718072
C	-1.265128753596	0.577851585457	0.324621778608
Cl	2.660155573902	-0.886190129217	0.221293979249
Cl	1.697087509157	1.861717971970	0.084420319720
H	1.143293303257	0.201217936081	1.645175884203
Cl	-0.331814736031	-1.959430531939	0.617138943429
Cl	0.069955986621	-0.404010420546	-1.849255167411
F	-1.225250909408	0.758848915339	1.651245119188
F	-1.179717327798	1.767443222583	-0.260350416640
Cl	-2.845895306506	-0.129684375811	-0.116315423227

Atom	Z	Z	Z
C	1.281041190304	-0.186278476599	0.562813574312
C	-0.044824638895	0.324285778486	-0.088006802879
C	-1.267277665993	-0.575289123574	0.341006733994
Cl	1.693321902747	-1.864955121213	0.112287153660
Cl	2.657839698635	0.884815659701	0.187810231134
H	1.147895526354	-0.172531334909	1.641378095523
Cl	0.057084607001	0.361224393438	-1.859282396984
Cl	-0.331791505365	1.967103430772	0.576654115652
F	-1.185150799567	-1.776678535711	-0.219828987184
F	-1.220748638962	-0.729014222765	1.670849823004
Cl	-2.850055676260	0.123638552373	-0.106395540232

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
51.4521	0.0258
73.8398	0.0155
133.9755	0.0649
169.2159	0.0210
196.8626	0.0927
205.0436	0.0285
222.2006	0.0425
245.1441	0.0309
266.5828	0.0647
325.6097	0.149
334.5485	0.174
382.4864	0.127
429.3632	0.0458
451.1242	0.318
585.1723	6.57
629.0864	2.30
699.2745	16.1
754.4690	20.2
842.4655	11.8
874.6251	2.48
977.8517	12.0
1044.5569	21.3
1166.1567	20.0
1199.1992	14.5
1231.1094	7.29
1279.0539	1.20
3160.2126	0.570

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
51.4526	0.0258
73.8406	0.0155
133.9759	0.0649
169.2168	0.0211
196.8628	0.0927
205.0429	0.0285
222.2009	0.0425
245.1442	0.0309
266.5823	0.0647
325.6098	0.149
334.5490	0.174
382.4866	0.127
429.3633	0.0458
451.1245	0.318
585.1727	6.57
629.0865	2.30
699.2755	16.1
754.4683	20.2
842.4660	11.8
874.6244	2.48
977.8537	12.0
1044.5586	21.3
1166.1575	20.0
1199.1967	14.5
1231.1080	7.29
1279.0525	1.20
3160.2140	0.570



$\Delta E = 1.79$ kcal mol^{-1}
Population = 0.019

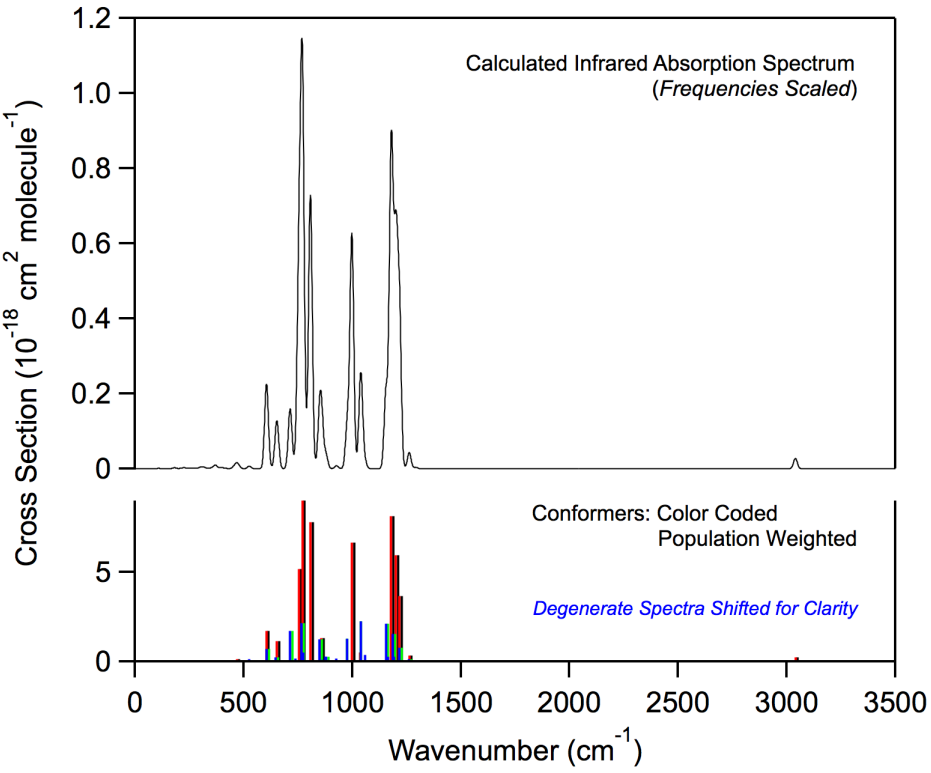
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.436370930174	-0.008394757851	-0.418566162515
C	-0.127226120132	-0.034504850965	-0.517003469796
C	-0.901239996196	0.062033677076	0.847343695771
Cl	2.091165215045	1.517629988550	0.244768746426
Cl	2.125637137541	-1.398254737467	0.470659144410
H	1.803301823990	-0.083107504679	-1.438979704144
Cl	-0.574500245344	-1.566808532298	-1.326858002185
Cl	-0.608909478526	1.343879905096	-1.552334231822
F	-0.555385512082	-0.955581324507	1.631554225899
F	-0.580809555711	1.196103269108	1.464880888183
Cl	-2.680711198758	0.024320867937	0.631933869773

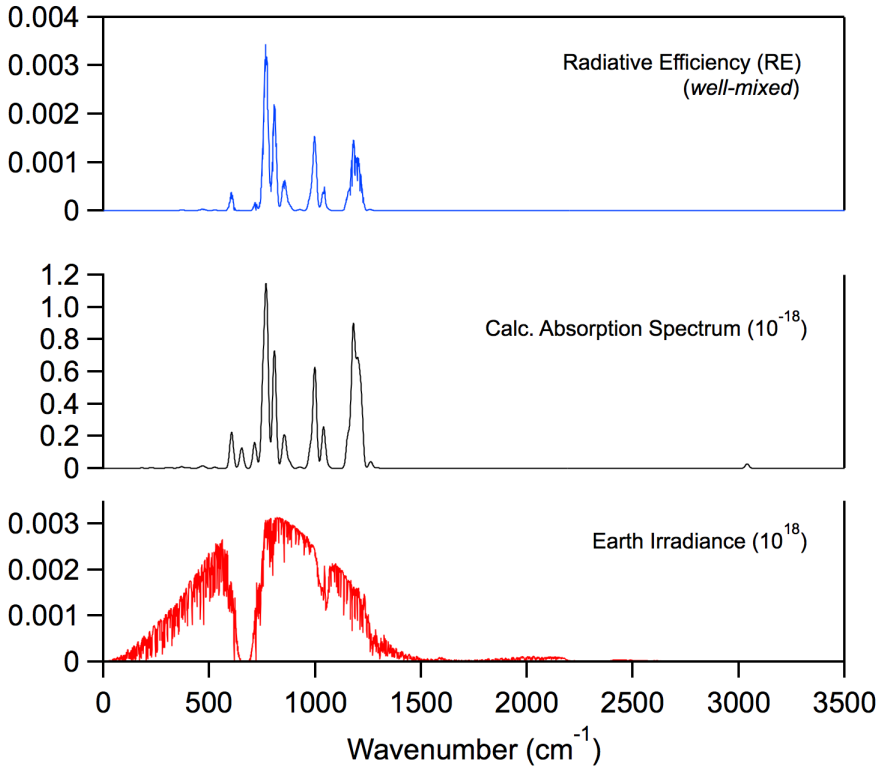
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
41.4719	0.00125
89.4357	0.0201
140.1776	0.00771
165.5848	0.00354
193.6991	0.0473
199.4770	0.0273
222.0867	0.00440
256.6817	0.00940
274.7535	0.0331
320.6809	0.0490
334.5631	0.00533
396.9913	0.0223
422.6582	0.0748
446.9446	0.336
499.8539	7.51
636.8580	2.43
725.3009	8.86
763.0518	27.6
857.1591	4.65
872.4978	14.6
925.1672	8.92
1063.5851	20.3
1176.8099	15.1
1204.2863	13.9
1228.3298	6.09
1311.2052	4.44
3153.5277	0.768

Infrared Spectrum

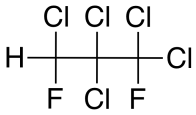


Radiative Efficiency



HCFC-222ab

Molecular Formula:	$CHClFCCl_2CCl_2F$
Name:	1,1,2,2,3-Pentachloro-1,3-difluoropropane
CAS number:	147728-31-2
Molecular Weight:	252.3



Global Atmospheric Lifetime (years):	2.67
Tropospheric Atmospheric Lifetime (years):	2.96
Stratospheric Atmospheric Lifetime (years):	27.3
Ozone Depletion Potential (ODP):	0.061

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.268	0.234
Global Warming Potential (GWP_H):		
GWP_{20}	638	557
GWP_{100}	173	151
Global Temperature Potentials (GTP_H)		
GTP_{20}		226
GTP_{50}		28
GTP_{100}		21

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 1.98 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 1.27 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 2.86$ years

$\tau^{OH}_{Trop} = 2.96$ years

$\tau^{OH}_{Strat} = 89.6$ years

Fractional Atmospheric Loss: 0.932

$O(^1D)$ Reactivity

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

$k_{Est}(T) = 2.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 185$ years

Fractional Atmospheric Loss: 0.014

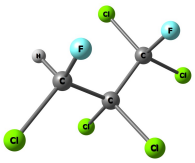
UV Photolysis

UV Spectrum: *No Recommendation*

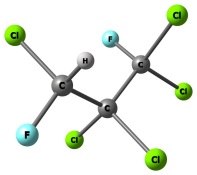
$\tau_{hv} = 50$ years

Fractional Atmospheric Loss: 0.053

Molecular Structure and Infrared Spectrum (5 conformers)



E = 0
Population = 0.531



$\Delta E = 0.54$ kcal mol^{-1}
Population = 0.212

Optimized Coordinates (Angstroms)

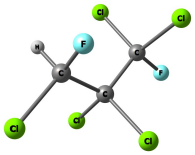
Atom	X	Y	Z
C	1.320553648038	0.827362967751	-0.150157395829
C	0.239824378338	-0.270920725702	0.090323364804
C	-1.191356060135	0.249437527664	-0.336317798715
Cl	2.968814316027	0.265535827399	0.252330900689
F	1.290483934836	1.206996926160	-1.442678537550
H	1.116520564307	1.682885723650	0.493180294134
Cl	0.237137438006	-0.676887511308	1.824729649119
Cl	0.603497336451	-1.703062719801	-0.910273694241
Cl	-2.470662725407	-0.936690453426	0.035927219816
Cl	-1.573137299069	1.806485488615	0.482607546403
F	-1.198008531391	0.469251949000	-1.650368548630

Atom	X	Y	Z
C	1.481333659833	0.168219352595	-0.686594463269
C	0.207671233854	-0.480294763989	-0.058750385564
C	-0.954721221803	0.535616004899	0.248741110826
Cl	2.215794765141	1.451014896499	0.321996431548
F	2.395507244740	-0.801181659704	-0.875451627229
H	1.222246730058	0.624882231299	-1.641230741890
Cl	0.647353690053	-1.309289071411	1.457136471881
Cl	-0.352226092062	-1.673924590649	-1.275600477266
Cl	-1.295731606107	1.555383749484	-1.193481139188
Cl	-2.451480269135	-0.296781617534	0.751370779823
F	-0.584811134572	1.341379468513	1.243326040327

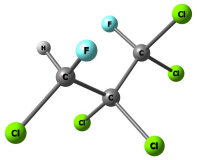
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
59.5839	0.0522
81.4214	0.0228
129.4381	0.0514
175.3555	0.0145
194.9483	0.0853
198.3951	0.0147
227.0377	0.0119
240.7699	0.0533
278.2697	0.0277
303.6089	0.166
347.9579	0.159
382.5796	0.00653
400.7387	0.247
435.9580	0.310
496.5885	0.617
612.6116	10.4
687.8687	22.1
784.3656	23.2
865.2811	12.3
891.6885	11.9
989.9965	2.92
1041.1596	11.8
1126.8793	2.76
1169.0350	27.8
1282.0389	2.27
1359.8654	1.73
3133.7224	0.404

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
58.0469	0.0284
90.8744	0.0290
135.1452	0.0556
174.0547	0.0405
185.6771	0.0932
200.3099	0.0239
227.5147	0.0191
259.0527	0.0479
275.9504	0.0448
308.8171	0.161
339.6862	0.318
380.3671	0.0169
394.5703	0.187
417.2587	0.717
498.9325	0.359
621.2976	8.08
737.1592	24.4
775.4269	22.1
816.3407	20.5
858.8112	6.76
1009.1174	0.719
1050.9090	10.9
1143.4862	12.8
1163.4680	18.1
1279.3513	4.82
1360.6678	1.18
3135.0003	0.419



$\Delta E = 0.76$ kcal mol^{-1}
Population = 0.148



$\Delta E = 1.15$ kcal mol^{-1}
Population = 0.076

Optimized Coordinates (Angstroms)

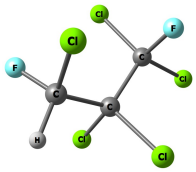
Atom	X	Y	Z
C	1.078025998453	0.320432494036	0.918775368040
C	0.275351936529	-0.198361518891	-0.307232667465
C	-1.292016573948	-0.090890756052	-0.116998991030
Cl	2.844139150260	0.149031276592	0.700735844657
F	0.795165669986	1.620512329283	1.131123179604
H	0.810738054660	-0.266112918283	1.798125658019
Cl	0.652747320403	-1.936982569614	-0.523631324626
Cl	0.715748051232	0.704195351867	-1.780350791142
Cl	-1.803433890222	-0.923032640704	1.395898032181
Cl	-1.884642658702	1.590941217461	-0.072017528382
F	-1.878268058650	-0.702861265695	-1.144888779857

Atom	X	Y	Z
C	1.339144030123	0.598593829855	0.603177618325
C	0.249865565968	-0.284139856173	-0.085932681109
C	-1.195865828172	0.137724934135	0.400556709765
Cl	3.000737107764	0.046373996451	0.240083577872
F	1.226579641241	1.877253767126	0.197021336478
H	1.209061657667	0.538075172880	1.684667372645
Cl	0.512425454557	-1.967483951683	0.474992284564
Cl	0.369079143536	-0.169193858744	-1.850818028420
Cl	-1.643642537591	1.796079793126	-0.086854014053
Cl	-2.450508492159	-0.984785954775	-0.192242502049
F	-1.182036742935	0.093326127802	1.744206325982

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
54.1865	0.0554
80.7277	0.0294
136.0325	0.0379
168.0025	0.0183
189.6667	0.0967
207.8844	0.00400
223.1551	0.0128
257.5442	0.0879
277.9939	0.0258
295.0799	0.191
334.4751	0.126
388.9739	0.140
392.1851	0.128
438.1679	0.345
480.8413	0.892
627.5541	6.99
720.0213	23.3
797.5183	31.2
809.5128	17.3
876.5334	0.834
991.4020	5.20
1051.1148	3.86
1139.6708	11.9
1166.6847	20.6
1282.2598	2.57
1361.9342	1.70
3128.0609	0.433

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
51.3879	0.0554
75.9773	0.0300
136.1288	0.0409
171.1025	0.00580
196.5382	0.0834
207.1791	0.118
230.1882	0.0231
240.5661	0.0980
263.3524	0.0312
295.8244	0.0460
365.8065	0.0611
384.9666	0.00269
393.4652	0.219
440.2000	0.459
498.1326	0.308
615.7196	12.7
700.9772	17.2
784.3303	29.4
859.6533	7.75
885.3035	6.00
987.5489	5.93
1038.8707	12.4
1120.8078	13.7
1143.0968	17.5
1280.0924	3.22
1360.4771	1.86
3120.9797	0.330



$\Delta E = 1.63$ kcal mol^{-1}
Population = 0.034

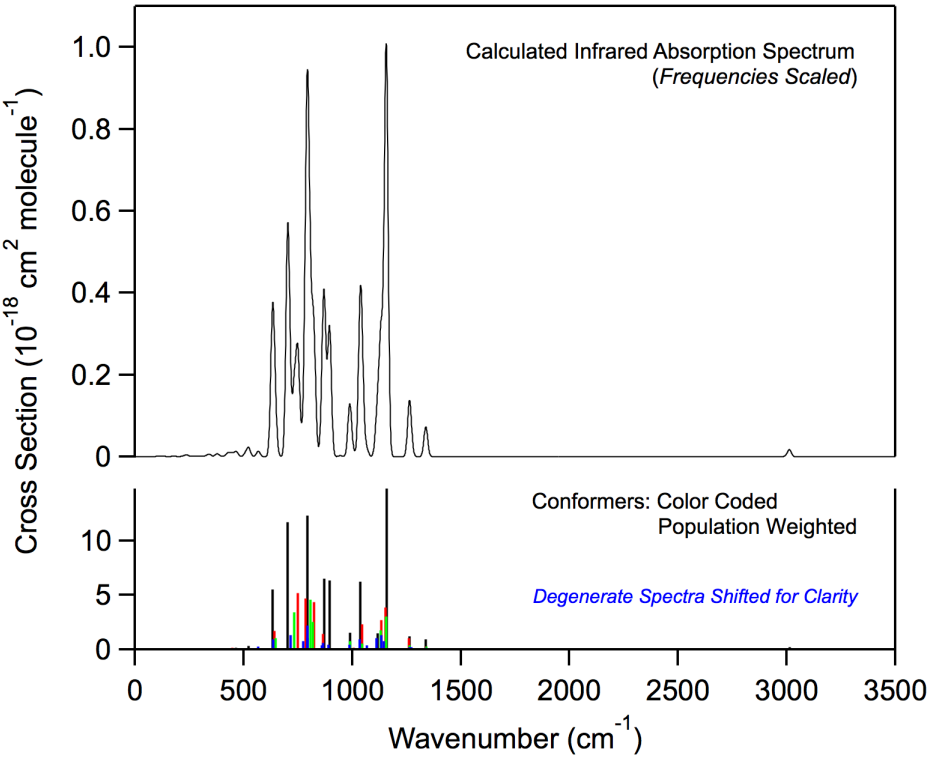
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.586427491283	0.031247417733	0.603992338606
C	0.138533388199	-0.504086597915	0.340846308560
C	-0.802999885878	0.388825609811	-0.551789749963
Cl	2.504133401023	0.429975683779	-0.882363572655
F	1.561145705624	1.116404708715	1.398439900238
H	2.133478753125	-0.771916549250	1.099788862792
Cl	-0.587759066625	-0.729513834139	1.960550086912
Cl	0.322786505116	-2.093321677735	-0.466165310266
Cl	-2.449935097108	-0.307500742971	-0.659839962565
Cl	-0.910199434912	2.059362771906	0.073313382665
F	-0.303511759847	0.436919210065	-1.788228284324

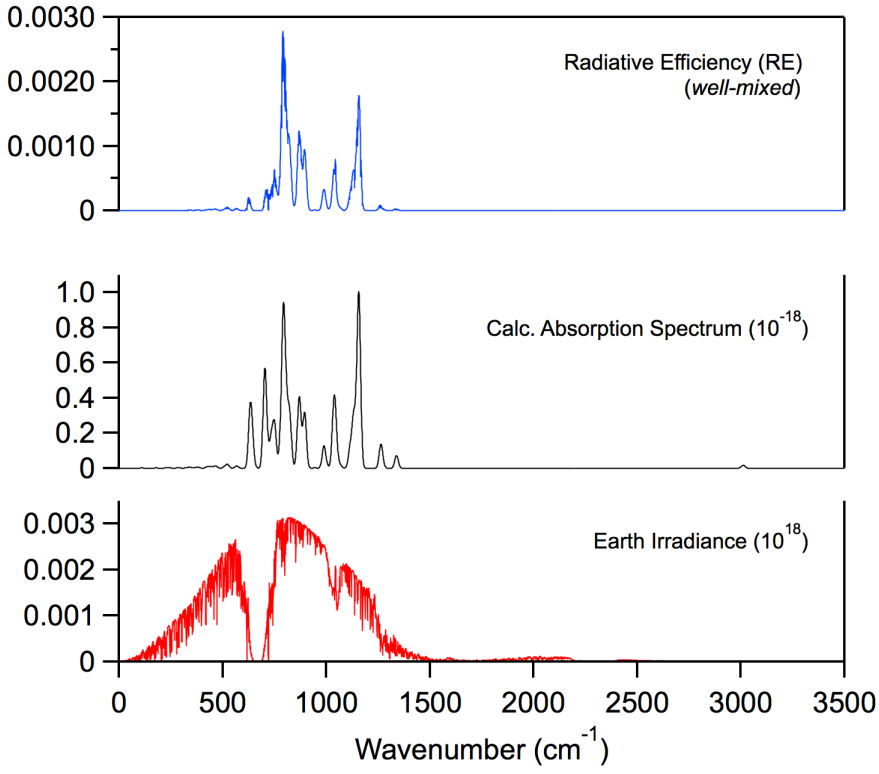
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
49.1856	0.0127
99.1050	0.0420
147.7054	0.0272
167.1247	0.0002
186.5871	0.00960
205.4880	0.0844
230.3517	0.0213
255.0992	0.0967
265.9094	0.0173
318.2985	0.0440
363.4324	0.0711
382.2268	0.0798
389.8813	0.0818
432.4961	0.574
488.9032	1.58
544.0182	8.53
761.8227	22.9
782.7004	31.3
854.9699	10.9
861.9646	5.26
943.0256	1.64
1072.1836	11.7
1143.9990	5.66
1154.9371	22.8
1291.3117	5.94
1373.6634	0.813
3115.9426	0.498

Infrared Spectrum

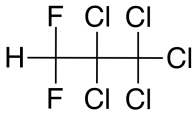


Radiative Efficiency



HCFC-222ac

Molecular Formula:	$CHF_2CCl_2CCl_3$
Name:	1,1,1,2,2-Pentachloro-3,3-difluoropropane
CAS number:	422-27-5
Molecular Weight:	252.3



Global Atmospheric Lifetime (years):	9.29
Tropospheric Atmospheric Lifetime (years):	12.6
Stratospheric Atmospheric Lifetime (years):	35.2
Ozone Depletion Potential (ODP):	0.191

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.232	0.221
Global Warming Potential (GWP_H):		
GWP_{20}	1698	1616
GWP_{100}	520	495
Global Temperature Potentials (GTP_H)		
GTP_{20}		1182
GTP_{50}		175
GTP_{100}		71

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 4.65 \times 10^{-15}$; $k_{SAR}(272\ K) \approx 2.97 \times 10^{-15}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 12.2$ years

$\tau^{OH}_{Trop} = 12.6$ years

$\tau^{OH}_{Strat} = 331.1$ years

Fractional Atmospheric Loss: 0.764

$O(^1D)$ Reactivity

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

$k_{Est}(T) = 2.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 185$ years

Fractional Atmospheric Loss: 0.050

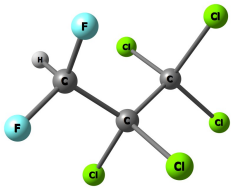
UV Photolysis

UV Spectrum: *No Recommendation*

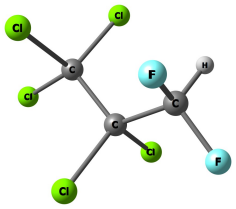
$\tau_{hv} = 50$ years

Fractional Atmospheric Loss: 0.186

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.467



E = 0
Population = 0.467

Optimized Coordinates (Angstroms)

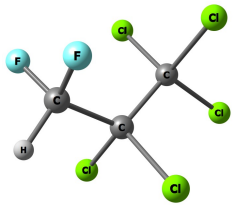
Atom	X	Y	Z
C	1.544171209543	0.591502571763	0.796884636578
C	0.582054565910	-0.256713420657	-0.098746971420
C	-0.943967065943	0.118309039880	0.062060953320
F	2.800355440207	0.156930103541	0.604572276578
F	1.497064878795	1.888745439253	0.449608865417
H	1.276429080483	0.482370499247	1.851488349533
Cl	0.822794679817	-1.958989310466	0.415659316537
Cl	1.077340738584	-0.064682034416	-1.800490093047
Cl	-1.969461184023	-1.003754714126	-0.873589135570
Cl	-1.402207753480	0.010028096319	1.799552433040
Cl	-1.271043589893	1.781368729661	-0.497867630966

Atom	X	Y	Z
C	1.544559730520	0.604750763983	-0.787424945729
C	0.583957630174	-0.257521059229	0.096331606504
C	-0.943081980274	0.114255739518	-0.062337488984
F	1.492504821061	1.897517173305	-0.424514420134
F	2.801918106350	0.172130248304	-0.598414883935
H	1.278812632124	0.507519313886	-1.843696310704
Cl	1.075959269083	-0.084469847633	1.801060504935
Cl	0.831287094023	-1.952606998021	-0.438293113811
Cl	-1.966194321028	-1.022537858961	0.858014507313
Cl	-1.276682609291	1.769286118410	0.517190090178
Cl	-1.398267372742	0.025504406438	-1.801738545636

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
54.5927	0.0801
92.3408	0.0627
149.8319	0.0350
168.0381	0.00384
199.8134	0.0939
204.4461	0.0790
221.7958	0.0110
238.5321	0.0425
266.8901	0.0445
299.2781	0.148
303.4165	0.0357
330.2153	0.225
401.1296	0.194
407.9254	0.238
563.4523	3.49
657.0645	12.3
714.6506	9.31
763.7359	26.6
771.4916	13.0
869.2059	2.20
993.0287	0.348
1043.1076	4.26
1163.3120	20.1
1171.5259	18.8
1376.1244	5.10
1392.5373	1.33
3099.7572	1.69

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
54.5926	0.0801
92.3411	0.0627
149.8324	0.0350
168.0378	0.00384
199.8131	0.0939
204.4461	0.0790
221.7956	0.0110
238.5319	0.0425
266.8901	0.0445
299.2781	0.148
303.4163	0.0357
330.2149	0.225
401.1295	0.194
407.9254	0.238
563.4524	3.49
657.0646	12.3
714.6506	9.31
763.7361	26.6
771.4921	13.0
869.2067	2.20
993.0290	0.348
1043.1072	4.26
1163.3121	20.1
1171.5265	18.8
1376.1236	5.10
1392.5370	1.33
3099.7570	1.69



$\Delta E = 1.17$ kcal mol^{-1}
Population = 0.065

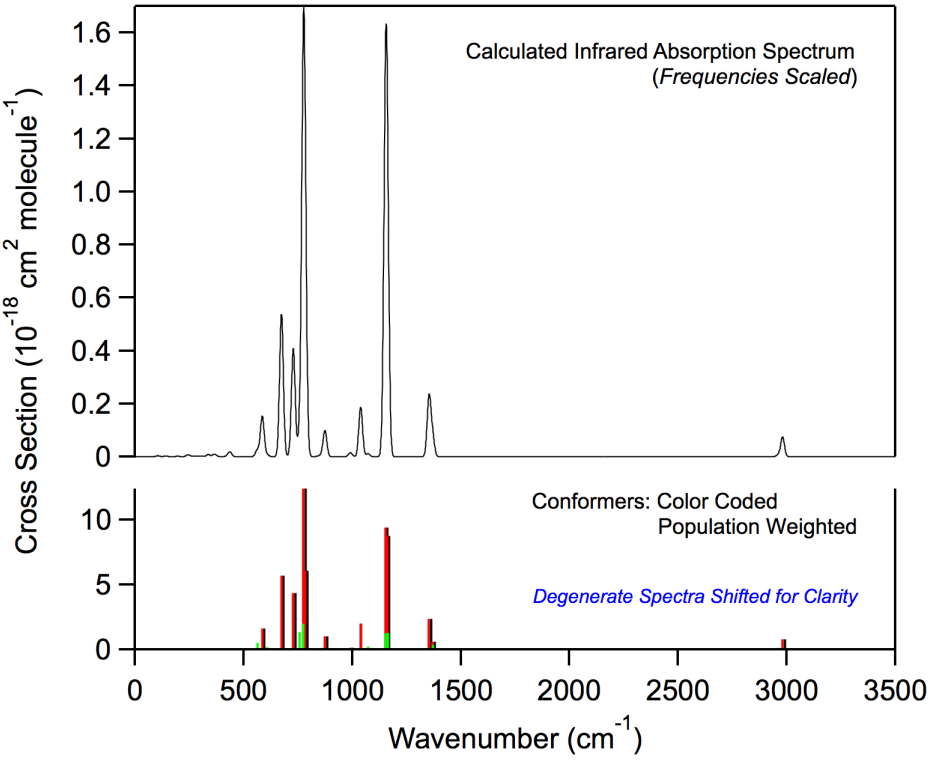
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.829539277626	0.535196261954	-0.006605531852
C	0.596853221208	-0.434708359592	-0.003744484602
C	-0.841521012421	0.216367618329	0.003907736343
F	1.826967592146	1.324859386201	-1.092690683297
F	1.836161811542	1.319592908881	1.083272247756
H	2.731315181776	-0.086381907599	-0.011920243548
Cl	0.800617313830	-1.457513947634	1.454209877786
Cl	0.788270242689	-1.450442644829	-1.468300941217
Cl	-2.093402856404	-1.066141662985	0.006094837174
Cl	-1.071225104164	1.230106209400	1.458483782517
Cl	-1.083487667828	1.237126137872	-1.443754597061

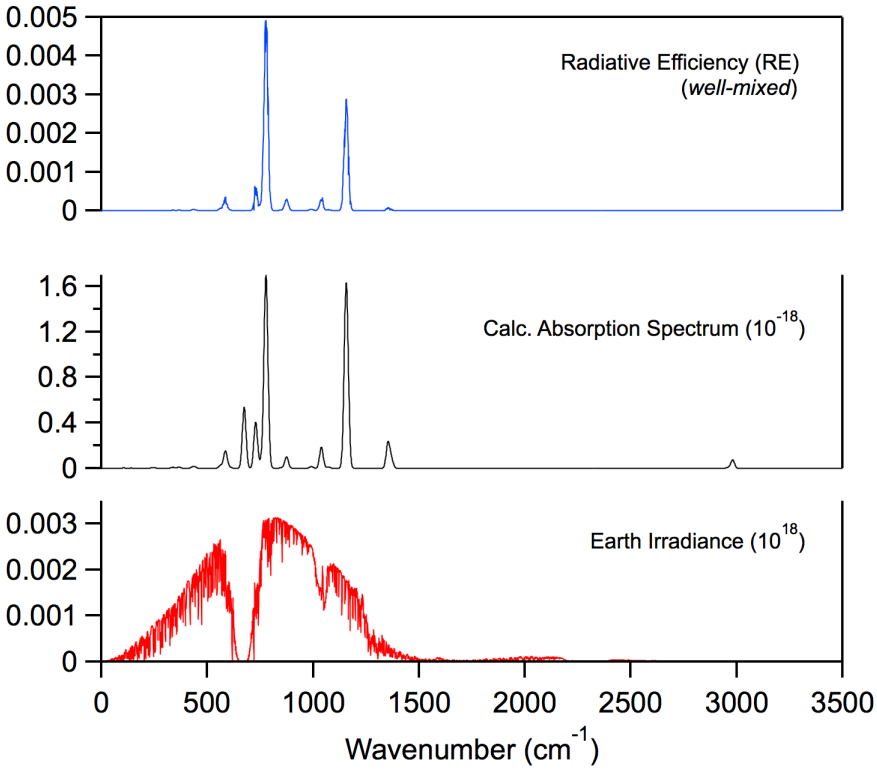
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
44.1503	0.0316
112.0155	0.0864
159.3900	0.0455
162.3644	0.00299
203.3078	0.0982
207.6976	0.00588
219.6246	0.0331
235.4786	0.0341
259.9670	0.0186
293.7120	0.0676
315.3267	0.0698
361.8196	0.351
391.5111	0.241
409.8836	0.156
539.0716	8.17
586.2891	2.59
744.4506	20.8
763.3352	30.8
837.3981	0.947
856.3740	2.07
919.5140	0.191
1078.7901	3.82
1164.3658	19.2
1176.0924	20.2
1395.3274	1.18
1395.8694	5.63
3077.7081	2.35

Infrared Spectrum

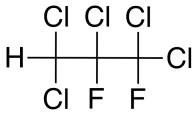


Radiative Efficiency



HCFC-222ba

Molecular Formula:	$CHCl_2CClFCCl_2F$
Name:	1,1,2,3,3-Pentachloro-1,2-difluoropropane
CAS number:	146254-26-4
Molecular Weight:	252.3



Global Atmospheric Lifetime (years):	1.11
Tropospheric Atmospheric Lifetime (years):	1.17
Stratospheric Atmospheric Lifetime (years):	20
Ozone Depletion Potential (ODP):	0.028

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.276	0.210
Global Warming Potential (GWP_H):		
GWP_{20}	273	207
GWP_{100}	74	56
Global Temperature Potentials (GTP_H)		
GTP_{20}		68
GTP_{50}		10
GTP_{100}		8

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 5.01 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 3.20 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 1.14$ years

$\tau^{OH}_{Trop} = 1.17$ years

$\tau^{OH}_{Strat} = 38.9$ years

Fractional Atmospheric Loss: 0.972

O(^{1}D) Reactivity

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

$k_{Est}(T) = 2.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 185$ years

Fractional Atmospheric Loss: 0.006

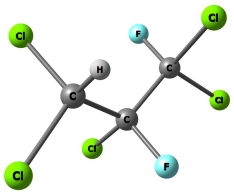
UV Photolysis

UV Spectrum: *No Recommendation*

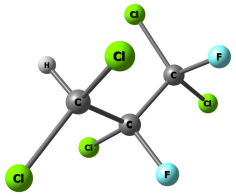
$\tau_{hv} = 50$ years

Fractional Atmospheric Loss: 0.022

Molecular Structure and Infrared Spectrum (2 conformers)



E = 0
Population = 0.942



$\Delta E = 1.65$ kcal mol^{-1}
Population = 0.058

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.305149181793	-0.524767171280	0.326095100890
C	0.083647999938	0.434903959238	0.239106946925
C	-1.263631013957	-0.266668075337	-0.178797108445
Cl	1.710391557444	-1.293089398170	-1.224843411242
Cl	2.708701110238	0.336878482003	1.013583874129
H	1.060200745629	-1.319232370370	1.025479504297
Cl	0.394933347593	1.780054055267	-0.893447831970
F	-0.106550136327	0.925411056239	1.480404608691
F	-1.219605659228	-0.648530357432	-1.450585005077
Cl	-1.539642700207	-1.720905131864	0.846547675201
Cl	-2.632204432917	0.857690951706	0.040415646601

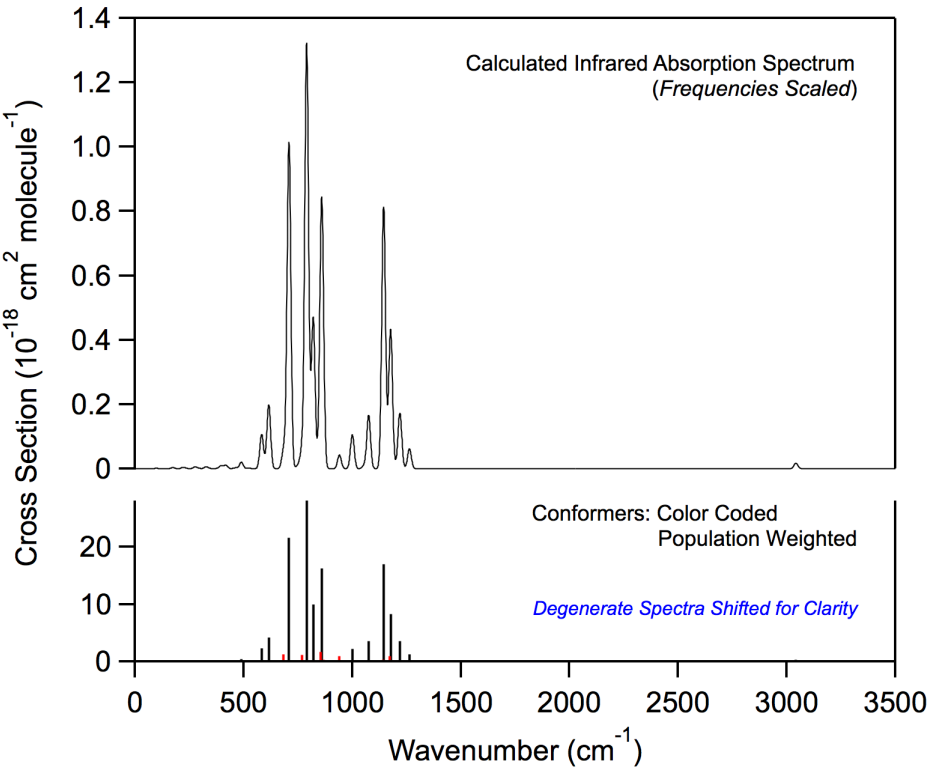
Atom	X	Y	Z
C	1.372650265933	-0.201278235599	-0.417887696764
C	0.113218087050	0.398956907285	0.273850009337
C	-1.211476357182	-0.442532978053	0.101330712075
Cl	2.802589383771	0.808208002027	-0.056894454305
Cl	1.701011844902	-1.886061735203	0.079762234646
H	1.232747332438	-0.201440157131	-1.494311053156
Cl	-0.142684249131	2.036669380674	-0.416260892320
F	0.323509193905	0.491946388697	1.596728353212
F	-1.077611227174	-1.590022575512	0.767569502496
Cl	-2.603799423283	0.417086218420	0.817960496511
Cl	-1.522619851228	-0.809221215606	-1.622131211732

Infrared Absorption Spectrum (unscaled frequencies)

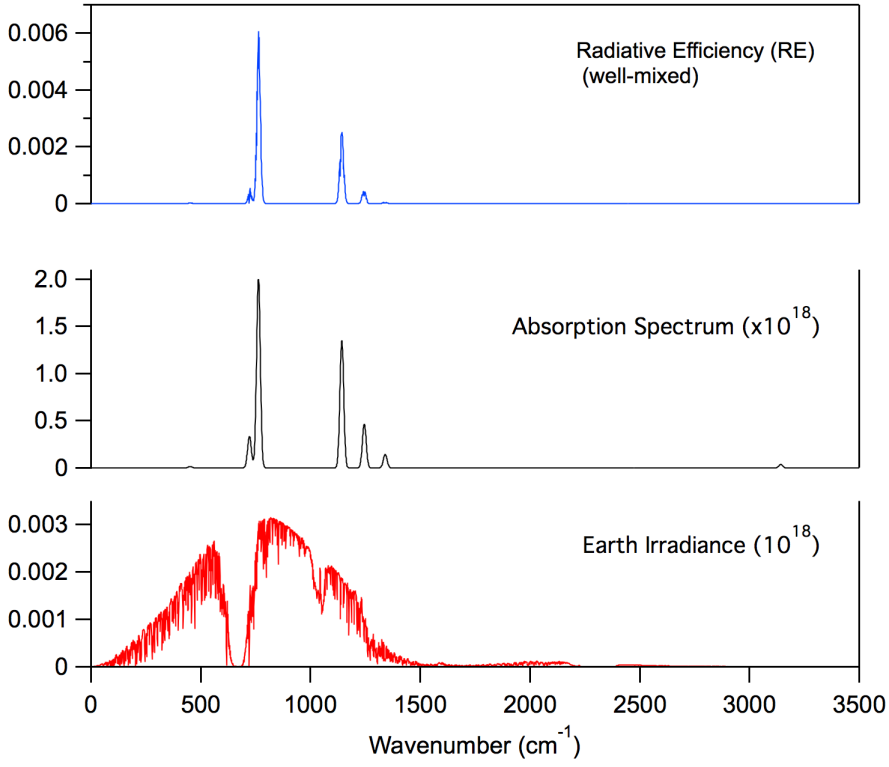
Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
46.1919	0.0285
78.1035	0.0141
127.3667	0.0764
175.4098	0.0583
182.1448	0.0444
200.9735	0.00923
235.4923	0.119
252.0954	0.0315
289.0840	0.122
293.9465	0.0184
362.0299	0.203
377.4588	0.0586
387.0594	0.198
461.4687	0.457
560.6068	2.41
595.0138	4.50
693.5829	23.0
779.8427	29.9
811.8317	10.6
853.3910	17.3
1002.3329	2.38
1082.0320	3.74
1155.0344	18.1
1189.5857	8.85
1234.6153	3.76
1280.6413	1.39
3163.8309	0.376

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
43.1125	0.0115
69.4810	0.0196
134.7934	0.0580
176.8367	0.0394
189.8248	0.0431
214.5726	0.0265
234.0684	0.0285
253.2157	0.0555
278.6935	0.0148
307.1793	0.196
335.2692	0.237
379.8828	0.128
389.8245	0.0599
431.7658	1.00
497.6876	0.699
667.4416	21.8
736.8325	3.54
756.2097	19.9
849.1264	29.7
862.0694	4.86
939.4717	15.6
1059.0756	3.35
1153.1546	5.07
1184.6220	17.1
1224.7706	4.43
1293.5879	0.507
3176.3705	0.549

Infrared Spectrum

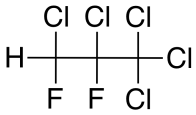


Radiative Efficiency



HCFC-222bb

Molecular Formula:	$CHClFCClFCCl_3$
Name:	1,1,1,2,3-Pentachloro-2,3-difluoropropane
CAS number:	147728-30-1
Molecular Weight:	252.3



Global Atmospheric Lifetime (years):	3.15
Tropospheric Atmospheric Lifetime (years):	3.54
Stratospheric Atmospheric Lifetime (years):	28.6
Ozone Depletion Potential (ODP):	0.071

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.224	0.199
Global Warming Potential (GWP_H):		
GWP_{20}	627	557
GWP_{100}	170	151
Global Temperature Potentials (GTP_H)		
GTP_{20}		243
GTP_{50}		28
GTP_{100}		21

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 1.66 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 1.06 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

τ^{OH}_{Global} = 3.42 years
τ^{OH}_{Trop} = 3.54 years
τ^{OH}_{Strat} = 105.3 years

Fractional Atmospheric Loss: 0.920

$O(^1D)$ Reactivity

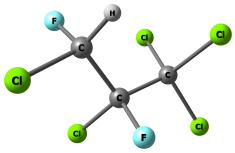
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 2.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)}$ = 185 years
Fractional Atmospheric Loss: 0.017

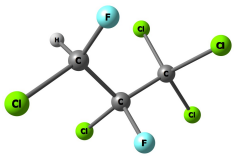
UV Photolysis

UV Spectrum: *No Recommendation*
τ_{hv} = 50 years
Fractional Atmospheric Loss: 0.063

Molecular Structure and Infrared Spectrum (2 conformers)



E = 0
Population = 0.882



$\Delta E = 1.26$ kcal mol^{-1}
Population = 0.104

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.425729585619	-0.790582863958	0.052797501935
C	-0.375272258481	0.307655309325	-0.290618533796
C	1.118683747324	-0.149592740550	-0.050931045554
Cl	-3.023304730456	-0.353955795717	-0.623381319236
H	-1.140448758372	-1.735143569968	-0.410595436386
F	-1.528219911307	-0.945556903665	1.384160303776
Cl	-0.725791929006	1.786482687344	0.645409332334
F	-0.476283978717	0.577049330835	-1.606213915291
Cl	2.223632880702	1.140276615742	-0.594887220610
Cl	1.433515931446	-0.540215255606	1.652594653452
Cl	1.423666592486	-1.611041813783	-1.060447320624

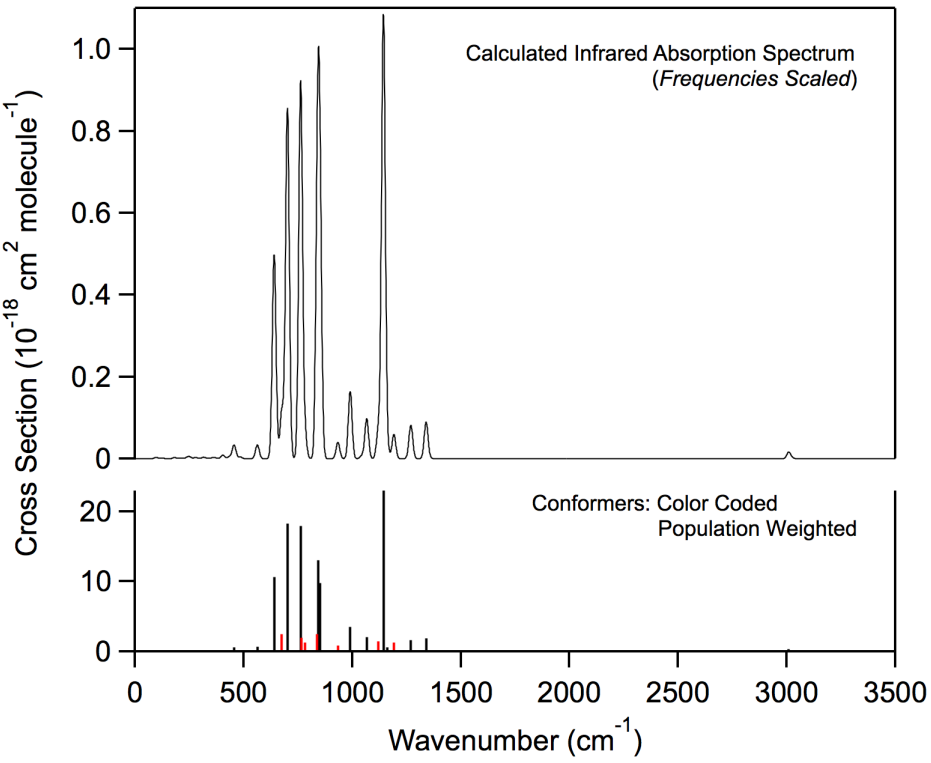
Atom	X	Y	Z
C	1.455836532082	0.544633094872	0.493181139368
C	0.384483200360	-0.271882990378	-0.293877733570
C	-1.108919771619	0.148041939976	0.012783904334
Cl	3.084210138666	0.221618383231	-0.175666581751
F	1.213145852925	1.867392628390	0.406513769304
H	1.464825018417	0.238578792434	1.537931115775
Cl	0.637578631631	-1.993196259465	0.154170545400
F	0.565630153704	-0.128958230442	-1.615440445359
Cl	-2.233224064957	-1.008578502273	-0.754155223241
Cl	-1.380997934341	0.177754995662	1.780235428014
Cl	-1.441931756867	1.761881147993	-0.677116918274

Infrared Absorption Spectrum (unscaled frequencies)

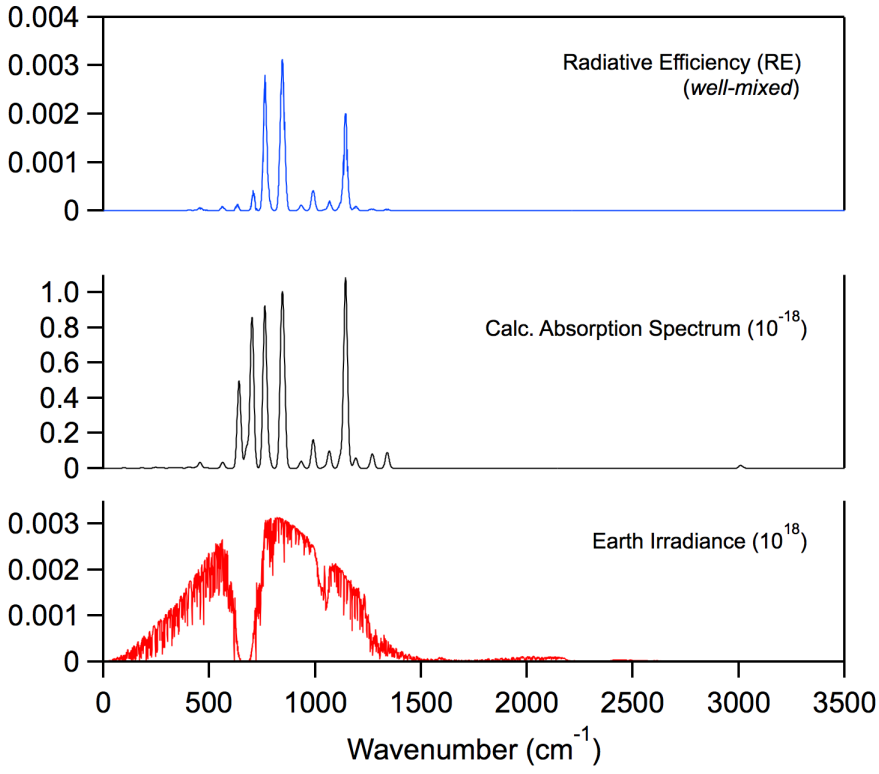
Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
45.9079	0.0682
78.5154	0.0275
136.0684	0.0686
168.9608	0.0337
197.2767	0.0521
208.6623	0.0964
217.1647	0.00169
238.8825	0.0645
276.8353	0.0848
304.0089	0.0356
328.4267	0.0711
372.1954	0.194
404.0528	0.105
426.3248	0.693
539.5740	0.813
621.3857	12.0
686.2399	20.7
749.9187	20.3
834.9136	14.8
845.0899	11.1
992.0405	3.97
1072.4556	2.36
1153.8644	26.1
1171.6235	0.681
1288.3671	1.82
1361.8742	2.16
3129.3230	0.387

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
45.8001	0.0580
69.3767	0.0297
138.8116	0.0203
173.4452	0.0298
197.5554	0.112
215.7311	0.00450
223.8615	0.0314
249.1139	0.0557
273.6123	0.0315
295.7668	0.0747
325.4668	0.138
360.9810	0.183
402.4472	0.0979
425.8353	0.940
456.5906	0.809
658.9808	23.9
754.8972	18.6
771.1298	12.3
831.3784	24.2
850.3991	1.27
932.2077	8.17
1048.6875	1.49
1128.7173	13.7
1205.0054	12.1
1281.4684	1.82
1376.3690	0.619
3144.3294	0.504

Infrared Spectrum

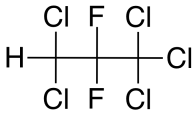


Radiative Efficiency



HCFC-222ca

Molecular Formula:	$CHCl_2CF_2CCl_3$
Name:	1,1,1,3,3-Pentachloro-2,2-difluoropropane
CAS number:	422-49-1
Molecular Weight:	252.3



Global Atmospheric Lifetime (years): 1.38
- Tropospheric Atmospheric Lifetime (years): 1.47
- Stratospheric Atmospheric Lifetime (years): 21.6

Ozone Depletion Potential (ODP): 0.034

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.259	0.205
Global Warming Potential (GWP_H):		
GWP_{20}	318	253
GWP_{100}	86	68
Global Temperature Potentials (GTP_H)		
GTP_{20}		86
GTP_{50}		12
GTP_{100}		10

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 3.98 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 2.54 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 1.43$ years

$\tau^{OH}_{Trop} = 1.47$ years

$\tau^{OH}_{Strat} = 47.8$ years

Fractional Atmospheric Loss: 0.965

O(^{1}D) Reactivity

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

$k_{Est}(T) = 2.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 185$ years

Fractional Atmospheric Loss: 0.007

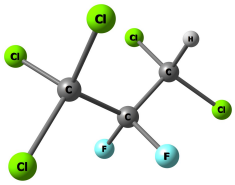
UV Photolysis

UV Spectrum: *No Recommendation*

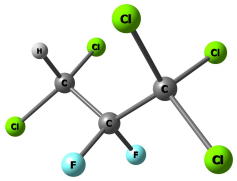
$\tau_{hv} = 50$ years

Fractional Atmospheric Loss: 0.028

Molecular Structure and Infrared Spectrum (2 conformers)



E = 0
Population = 0.499



E = 0
Population = 0.499

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.469108028834	0.046191331243	0.481903104484
C	0.240493118675	-0.587771843934	-0.233242124087
C	-1.182889098177	0.038574496134	0.062217245122
Cl	2.881682157218	-1.024562622065	0.231409577681
Cl	1.844072988955	1.693892617229	-0.069509402286
H	1.286589975195	0.086936607995	1.551216526290
F	0.176184109822	-1.862900543301	0.198940539018
F	0.423289295852	-0.590837624999	-1.557864291614
Cl	-2.410194253593	-1.091012277770	-0.586118882520
Cl	-1.400739200886	0.192992820677	1.834044693145
Cl	-1.403377121896	1.616017038791	-0.721703985232

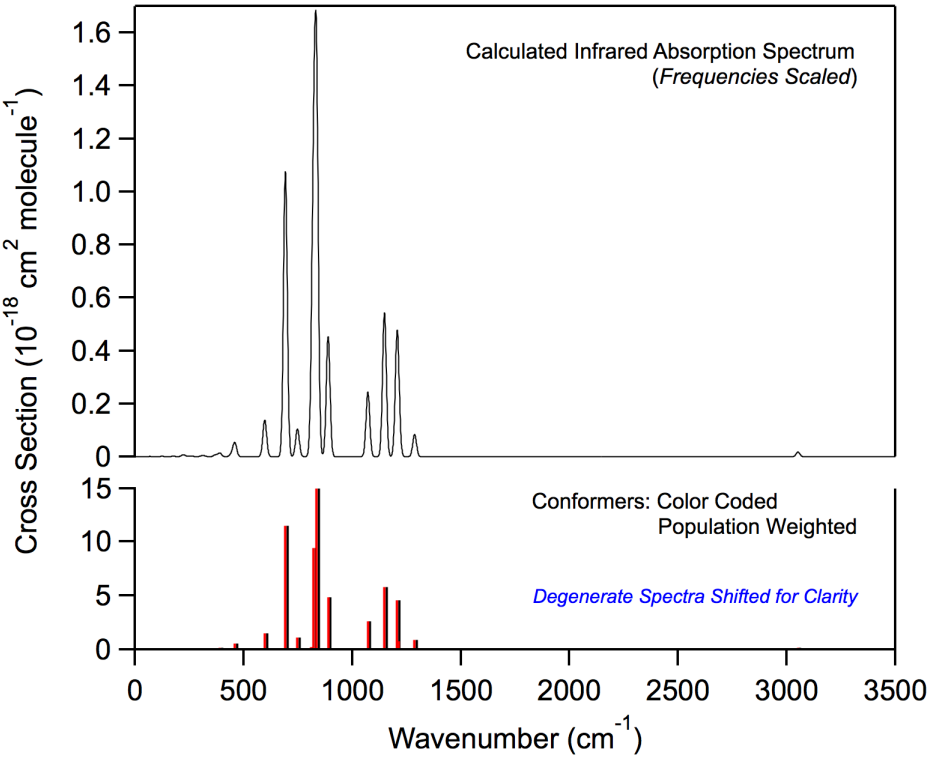
Atom	X	Y	Z
C	1.467785274442	-0.044759306842	0.469263656337
C	0.238830648462	0.573483161433	-0.258941266795
C	-1.185905148830	-0.037883332758	0.060401853635
Cl	1.833487230532	-1.709380845749	-0.035585292971
Cl	2.883772577954	1.012155809012	0.181974947031
H	1.289621239386	-0.053656069816	1.540049634204
F	0.416043477933	0.537335610302	-1.583832330573
F	0.181696346741	1.860877110419	0.136310090502
Cl	-2.411189176431	1.077716140125	-0.615393600211
Cl	-1.416317999482	-1.636425156706	-0.676515385399
Cl	-1.396913470706	-0.139922119420	1.836841694241

Infrared Absorption Spectrum (unscaled frequencies)

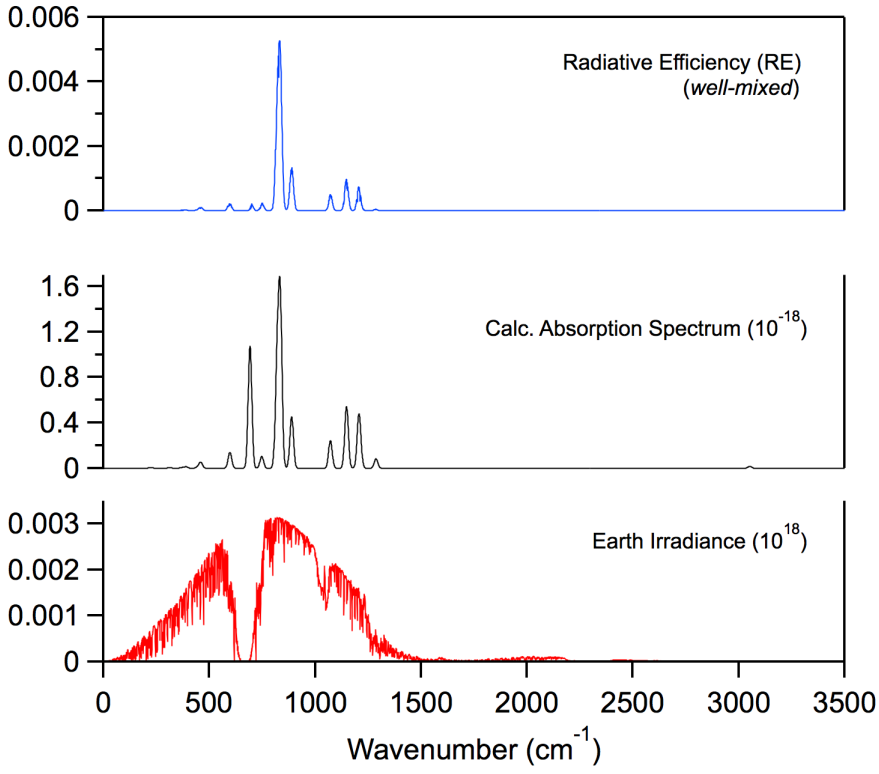
Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
15.2238	0.0252
75.0785	0.0330
130.0989	0.0421
172.1765	0.0479
181.4255	0.125
208.2396	0.0234
227.0038	0.0236
264.7494	0.0336
277.3052	0.0871
292.9613	0.00453
334.2882	0.147
356.1008	0.298
413.0946	0.212
429.6644	1.13
575.5794	2.97
676.1242	23.0
735.0476	2.22
800.3721	0.478
812.4370	18.8
827.4369	29.9
884.5551	9.69
1078.2464	5.21
1158.8517	11.6
1220.4066	9.12
1228.3471	1.57
1306.0346	1.78
3174.8061	0.378

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
15.2269	0.0252
75.0782	0.0330
130.0984	0.0421
172.1771	0.0479
181.4253	0.125
208.2394	0.0234
227.0031	0.0236
264.7503	0.0336
277.3046	0.0871
292.9609	0.00453
334.2886	0.147
356.1009	0.298
413.0948	0.212
429.6637	1.13
575.5800	2.97
676.1243	23.0
735.0470	2.22
800.3723	0.478
812.4378	18.8
827.4370	29.9
884.5556	9.69
1078.2481	5.21
1158.8511	11.6
1220.4070	9.12
1228.3473	1.57
1306.0345	1.78
3174.8059	0.378

Infrared Spectrum

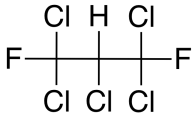


Radiative Efficiency



HCFC-222da

Molecular Formula:	$CCl_2FCHClCCl_2F$
Name:	1,1,2,3,3-Pentachloro-1,3-difluoropropane
CAS number:	431-82-3
Molecular Weight:	252.3



Global Atmospheric Lifetime (years):	4.48
Tropospheric Atmospheric Lifetime (years):	5.23
Stratospheric Atmospheric Lifetime (years):	31.2
Ozone Depletion Potential (ODP):	0.097

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.309	0.283
Global Warming Potential (GWP_H):		
GWP_{20}	1222	1118
GWP_{100}	335	306
Global Temperature Potentials (GTP_H)		
GTP_{20}		580
GTP_{50}		62
GTP_{100}		43

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 1.12 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 0.715 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 5.06$ years

$\tau^{OH}_{Trop} = 5.23$ years

$\tau^{OH}_{Strat} = 149.8$ years

Fractional Atmospheric Loss: 0.886

$O(^1D)$ Reactivity

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

$k_{Est}(T) = 2.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 185$ years

Fractional Atmospheric Loss: 0.024

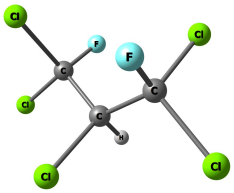
UV Photolysis

UV Spectrum: *No Recommendation*

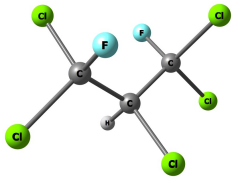
$\tau_{hv} = 50$ years

Fractional Atmospheric Loss: 0.090

Molecular Structure and Infrared Spectrum (7 conformers)



E = 0
Population = 0.323



E = 0
Population = 0.323

Optimized Coordinates (Angstroms)

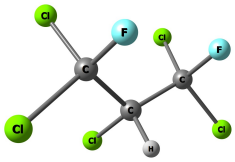
Atom	X	Y	Z
C	1.278424293231	-0.415547691450	-0.224449124838
C	-0.012431140141	0.438095967126	-0.425651341836
C	-1.342496222558	-0.143339323079	0.145950870757
Cl	2.673071106401	0.424403747857	-0.990428481707
Cl	1.642221560002	-0.757307310204	1.487428423804
F	1.139876827616	-1.580253044903	-0.869699469658
H	-0.137158889424	0.543810790137	-1.503620314051
Cl	0.220401445340	2.070929111967	0.262522503022
F	-1.335790158730	-0.135384914495	1.477570181017
Cl	-2.710489644270	0.884094354492	-0.419507539078
Cl	-1.659399177466	-1.819448687448	-0.404882707431

Atom	X	Y	Z
C	1.342761353596	-0.136594212818	0.161567472522
C	0.014657144113	0.425354963624	-0.433597393248
C	-1.276685562324	-0.421816747667	-0.209473559619
Cl	1.662198453680	-1.829632510707	-0.333173012332
Cl	2.712542420404	0.872433435911	-0.432007615706
F	1.331110176259	-0.085252058725	1.492186014778
H	0.143357306511	0.495945914511	-1.513969142796
Cl	-0.221211390908	2.079644455307	0.200146038214
F	-1.135402152179	-1.606863142592	-0.815927448610
Cl	-1.646734102181	-0.707786539101	1.511269692767
Cl	-2.668726646971	0.392161442257	-1.007562045970

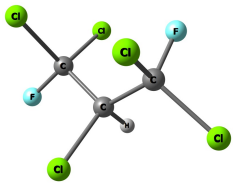
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
29.3929	0.00111
74.5972	0.00998
147.5652	0.0560
179.1164	0.0624
187.8647	0.0253
207.8870	0.0221
237.3801	0.100
245.1418	0.0681
281.9561	0.0401
320.4468	0.0408
370.6419	0.0371
383.1380	0.118
390.2730	0.201
457.6533	0.710
496.9664	0.530
609.7148	15.1
702.4354	22.0
777.9321	26.5
838.8536	2.57
879.3509	17.4
946.2511	3.97
1044.5943	23.8
1137.8575	17.6
1174.1633	15.7
1239.0977	4.72
1321.6256	1.73
3128.2717	0.569

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
29.3952	0.00111
74.5969	0.00998
147.5645	0.0560
179.1163	0.0624
187.8654	0.0253
207.8866	0.0221
237.3803	0.100
245.1420	0.0681
281.9555	0.0401
320.4471	0.0408
370.6420	0.0371
383.1382	0.118
390.2731	0.201
457.6534	0.710
496.9663	0.530
609.7151	15.1
702.4355	22.0
777.9322	26.5
838.8535	2.57
879.3508	17.4
946.2517	3.97
1044.5950	23.8
1137.8576	17.6
1174.1638	15.7
1239.0970	4.72
1321.6251	1.73
3128.2710	0.569



$\Delta E = 0.49$ kcal mol^{-1}
Population = 0.142



$\Delta E = 0.92$ kcal mol^{-1}
Population = 0.068

Optimized Coordinates (Angstroms)

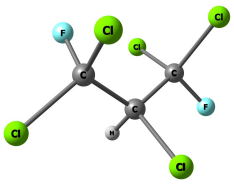
Atom	X	Y	Z
C	1.326367695049	-0.192784279951	-0.421221866602
C	-0.000448551551	0.604577958259	-0.222076859987
C	-1.327207205710	-0.192821781627	-0.421463102825
Cl	2.678145676005	0.991205282854	-0.562128918621
Cl	1.699103727607	-1.359527974622	0.871084045646
F	1.262146347753	-0.854704932202	-1.582956642117
H	-0.000385735193	1.348575995269	-1.021249094123
Cl	-0.000601303470	1.484284484259	1.319990940346
F	-1.262748145422	-0.854759778908	-1.583174871540
Cl	-1.700161537748	-1.359555089614	0.870789245217
Cl	-2.678987967320	0.991132116283	-0.562645875393

Atom	X	Y	Z
C	1.431373354136	0.111198866081	-0.318777331169
C	-0.067996691689	0.408151236406	-0.629757750880
C	-1.154012583883	-0.515651643642	0.001341634925
Cl	1.843104597230	0.085112259635	1.413029908999
Cl	1.930517192980	-1.434138438382	-1.093884303854
F	2.152253677109	1.077955027097	-0.902342755352
H	-0.156049281303	0.280763108525	-1.709742229528
Cl	-0.423115381132	2.123973906756	-0.293223717160
F	-0.763290502037	-1.791526691754	-0.094394351474
Cl	-1.523264565951	-0.179521816039	1.712290376301
Cl	-2.663465815459	-0.339577814684	-0.968882480809

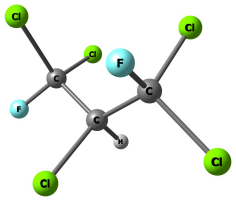
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
23.0084	0.0
78.6677	0.00641
147.9690	0.0778
172.6760	0.0411
181.1487	0.0138
195.4277	0.0129
204.7475	0.0250
249.1832	0.0001
306.3483	0.0754
342.2704	0.0141
377.4660	0.00450
382.3338	0.0216
396.7639	0.203
485.9452	0.441
503.0856	0.558
608.8111	14.2
620.6948	17.5
755.0050	9.24
869.5341	26.5
880.4012	12.4
1004.2331	23.0
1061.9689	14.7
1125.9340	0.365
1158.3848	31.8
1241.9166	2.77
1325.2249	0.387
3107.2220	0.675

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
25.0275	0.00161
78.0523	0.00659
147.3756	0.0882
164.3499	0.0215
180.1348	0.0265
195.3697	0.0158
230.1514	0.0658
255.3311	0.0484
305.1461	0.0661
323.2841	0.193
372.2190	0.0116
384.2585	0.0364
391.9287	0.107
472.3583	1.22
498.1874	0.444
608.3464	13.6
673.4232	10.0
774.8446	17.0
811.8268	21.5
870.5888	23.0
1012.9095	17.5
1067.4890	10.5
1133.6382	12.4
1155.8083	22.4
1245.2162	1.63
1322.7139	0.982
3115.6702	0.741



$\Delta E = 0.92$ kcal mol^{-1}
Population = 0.068



$\Delta E = 1.27$ kcal mol^{-1}
Population = 0.038

Optimized Coordinates (Angstroms)

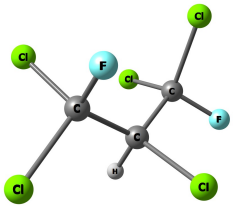
Atom	X	Y	Z
C	1.154576594278	-0.519108051983	-0.042665784601
C	0.072754541707	0.454295211374	-0.602375834839
C	-1.428604693511	0.133855140450	-0.326267337449
Cl	2.670129990319	-0.264926561690	-0.985680260352
Cl	1.513160147865	-0.325164014032	1.692407726822
F	0.764171063084	-1.782489320014	-0.245489408020
H	0.167571191200	0.416150205150	-1.688608797994
Cl	0.426121229839	2.136342326868	-0.123565409018
F	-2.145593079429	1.145887900605	-0.832776033163
Cl	-1.923194951028	-1.342080017297	-1.229040043093
Cl	-1.851223034324	-0.034374819432	1.394910181707

Atom	X	Y	Z
C	1.405544350795	0.074484322753	-0.294157678750
C	-0.087424363258	0.444227865708	-0.582499465089
C	-1.208657608632	-0.196847471049	0.288096458948
Cl	1.816151794818	0.066363974687	1.441405237595
Cl	1.824386193532	-1.505154318782	-1.046099467041
F	2.180325717044	0.982189806753	-0.899147067370
H	-0.276207184704	0.181077976341	-1.622405932499
Cl	-0.259447009567	2.227373311958	-0.451154857352
F	-1.207678413746	0.315427593940	1.517933069924
Cl	-2.800483047215	0.171579843750	-0.473224819773
Cl	-1.065812429065	-1.974803906059	0.430465521407

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
25.0286	0.00161
78.0503	0.00659
147.3745	0.0882
164.3502	0.0215
180.1358	0.0265
195.3700	0.0158
230.1512	0.0658
255.3312	0.0484
305.1466	0.0661
323.2845	0.193
372.2185	0.0116
384.2588	0.0364
391.9287	0.107
472.3585	1.22
498.1868	0.444
608.3468	13.6
673.4239	10.0
774.8447	17.0
811.8268	21.5
870.5895	23.0
1012.9097	17.5
1067.4905	10.5
1133.6402	12.4
1155.8100	22.4
1245.2166	1.63
1322.7138	0.983
3115.6709	0.741

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
45.6591	0.00334
70.3218	0.00493
143.9325	0.0685
169.0915	0.0339
190.6757	0.00702
213.7449	0.00110
227.3706	0.0701
268.9495	0.0150
294.5733	0.183
314.5980	0.0993
355.1401	0.155
386.0969	0.0577
393.8012	0.113
455.1690	0.594
483.8248	1.33
633.7135	12.2
747.6677	14.6
753.6786	31.0
813.6023	10.5
849.1863	11.5
965.9222	11.3
1037.0171	19.8
1138.2489	15.2
1181.2972	15.2
1239.4575	3.07
1323.6115	2.19
3138.4260	0.592



$\Delta E = 1.27$ kcal mol^{-1}
Population = 0.038

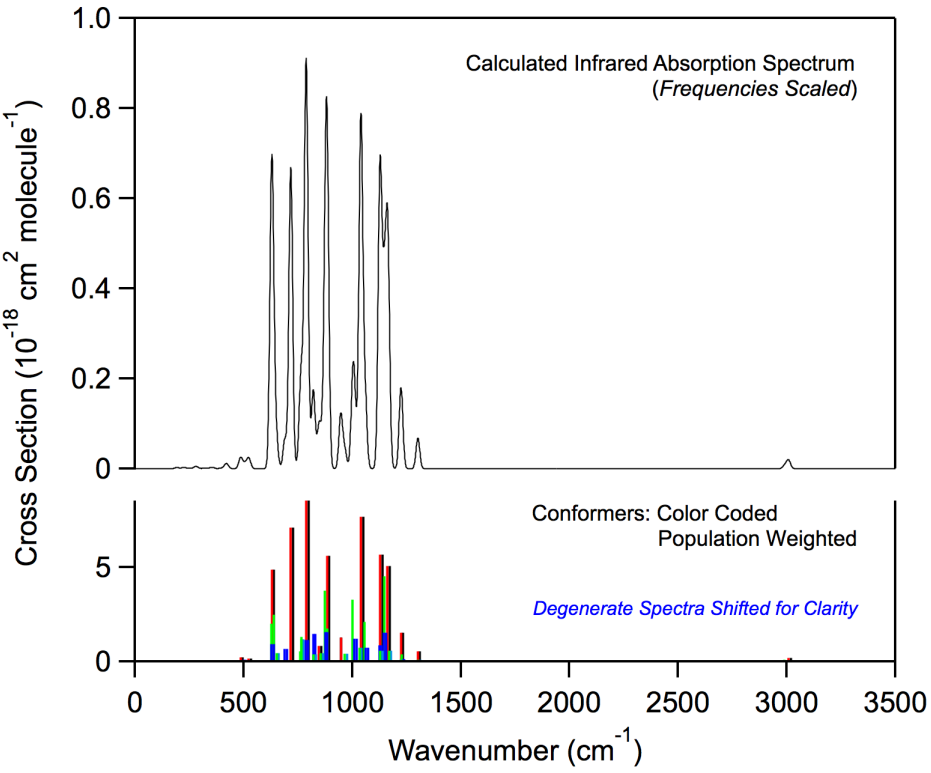
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.209326885758	-0.191230786166	0.290805647058
C	0.088893948764	0.447064001946	-0.582858614519
C	-1.404095181515	0.075415123087	-0.297085636494
Cl	1.068884133051	-1.969222973707	0.435099123993
Cl	2.802134689813	0.178663390480	-0.467744845702
F	1.205077119064	0.322570751114	1.519998717348
H	0.280184614899	0.182914351921	-1.622052921445
Cl	0.257948644280	2.230629882670	-0.453378731684
F	-2.179020701428	0.981189059595	-0.904778836978
Cl	-1.819014648269	-1.505793229846	-1.047901549229
Cl	-1.818212504417	0.068831428908	1.437649647652

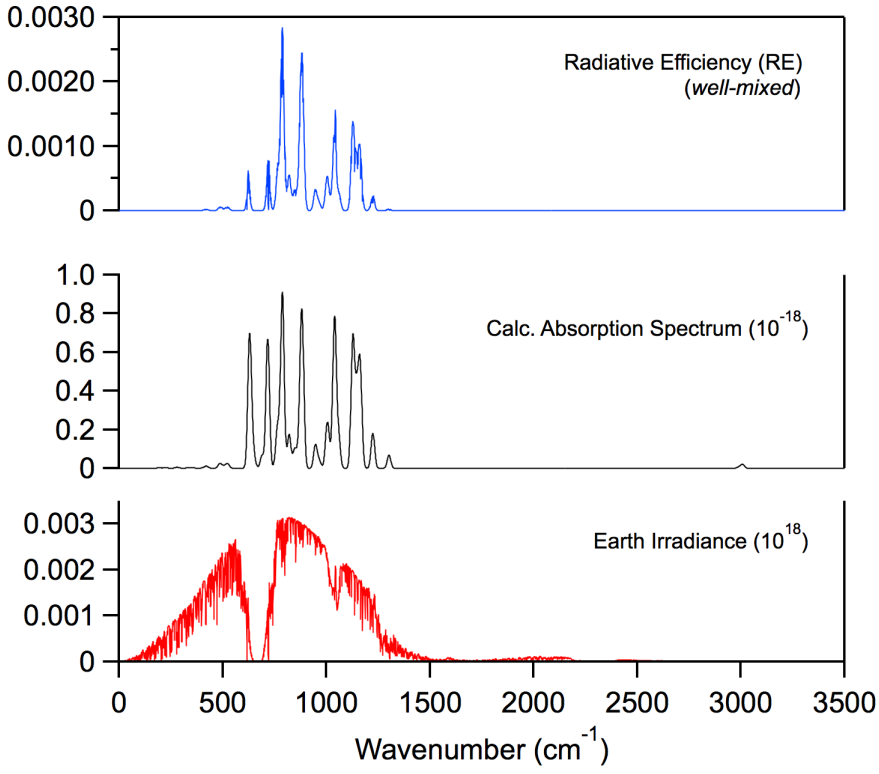
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
45.6599	0.00334
70.3228	0.00493
143.9331	0.0685
169.0918	0.0339
190.6755	0.00702
213.7447	0.00110
227.3711	0.0701
268.9494	0.0150
294.5734	0.183
314.5981	0.0993
355.1401	0.155
386.0971	0.0576
393.8012	0.113
455.1691	0.594
483.8249	1.33
633.7134	12.2
747.6681	14.6
753.6787	31.0
813.6029	10.5
849.1863	11.5
965.9226	11.3
1037.0179	19.8
1138.2501	15.2
1181.2967	15.2
1239.4547	3.07
1323.6087	2.19
3138.4278	0.592

Infrared Spectrum

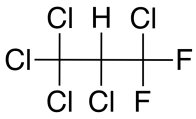


Radiative Efficiency



HCFC-222db

Molecular Formula:	$CCl_3CHClCClF_2$
Name:	1,1,1,2,3-Pentachloro-3,3-difluoropropane
CAS number:	431-80-1
Molecular Weight:	252.3



Global Atmospheric Lifetime (years):	4.62
Tropospheric Atmospheric Lifetime (years):	5.42
Stratospheric Atmospheric Lifetime (years):	31.4
Ozone Depletion Potential (ODP):	0.100

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.289	0.265
Global Warming Potential (GWP_H):		
GWP_{20}	1175	1077
GWP_{100}	322	296
Global Temperature Potentials (GTP_H)		
GTP_{20}		568
GTP_{50}		61
GTP_{100}		41

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 1.08 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 0.691 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

τ^{OH}_{Global} = 5.24 years
τ^{OH}_{Trop} = 5.42 years
τ^{OH}_{Strat} = 154.6.3 years

Fractional Atmospheric Loss: 0.883

O(^{1}D) Reactivity

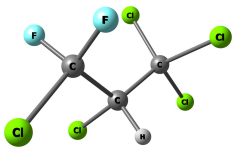
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 2.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)}$ = 185 years
Fractional Atmospheric Loss: 0.025

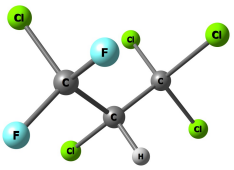
UV Photolysis

UV Spectrum: *No Recommendation*
τ_{hv} = 50 years
Fractional Atmospheric Loss: 0.092

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.908



$\Delta E = 1.70$ kcal mol^{-1}
Population = 0.052

Optimized Coordinates (Angstroms)

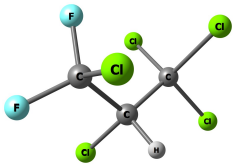
Atom	X	Y	Z
C	1.166322956414	-0.139696761217	-0.113089606711
C	-0.276803509025	0.351229497519	-0.452398677813
C	-1.447051394545	-0.477467825560	0.164107223023
Cl	1.454136878321	-1.728161612965	-0.903637812532
Cl	2.357505489855	1.009150162127	-0.807610815398
Cl	1.438431548695	-0.283308912439	1.642182650373
H	-0.369260554137	0.305833911323	-1.536804616782
Cl	-0.513187833720	2.056287975731	0.031004800961
F	-1.242135169486	-1.787788333916	0.035013057095
F	-1.611765872067	-0.214491800236	1.455618374945
Cl	-2.980267540306	-0.080889300366	-0.701545577159

Atom	X	Y	Z
C	1.084017912442	-0.185551028622	0.013477241942
C	-0.181205493262	0.481892092966	-0.605845812346
C	-1.563794714726	-0.236466340837	-0.534110489365
Cl	2.515396096681	0.739932859003	-0.573530664448
Cl	1.097188951990	-0.185031533185	1.792933933998
Cl	1.256835951956	-1.869404897788	-0.575858175057
H	0.018927067470	0.555862611052	-1.677235487912
Cl	-0.371940509864	2.152024500277	-0.000334916569
F	-2.440665573629	0.542037709564	-1.177890975252
F	-1.510596949468	-1.394550639881	-1.197508972546
Cl	-2.194821739589	-0.547881332548	1.106753317555

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
33.6810	0.000
72.2269	0.00560
146.7991	0.105
168.7157	0.0254
198.2766	0.0163
211.5183	0.0473
221.7897	0.0216
242.2255	0.0644
292.4213	0.0516
300.3494	0.0837
340.2486	0.115
390.0118	0.268
421.3354	0.263
428.9150	0.211
600.9881	10.6
603.9951	5.49
710.2278	17.6
747.6849	22.4
834.3318	2.77
867.2231	2.36
927.5466	22.5
1027.1748	17.5
1176.4622	20.8
1215.6451	20.8
1254.2629	4.82
1326.2989	3.27
3137.0369	0.683

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
23.2762	0.000
83.0236	0.00337
152.6400	0.0526
173.7152	0.0248
180.6715	0.0159
200.0449	0.0661
226.3707	0.0182
268.4066	0.162
283.4046	0.0231
304.4193	0.0382
334.3528	0.0944
398.9706	0.113
426.6693	0.00277
440.0321	0.205
601.3885	9.16
611.5727	10.7
687.3866	3.14
757.7937	21.3
768.8406	7.13
856.3740	5.93
1015.7952	21.7
1057.1904	16.9
1157.9328	22.5
1178.5214	22.5
1240.5547	3.21
1329.3857	2.72
3103.5151	0.561



$\Delta E = 1.84$ kcal mol^{-1}
Population = 0.041

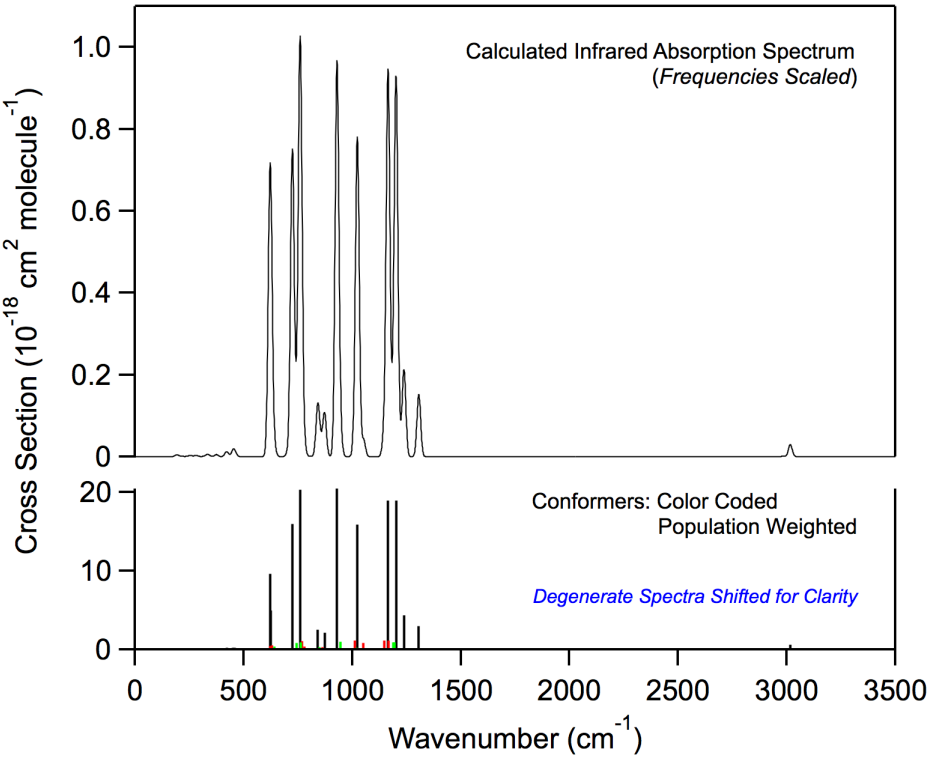
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.019591125987	-0.231369063339	0.068291814413
C	-0.183712055388	0.521205032803	-0.577821208618
C	-1.603035146228	0.198268700303	0.017221150012
Cl	2.470875367728	0.068813447085	-0.950084688401
Cl	1.359192860318	0.307110007186	1.733926073493
Cl	0.712955602903	-1.997064969042	0.070097637426
H	-0.197762004930	0.242776288808	-1.629589449632
Cl	0.106995137275	2.288827626384	-0.530806059694
F	-1.539281337993	-0.181919057173	1.290637123488
F	-2.398265098905	1.260647458555	-0.054505246936
Cl	-2.402223450767	-1.111544471570	-0.937095145551

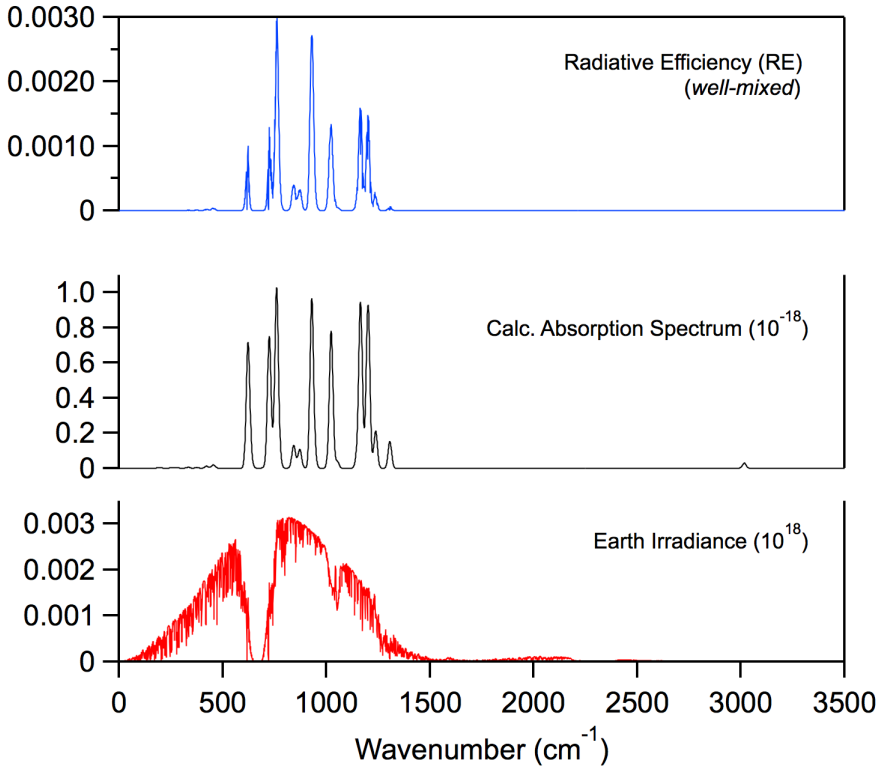
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
40.2242	0.00573
69.4460	0.00676
145.9004	0.0234
169.5175	0.0737
181.3877	0.0403
218.4810	0.00151
233.6260	0.0870
274.6528	0.0473
286.0269	0.223
292.8962	0.0236
329.8804	0.0763
386.0546	0.464
420.0886	0.261
423.5616	0.154
591.4382	4.44
623.4270	8.60
730.3555	20.2
751.6011	22.7
803.1918	0.469
840.8221	8.13
944.4082	25.2
1024.6217	6.10
1200.8418	22.8
1208.0432	21.7
1251.0555	2.47
1327.0656	3.53
3146.8123	0.712

Infrared Spectrum

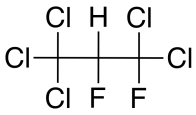


Radiative Efficiency



HCFC-222ea

Molecular Formula:	$CCl_3CHFCCl_2F$
Name:	1,1,1,3,3-Pentachloro-2,3-difluoropropane
CAS number:	146254-25-3
Molecular Weight:	252.3



Global Atmospheric Lifetime (years):	4.68
Tropospheric Atmospheric Lifetime (years):	5.49
Stratospheric Atmospheric Lifetime (years):	31.5
Ozone Depletion Potential (ODP):	0.101

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.267	0.245
Global Warming Potential (GWP_H):		
GWP_{20}	1097	1007
GWP_{100}	301	276
Global Temperature Potentials (GTP_H)		
GTP_{20}		534
GTP_{50}		57
GTP_{100}		39

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 1.07 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 0.681 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

τ^{OH}_{Global} = 5.31 years
τ^{OH}_{Trop} = 5.49 years
τ^{OH}_{Strat} = 156.5.6 years

Fractional Atmospheric Loss: 0.881

$O(^1D)$ Reactivity

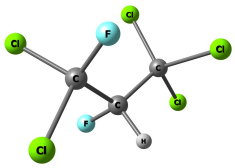
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 2.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)}$ = 185 years
Fractional Atmospheric Loss: 0.025

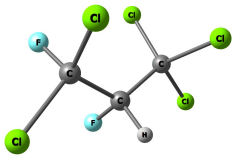
UV Photolysis

UV Spectrum: *No Recommendation*
τ_{hv} = 50 years
Fractional Atmospheric Loss: 0.094

Molecular Structure and Infrared Spectrum (2 conformers)



E = 0
Population = 0.791



$\Delta E = 0.82$ kcal mol^{-1}
Population = 0.199

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.259905834400	0.092162322314	0.140810077082
C	0.116124685215	0.733615073410	-0.219427862171
C	1.412205961892	-0.027979556258	0.217477591264
Cl	-1.512270755638	0.194740411030	1.910717303441
Cl	-2.516702269057	1.090555013976	-0.666794087680
Cl	-1.422120895010	-1.592803718519	-0.404065795372
H	0.126415849332	1.703078510957	0.287428385387
F	0.187568076107	0.925720714699	-1.559064239636
F	1.255268394868	-0.601969913699	1.411365920642
Cl	1.908534027008	-1.271480951948	-0.959528326945
Cl	2.730562759681	1.195660094037	0.356129033987

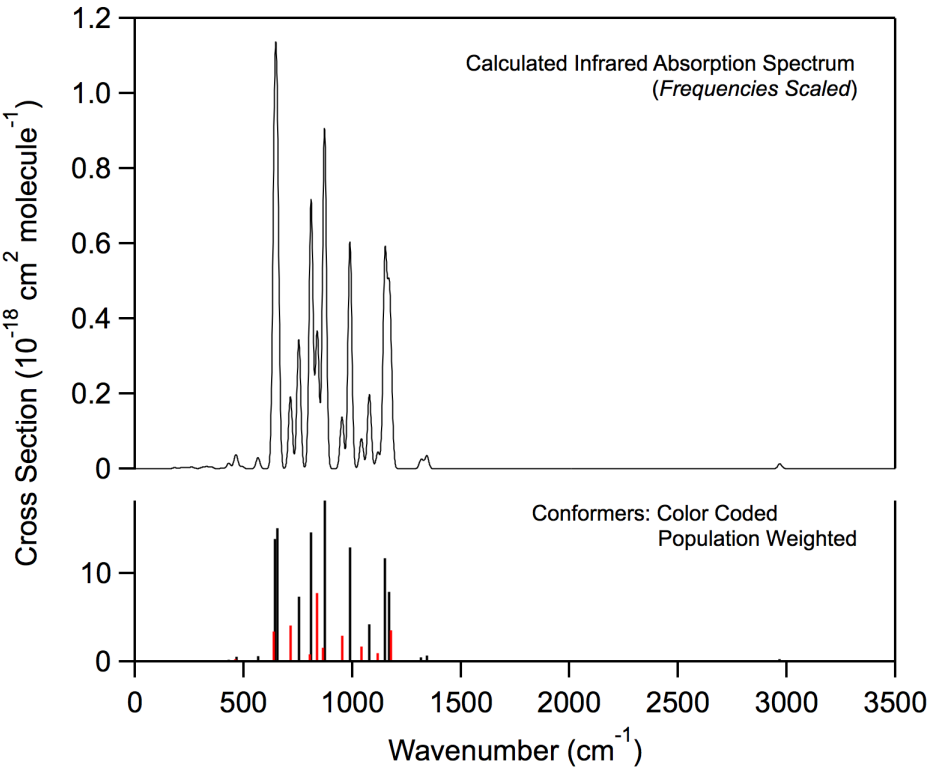
Atom	X	Y	Z
C	-1.254600288482	-0.043577599054	0.078558714970
C	0.129069479023	0.554745729656	0.491599885498
C	1.433191457713	0.056676653246	-0.206653505716
Cl	-2.507305809504	1.021625008803	0.810230673850
Cl	-1.485858004440	-0.077729681724	-1.686716480482
Cl	-1.470049093051	-1.679872822913	0.763565886596
H	0.232904184904	0.397261394040	1.568513106756
F	0.091587070158	1.888574130148	0.213884668498
F	1.436711377486	0.426177683498	-1.487122901248
Cl	2.805149831812	0.897577191307	0.611602570788
Cl	1.702197794381	-1.701235687008	-0.113959619508

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
23.8456	0.0112
73.8474	0.0130
136.5379	0.0684
169.9399	0.0662
192.4803	0.0540
195.9130	0.00956
217.7438	0.116
269.4766	0.0729
284.7785	0.0486
293.6683	0.0931
315.4549	0.119
375.5626	0.0129
401.1417	0.277
437.2148	0.678
542.4515	0.799
624.3021	17.5
636.9731	19.1
741.6331	9.26
801.6510	18.5
867.1905	23.1
990.8736	16.3
1085.5468	5.33
1161.2840	14.8
1180.8635	9.97
1337.3979	0.570
1366.1623	0.893
3085.0328	0.323

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
22.2563	0.001
88.4801	0.00922
135.1823	0.0603
169.7617	0.0545
183.7306	0.0259
201.9853	0.0154
234.4390	0.127
270.3378	0.0459
285.0024	0.0409
299.8889	0.109
332.1725	0.0181
368.0867	0.143
398.7400	0.504
431.1447	1.51
465.0509	0.641
619.3621	17.2
700.6219	20.6
795.4302	4.21
831.4561	39.0
859.4331	7.75
952.1257	14.7
1046.7847	8.58
1127.0413	4.73
1191.0611	17.6
1340.6092	0.116
1349.5560	0.734
3096.9434	0.231

Infrared Spectrum



Radiative Efficiency