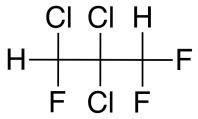
HCFC-233aa

Molecular Formula:	$CHClFCCl_2CHF_2$
Name:	1,2,2-Trichloro-1,3,3-trifluoropropane
CAS number:	–
Molecular Weight:	201.4



Global Atmospheric Lifetime (years):	2.63
Tropospheric Atmospheric Lifetime (years):	2.87
Stratospheric Atmospheric Lifetime (years):	31.6
Ozone Depletion Potential (ODP):	0.043

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.212	0.185
Global Warming Potential (GWP_H):		
GWP_{20}	621	542
GWP_{100}	168	147
Global Temperature Potentials (GTP_H)		
GTP_{20}		219
GTP_{50}		27
GTP_{100}		20

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 2.05 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 1.31 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 2.77$ years

$\tau^{OH}_{Trop} = 2.87$ years

$\tau^{OH}_{Strat} = 87.1$ years

Fractional Atmospheric Loss: 0.947

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: 0.014

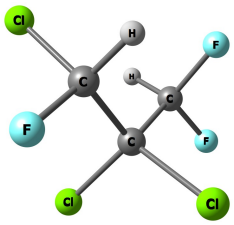
UV Photolysis

UV Spectrum: *No Recommendation*

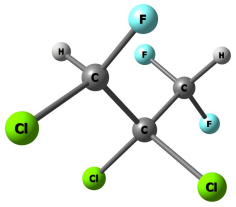
$\tau_{hv} = 68$ years

Fractional Atmospheric Loss: 0.039

Molecular Structure and Infrared Spectrum (6 conformers)



E = 0
Population = 0.378



$\Delta E = 0.12$ kcal mol^{-1}
Population = 0.307

Optimized Coordinates (Angstroms)

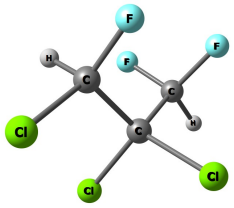
Atom	X	Y	Z
C	1.054185237607	0.164074024069	0.748342157599
C	-0.268849394159	0.195454117529	-0.047116753046
C	-0.904553770237	-1.209462214394	-0.170121474526
Cl	2.237614729625	-0.990136928985	0.030434593975
F	1.604187193745	1.387501356221	0.777455520718
H	0.858133520019	-0.187745084871	1.761663641579
Cl	-0.012323402922	0.844876721907	-1.688616541669
Cl	-1.385164855945	1.255285453902	0.877905398698
H	-0.293950446546	-1.854144087971	-0.808768104271
F	-0.983213821324	-1.750656189597	1.068230782130
F	-2.141694989862	-1.115238167810	-0.676300221186

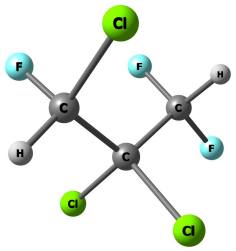
Atom	X	Y	Z
C	0.953980896362	-0.782579738282	-0.310082079632
C	-0.241044169306	0.122961779577	0.062882297756
C	-1.519949049396	-0.753158369806	0.146555849325
Cl	2.517810913299	0.069888681644	-0.339662432843
F	1.009915526141	-1.792907993040	0.594124334163
H	0.791093317073	-1.195952366654	-1.306141570432
Cl	-0.460046495123	1.356884989066	-1.205661706846
Cl	-0.007687018917	0.868083654060	1.668862538613
H	-1.429443332843	-1.477369321448	0.961610190147
F	-2.600073125241	0.014539874032	0.339728170654
F	-1.665909462050	-1.415214189151	-1.025206590906

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
73.1142	0.159
90.0896	0.176
139.6370	0.0231
174.5203	0.0618
200.0686	0.404
224.6424	0.0242
243.6143	0.116
315.5636	0.312
336.7078	0.00153
396.8613	0.239
435.1927	0.239
568.1273	1.40
627.0139	8.80
657.4953	10.4
761.4861	17.8
871.7741	11.7
1050.3990	4.18
1055.0598	0.985
1137.0136	12.8
1169.4949	23.6
1191.5291	16.8
1275.1111	3.16
1365.3605	1.64
1376.5425	5.07
1396.1372	1.98
3097.8075	1.81
3126.9486	0.388

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
76.7934	0.126
85.3146	0.211
135.8057	0.0357
176.1698	0.0524
201.1298	0.0190
211.8240	0.462
258.8612	0.0881
294.2464	0.164
353.7172	0.111
406.9289	0.174
438.6215	0.249
554.7214	3.18
622.7051	7.46
680.6899	8.84
791.6920	15.2
881.5945	12.7
1034.6335	2.88
1064.0601	6.34
1115.9666	13.3
1140.9176	19.0
1190.0643	20.1
1283.1525	3.55
1357.1075	1.66
1372.8227	6.84
1396.2226	1.99
3094.1435	1.84
3124.0466	0.410





$\Delta E = 0.75$ kcal mol^{-1}
Population = 0.106

$\Delta E = 0.81$ kcal mol^{-1}
Population = 0.097

Optimized Coordinates (Angstroms)

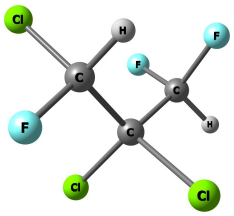
Atom	X	Y	Z
C	0.688836666977	-0.574894413708	-0.719574955363
C	-0.248269031160	0.260464343024	0.184056975046
C	-1.740480443251	-0.076913539174	-0.102154579370
Cl	2.419037046012	-0.196067620028	-0.478588421233
F	0.483979474967	-1.883719870797	-0.464924743671
H	0.456433992377	-0.361451493724	-1.763944594993
Cl	-0.042539674419	1.997029265968	-0.207184085655
Cl	0.063606093731	-0.049331126098	1.909829230224
H	-2.393715631515	0.623093040689	0.428403744633
F	-1.954119041621	0.025390318368	-1.434660279825
F	-2.025743452097	-1.334259904520	0.269620710204

Atom	X	Y	Z
C	1.091304248688	-0.287687077963	-0.714028909143
C	-0.286847640309	0.199472670954	-0.200994308830
C	-0.664609501573	-0.334533434334	1.202694758934
Cl	2.411753353848	0.088870053853	0.455669836052
F	1.068592828439	-1.616564462641	-0.914379453641
H	1.338983237635	0.229677774242	-1.641899383056
Cl	-1.508966927945	-0.352474598852	-1.388550887115
Cl	-0.266636142039	1.988106718047	-0.128336783013
H	0.043974567575	0.030953502828	1.952276824577
F	-1.904227033783	0.072389876683	1.521963713815
F	-0.644627990535	-1.680695022818	1.182888591420

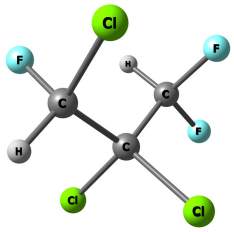
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
63.7850	0.0899
96.5663	0.111
146.7133	0.0390
170.5769	0.0267
208.3609	0.231
214.9233	0.0906
254.5974	0.0618
308.9263	0.0287
377.2131	0.479
395.0159	0.269
436.5505	0.507
539.7889	7.49
582.8125	3.63
670.2909	8.46
842.4676	11.5
879.7378	13.4
975.6948	3.89
1100.9248	7.45
1132.8431	14.6
1138.6560	8.43
1179.7037	28.9
1280.4725	4.69
1358.3855	1.22
1382.4292	3.73
1394.9997	4.79
3085.9326	2.51
3120.0693	0.374

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
61.5183	0.123
98.2668	0.0668
148.7970	0.0565
171.8802	0.0805
199.7776	0.170
243.8871	0.164
245.9129	0.113
316.0189	0.331
342.4142	0.134
387.3778	0.262
434.2920	0.444
526.3131	3.29
641.4227	6.54
670.8172	9.52
759.6028	14.2
877.4437	18.0
995.7250	0.941
1095.6528	1.87
1143.5720	2.49
1165.3612	28.5
1181.0443	21.5
1281.3669	3.33
1363.4703	2.17
1388.2608	4.49
1395.9750	2.13
3091.2689	1.96
3119.5869	0.511



$\Delta E = 1.12$ kcal mol^{-1}
Population = 0.057



$\Delta E = 1.40$ kcal mol^{-1}
Population = 0.036

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	0.666840687930	0.578847925667	0.811799818405
C	-0.448843082605	0.101931906885	-0.146403791930
C	-0.653816101274	-1.436220292744	-0.167247834663
Cl	2.282561025695	-0.052978452704	0.364858978556
F	0.712630367306	1.923818949166	0.811731199357
H	0.452853397866	0.210887718907	1.815732695091
Cl	-0.182026949053	0.682333273923	-1.806243794126
Cl	-1.986666080459	0.790614023246	0.506087590256
H	-1.604900426403	-1.679624561795	-0.651406651485
F	0.347139271018	-2.054128130445	-0.812626313726
F	-0.669368110021	-1.878652360105	1.111808104265

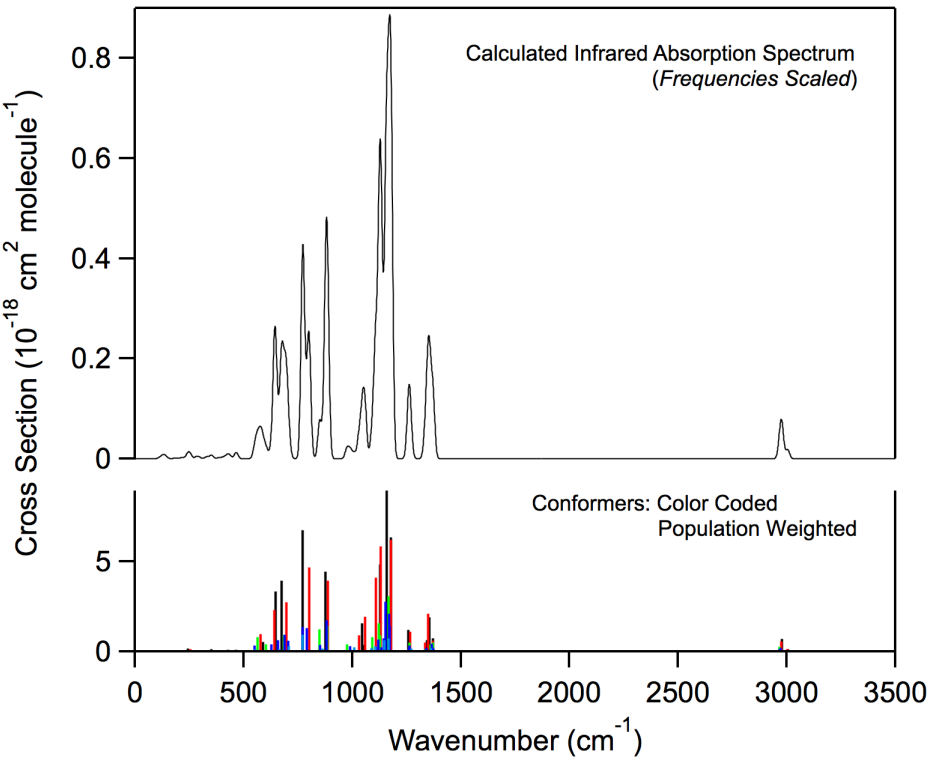
Atom	X	Y	Z
C	0.997965614090	0.895327232262	0.089918421130
C	-0.367857099173	0.168443455632	0.171743931481
C	-0.638495538680	-0.776175254912	-1.027367759630
Cl	2.414274014666	-0.186019229871	0.258278134828
F	1.070693828174	1.511406337865	-1.115623287761
H	1.065933922186	1.633293894830	0.889783177951
Cl	-1.610439338320	1.474571061432	0.092066336920
Cl	-0.511432593393	-0.714150069240	1.708016594992
H	-0.501585683431	-0.229817047604	-1.966563655695
F	0.207021765684	-1.821893671754	-0.986792918526
F	-1.893767891802	-1.248983708641	-0.956643975689

Infrared Absorption Spectrum (unscaled frequencies)

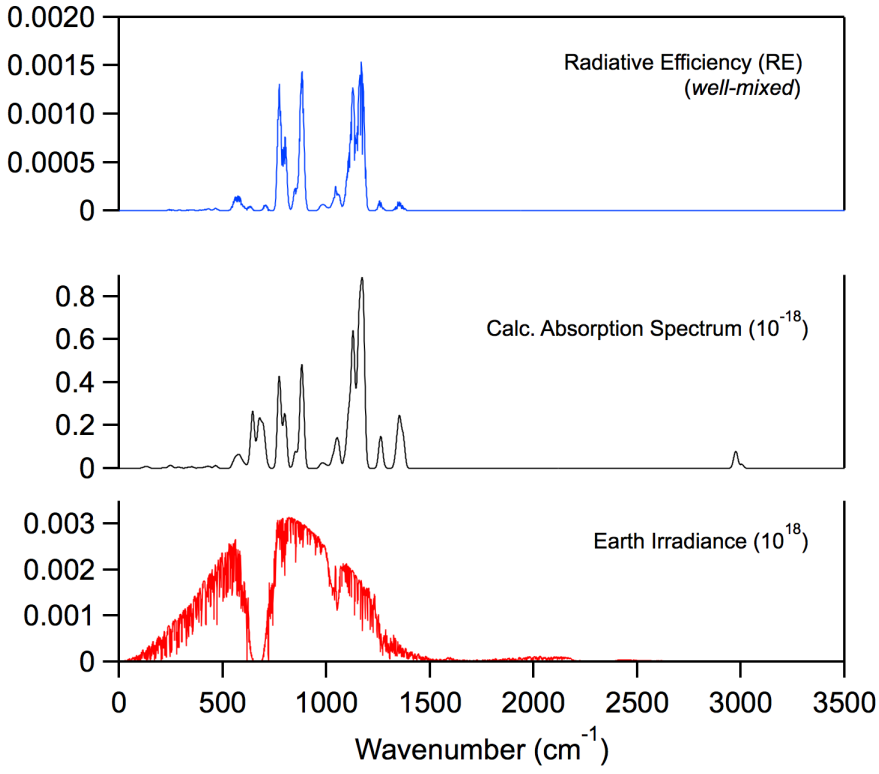
Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
60.6458	0.107
99.1635	0.0770
148.1686	0.0316
167.9553	0.142
198.7972	0.124
245.1708	0.169
249.4192	0.123
291.1812	0.423
369.5099	0.406
392.6575	0.267
406.5507	0.644
567.0222	1.21
606.4520	6.74
690.9066	10.4
781.2469	22.7
846.0757	6.15
990.8907	5.16
1117.7809	4.41
1129.4471	11.7
1155.0114	13.1
1185.6750	24.9
1279.3190	3.79
1362.5353	2.42
1385.7834	2.41
1397.8291	2.55
3085.6026	2.62
3125.1083	0.385

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
58.2380	0.136
93.9325	0.0653
153.6506	0.0729
158.9588	0.00623
201.4490	0.208
240.9994	0.0690
253.2874	0.382
288.1518	0.268
359.7254	0.157
388.3352	0.365
435.8033	0.244
528.1467	3.55
646.5693	3.61
694.1344	8.01
760.7460	26.1
855.4678	4.83
1010.8221	6.32
1096.8664	5.39
1115.2497	8.52
1158.4758	17.4
1179.5068	20.4
1291.2614	4.43
1354.5470	0.935
1386.5811	5.70
1395.2771	2.17
3082.7236	1.91
3122.9936	0.500

Infrared Spectrum

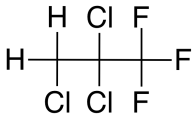


Radiative Efficiency



HCFC-233ab

Molecular Formula:	$CH_2ClCCl_2CF_3$
Name:	2,2,3-Trichloro-1,1,1-trifluoropropane
CAS number:	7125-83-9
Molecular Weight:	201.4



Global Atmospheric Lifetime (years):	2.57
Tropospheric Atmospheric Lifetime (years):	2.80
Stratospheric Atmospheric Lifetime (years):	31.4
Ozone Depletion Potential (ODP):	0.042

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.223	0.194
Global Warming Potential (GWP_H):		
GWP_{20}	639	556
GWP_{100}	173	151
Global Temperature Potentials (GTP_H)		
GTP_{20}		223
GTP_{50}		27
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*

$k_{SAR}(298\ K) = 2.09 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 1.34 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 2.71$ years

$\tau^{OH}_{Trop} = 2.80$ years

$\tau^{OH}_{Strat} = 85.3$ years

Fractional Atmospheric Loss: 0.948

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: 0.014

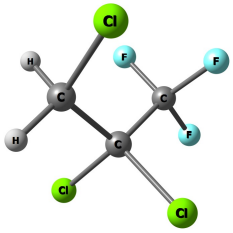
UV Photolysis

UV Spectrum: *No Recommendation*

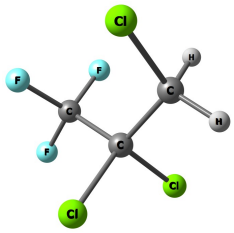
$\tau_{hv} = 68$ years

Fractional Atmospheric Loss: 0.038

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.350



E = 0
Population = 0.350

Optimized Coordinates (Angstroms)

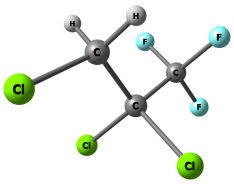
Atom	X	Y	Z
C	-1.001384326228	-0.693802901826	-0.944935904132
C	0.210207063780	-0.422366133611	-0.044333708297
C	0.575947007181	1.086200815311	0.083695291320
Cl	-2.552952558759	-0.028954833069	-0.337740426277
H	-0.815159071285	-0.249059698494	-1.921505413902
H	-1.124403646907	-1.770479332968	-1.042517891293
Cl	1.599320822994	-1.234290879055	-0.862670037598
Cl	-0.009376968795	-1.099101525665	1.591163047145
F	1.749613826007	1.245503069608	0.683226766354
F	0.643010073351	1.626780742093	-1.137798580994
F	-0.343625221340	1.743825677677	0.781604857673

Atom	X	Y	Z
C	-1.001833238343	-0.694521968504	0.943906746563
C	0.210143055382	-0.422479759654	0.044005413035
C	0.576033296507	1.086160171127	-0.082727514775
Cl	-2.553110497717	-0.029111408157	0.336584023373
H	-1.124962235235	-1.771264235322	1.040620108056
H	-0.815977496796	-0.250533328923	1.920889913896
Cl	-0.008817784628	-1.097957293975	-1.592094764453
Cl	1.598870122367	-1.235117072915	0.862290771269
F	1.749954938395	1.245841413663	-0.681658960448
F	-0.343211372960	1.744375527882	-0.780511961656
F	0.642633213027	1.625806954779	1.139204225139

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
58.1792	0.0511
108.5667	0.147
146.0255	0.0161
190.4922	0.162
216.4035	0.279
255.5710	0.186
276.7282	0.218
298.9455	0.203
360.4100	0.144
388.7390	0.0348
504.9019	2.65
554.6346	1.42
587.5598	1.12
704.8269	4.78
748.2421	14.1
803.9389	5.18
856.4807	6.19
989.2948	8.72
1080.8588	3.60
1195.5626	19.4
1223.5972	20.1
1248.7516	25.1
1280.1045	12.8
1318.6918	9.40
1458.8848	1.69
3112.1762	0.650
3181.3465	0.0445

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
58.1792	0.0511
108.5666	0.147
146.0255	0.0161
190.4922	0.162
216.4036	0.279
255.5710	0.186
276.7282	0.218
298.9455	0.203
360.4100	0.144
388.7390	0.0348
504.9019	2.65
554.6346	1.42
587.5598	1.12
704.8269	4.78
748.2421	14.1
803.9389	5.18
856.4807	6.19
989.2948	8.72
1080.8588	3.60
1195.5627	19.4
1223.5971	20.1
1248.7516	25.1
1280.1046	12.8
1318.6918	9.40
1458.8848	1.69
3112.1762	0.650
3181.3465	0.0445



$\Delta E = 0.09$ kcal mol^{-1}
Population = 0.299

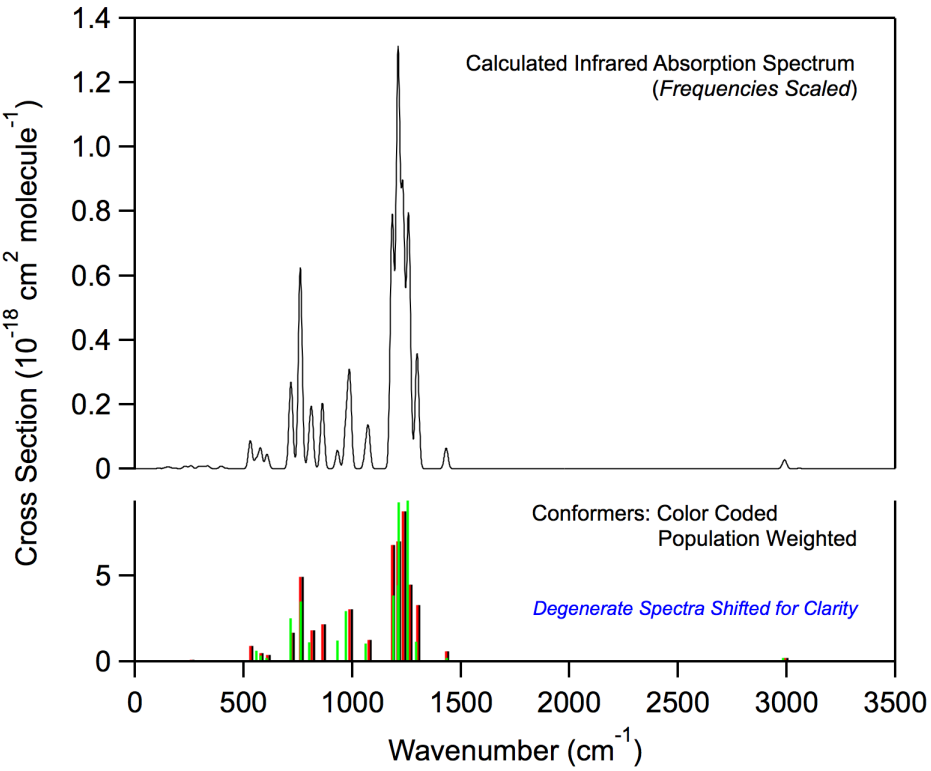
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.420622968022	0.225791207218	0.000000000000
C	0.079003064894	-0.091985588687	0.000000000000
C	0.872493930978	1.248794632283	0.000000000000
Cl	-2.466702759334	-1.219758578665	0.000000000000
H	-1.655305595132	0.805355470489	0.892359349206
H	-1.655305595132	0.805355470489	-0.892359349206
Cl	0.546576704630	-1.000466906134	-1.469349489154
Cl	0.546576704630	-1.000466906134	1.469349489154
F	2.180770333989	1.050476516750	0.000000000000
F	0.547218589283	1.965966841150	-1.080160649028
F	0.547218589283	1.965966841150	1.080160649028

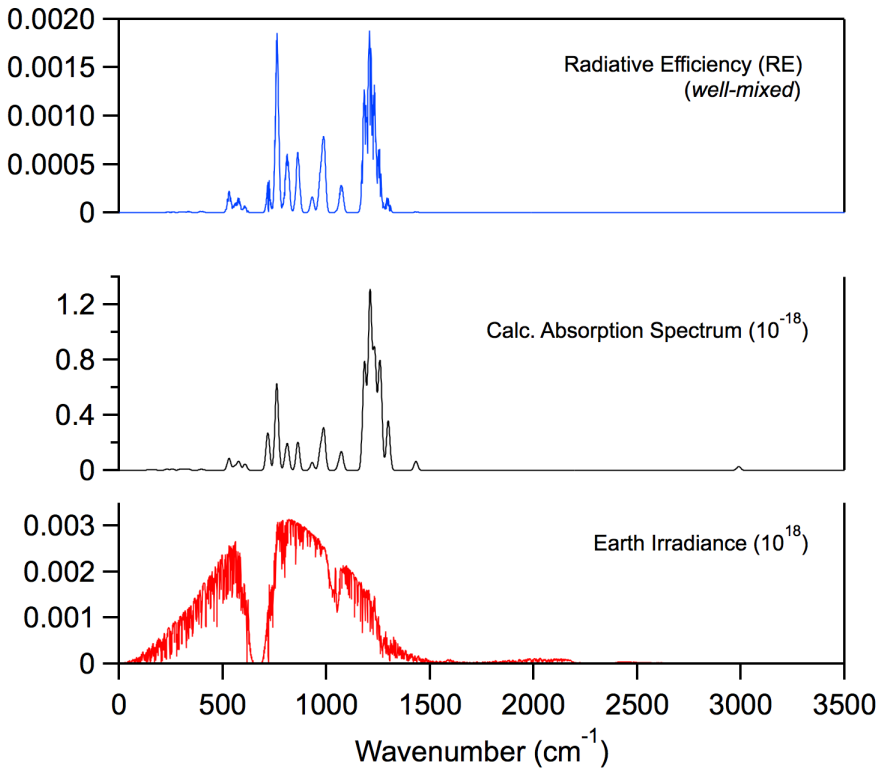
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
73.5938	0.00211
91.3323	0.229
132.0810	0.150
183.1713	0.237
204.5211	0.0527
258.4568	0.111
296.1597	0.0578
298.7900	0.0647
365.0176	0.229
373.0476	0.0898
533.7844	2.06
554.1919	1.17
583.3707	0.650
700.6199	8.45
750.1259	11.7
791.9825	3.76
929.8245	4.07
971.6966	9.82
1067.2991	3.49
1202.7156	12.8
1225.3756	14.9
1227.9910	31.1
1272.3688	31.4
1314.3494	3.91
1463.9733	0.739
3101.9135	0.684
3168.7132	0.0116

Infrared Spectrum

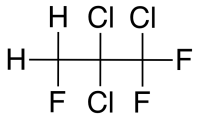


Radiative Efficiency



HCFC-233ac

Molecular Formula:	$CH_2FCCl_2CClF_2$
Name:	1,2,2-Trichloro-1,1,3-trifluoropropane
CAS number:	–
Molecular Weight:	201.4



Global Atmospheric Lifetime (years):	3.71
Tropospheric Atmospheric Lifetime (years):	4.14
Stratospheric Atmospheric Lifetime (years):	35.3
Ozone Depletion Potential (ODP):	0.057

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.277	0.250
Global Warming Potential (GWP_H):		
GWP_{20}	1142	1030
GWP_{100}	311	280
Global Temperature Potentials (GTP_H)		
GTP_{20}		485
GTP_{50}		54
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*

$k_{SAR}(298\ K) = 1.42 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 0.904 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 4.01$ years

$\tau^{OH}_{Trop} = 4.14$ years

$\tau^{OH}_{Strat} = 121.4$ years

Fractional Atmospheric Loss: 0.925

$O(^1D)$ 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: 0.020

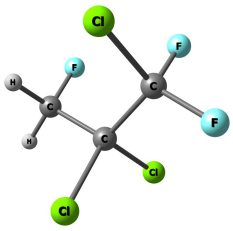
UV Photolysis

UV Spectrum: *No Recommendation*

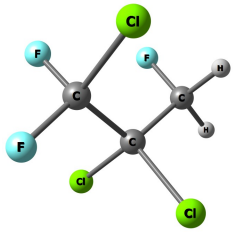
$\tau_{hv} = 68$ years

Fractional Atmospheric Loss: 0.055

Molecular Structure and Infrared Spectrum (9 conformers)



E = 0
Population = 0.195



E = 0
Population = 0.195

Optimized Coordinates (Angstroms)

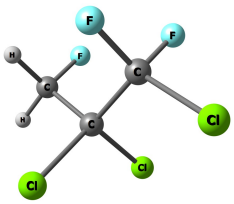
Atom	X	Y	Z
C	0.782063037928	-0.579223305604	1.483916340513
C	0.531124150720	0.188562501816	0.179346277873
C	-0.764864954870	-0.240339437122	-0.578601527639
H	-0.046892510210	-0.395481818423	2.173440752325
F	0.879753405694	-1.918328367327	1.232079688056
H	1.716523722881	-0.213355036046	1.918682895719
Cl	1.900703839056	-0.092138037820	-0.948324415896
Cl	0.426323514700	1.925054632849	0.597933267944
Cl	-2.227340056488	-0.102772177737	0.465825256255
F	-0.945416390762	0.522030541774	-1.651700233912
F	-0.657843758649	-1.506264496361	-0.970684301237

Atom	X	Y	Z
C	0.778921113914	0.583633754096	1.484153985827
C	0.532834358433	-0.185893844653	0.179685920775
C	-0.764914088531	0.235942769329	-0.579215700005
H	1.715018180064	0.222823092456	1.919626425244
F	0.869734680382	1.923149574329	1.231928735818
H	-0.049489354732	0.395770291897	2.173222659347
Cl	0.436892012082	-1.922772714224	0.598792262804
Cl	1.901626544648	0.101619162377	-0.947224347539
Cl	-2.227300929246	0.091040291004	0.464342336229
F	-0.664299049693	1.502282556913	-0.971655371282
F	-0.940784467322	-0.527720933525	-1.652171907218

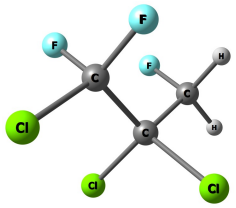
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
59.5816	0.0527
119.8879	0.218
158.3300	0.0157
187.7554	0.0723
233.2800	0.393
243.6487	0.124
283.6774	0.456
308.8969	0.0148
344.8913	0.207
390.9529	0.164
423.3443	0.186
433.2716	0.349
552.8127	4.37
661.2490	3.25
719.0768	20.1
872.8170	16.0
943.0206	26.1
1071.5394	1.22
1107.8546	3.81
1127.8267	9.04
1212.0228	18.2
1222.1438	23.0
1290.3972	1.84
1418.5862	1.55
1494.8751	1.43
3063.6755	1.39
3122.5945	1.28

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
59.5817	0.0527
119.8878	0.218
158.3300	0.0157
187.7554	0.0723
233.2799	0.393
243.6487	0.124
283.6773	0.456
308.8968	0.0148
344.8911	0.207
390.9529	0.164
423.3443	0.186
433.2716	0.349
552.8128	4.37
661.2490	3.25
719.0767	20.1
872.8169	16.0
943.0207	26.1
1071.5394	1.22
1107.8546	3.81
1127.8269	9.04
1212.0229	18.2
1222.1437	23.0
1290.3975	1.84
1418.5863	1.55
1494.8751	1.43
3063.6753	1.39
3122.5943	1.28



$\Delta E = 0.20$ kcal mol^{-1}
Population = 0.139



$\Delta E = 0.20$ kcal mol^{-1}
Population = 0.139

Optimized Coordinates (Angstroms)

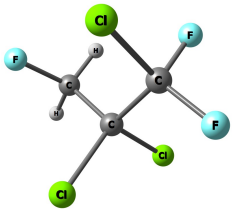
Atom	X	Y	Z
C	1.771575406806	-0.281682666059	0.742046009266
C	0.528319175470	0.288805095389	0.031994101687
C	-0.724649857508	-0.608984783023	0.282991966651
H	1.548999843744	-0.384117822285	1.808518564409
F	2.105465823176	-1.500166132721	0.224796591159
H	2.597608124221	0.419954523699	0.598008675871
Cl	0.833828678762	0.401624240129	-1.720914979278
Cl	0.250394013569	1.907449250151	0.746966540810
Cl	-2.237461189384	0.055880588192	-0.399044712550
F	-0.515693551069	-1.814282483154	-0.241037553630
F	-0.879195467787	-0.753426810318	1.605503795604

Atom	X	Y	Z
C	1.774054688699	-0.287359550367	-0.735459301934
C	0.530155531759	0.287082670216	-0.029735152461
C	-0.724103039993	-0.608397027646	-0.282537601684
H	2.601236110463	0.412716765204	-0.590423064313
F	2.103884255309	-1.505669664264	-0.215205042565
H	1.554112645795	-0.391161875565	-1.802345893392
Cl	0.257699248060	1.905085714472	-0.748254466159
Cl	0.831214699419	0.402280924523	1.723788842221
Cl	-2.237274654893	0.060963744171	0.394282883000
F	-0.875420547446	-0.754800839350	-1.605206791238
F	-0.519196937173	-1.813235861392	0.244139588525

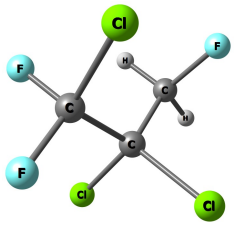
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
61.1906	0.0432
123.6971	0.296
160.8117	0.0540
181.8035	0.135
212.3214	0.229
246.9908	0.0814
292.8864	0.415
313.8515	0.286
336.9734	0.227
409.1034	0.0685
425.7521	0.00772
449.2551	0.507
529.4427	8.62
630.2838	2.61
765.0309	9.89
879.2657	17.2
963.6655	20.8
1068.7545	7.94
1091.2762	8.69
1130.0548	17.1
1183.2629	16.7
1208.9049	19.7
1292.7960	0.599
1413.9891	2.33
1494.6001	0.951
3061.7665	1.55
3122.4177	1.09

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
61.1906	0.0432
123.6971	0.296
160.8117	0.0540
181.8035	0.135
212.3214	0.229
246.9908	0.0814
292.8866	0.415
313.8516	0.286
336.9735	0.227
409.1035	0.0685
425.7523	0.00772
449.2552	0.507
529.4428	8.62
630.2840	2.61
765.0312	9.89
879.2660	17.2
963.6658	20.8
1068.7545	7.94
1091.2764	8.69
1130.0552	17.1
1183.2636	16.7
1208.9052	19.7
1292.7958	0.599
1413.9888	2.33
1494.5997	0.951
3061.7670	1.55
3122.4181	1.09



$\Delta E = 0.40$ kcal mol^{-1}
Population = 0.099



$\Delta E = 0.40$ kcal mol^{-1}
Population = 0.099

Optimized Coordinates (Angstroms)

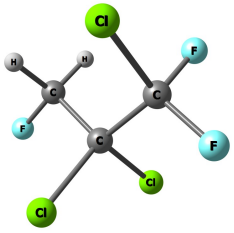
Atom	X	Y	Z
C	0.544697847878	1.224264504122	1.189549753325
C	0.581101799403	0.205616321246	0.038313883884
C	-0.608456283587	-0.804108722770	0.045035947918
H	1.506783941807	1.742820966640	1.211376785506
F	-0.457693511614	2.134115246203	1.016614806361
H	0.392472494774	0.681324015235	2.128076641846
Cl	2.075173241400	-0.771585274556	0.299959260404
Cl	0.659980109342	1.035941519453	-1.535495213126
Cl	-2.196998445189	-0.014376703434	-0.191442637830
F	-0.445662292064	-1.718413364390	-0.905375191823
F	-0.628007902149	-1.425005507751	1.231490963535

Atom	X	Y	Z
C	0.553316582581	-1.218566382760	1.190430103788
C	0.583110670189	-0.200064204499	0.038879247434
C	-0.611847116731	0.803256294180	0.046500630411
H	0.399090522712	-0.676188259966	2.128955791944
F	-0.444331982959	-2.133847353412	1.018726462160
H	1.518200004923	-1.731932888060	1.211454682103
Cl	0.664896171406	-1.030395436948	-1.534777450279
Cl	2.072166886442	0.785222890049	0.298783606817
Cl	-2.196355294460	0.004937797491	-0.188200171473
F	-0.633565832615	1.424363567330	1.232807959351
F	-0.454901611488	1.718160976596	-0.904316862256

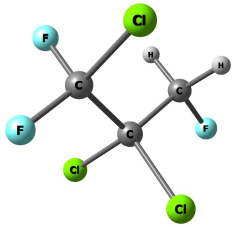
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
61.6837	0.0744
124.4767	0.312
163.6278	0.0262
180.1269	0.102
225.2132	0.329
253.1178	0.483
267.3068	0.172
302.8173	0.181
334.4109	0.0727
393.7036	0.155
429.7241	0.0391
440.6234	0.556
560.6518	4.45
647.6371	4.12
760.2899	18.3
830.1984	19.5
952.5552	14.1
1069.9617	3.62
1107.4035	12.1
1133.8954	13.1
1189.2840	12.8
1220.0462	21.2
1298.9931	0.973
1418.5925	1.16
1494.3739	0.820
3059.2089	1.43
3120.6440	1.15

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
61.6845	0.0744
124.4776	0.312
163.6282	0.0262
180.1267	0.102
225.2137	0.329
253.1188	0.483
267.3072	0.172
302.8192	0.181
334.4116	0.0727
393.7047	0.155
429.7243	0.0391
440.6239	0.556
560.6528	4.45
647.6374	4.12
760.2903	18.3
830.2006	19.5
952.5565	14.1
1069.9660	3.62
1107.4050	12.1
1133.8958	13.1
1189.2845	12.8
1220.0471	21.2
1298.9944	0.973
1418.5938	1.16
1494.3738	0.820
3059.2069	1.43
3120.6427	1.15



$\Delta E = 0.82$ kcal mol^{-1}
Population = 0.049



$\Delta E = 0.82$ kcal mol^{-1}
Population = 0.049

Optimized Coordinates (Angstroms)

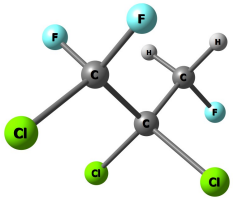
Atom	X	Y	Z
C	0.885432355105	0.780126387503	1.249809303729
C	0.461306520968	0.014979782099	-0.011998983989
C	-1.009076155839	-0.489515313658	0.082930426711
H	0.721645830447	0.137371773106	2.120949269434
F	2.204588196637	1.109785485009	1.162978628858
H	0.287396015142	1.691423380684	1.337104971934
Cl	1.498566095482	-1.444831222329	-0.181876702058
Cl	0.650131841344	1.050564900934	-1.455849199019
Cl	-2.175488608380	0.864710095706	0.307202766486
F	-1.351817736341	-1.162833839867	-1.005550398991
F	-1.121020354567	-1.300260429186	1.140590916905

Atom	X	Y	Z
C	0.883544512533	-0.782705513499	1.249042366398
C	0.460474349058	-0.014779392065	-0.011430920765
C	-1.009657428650	0.490388626365	0.083804959478
H	0.284933167362	-1.693825156656	1.334222008648
F	2.202549016204	-1.112962347302	1.162183661990
H	0.719714591856	-0.141604177382	2.121391659727
Cl	0.649386360286	-1.047576326123	-1.457265673763
Cl	1.498672286637	1.444759329691	-0.177881123871
Cl	-2.176972308733	-0.863597880648	0.304800324182
F	-1.121634490387	1.299076268984	1.143035974482
F	-1.351480056167	1.166090568635	-1.003487236507

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
70.3159	0.0337
105.6610	0.337
155.1554	0.259
168.4385	0.157
222.3820	0.00530
237.7201	0.155
287.7265	0.145
329.9702	0.115
337.0641	0.285
354.4112	0.169
423.5845	0.104
452.5012	0.192
587.4595	4.58
633.5192	1.79
733.0063	23.3
822.0190	21.0
1011.7045	17.0
1066.8221	2.57
1079.8370	4.25
1141.7698	12.7
1188.4937	18.2
1236.7338	19.3
1284.0568	2.21
1418.4288	0.684
1500.7383	0.482
3056.1333	1.85
3117.9030	1.13

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
70.3161	0.0337
105.6614	0.337
155.1554	0.259
168.4386	0.157
222.3822	0.00530
237.7200	0.155
287.7266	0.145
329.9703	0.115
337.0641	0.285
354.4112	0.169
423.5846	0.104
452.5011	0.192
587.4595	4.58
633.5192	1.79
733.0064	23.3
822.0189	21.0
1011.7046	17.0
1066.8224	2.57
1079.8368	4.25
1141.7697	12.7
1188.4938	18.2
1236.7338	19.3
1284.0563	2.21
1418.4286	0.684
1500.7380	0.482
3056.1332	1.85
3117.9031	1.13



$\Delta E = 1.02$ kcal mol^{-1}
Population = 0.035

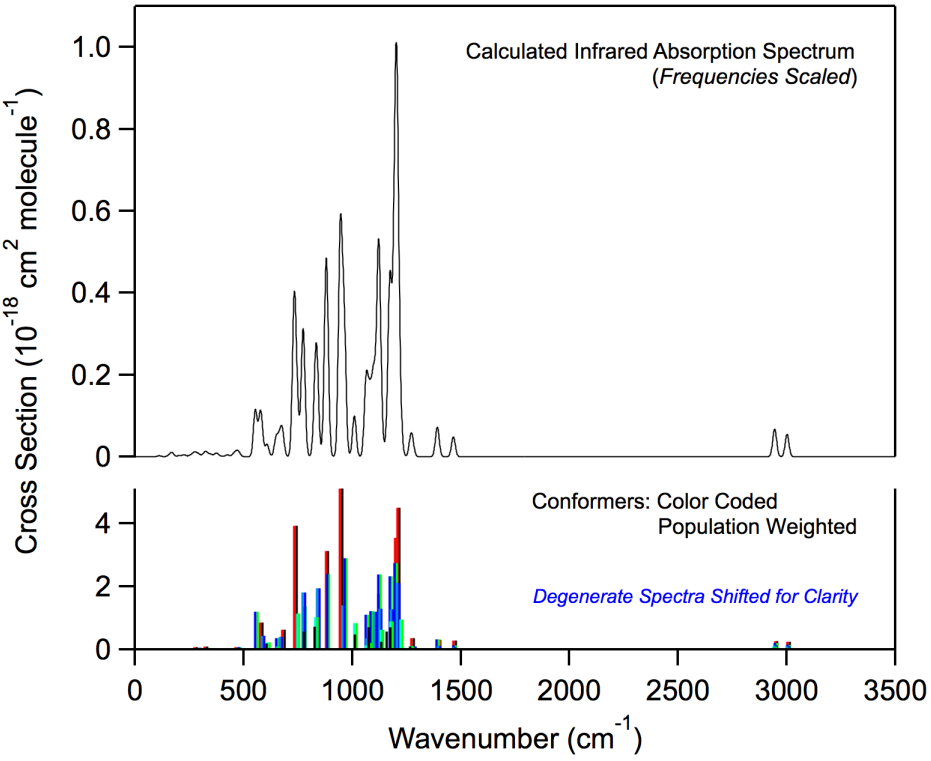
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.503524103318	-0.005052206018	1.145313558100
C	0.481220570247	0.000042965425	-0.007573516942
C	-0.955966200932	-0.002750248517	0.595525369516
H	1.349408642281	-0.904930735060	1.748301381800
F	2.768115734695	-0.002718105357	0.641271034528
H	1.349296733970	0.889375476409	1.756329217464
Cl	0.714272564852	-1.464063625881	-1.005940004551
Cl	0.714083096652	1.473061471577	-0.992788790927
Cl	-2.261934479211	0.002596531073	-0.614795732517
F	-1.089624291612	-1.086689733666	1.370567901123
F	-1.089757474259	1.074179210015	1.380256582407

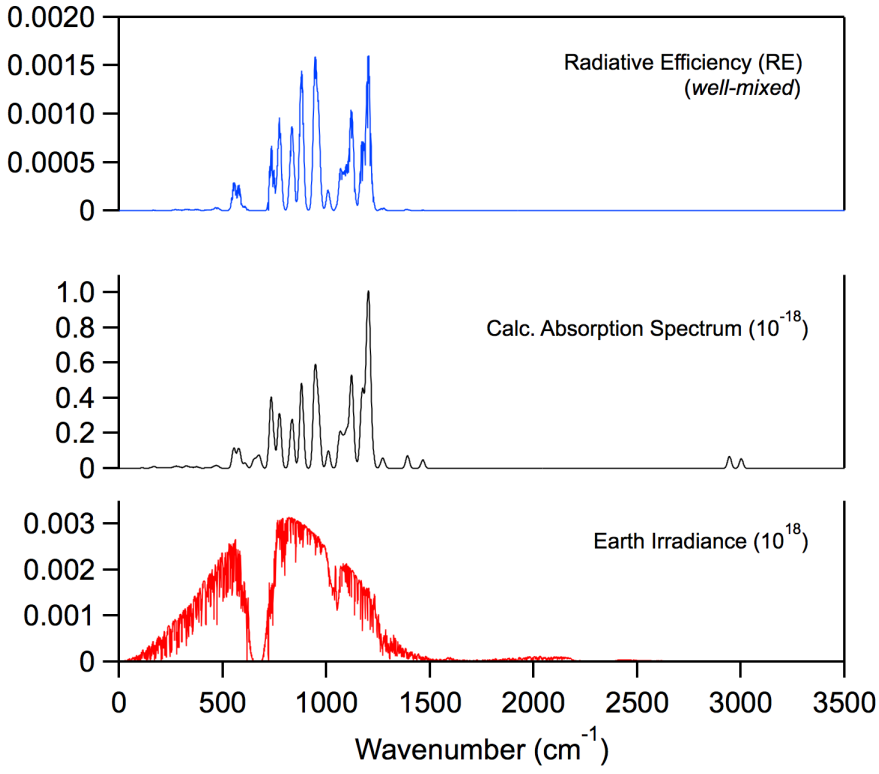
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
69.9798	0.0478
107.5446	0.377
146.1049	0.254
180.5626	0.181
196.6179	0.0657
255.1082	0.0611
302.2837	0.0169
312.5096	0.423
338.7286	0.203
366.6474	0.228
430.9358	0.0388
448.9556	0.556
584.9635	5.31
632.8961	1.62
766.8878	16.2
820.0340	20.7
1014.3952	13.6
1081.4018	20.5
1082.2101	5.68
1144.8224	7.37
1169.9385	16.4
1188.6169	20.1
1285.2660	2.84
1417.7502	0.899
1503.9283	0.431
3056.9822	1.78
3117.0247	1.23

Infrared Spectrum

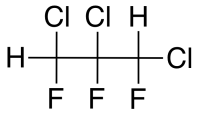


Radiative Efficiency



HCFC-233ba

Molecular Formula:	CHClFCClFCHClF
Name:	1,2,3-Trichloro-1,2,3-trifluoropropane
CAS number:	–
Molecular Weight:	201.4



Global Atmospheric Lifetime (years):	2.10
Tropospheric Atmospheric Lifetime (years):	2.23
Stratospheric Atmospheric Lifetime (years):	37.8
Ozone Depletion Potential (ODP):	0.031

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.238	0.202
Global Warming Potential (GWP_H):		
GWP_{20}	560	475
GWP_{100}	152	129
Global Temperature Potentials (GTP_H)		
GTP_{20}		178
GTP_{50}		23
GTP_{100}		18

* 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) = 2.63×10^{-14}; k_{SAR}(272 K) ≈ 1.68×10^{-14} cm^3 $molecule^{-1}$ s^{-1}

τ^{OH}_{Global} = 2.16 years

τ^{OH}_{Trop} = 2.23 years

τ^{OH}_{Strat} = 69.4 years

Fractional Atmospheric Loss: 0.975

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: 0.011

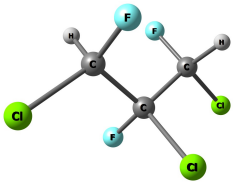
UV Photolysis

UV Spectrum: *No Recommendation*

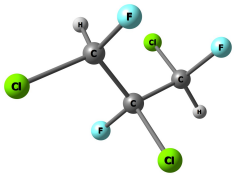
τ_{hv} = 150 years

Fractional Atmospheric Loss: 0.014

Molecular Structure and Infrared Spectrum (11 conformers)



E = 0
Population = 0.223



$\Delta E = 0.02$ kcal mol^{-1}
Population = 0.214

Optimized Coordinates (Angstroms)

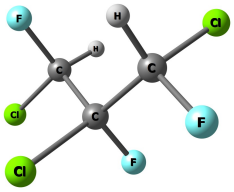
Atom	X	Y	Z
C	-1.270218590223	0.594727627967	-0.382372018038
C	-0.007889707089	-0.094453990726	0.189918790599
C	1.236993336107	0.749096781288	-0.170405404832
Cl	-2.765884782683	-0.155304701981	0.230269191038
F	-1.240199988573	1.898362646161	0.002595639491
H	-1.281887417745	0.534168548110	-1.470224518880
Cl	0.112225805753	-1.739705384027	-0.498181567607
F	-0.091678474172	-0.154539531566	1.531936457395
H	1.127211280300	1.742287924133	0.266791378519
Cl	2.735495417974	0.051501765125	0.493525457781
F	1.319794120349	0.849495315515	-1.516546405466

Atom	X	Y	Z
C	-1.482960059249	-0.480283838054	0.059294563821
C	0.012790556627	-0.295854343263	0.414418690684
C	0.726272328036	0.772834144460	-0.442315331760
Cl	-2.394574321395	1.046525372173	0.355832833829
F	-1.626037828677	-0.839734290619	-1.225957153700
H	-1.918087927183	-1.232745596306	0.719223400579
Cl	0.793131751067	-1.898829173885	0.206516564076
F	0.077415012201	0.066745790088	1.711027335213
H	0.187566872605	1.718900071077	-0.362296116402
Cl	2.383775250262	1.077958962760	0.154847911850
F	0.761809365707	0.373429901570	-1.726793698190

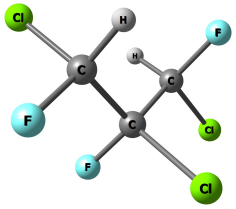
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
62.8043	0.0736
70.0613	0.191
126.3104	0.0696
181.9234	0.0284
205.7939	0.498
232.8408	0.0122
249.0385	0.0670
324.4596	0.116
361.4311	0.0962
405.9318	0.228
438.1627	0.524
510.2947	1.12
619.9318	11.5
715.8930	26.1
789.1519	4.74
862.7304	3.68
973.9027	12.5
1091.9238	4.94
1094.9886	17.2
1138.4646	17.3
1206.6376	11.7
1282.5609	0.366
1296.2310	4.16
1357.6649	2.92
1363.5732	0.495
3123.1745	0.425
3135.7459	0.518

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
49.1208	0.145
84.5818	0.0600
144.8320	0.117
170.9643	0.0640
196.4681	0.0902
228.3820	0.196
269.1316	0.0421
338.5438	0.0748
373.5393	0.0692
395.8880	0.517
445.2147	0.541
539.3222	9.26
588.5024	0.959
641.8113	11.8
758.8033	22.0
838.3478	10.1
987.1271	4.02
1122.2152	3.49
1158.1255	13.1
1172.4592	3.86
1174.6104	31.5
1283.7945	2.84
1295.0923	1.90
1354.8054	2.26
1378.9467	1.98
3113.0527	0.595
3115.0363	0.694



$\Delta E = 0.12$ kcal mol^{-1}
Population = 0.180



$\Delta E = 0.12$ kcal mol^{-1}
Population = 0.180

Optimized Coordinates (Angstroms)

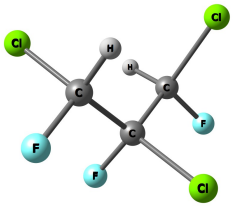
Atom	X	Y	Z
C	-1.434121274903	-0.230328634958	-0.395005440646
C	-0.016999674166	-0.309532228717	0.220051498982
C	0.886991746007	0.838115305028	-0.273099524661
Cl	-2.229201031223	1.324903350334	0.054624400907
H	-1.385586752097	-0.261375495937	-1.483224589686
F	-2.180059837223	-1.242211017278	0.077097361376
Cl	0.660912771376	-1.901000122884	-0.267219001069
F	-0.104887889255	-0.249268509510	1.560661214311
H	0.467454611394	1.792775285832	0.047046251704
Cl	2.526655110240	0.743945297788	0.418882942082
F	0.940416219850	0.794167770302	-1.624293113300

Atom	X	Y	Z
C	-0.881758921605	0.846309761054	-0.249268945343
C	0.015229001810	-0.316553870568	0.220470643587
C	1.434557163308	-0.230398476607	-0.388533760674
Cl	-2.523928007813	0.744533891831	0.435658958246
H	-0.458609434874	1.791453139965	0.093556118858
F	-0.931332701464	0.833111463640	-1.601259420155
Cl	-0.668847166975	-1.893309867430	-0.304553130886
F	0.099378064228	-0.286970490461	1.562348018504
H	1.389148309790	-0.236671963818	-1.477312429380
Cl	2.235731271123	1.310419546051	0.098361076222
F	2.174209422473	-1.256280133659	0.062788871023

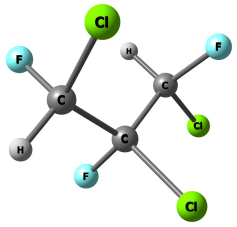
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
58.9856	0.128
73.5784	0.144
129.9405	0.0720
182.4446	0.109
193.9880	0.308
241.4179	0.0845
264.6905	0.105
313.9257	0.149
359.3375	0.110
401.5825	0.425
419.3795	0.609
507.2969	0.858
623.4026	8.94
739.6683	29.8
773.7765	10.3
813.1835	8.23
961.3343	4.69
1102.3165	8.52
1129.1702	18.7
1160.2183	10.3
1215.0749	13.6
1276.3881	1.70
1296.6756	2.01
1358.3554	1.41
1377.2071	1.80
3122.2984	0.606
3134.9190	0.445

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
58.9853	0.128
73.5780	0.144
129.9402	0.0720
182.4445	0.109
193.9876	0.308
241.4181	0.0845
264.6901	0.105
313.9251	0.149
359.3371	0.110
401.5825	0.425
419.3793	0.609
507.2967	0.858
623.4021	8.94
739.6686	29.8
773.7758	10.3
813.1839	8.23
961.3337	4.69
1102.3164	8.52
1129.1696	18.7
1160.2182	10.3
1215.0738	13.6
1276.3884	1.70
1296.6760	2.01
1358.3559	1.41
1377.2065	1.80
3122.2979	0.606
3134.9195	0.445



$\Delta E = 0.64$ kcal mol^{-1}
Population = 0.075



$\Delta E = 1.15$ kcal mol^{-1}
Population = 0.032

Optimized Coordinates (Angstroms)

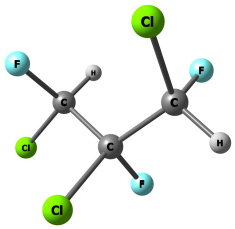
Atom	X	Y	Z
C	0.986625111041	-0.672992608343	0.602486433604
C	-0.014118896869	0.462248959530	0.299244732343
C	-1.204799210405	0.069409899478	-0.597356618035
Cl	1.606438583182	-1.444507667202	-0.892679566691
F	2.009761024128	-0.171259555163	1.314908322981
H	0.483226871115	-1.451466956280	1.177767725912
Cl	0.827095976663	1.839794193369	-0.488573500279
F	-0.490231381968	0.876943190965	1.495444351513
H	-0.875080048059	-0.241355348041	-1.587578984223
Cl	-2.095100686919	-1.322143452335	0.126137908357
F	-2.042453341909	1.116989344023	-0.683159805481

Atom	X	Y	Z
C	0.842034759850	-0.855699059243	0.137204483323
C	0.068637467246	0.466575945421	0.344011807996
C	-1.440773302636	0.252366773313	0.625151665637
Cl	2.606544191268	-0.595812536934	0.268233224719
H	0.563906068751	-1.553444686752	0.929844601691
F	0.549294545184	-1.384949087954	-1.064063746768
Cl	0.284337834813	1.583021409657	-1.028344033470
F	0.540988722254	1.050812648265	1.473203123395
H	-1.897089026218	1.219236906949	0.844413119281
Cl	-2.350619102505	-0.483074124417	-0.719383066180
F	-1.529854158007	-0.550584188306	1.715464820376

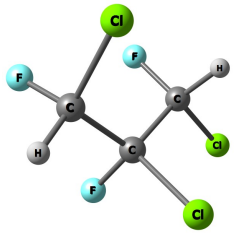
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
60.4903	0.0921
84.1375	0.142
132.2359	0.0219
178.9184	0.411
198.9630	0.0988
253.7689	0.0547
273.8488	0.0387
321.3893	0.193
351.0421	0.159
397.9997	0.524
429.2913	0.958
460.2138	0.0379
626.3728	10.0
749.2797	21.5
764.4713	7.73
823.9813	14.4
975.5005	10.5
1079.6926	11.8
1146.8110	7.86
1169.6380	19.1
1192.7543	13.9
1269.4908	1.55
1282.2860	1.96
1366.0679	0.711
1381.0548	2.13
3120.6895	0.617
3143.7197	0.494

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
49.8971	0.114
83.7786	0.0508
142.9030	0.0833
169.5050	0.0432
194.7812	0.102
216.9274	0.236
313.2313	0.199
328.5083	0.0975
375.4465	0.102
407.2838	0.566
435.9080	0.775
541.7863	0.338
550.3715	10.2
658.4297	7.88
827.3267	21.8
838.4920	6.34
1003.3291	13.8
1096.1038	3.48
1135.4491	21.1
1139.5513	5.71
1160.7060	19.0
1285.5727	4.71
1293.4560	1.53
1352.9725	1.73
1373.6110	2.25
3109.4092	0.504
3113.9380	0.745



$\Delta E = 1.15$ kcal mol^{-1}
Population = 0.032



$\Delta E = 1.28$ kcal mol^{-1}
Population = 0.026

Optimized Coordinates (Angstroms)

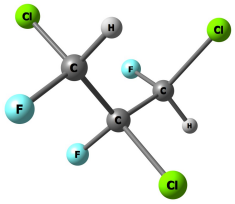
Atom	X	Y	Z
C	-1.433723830470	-0.184665008992	0.660454773559
C	0.071031468018	-0.431773658992	0.381353104097
C	0.842368047005	0.858521302606	0.021489788280
Cl	-2.363311785786	0.403801618756	-0.741701005088
H	-1.887512637553	-1.121086397083	0.989586002354
F	-1.505439838441	0.731411902988	1.659009192594
Cl	0.264787205336	-1.690245555841	-0.865662054207
F	0.560026979458	-0.892025195297	1.559729978623
H	0.576994232355	1.638382643374	0.738341034702
Cl	2.608437274805	0.609794779147	0.153186430351
F	0.531814885272	1.255875569334	-1.225311245266

Atom	X	Y	Z
C	0.838909074100	-0.553946928019	-0.586462558963
C	0.044953656939	0.221054629700	0.487025615290
C	-1.458230883711	-0.159481322848	0.567350102650
Cl	2.596523940356	-0.274846345131	-0.408999690021
F	0.582556031952	-1.872020499697	-0.434668216455
H	0.554788017077	-0.231637150404	-1.587362684978
Cl	0.164209962560	1.982394726017	0.166676679461
F	0.552121258353	-0.043608166906	1.709264852603
H	-1.971040597744	0.549949095584	1.219389519686
Cl	-2.264898286932	-0.082179229176	-1.033908757600
F	-1.570973172950	-1.402540809121	1.068216138326

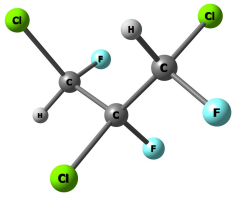
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
49.8999	0.114
83.7792	0.0508
142.9044	0.0833
169.5039	0.0432
194.7826	0.102
216.9287	0.236
313.2315	0.199
328.5081	0.0975
375.4467	0.102
407.2834	0.566
435.9076	0.775
541.7862	0.338
550.3706	10.2
658.4310	7.88
827.3259	21.8
838.4898	6.34
1003.3285	13.8
1096.1025	3.48
1135.4497	21.1
1139.5505	5.71
1160.7053	19.0
1285.5704	4.71
1293.4526	1.53
1352.9701	1.73
1373.6094	2.25
3109.4107	0.503
3113.9418	0.744

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
55.9341	0.0588
79.6631	0.0509
141.9731	0.0727
180.5287	0.0479
199.6007	0.228
233.1867	0.0880
307.6654	0.146
321.5781	0.155
366.2129	0.103
411.1857	0.849
418.1896	0.435
456.7153	0.970
563.7534	11.7
763.8753	1.31
822.3679	22.9
855.6033	6.34
928.3109	23.4
1097.7748	1.14
1113.2170	11.2
1162.5048	18.1
1176.4475	18.0
1287.6040	4.85
1289.9240	0.673
1362.0020	1.60
1382.5247	1.58
3112.2020	0.735
3139.4035	0.584



$\Delta E = 1.69$ kcal mol^{-1}
Population = 0.013



$\Delta E = 1.69$ kcal mol^{-1}
Population = 0.013

Optimized Coordinates (Angstroms)

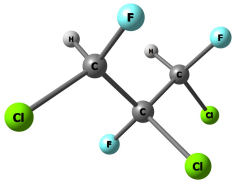
Atom	X	Y	Z
C	1.114603737014	-0.578460248473	0.642711187837
C	0.014261824645	0.490009891336	0.425287820174
C	-1.027517718638	0.230289288385	-0.682763568898
Cl	1.891365428049	-1.071780537568	-0.898512494042
H	1.897962125504	-0.154681502262	1.273451344279
F	0.584535926354	-1.657248140718	1.246148731334
Cl	0.841734710751	2.044618388198	0.025523706019
F	-0.620787823644	0.635877720036	1.605927173002
H	-0.546035220497	0.112754431645	-1.652448033529
Cl	-1.954707400848	-1.270162131644	-0.360721841208
F	-1.885162588689	1.269851841065	-0.707338024967

Atom	X	Y	Z
C	1.029014417949	0.224717481430	-0.680822472253
C	-0.010953798563	0.491610948020	0.427224425225
C	-1.114940004676	-0.572224555495	0.648820358919
Cl	1.951028938757	-1.278072172747	-0.354870076521
H	0.546353769952	0.105939100088	-1.649768447323
F	1.890382342519	1.261099193649	-0.709259019630
Cl	-0.833172686488	2.047920286932	0.023288258789
F	0.625542797240	0.638855834344	1.606912723221
H	-1.896269148077	-0.143682894387	1.278861696012
Cl	-1.894691251897	-1.067542371595	-0.890248291581
F	-0.588256376717	-1.651024850239	1.255194845141

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
49.7764	0.0630
88.1676	0.0365
143.8667	0.0958
175.5847	0.0402
208.3920	0.355
251.2756	0.0239
289.0418	0.422
308.5884	0.161
366.0972	0.0365
399.3958	0.428
412.5688	1.21
441.6223	0.656
631.7196	8.04
767.7338	5.23
775.4228	25.4
827.3452	14.4
919.0192	11.1
1110.7725	5.29
1126.3586	8.88
1171.1006	27.8
1183.8210	8.76
1281.9441	1.56
1292.0142	1.53
1373.9139	2.10
1381.0834	0.399
3113.7763	0.701
3141.4742	0.540

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
49.7778	0.0630
88.1674	0.0365
143.8684	0.0958
175.5879	0.0402
208.3914	0.355
251.2752	0.0239
289.0404	0.422
308.5930	0.161
366.0991	0.0365
399.3964	0.428
412.5696	1.21
441.6257	0.656
631.7237	8.04
767.7354	5.23
775.4273	25.4
827.3500	14.4
919.0264	11.1
1110.7751	5.29
1126.3574	8.88
1171.1033	27.8
1183.8254	8.76
1281.9441	1.56
1292.0191	1.53
1373.9123	2.10
1381.0853	0.399
3113.7615	0.701
3141.4817	0.540



$\Delta E = 1.95$ kcal mol^{-1}
Population = 0.008

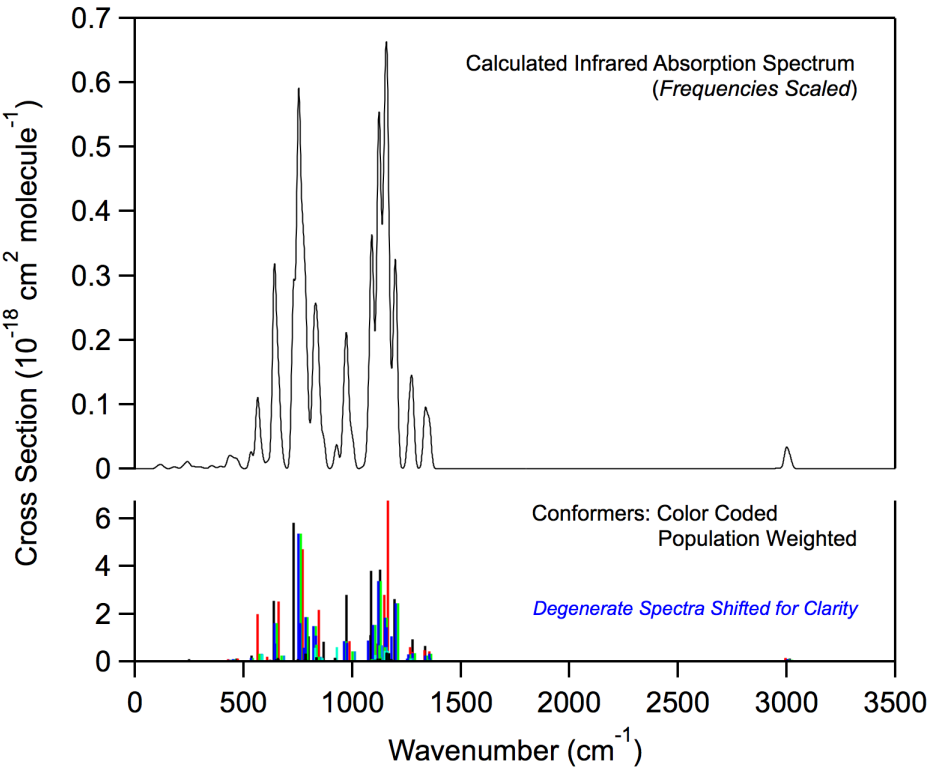
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.266719662237	0.625238827445	0.487297912557
C	0.002570672766	-0.219314786804	0.207501632580
C	1.272160063163	0.631802953055	0.465176613380
Cl	-2.743659912216	-0.378726830669	0.442254477469
H	-1.207372600704	1.034358874760	1.500640077764
F	-1.361534634006	1.629228489888	-0.402098335729
Cl	-0.010351213849	-0.842491544173	-1.460337418071
F	0.012931639162	-1.238035323680	1.094358240796
H	1.228362069999	1.040660823456	1.479415587125
Cl	2.753261637953	-0.364517338551	0.394371112220
F	1.346275939971	1.636224855273	-0.425695900091

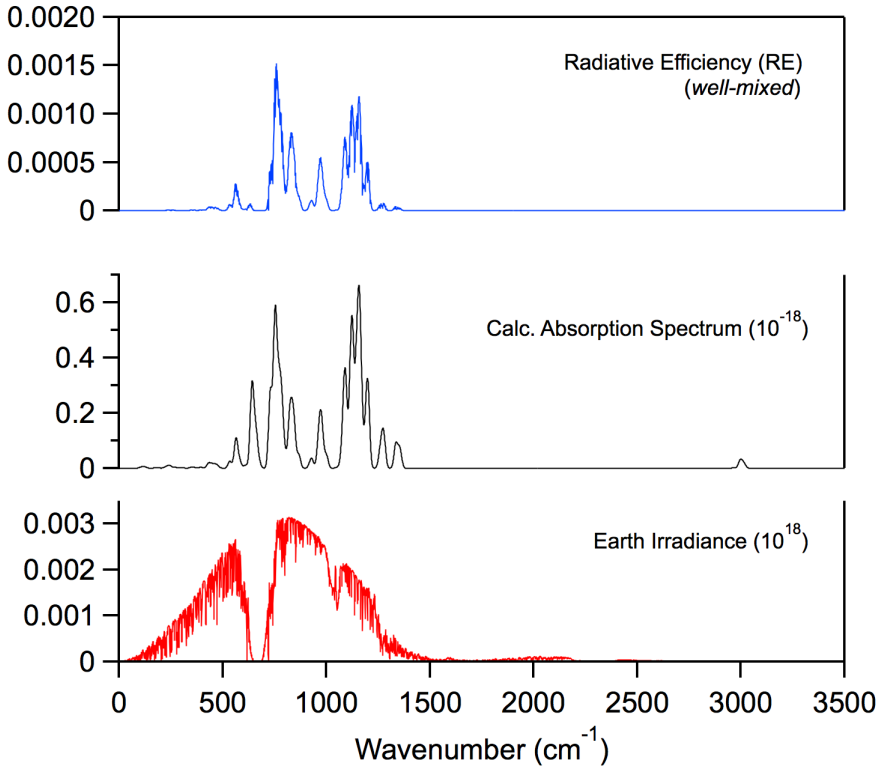
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
48.2350	0.0299
73.4313	0.0523
130.6767	0.119
181.4064	0.0143
209.5427	0.334
228.0927	0.196
242.4278	0.0135
333.3286	0.0315
359.0791	0.246
413.3877	0.302
447.1855	0.412
586.5848	0.356
601.8195	9.85
641.2543	17.6
735.7694	12.4
857.8804	6.91
1054.8563	7.32
1072.6090	1.19
1140.5015	0.996
1168.9969	45.7
1183.9716	1.91
1287.6194	7.33
1304.3260	1.32
1346.3118	0.187
1369.8166	3.88
3070.3869	1.00
3080.2998	2.87

Infrared Spectrum

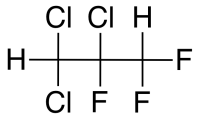


Radiative Efficiency



HCFC-233bb

Molecular Formula:	$CHCl_2CClFCHF_2$
Name:	1,1,2-Trichloro-2,3,3-trifluoropropane
CAS number:	13058-99-6
Molecular Weight:	201.4



Global Atmospheric Lifetime (years):	1.27
Tropospheric Atmospheric Lifetime (years):	1.34
Stratospheric Atmospheric Lifetime (years):	23.3
Ozone Depletion Potential (ODP):	0.023

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.219	0.171
Global Warming Potential (GWP_H):		
GWP_{20}	310	242
GWP_{100}	84	66
Global Temperature Potentials (GTP_H)		
GTP_{20}		81
GTP_{50}		11
GTP_{100}		9

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 4.37 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 2.79 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 1.30$ years

$\tau^{OH}_{Trop} = 1.34$ years

$\tau^{OH}_{Strat} = 44.0$ years

Fractional Atmospheric Loss: 0.974

$O(^1D)$ 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: 0.007

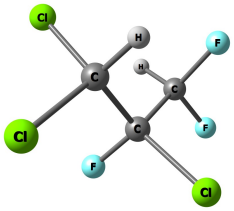
UV Photolysis

UV Spectrum: *No Recommendation*

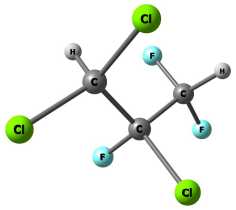
$\tau_{hv} = 68$ years

Fractional Atmospheric Loss: 0.019

Molecular Structure and Infrared Spectrum (6 conformers)



E = 0
Population = 0.463



$\Delta E = 0.42$ kcal mol^{-1}
Population = 0.229

Optimized Coordinates (Angstroms)

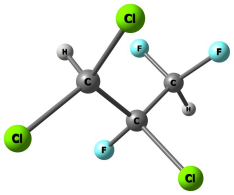
Atom	X	Y	Z
C	-0.932319663830	-0.114775288518	-0.469730551059
C	0.385421072558	0.162003517805	0.282951046368
C	1.467870275744	-0.907712297965	-0.007202468176
Cl	-1.510411122943	-1.780676389920	-0.108146338273
Cl	-2.189343450287	1.070409615838	-0.046191748086
H	-0.760963661082	-0.065045664975	-1.541019046173
F	0.174529895888	0.171811935133	1.613512213217
Cl	1.014543160222	1.762616100736	-0.235940568178
H	1.178179748349	-1.868443674383	0.428647353134
F	1.607456570518	-1.038851914619	-1.344134498914
F	2.637604174862	-0.518189939133	0.521311606141

Atom	X	Y	Z
C	-0.878778565768	0.442726836939	-0.454423113470
C	0.415297798461	-0.338959957881	-0.145539673876
C	1.632393269664	0.602386700944	0.037564025547
Cl	-2.231440102281	-0.654343690224	-0.813273766808
Cl	-1.283348629856	1.593490664097	0.851167012154
H	-0.696293629525	1.032430675792	-1.350045931509
F	0.669425577603	-1.120135645981	-1.219615483665
Cl	0.274133949827	-1.367402012916	1.310190915348
H	1.568220650665	1.187872912856	0.957793768207
F	2.751240079722	-0.137122135026	0.038501413069
F	1.672952601487	1.437610651400	-1.029863164996

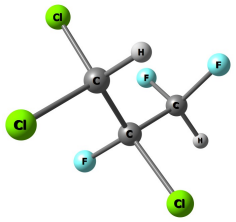
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
56.2941	0.0577
73.8589	0.234
144.2075	0.0524
198.8818	0.326
204.8299	0.205
215.8557	0.0122
256.4272	0.0333
300.3111	0.274
334.6903	0.0554
381.1900	0.190
475.9983	0.288
566.0454	3.48
655.9859	14.9
728.9240	12.8
741.0838	2.09
776.9581	11.7
985.0241	9.19
1086.2036	0.558
1156.5662	22.7
1189.4269	10.1
1195.8870	18.1
1225.4347	2.57
1288.3532	0.592
1379.6673	5.35
1400.0466	2.09
3095.0605	2.33
3171.8720	0.548

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
62.4953	0.115
79.0873	0.144
137.1929	0.0480
167.9255	0.0611
193.3942	0.306
236.8821	0.0335
272.1095	0.157
325.9337	0.0506
341.2120	0.397
383.3196	0.214
447.9290	1.16
559.9274	2.57
599.2075	4.67
751.6475	11.3
794.0039	14.4
835.3568	10.4
958.8414	17.9
1095.4484	3.38
1121.8456	14.3
1167.1361	9.39
1206.5437	22.8
1239.9847	2.84
1277.0215	2.33
1387.7328	3.03
1403.4909	2.34
3109.6007	2.24
3151.6003	0.465



$\Delta E = 0.73$ kcal mol^{-1}
Population = 0.136



$\Delta E = 1.13$ kcal mol^{-1}
Population = 0.069

Optimized Coordinates (Angstroms)

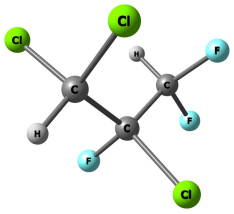
Atom	X	Y	Z
C	-0.706978494179	0.431786301260	-0.554256523070
C	0.346193256255	-0.602554503882	-0.100011523220
C	1.808322830484	-0.097080650985	-0.205666621938
Cl	-2.314314176803	-0.327269196427	-0.707327560634
Cl	-0.757943698429	1.867938989541	0.494301476566
H	-0.420309850093	0.769561441833	-1.547655900330
F	0.278879936041	-1.640861151703	-0.974306484233
Cl	0.065015825999	-1.218835980095	1.550104946814
H	2.484216618107	-0.955192614545	-0.117032230388
F	1.964655453146	0.468936266606	-1.426906856671
F	2.103947299471	0.815151098397	0.728722277103

Atom	X	Y	Z
C	-0.767631427369	-0.179128233108	-0.505228751248
C	0.387738582151	0.356991536305	0.366075654169
C	1.765707749005	-0.311972443865	0.100347401961
Cl	-0.988358746399	-1.938938912676	-0.266171255429
Cl	-2.292224102072	0.678036090573	-0.148445232551
H	-0.531981943713	-0.023283753794	-1.553768356550
F	0.106743563247	0.226429471625	1.672570401919
Cl	0.623223705840	2.109058573026	-0.018168997899
H	2.566142153647	0.304444079148	0.522623095930
F	1.810455114120	-1.531793242492	0.659715965143
F	1.941455351543	-0.433541164741	-1.233277925444

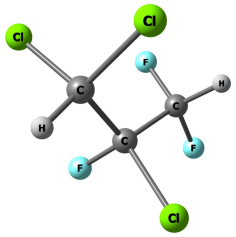
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
50.9158	0.0896
92.8830	0.116
148.2412	0.112
166.3318	0.00626
191.8014	0.127
226.6803	0.146
275.6390	0.297
318.8507	0.143
358.9842	0.342
404.2994	0.125
487.7731	1.61
548.1204	6.85
600.6944	2.72
649.0911	6.98
810.8129	13.3
826.3214	9.05
983.4794	14.1
1107.4195	7.16
1142.9324	6.89
1156.4317	20.9
1197.6486	12.1
1236.8486	3.92
1284.4392	2.23
1386.9779	2.49
1395.2338	5.97
3073.6861	3.34
3151.0629	0.403

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
45.6439	0.0327
81.6444	0.161
153.0358	0.0759
200.2835	0.225
203.9631	0.166
217.2745	0.0317
251.3356	0.0937
310.9666	0.127
322.5639	0.372
398.7204	0.230
467.1285	0.660
560.0131	5.99
602.0388	7.52
742.7393	5.47
754.6940	21.3
841.1530	0.666
900.4500	10.6
1110.5224	4.13
1149.4691	17.6
1186.5847	9.55
1199.2972	15.7
1226.7546	6.81
1301.2102	2.08
1387.8855	3.42
1400.6541	3.76
3081.4124	2.98
3171.5766	0.482



$\Delta E = 1.18$ kcal mol^{-1}
Population = 0.063



$\Delta E = 1.61$ kcal mol^{-1}
Population = 0.031

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.041588670585	0.114775360816	0.527435972391
C	0.456940587452	-0.256412686376	0.424034192354
C	0.985058815701	-0.611387621298	-0.986254947174
Cl	-1.489910979598	1.574658247149	-0.380740447200
Cl	-2.047336786504	-1.288222454308	0.021665012086
H	-1.268534987293	0.294021778032	1.575882492413
F	0.631756490090	-1.361857320208	1.189174948850
Cl	1.436628348911	1.070557010030	1.126332408468
H	0.365730457748	-1.395886002559	-1.435210504986
F	0.988016927653	0.471619010539	-1.780868997511
F	2.246466796424	-1.060936321818	-0.858427129690

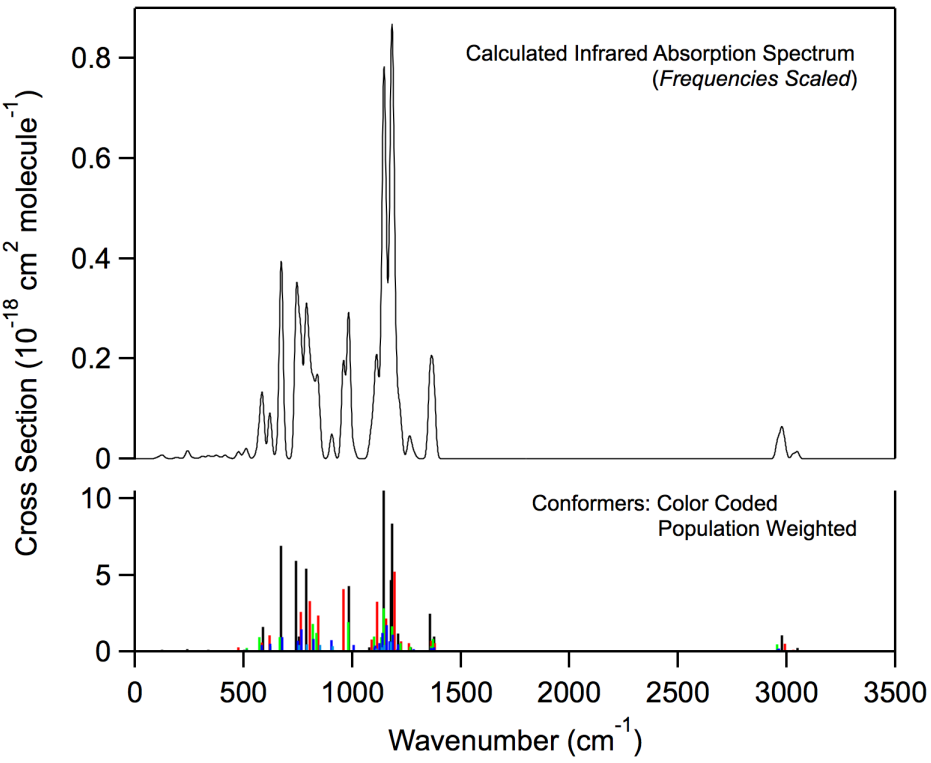
Atom	X	Y	Z
C	-0.990706674156	-0.382219830186	-0.436635035171
C	0.517149748299	-0.030436866364	-0.399838398367
C	1.033780328738	0.682873195391	0.872761122934
Cl	-1.499600006885	-1.247954997227	1.044160006450
Cl	-1.998775803529	1.063954589747	-0.717874454239
H	-1.165547198639	-1.052640800150	-1.274334515759
F	0.790561766327	0.747716466013	-1.465319052617
Cl	1.442314392849	-1.571269774228	-0.572893803007
H	0.926900196936	0.054282103345	1.760455021396
F	2.329250138914	0.990157566722	0.682115013359
F	0.347162111147	1.830217346936	1.042247095020

Infrared Absorption Spectrum (unscaled frequencies)

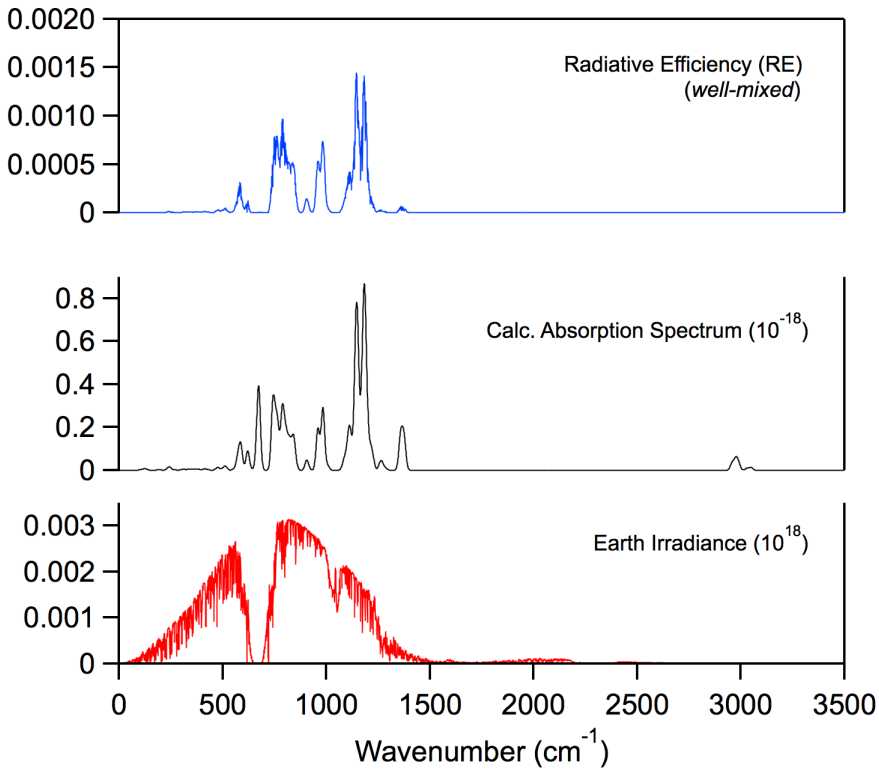
Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
48.5119	0.152
85.2721	0.0802
150.0146	0.110
168.0725	0.0229
195.0464	0.157
236.4515	0.0871
272.6024	0.512
309.3361	0.0160
350.8242	0.0867
383.5064	0.171
486.5847	2.18
563.8771	1.93
632.9347	1.49
661.1921	14.7
736.3468	11.5
813.6659	13.2
1009.1489	6.83
1115.6054	6.21
1135.3100	8.66
1171.2166	27.3
1185.4975	10.7
1223.8461	2.71
1302.5434	0.128
1393.5374	3.39
1398.9505	3.38
3076.6906	2.49
3149.7221	0.477

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
45.5155	0.0968
80.5103	0.0415
149.4400	0.0325
169.7664	0.0540
211.8002	0.353
231.1993	0.0599
268.6029	0.138
322.6871	0.209
339.8872	0.542
368.2440	0.124
438.8434	1.30
528.7402	3.11
633.3447	0.971
742.7447	14.5
780.7593	15.5
845.7636	14.1
906.2776	11.5
1119.7640	6.27
1146.1126	9.47
1159.2510	13.7
1191.0025	20.0
1231.0401	0.759
1309.3361	2.26
1398.2887	1.47
1405.5375	3.16
3104.9678	2.29
3153.6802	0.457

Infrared Spectrum

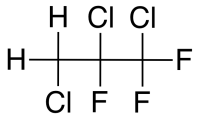


Radiative Efficiency



HCFC-233bc

Molecular Formula:	$CH_2ClCClFCClF_2$
Name:	1,2,3-Trichloro-1,1,2-trifluoropropane
CAS number:	421-95-4
Molecular Weight:	201.4



Global Atmospheric Lifetime (years):	4.75
Tropospheric Atmospheric Lifetime (years):	5.21
Stratospheric Atmospheric Lifetime (years):	53.3
Ozone Depletion Potential (ODP):	0.057

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.284	0.261
Global Warming Potential (GWP_H):		
GWP_{20}	1485	1365
GWP_{100}	408	375
Global Temperature Potentials (GTP_H)		
GTP_{20}		729
GTP_{50}		78
GTP_{100}		53

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 1.12 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 0.718 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 5.04$ years

$\tau^{OH}_{Trop} = 5.21$ years

$\tau^{OH}_{Strat} = 149.4$ years

Fractional Atmospheric Loss: 0.943

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

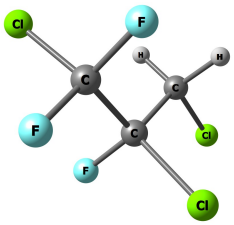
UV Photolysis

UV Spectrum: *No Recommendation*

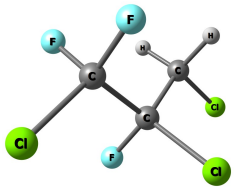
$\tau_{hv} = 150$ years

Fractional Atmospheric Loss: 0.032

Molecular Structure and Infrared Spectrum (7 conformers)



E = 0
Population = 0.308



$\Delta E = 0.25$ kcal mol^{-1}
Population = 0.202

Optimized Coordinates (Angstroms)

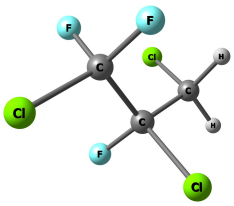
Atom	X	Y	Z
C	-1.017542442228	-0.840836796314	0.589524210687
C	-0.222154264899	0.169110477670	-0.236801069867
C	1.285619101966	0.184394678960	0.165799646199
Cl	-2.719936240810	-0.949574237276	0.057045367147
H	-0.575821766995	-1.828748572199	0.461073416656
H	-0.999777036290	-0.557003796064	1.639889732477
Cl	-0.848036815165	1.838667740089	0.017591580667
F	-0.288675578194	-0.121278990771	-1.549396478217
Cl	2.064579060107	-1.393508973243	-0.218916430459
F	1.934371490779	1.134867638352	-0.492181409757
F	1.397832491730	0.406411830794	1.476651434468

Atom	X	Y	Z
C	-1.351473729297	-0.840220097045	0.367910994792
C	-0.238092451460	0.057938293029	-0.181489983126
C	1.147773502473	-0.534433140328	0.225618768149
Cl	-2.969278878419	-0.322923172028	-0.183977912456
H	-1.189687997263	-1.853501862867	0.001460320633
H	-1.335609191408	-0.828656130750	1.456100615808
Cl	-0.380288111840	1.726672845994	0.452050268408
F	-0.282818321124	0.084092987687	-1.527657749630
Cl	2.515568517257	0.359054011541	-0.481788083889
F	1.257331624724	-0.550507942784	1.555275480832
F	1.200058036355	-1.802386792450	-0.209395719521

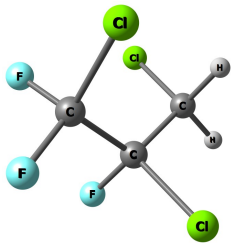
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
63.0621	0.0391
75.8514	0.328
138.4363	0.201
175.6275	0.0963
227.1918	0.174
249.8820	0.103
302.7255	0.0698
314.0786	0.128
359.4733	0.166
391.7302	0.229
421.6779	0.0905
501.4319	0.134
606.6161	5.38
660.1861	3.56
760.0834	25.0
804.4803	17.8
902.7522	7.80
1011.7918	1.08
1051.4738	18.6
1176.6285	16.3
1213.9387	12.6
1241.0415	18.1
1253.8190	7.98
1319.3821	1.82
1464.0767	0.979
3108.7979	0.826
3178.3907	0.0189

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
61.0394	0.0212
81.7518	0.419
128.4277	0.209
182.8003	0.102
218.6140	0.0671
249.8773	0.198
306.7039	0.0402
312.4658	0.184
352.7949	0.0374
416.8955	0.375
430.7981	0.0808
487.4951	1.04
623.3558	5.93
652.2906	3.25
733.3472	20.1
852.1289	7.88
910.4701	4.92
1003.0685	20.2
1078.3988	21.8
1167.8584	8.04
1178.8583	17.9
1215.1504	10.6
1254.1157	11.2
1317.5882	1.69
1464.1371	0.879
3108.5643	0.620
3177.5380	0.0280



$\Delta E = 0.36$ kcal mol^{-1}
Population = 0.167



$\Delta E = 0.70$ kcal mol^{-1}
Population = 0.095

Optimized Coordinates (Angstroms)

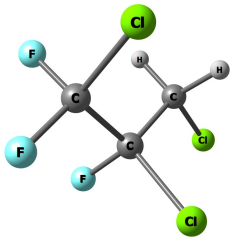
Atom	X	Y	Z
C	-1.532128584808	0.782368140490	0.324075256395
C	-0.132173367000	0.562711127215	-0.265246811852
C	0.604594923017	-0.683796242589	0.313550231353
Cl	-2.745760803357	-0.408701670939	-0.249663089877
H	-1.484412450823	0.730931536245	1.410498356287
H	-1.880647076141	1.765456262264	0.013942389685
Cl	0.816869436795	2.039503816757	0.157060501363
F	-0.184104776171	0.435562603068	-1.600769230701
Cl	2.241231391351	-0.886868076252	-0.375134979871
F	0.689289736812	-0.565305851326	1.641196458607
F	-0.101552429675	-1.779307644933	0.036212918610

Atom	X	Y	Z
C	-1.233322507571	0.689896010081	0.785619352525
C	-0.073083515841	0.688018454509	-0.206972290819
C	0.663493044884	-0.669544318439	-0.447087993467
Cl	-2.608802400707	-0.339745081401	0.264316838497
H	-0.898516809399	0.343980998128	1.760666965922
H	-1.604516450734	1.711055988528	0.858131969800
Cl	1.125318378200	1.891823460373	0.403079210959
F	-0.496835396294	1.086185329039	-1.425633588579
Cl	1.182402200213	-1.447197862209	1.084228571378
F	-0.151151611582	-1.497882249414	-1.095872396165
F	1.731728068831	-0.461629729197	-1.211608640051

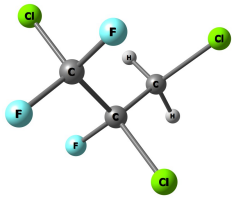
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
43.9919	0.0598
104.2828	0.270
160.7057	0.206
176.8051	0.134
202.0143	0.171
270.5971	0.0239
291.1866	0.568
309.8632	0.156
344.0390	0.0555
418.8380	0.437
426.4774	0.0909
492.6661	1.28
565.2359	7.71
661.2661	3.25
750.7533	13.6
837.9407	6.42
929.1444	13.4
943.7134	24.4
1084.3555	18.6
1177.9223	6.87
1196.3882	16.8
1208.4801	18.0
1295.1048	0.540
1314.0235	5.97
1459.0373	1.30
3115.0412	0.685
3182.9325	0.0498

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
46.1586	0.0639
107.7102	0.173
159.3847	0.0951
175.6754	0.0407
225.6920	0.490
266.1773	0.0281
306.3682	0.212
314.9919	0.351
359.8921	0.0527
399.5078	0.502
426.6377	0.578
451.1343	0.655
569.7189	4.05
680.4333	1.39
750.3358	14.2
861.5155	11.1
901.1512	12.5
964.2438	34.3
1068.4029	4.69
1173.8022	23.3
1195.2018	11.3
1221.6821	10.8
1291.0641	4.09
1313.8789	6.34
1457.4711	2.39
3117.0779	0.698
3188.2720	0.0259



$\Delta E = 0.74$ kcal mol^{-1}
Population = 0.088



$\Delta E = 0.82$ kcal mol^{-1}
Population = 0.077

Optimized Coordinates (Angstroms)

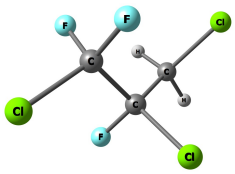
Atom	X	Y	Z
C	-1.085272826639	-0.940942563260	0.309196272201
C	-0.242594979194	0.161714171119	-0.330194983898
C	1.272259459716	-0.218148825013	-0.373822034727
Cl	-2.834523367511	-0.655468012502	0.078941071848
H	-0.840219005525	-1.887236274300	-0.174237021307
H	-0.886080689205	-1.002757819855	1.376315826068
Cl	-0.442595586957	1.731252549769	0.506970630931
F	-0.593446584723	0.317027056252	-1.628016071773
Cl	1.959511469753	-0.534013939344	1.251540181848
F	1.392826665553	-1.331166102699	-1.108405773301
F	1.965364444732	0.746142759832	-0.963027097891

Atom	X	Y	Z
C	1.126139234909	0.587351275295	-1.020825938015
C	0.183889940493	-0.503308797790	-0.507285231703
C	-0.964008543813	-0.057519465618	0.448083794780
Cl	2.063538275950	1.435671380810	0.240246254489
H	1.829475453391	0.111740649953	-1.703577058430
H	0.536103907403	1.329969951725	-1.556895747449
Cl	1.094445370223	-1.814634666011	0.317391809324
F	-0.417210210831	-1.027355207833	-1.604822904547
Cl	-1.944082430053	1.250550314644	-0.313138272516
F	-1.765907902450	-1.093478450413	0.675816231298
F	-0.489586095223	0.381287015237	1.605950062770

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
67.3575	0.0143
81.3183	0.335
135.5334	0.195
173.6539	0.0627
207.5924	0.113
290.5925	0.0794
302.8192	0.337
308.7520	0.139
372.0466	0.0245
395.3102	0.532
429.7161	0.514
454.6269	0.431
622.2575	4.28
638.3348	4.13
776.6008	11.0
834.8435	9.79
929.6913	20.4
1007.8264	29.6
1044.6022	6.02
1162.7389	9.35
1193.5928	9.11
1237.3947	16.2
1243.3675	18.3
1318.7947	1.52
1463.2702	0.899
3106.1363	0.858
3182.6194	0.119

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
46.5599	0.0572
96.6677	0.106
150.4523	0.0149
183.4225	0.130
242.1969	0.578
253.3617	0.0901
304.5926	0.251
327.9269	0.122
369.0630	0.0290
390.1578	0.335
421.4840	0.140
506.2579	1.83
572.1654	2.24
661.9536	1.38
726.5552	23.9
808.0183	6.89
906.5043	27.1
1013.1876	0.108
1106.9162	21.6
1142.7906	14.3
1196.5543	6.67
1226.7030	22.8
1276.2362	4.63
1318.7711	2.25
1464.4382	2.18
3104.4462	0.823
3169.9995	0.00405



$\Delta E = 0.94$ kcal mol^{-1}
Population = 0.063

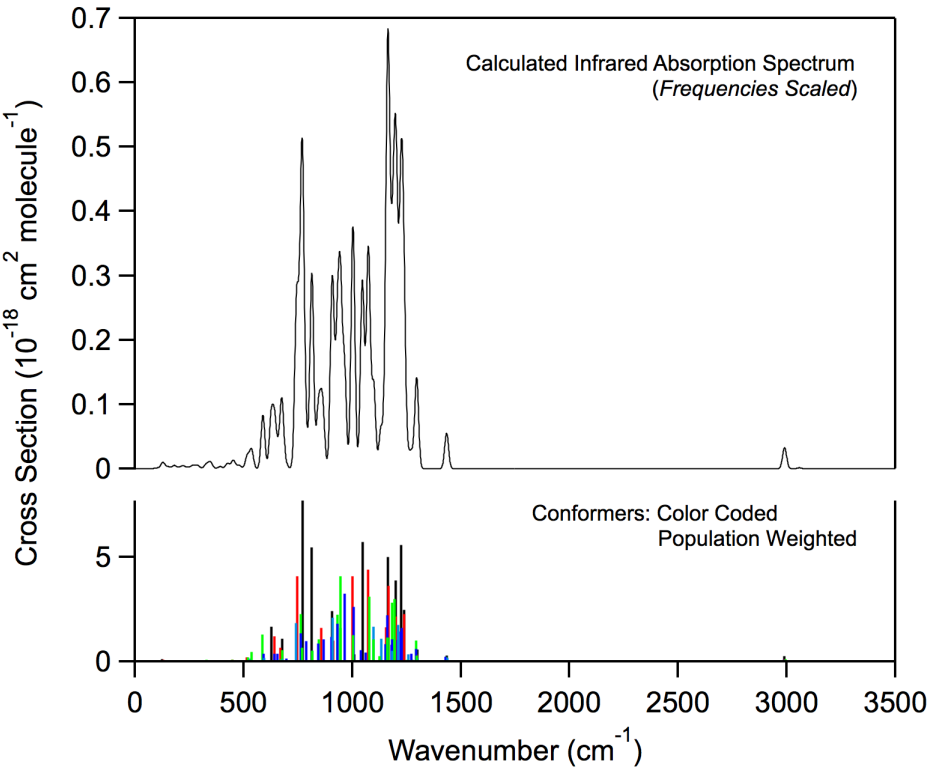
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.527693672286	0.033042618114	-0.946457147430
C	-0.135448063790	0.486778878356	-0.485179333653
C	0.757538214932	-0.675993444420	0.048373832391
Cl	-2.578185514268	-0.628405751601	0.337059332297
H	-2.025991332490	0.899395436213	-1.379513518850
H	-1.396635108675	-0.738678455615	-1.704238693533
Cl	-0.231609449572	1.790648776605	0.730928491984
F	0.468012625445	0.967271888758	-1.602099139323
Cl	2.475341766255	-0.192958054919	0.166999965699
F	0.338182726281	-1.095344156569	1.235190884314
F	0.663517808168	-1.695218734920	-0.818184673895

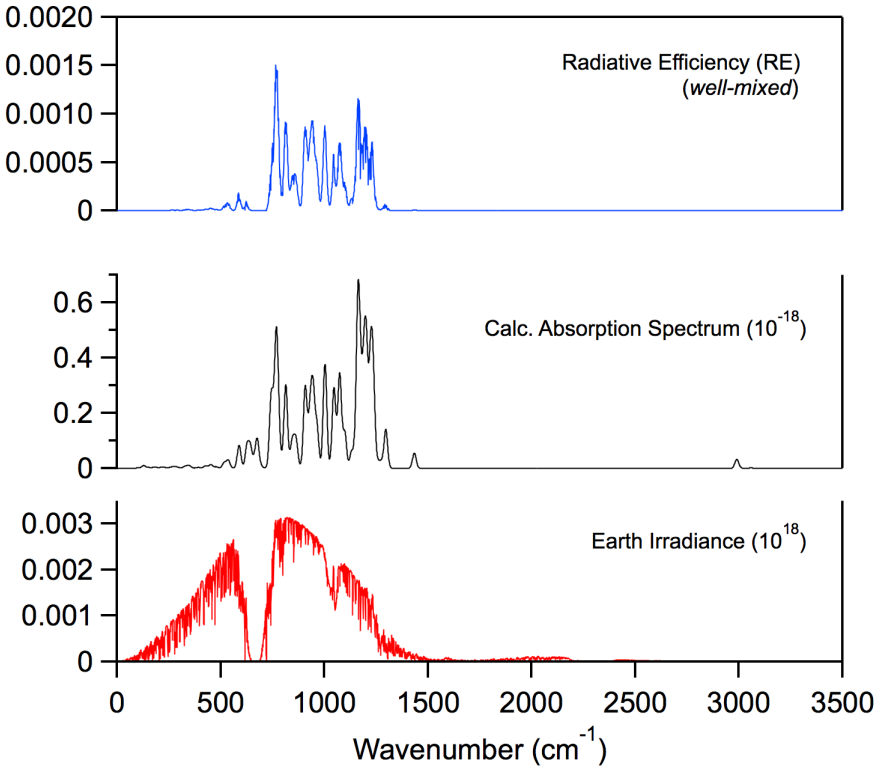
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
48.9014	0.0447
92.3193	0.143
146.4743	0.0579
187.3030	0.175
208.4837	0.165
284.8969	0.662
312.8057	0.113
322.9848	0.0355
358.5072	0.108
421.5328	0.0828
443.0675	0.285
512.4325	7.47
517.8637	0.413
652.3064	1.95
756.5517	10.4
807.1545	8.24
945.5932	25.9
1006.7536	20.4
1106.6263	16.9
1136.0423	4.16
1171.7648	18.3
1209.3063	17.6
1268.4379	1.46
1315.8972	4.61
1462.7555	1.06
3104.8380	0.859
3172.2420	0.0186

Infrared Spectrum

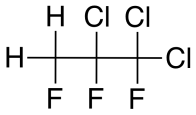


Radiative Efficiency



HCFC-233bd

Molecular Formula: $CH_2FCClFCCl_2F$
Name: 1,1,2-Trichloro-1,2,3-trifluoropropane
CAS number: –
Molecular Weight: 201.4



Global Atmospheric Lifetime (years): 3.71
  Tropospheric Atmospheric Lifetime (years): 4.14
  Stratospheric Atmospheric Lifetime (years): 35.3
Ozone Depletion Potential (ODP): 0.057

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.285	0.257
Global Warming Potential (GWP_H):		
GWP_{20}	1174	1058
GWP_{100}	319	288
Global Temperature Potentials (GTP_H)		
GTP_{20}		498
GTP_{50}		55
GTP_{100}		40

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 1.42 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 0.904 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 4.01$ years
$\tau^{OH}_{Trop} = 4.14$ years
$\tau^{OH}_{Strat} = 121.4$ years

Fractional Atmospheric Loss: 0.925

O(^{1}D) Reactivity

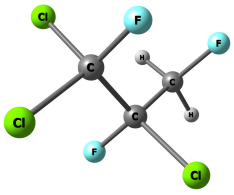
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 2.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)} = 185$ years
Fractional Atmospheric Loss: 0.020

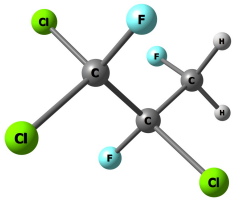
UV Photolysis

UV Spectrum: *No Recommendation*
$\tau_{hv} = 68$ years
Fractional Atmospheric Loss: 0.055

Molecular Structure and Infrared Spectrum (9 conformers)



E = 0
Population = 0.225



$\Delta E = 0.16$ kcal mol^{-1}
Population = 0.171

Optimized Coordinates (Angstroms)

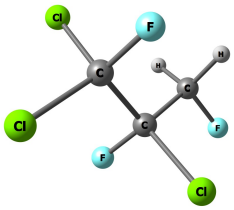
Atom	X	Y	Z
C	-1.515473027554	-1.239077066456	-0.428596630920
C	-0.653493533012	0.030387477141	-0.490942353128
C	0.678091147882	-0.048786110994	0.322767694499
H	-0.943892724874	-2.079742354128	-0.832201684031
F	-1.888198552366	-1.508367299053	0.855163584619
H	-2.399350155896	-1.060311361867	-1.049226451856
Cl	-1.617750706212	1.414974289612	0.128177983505
F	-0.346151073332	0.241938737948	-1.787787479686
Cl	1.634180312873	-1.472761743013	-0.227548206316
Cl	1.662401106290	1.422900043221	0.096121049551
F	0.401682206200	-0.201997612411	1.615019493765

Atom	X	Y	Z
C	-1.646174581888	-1.111400991055	0.284896722209
C	-0.769194958852	0.021239373363	-0.275203755719
C	0.667706677331	0.097805649899	0.331182733108
H	-2.669673157956	-0.934127008030	-0.057345236822
F	-1.225176751346	-2.325160059806	-0.179044815887
H	-1.611326716327	-1.089877496721	1.377971554595
Cl	-1.638120947159	1.550848971599	0.139170715684
F	-0.666438959995	-0.089827769751	-1.609256078854
Cl	1.576586073366	-1.404251921245	-0.011100750763
Cl	1.578049554492	1.486196539006	-0.326030629105
F	0.556125768334	0.231472712740	1.659070541554

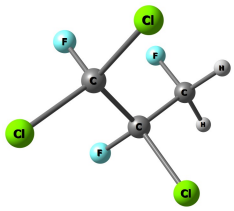
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
47.0400	0.0772
101.4361	0.253
166.5646	0.0606
196.2235	0.123
207.7340	0.172
248.0796	0.0791
287.7396	0.0953
309.5267	0.745
369.5846	0.109
379.9882	0.0331
389.3634	0.310
474.5572	0.676
537.9510	8.01
595.6735	0.540
707.2505	24.1
822.3744	26.3
951.6376	6.55
1079.2264	4.93
1127.5474	1.04
1160.6626	29.5
1178.0413	10.5
1203.8815	4.44
1277.2802	1.79
1420.4021	1.34
1500.3241	1.47
3058.3424	2.12
3116.7544	1.63

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
45.6568	0.0915
122.5900	0.580
168.3290	0.0666
194.0080	0.0306
208.3111	0.323
238.3732	0.0675
279.8576	0.333
301.2833	0.409
329.6050	0.0982
381.7189	0.0385
399.3028	0.0937
438.7361	0.351
536.7720	3.93
601.4367	8.07
788.2174	42.8
847.0039	7.07
941.7851	2.71
982.9456	10.6
1119.4662	9.70
1132.9957	13.3
1187.8780	9.16
1225.6758	11.7
1312.7446	1.55
1419.6730	0.929
1491.6404	0.733
3063.2661	1.44
3123.0771	1.27



$\Delta E = 0.32$ kcal mol^{-1}
Population = 0.131



$\Delta E = 0.38$ kcal mol^{-1}
Population = 0.118

Optimized Coordinates (Angstroms)

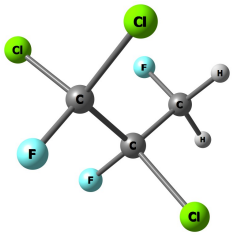
Atom	X	Y	Z
C	-1.493445280673	-1.162645100072	0.379386602165
C	-0.647724659438	-0.026243655712	-0.215510662573
C	0.813583949569	-0.028542941238	0.330824314467
H	-1.425426348832	-1.136299706461	1.470666189730
F	-2.790424930115	-1.009836838502	-0.015032638676
H	-1.114658252601	-2.115957536777	0.000854188557
Cl	-1.413070517625	1.545970635101	0.203905003170
F	-0.600634294218	-0.143090419724	-1.556734922712
Cl	1.582942147852	-1.621355178288	-0.012296816474
Cl	1.796991309218	1.257191720563	-0.406665995990
F	0.780771876865	0.138495021111	1.657052738335

Atom	X	Y	Z
C	-1.949556907592	-0.352766998835	0.333688716468
C	-0.711903755168	0.394943289906	-0.179874228049
C	0.608016684426	-0.446116865895	-0.178911447834
H	-2.799118461526	0.331367360727	0.240745942376
F	-2.173820012943	-1.465047206349	-0.428966643211
H	-1.812767273169	-0.635983517325	1.379813438931
Cl	-0.538556422543	1.871640636168	0.823345665600
F	-0.921858813420	0.751172186179	-1.466308969756
Cl	1.972220455483	0.501618903667	-0.835797725177
Cl	1.001634956275	-1.048767014905	1.459463261553
F	0.413359550176	-1.497732773338	-0.979891010902

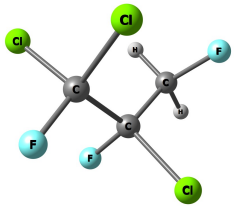
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
63.2753	0.105
89.3107	0.541
153.8493	0.268
188.1379	0.137
214.5172	0.0426
245.9835	0.0506
282.2913	0.110
300.4161	0.203
335.5645	0.216
380.5606	0.0275
392.9314	0.145
433.2942	0.469
542.8882	1.33
641.3675	8.48
761.5232	30.1
818.0383	29.7
928.9985	3.15
1068.1407	3.88
1108.8052	6.54
1136.7657	12.1
1173.8960	18.0
1213.5173	4.37
1299.6657	3.87
1422.0956	0.432
1498.5207	0.260
3063.9349	1.82
3125.1834	1.31

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
48.8508	0.0665
120.5285	0.349
171.3643	0.0276
183.2316	0.200
200.0898	0.191
254.9302	0.118
307.1914	0.272
320.2318	0.525
339.2494	0.0981
374.2453	0.101
396.4868	0.242
444.0284	0.864
491.7792	1.28
578.6215	10.4
840.0961	23.4
875.8714	19.0
948.2141	23.8
976.7324	9.57
1101.6609	0.480
1136.2075	15.0
1181.6498	0.121
1201.0065	19.4
1303.2411	2.55
1419.6829	1.51
1490.9926	1.18
3062.9983	1.52
3128.4810	1.34



$\Delta E = 0.50$ kcal mol^{-1}
Population = 0.097



$\Delta E = 0.55$ kcal mol^{-1}
Population = 0.088

Optimized Coordinates (Angstroms)

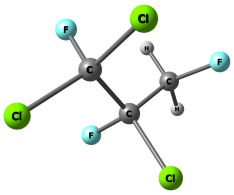
Atom	X	Y	Z
C	-0.860632439073	-1.350348771781	0.986319642597
C	-0.718517324410	-0.404731182130	-0.208896949268
C	0.561648753237	0.494004547736	-0.268966239021
H	-1.812904776580	-1.876481671154	0.865888821958
F	0.160264834091	-2.259828927941	1.002850337847
H	-0.868009018263	-0.778765886713	1.917158530759
Cl	-2.166814744834	0.671793658076	-0.184983192300
F	-0.738389104767	-1.116633627731	-1.356127864171
Cl	0.773275791124	1.430604535542	1.242103861819
Cl	2.012639685243	-0.503032142274	-0.573995079407
F	0.432774344233	1.347280468370	-1.287363870814

Atom	X	Y	Z
C	-1.028413175657	-0.222516606578	1.563221402545
C	-0.654485877870	-0.557799805896	0.114299300133
C	0.726904796804	-0.034392101069	-0.396394010837
H	-0.189303377007	-0.478781014750	2.217934735892
F	-1.347277342751	1.093257506628	1.716754239295
H	-1.892733896153	-0.847084947683	1.811703431709
Cl	-1.936416354017	0.020077054590	-1.000564011194
F	-0.597462861150	-1.910667075100	0.033513611497
Cl	0.856883613100	1.737342411091	-0.312348092207
Cl	2.038836801643	-0.786473801303	0.583295856412
F	0.891080673058	-0.426889619931	-1.660038463244

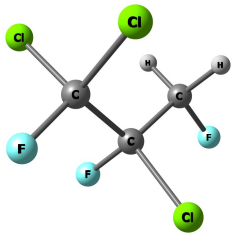
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
47.0103	0.105
117.0446	0.336
169.2254	0.0351
182.9417	0.112
224.6625	0.128
238.4585	0.393
301.4421	0.359
313.7587	0.287
333.1402	0.270
374.7009	0.0462
394.2548	0.113
446.6254	0.857
469.5904	0.995
638.3243	7.57
797.7912	36.5
865.1693	23.9
951.3954	4.16
959.3314	8.45
1115.7245	9.70
1135.6835	11.4
1192.5124	7.60
1211.0870	9.60
1308.5990	1.86
1425.0249	0.778
1490.8698	1.07
3064.3366	1.49
3129.2519	1.30

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
56.2640	0.106
111.7626	0.317
165.8010	0.0216
180.7674	0.0672
219.8077	0.320
255.9528	0.440
281.8321	0.359
316.1066	0.163
335.9015	0.190
387.1724	0.0874
393.7963	0.0731
461.4247	1.34
523.9202	0.633
611.9502	4.95
720.6667	27.5
849.8183	25.8
934.0233	8.35
1068.7381	8.26
1134.7325	25.1
1143.6696	7.09
1168.6280	0.340
1201.5885	8.13
1287.2173	2.24
1422.8055	0.516
1499.5732	1.13
3053.3136	1.99
3110.5531	1.69



$\Delta E = 0.64$ kcal mol^{-1}
Population = 0.076



$\Delta E = 0.90$ kcal mol^{-1}
Population = 0.050

Optimized Coordinates (Angstroms)

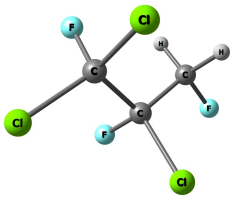
Atom	X	Y	Z
C	-1.842202825120	-0.284134466979	-0.817904007361
C	-0.628096136731	0.515069566810	-0.314705735509
C	0.706919337621	-0.297857009607	-0.316718815967
H	-1.561067082575	-0.796118448277	-1.743731844589
F	-2.276698103749	-1.191918138774	0.099573515981
H	-2.631621078920	0.445888186877	-1.023201684676
Cl	-0.964866599676	1.218399674521	1.288889679633
F	-0.452329076829	1.514925944770	-1.216431382732
Cl	2.102486961969	0.757966370548	0.033529183498
Cl	0.665155139712	-1.676457311541	0.806852644935
F	0.853891464298	-0.775388368348	-1.567098553213

Atom	X	Y	Z
C	-1.150684512574	-0.879911426804	1.057232732623
C	-0.649499250077	-0.196861600194	-0.218097056723
C	0.873923396386	0.148424834729	-0.222331787337
H	-1.006297383297	-0.226009837319	1.920159090842
F	-2.477522512951	-1.161082423979	0.899762212957
H	-0.598069954519	-1.814786622580	1.196207164428
Cl	-1.581258989096	1.314050589911	-0.509187292472
F	-0.857446353038	-1.018306725420	-1.272114934981
Cl	1.322761645691	1.204692686514	1.148250721296
Cl	1.831313785072	-1.372416195885	-0.149441910686
F	1.175981128402	0.765128721026	-1.362314939947

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
55.9698	0.0994
111.7894	0.343
163.8275	0.0532
173.9681	0.0507
212.0750	0.330
252.9231	0.193
293.2888	0.610
309.7910	0.243
362.5823	0.0793
386.3670	0.0547
397.9706	0.130
483.2937	1.59
520.9547	2.28
559.1909	7.50
763.6561	12.0
867.0945	34.0
951.4148	9.34
1075.5327	15.4
1099.3007	9.68
1135.0891	17.1
1159.3784	3.35
1183.8959	6.72
1285.5294	1.34
1418.8247	1.40
1501.0512	0.877
3054.2182	2.19
3112.6689	1.50

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
65.5454	0.143
90.2695	0.412
160.6952	0.268
165.0459	0.0428
229.7058	0.0465
236.8477	0.0716
294.4610	0.123
301.1280	0.300
349.3428	0.217
375.1093	0.0711
392.8633	0.0316
434.1987	0.941
498.2690	0.316
644.4900	9.26
768.9493	31.7
844.9474	22.5
940.2128	12.4
1053.8961	7.41
1091.3867	6.19
1139.4395	9.75
1197.5767	10.6
1199.2537	10.3
1290.8113	2.69
1425.2749	0.298
1499.2983	0.406
3061.7146	1.93
3127.5275	1.24



$\Delta E = 0.95$ kcal mol^{-1}
Population = 0.045

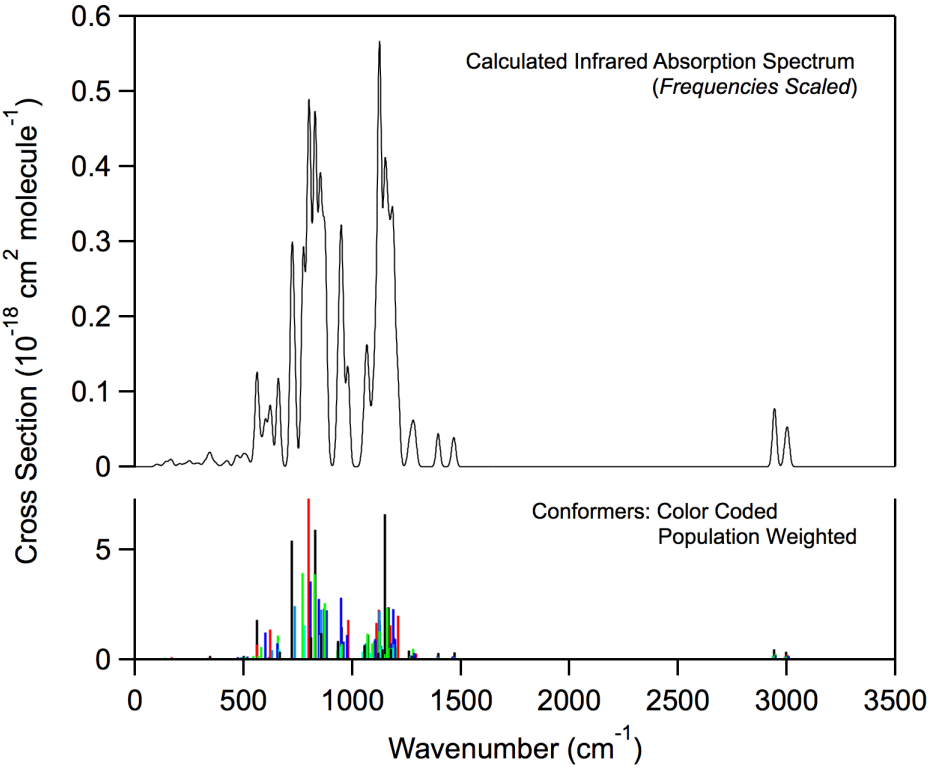
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.624600585321	-1.023244798457	-0.330944690280
C	-0.668404220784	0.172121685658	-0.211038734016
C	0.828328138855	-0.267055883993	-0.298129007497
H	-1.484153200561	-1.710059494091	0.506576121569
F	-2.905586807915	-0.553903921867	-0.341396003202
H	-1.416225084843	-1.532987518877	-1.277242416775
Cl	-0.996225318924	1.081470350713	1.293190967401
F	-0.882232653167	0.991926039373	-1.266506069488
Cl	1.917413710953	1.138552609114	-0.355595684545
Cl	1.282589941565	-1.360261380194	1.041900583652
F	0.960283080142	-0.946904687380	-1.452138066818

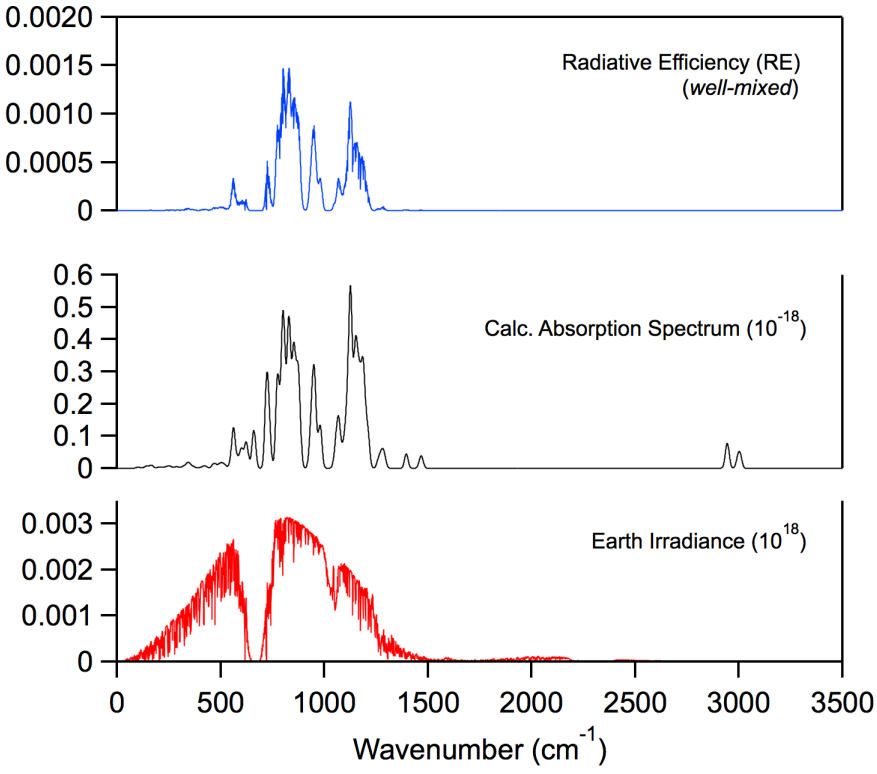
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
67.5002	0.142
93.7038	0.471
150.9848	0.305
168.6845	0.0370
214.4049	0.0884
244.7164	0.0303
299.8813	0.302
322.2318	0.346
339.4072	0.0456
376.2795	0.102
396.8953	0.0322
429.0019	1.19
497.8440	0.634
648.6403	8.22
800.2549	22.6
850.0705	26.8
933.5084	19.0
1061.8397	14.5
1103.5497	0.908
1128.9653	6.53
1149.7397	10.4
1191.2485	11.1
1292.4621	3.94
1422.5184	0.491
1501.8215	0.293
3061.2635	1.82
3128.2909	1.35

Infrared Spectrum

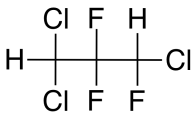


Radiative Efficiency



HCFC-233ca

Molecular Formula:	$CHCl_2CF_2CHClF$
Name:	1,1,3-Trichloro-2,2,3-trifluoropropane
CAS number:	131221-36-8
Molecular Weight:	201.4



Global Atmospheric Lifetime (years):	1.27
Tropospheric Atmospheric Lifetime (years):	1.34
Stratospheric Atmospheric Lifetime (years):	23.3
Ozone Depletion Potential (ODP):	0.023

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.223	0.174
Global Warming Potential (GWP_H):		
GWP_{20}	317	247
GWP_{100}	86	67
Global Temperature Potentials (GTP_H)		
GTP_{20}		83
GTP_{50}		12
GTP_{100}		9

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 4.37 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 2.79 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 1.30$ years

$\tau^{OH}_{Trop} = 1.34$ years

$\tau^{OH}_{Strat} = 43.9$ years

Fractional Atmospheric Loss: 0.974

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

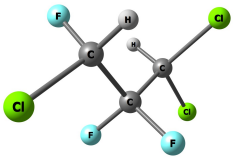
UV Photolysis

UV Spectrum: *No Recommendation*

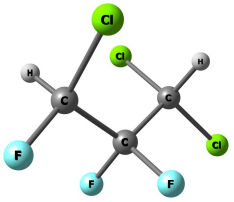
$\tau_{hv} = 68$ years

Fractional Atmospheric Loss: 0.019

Molecular Structure and Infrared Spectrum (4 conformers)



E = 0
Population = 0.682



$\Delta E = 0.78$ kcal mol^{-1}
Population = 0.182

Optimized Coordinates (Angstroms)

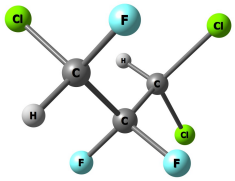
Atom	X	Y	Z
C	1.169887813651	0.132402120756	-0.444924211725
C	-0.172287149025	-0.390881900751	0.117023952161
C	-1.343318357261	0.568878486151	-0.187301543118
Cl	1.569713194369	1.727514899153	0.261074264828
Cl	2.461999146221	-1.053376492589	-0.144357304491
H	1.081121722395	0.265963308090	-1.519582203659
F	-0.092581174127	-0.566204602369	1.445262816037
F	-0.413001847585	-1.580604203664	-0.466773531688
H	-1.242939242885	1.497863752961	0.372676832771
F	-1.340360270510	0.827571344205	-1.518210755891
Cl	-2.894270835242	-0.174699711944	0.284735684776

Atom	X	Y	Z
C	0.960852890060	-0.294911704394	-0.401190814559
C	-0.135358631379	0.597415757939	0.214338253918
C	-1.482924145895	-0.109398915842	0.491824762710
Cl	2.440696748609	0.661522294266	-0.658110064064
Cl	1.272101889979	-1.714889957591	0.642597843813
H	0.636501877379	-0.667052493224	-1.368847091731
F	-0.357714913708	1.626804841236	-0.624593629405
F	0.283481519913	1.096961117221	1.394207533397
H	-1.366009001639	-0.916808517129	1.213898164596
F	-2.333779169065	0.819019059061	0.966261907440
Cl	-2.154176064254	-0.826011481543	-1.011257866115

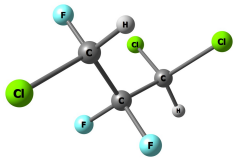
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
49.6542	0.103
65.7004	0.106
119.5870	0.0824
187.9566	0.336
210.9829	0.145
235.2758	0.0512
257.1738	0.0339
308.2645	0.198
359.5957	0.271
385.3737	0.303
469.9615	0.878
568.4320	1.86
691.6889	26.3
749.4174	2.19
764.2117	4.83
835.3680	19.7
865.0623	1.38
1067.7808	8.12
1113.9590	17.7
1202.4402	15.4
1230.1250	8.85
1248.9189	2.57
1279.1380	1.73
1314.4214	1.39
1369.3594	0.735
3138.5299	0.703
3165.2830	0.393

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
48.1539	0.0619
77.1097	0.139
127.0340	0.0591
178.9557	0.378
207.9894	0.0489
251.0161	0.0290
277.6015	0.186
319.3816	0.196
341.9185	0.0869
400.6514	0.499
420.0134	1.07
553.3829	2.28
721.0403	10.0
748.6204	5.17
781.6689	13.3
805.3226	14.7
868.2244	10.4
1066.5250	11.6
1138.9718	21.0
1196.7140	7.16
1224.3592	12.1
1248.2525	6.63
1269.3689	3.96
1305.7836	0.251
1383.3031	2.09
3137.3579	0.669
3168.2038	0.457



$\Delta E = 1.29$ kcal mol^{-1}
Population = 0.077



$\Delta E = 1.45$ kcal mol^{-1}
Population = 0.059

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	0.853282201911	0.062272101823	-0.527470094195
C	-0.088499281968	-0.540691605436	0.534079715138
C	-1.554093864827	-0.040141027537	0.557067422915
Cl	1.032774323511	1.822207007833	-0.319216907354
Cl	2.434752211580	-0.765106493323	-0.450972701052
H	0.444611152337	-0.112429795762	-1.518765694946
F	0.404745065507	-0.336691046775	1.769770658227
F	-0.155988712868	-1.874233427579	0.319344134256
H	-2.113425147814	-0.703637297520	1.221167846236
F	-1.630533827732	1.223573139897	1.002175254633
Cl	-2.313859119637	-0.169472555622	-1.064343633859

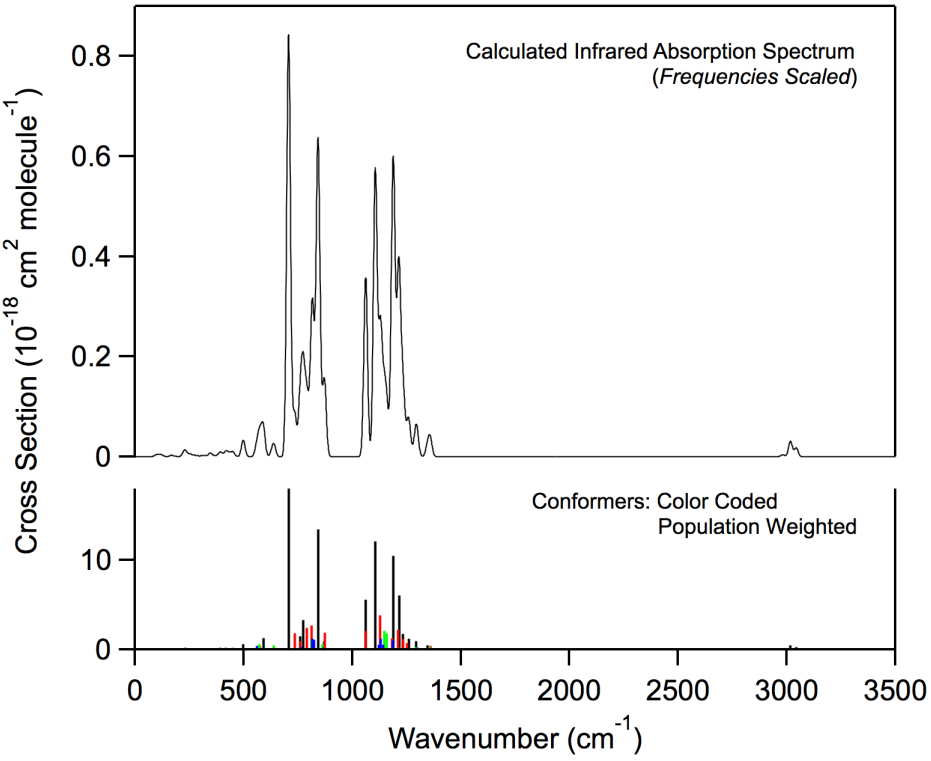
Atom	Z	Z	Z
C	1.300078807246	0.168466394808	0.461682305019
C	-0.243497577105	0.223595205773	0.602790264164
C	-1.062890247048	-0.075680769963	-0.668552588090
Cl	1.920345502450	-1.480951900619	0.231345261630
Cl	1.857173080544	1.278042518405	-0.827559996660
H	1.711279017855	0.541752798835	1.397871254446
F	-0.539409886870	1.479087141214	1.006378749270
F	-0.590150234013	-0.628456240165	1.583512083442
H	-0.818497093572	0.632591670968	-1.460335801672
F	-0.814628484717	-1.335188578158	-1.078246871997
Cl	-2.808555884769	0.108340758902	-0.315059659553

Infrared Absorption Spectrum (unscaled frequencies)

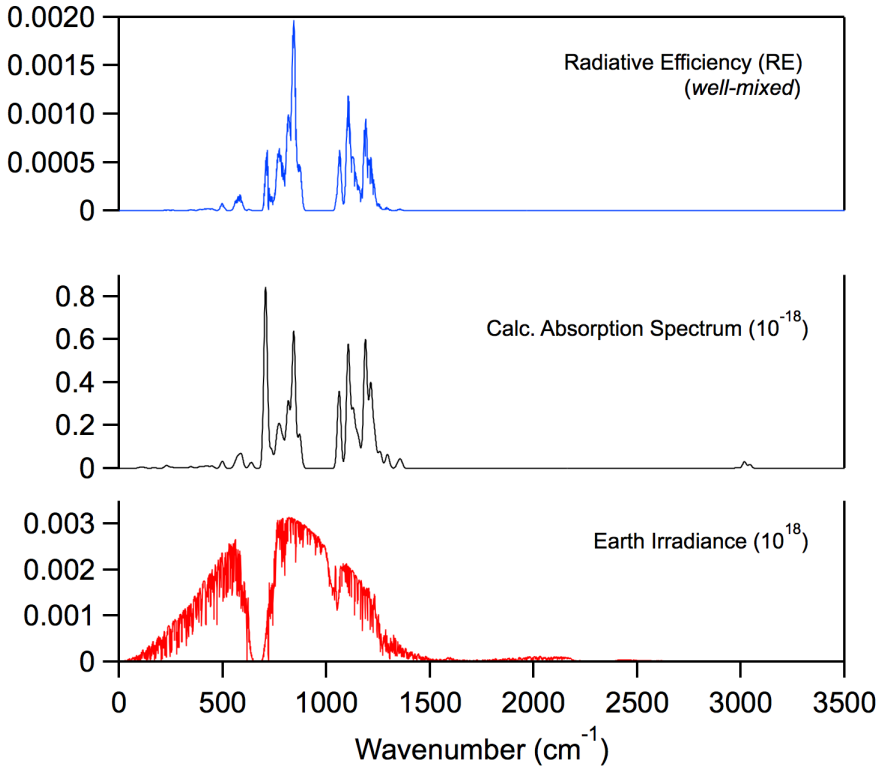
Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
38.2473	0.0633
82.2577	0.0727
143.1196	0.151
177.1147	0.121
212.5248	0.0332
229.6548	0.275
278.6427	0.243
318.2741	0.139
349.4502	0.200
409.4192	0.405
475.8288	0.418
549.3953	7.77
620.4037	6.32
736.7013	1.23
804.1493	13.0
809.7799	16.1
857.8192	8.15
1121.8638	1.26
1158.2773	26.7
1171.1057	23.2
1200.3447	2.50
1232.4849	2.79
1300.8408	1.09
1311.5769	3.37
1381.8828	3.64
3100.6021	1.13
3166.1357	0.393

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
33.6084	0.0955
75.1582	0.0523
135.7840	0.0375
181.5706	0.199
202.0201	0.135
237.0418	0.129
257.7383	0.0774
335.1470	0.176
368.7408	0.142
395.8917	0.552
474.1019	1.32
536.2818	7.27
609.9534	2.65
755.2797	4.03
807.1637	20.4
815.9809	17.8
859.3705	3.30
1130.6104	8.75
1140.3898	20.7
1152.4785	9.12
1198.2778	16.7
1230.5459	0.324
1299.7874	0.677
1322.9732	3.28
1384.4369	1.04
3130.1806	0.717
3139.7238	0.507

Infrared Spectrum

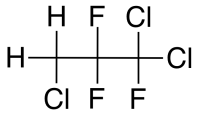


Radiative Efficiency



HCFC-233cb

Molecular Formula:	$CH_2ClCF_2CCl_2F$
Name:	1,1,3-Trichloro-1,2,2-trifluoropropane
CAS number:	421-99-8
Molecular Weight:	201.4



Global Atmospheric Lifetime (years):	4.57
Tropospheric Atmospheric Lifetime (years):	5.21
Stratospheric Atmospheric Lifetime (years):	37.3
Ozone Depletion Potential (ODP):	0.069

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.273	0.250
Global Warming Potential (GWP_H):		
GWP_{20}	1380	1264
GWP_{100}	378	347
Global Temperature Potentials (GTP_H)		
GTP_{20}		663
GTP_{50}		71
GTP_{100}		49

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 1.12 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 0.718 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 5.04$ years

$\tau^{OH}_{Trop} = 5.21$ years

$\tau^{OH}_{Strat} = 149.4$ years

Fractional Atmospheric Loss: 0.908

$O(^1D)$ 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

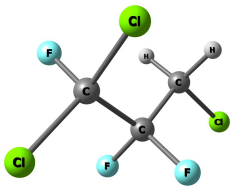
UV Photolysis

UV Spectrum: *No Recommendation*

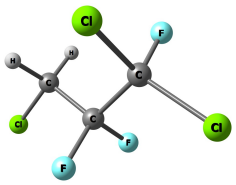
$\tau_{hv} = 68$ years

Fractional Atmospheric Loss: 0.067

Molecular Structure and Infrared Spectrum (5 conformers)



E = 0
Population = 0.378



E = 0
Population = 0.378

Optimized Coordinates (Angstroms)

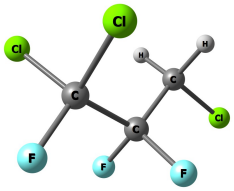
Atom	X	Y	Z
C	-1.485984112339	0.634900016275	0.426340746033
C	-0.425285361349	-0.326406334285	-0.109620427033
C	1.020431642918	0.094016212287	0.315827273149
Cl	-3.126842225674	0.051082830118	0.016237006795
H	-1.406746907824	0.697237667285	1.510361097875
H	-1.358519835585	1.619577488391	-0.018077369755
F	-0.472090295413	-0.400221011553	-1.449088337660
F	-0.629706428235	-1.560196763114	0.393178248983
Cl	2.199398904894	-1.129131732106	-0.212899545623
Cl	1.441639630890	1.693988753416	-0.368662809435
F	1.049413987717	0.179152873284	1.653779116670

Atom	Z	Z	Z
C	-1.487001957274	0.626733559397	-0.438662004925
C	-0.425608494148	-0.324340458180	0.113920783649
C	1.019988889901	0.090943153185	-0.316945296231
Cl	-3.127517321278	0.047577576109	-0.020653658853
H	-1.361219531135	1.618692012654	-0.010244639371
H	-1.406787711122	0.671482325592	-1.523478957457
F	-0.627973668313	-1.566428540073	-0.368882427463
F	-0.473628049238	-0.376359502971	1.454369101704
Cl	1.438500651319	1.702403826754	0.341763123230
Cl	2.199988574931	-1.121906336362	0.232785065311
F	1.050169616356	0.154287383894	-1.656079089594

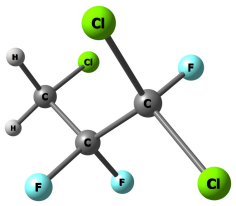
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
63.8001	0.330
65.4896	0.271
122.7436	0.206
191.6926	0.0178
224.2522	0.115
236.9169	0.184
283.0263	0.0303
316.6726	0.329
349.9699	0.0853
385.1844	0.0516
437.2953	0.260
513.4411	0.790
567.3542	2.06
705.2763	23.4
770.4037	3.17
859.8365	29.1
890.3381	8.70
912.7394	4.69
1104.9932	14.5
1116.2917	8.57
1171.1244	10.8
1247.5272	7.35
1285.0901	10.2
1323.8337	1.22
1465.1359	1.15
3117.5496	0.846
3186.3740	0.0179

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
63.7994	0.330
65.4894	0.271
122.7435	0.206
191.6925	0.0178
224.2523	0.115
236.9169	0.184
283.0264	0.0303
316.6726	0.329
349.9700	0.0853
385.1844	0.0516
437.2954	0.260
513.4411	0.790
567.3543	2.06
705.2762	23.4
770.4039	3.17
859.8364	29.1
890.3382	8.70
912.7396	4.69
1104.9940	14.5
1116.2915	8.57
1171.1254	10.8
1247.5276	7.35
1285.0899	10.2
1323.8339	1.22
1465.1364	1.15
3117.5498	0.846
3186.3743	0.0179



$\Delta E = 0.76$ kcal mol^{-1}
Population = 0.104



$\Delta E = 1.00$ kcal mol^{-1}
Population = 0.070

Optimized Coordinates (Angstroms)

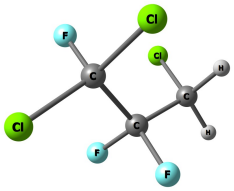
Atom	X	Y	Z
C	-1.284180348782	-0.022841994825	-0.826547304898
C	-0.442857766722	0.008894940706	0.444251592874
C	1.106507892822	-0.000933679219	0.207479711085
Cl	-3.027309116277	-0.008007027467	-0.417742623893
H	-1.074083426104	0.853856190908	-1.436023500924
H	-1.078183985255	-0.931538289192	-1.388719983270
F	-0.711969860749	-1.059288733600	1.220311425290
F	-0.706973562346	1.117895990999	1.162629569786
Cl	1.610247266048	-1.494487764536	-0.639529892169
Cl	1.616993262624	1.443364635363	-0.717338777000
F	1.695239644742	0.029363730863	1.402477783116

Atom	X	Y	Z
C	-1.637804288268	-0.122472158497	0.859663220199
C	-0.278412096318	-0.709247099228	0.467701963515
C	0.710822476386	0.238762234290	-0.283281676733
Cl	-2.711589764782	0.214458032818	-0.529360334958
H	-2.125863775657	-0.870765393222	1.484731487346
H	-1.503153664131	0.797911285587	1.423707166265
F	-0.449969489206	-1.795597479996	-0.307087348456
F	0.317490493341	-1.096622865344	1.617620844996
Cl	1.020332077562	1.713244344027	0.687648307359
Cl	2.245903802631	-0.621739290361	-0.589409514529
F	0.179612228441	0.595763389924	-1.451978115002

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
62.0234	0.451
69.4940	0.0781
131.8456	0.167
181.2515	0.0254
207.9909	0.0834
254.9036	0.109
300.9659	0.157
316.8993	0.529
365.8461	0.00430
372.3526	0.0242
432.0428	0.550
483.7391	1.00
548.7391	1.64
731.1859	12.1
780.7408	4.47
846.2287	35.1
910.7278	6.33
910.9499	15.5
1080.3509	9.15
1109.7650	8.98
1196.7318	13.9
1251.7790	15.9
1273.8133	6.80
1326.8703	1.12
1464.7028	1.45
3118.8584	1.07
3186.8628	0.00261

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
34.6671	0.0824
94.7654	0.158
171.0640	0.185
185.9848	0.350
197.5848	0.0294
270.5357	0.237
301.9113	0.305
317.5296	0.224
344.1392	0.0834
384.4598	0.0379
436.4424	1.02
512.4816	0.780
573.4420	8.70
618.1113	1.15
798.2378	12.4
834.4664	21.1
893.7191	17.1
923.1649	11.4
1103.4587	4.91
1160.6457	24.8
1172.5179	12.7
1220.3700	6.11
1296.7366	6.80
1319.1971	2.61
1463.4880	1.94
3106.3659	0.878
3178.5717	0.0113



ΔE = 1.0 kcal mol^{-1}
Population = 0.070

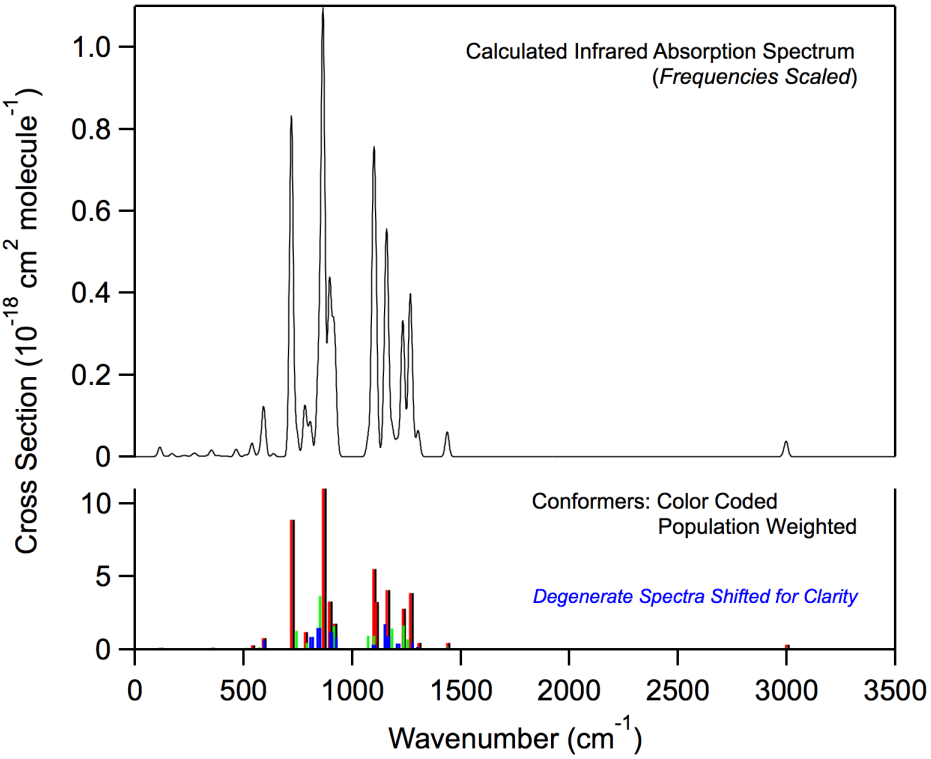
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.638199907302	-0.140585658308	-0.854083756927
C	-0.273851058507	-0.716322751311	-0.462984159285
C	0.711824863286	0.242575659094	0.278795803427
Cl	-2.709548747552	0.198210519513	0.536366285051
H	-1.511218878244	0.777096169999	-1.424275075708
H	-2.123555247215	-0.895822030193	-1.472875891714
F	0.320717732401	-1.107111162681	-1.612438912222
F	-0.435998697583	-1.798870628609	0.319118675407
Cl	2.253307738866	-0.606308546758	0.585190421809
Cl	1.008827206102	1.712877578450	-0.702325999690
F	0.182199995748	0.603523850806	1.446998609853

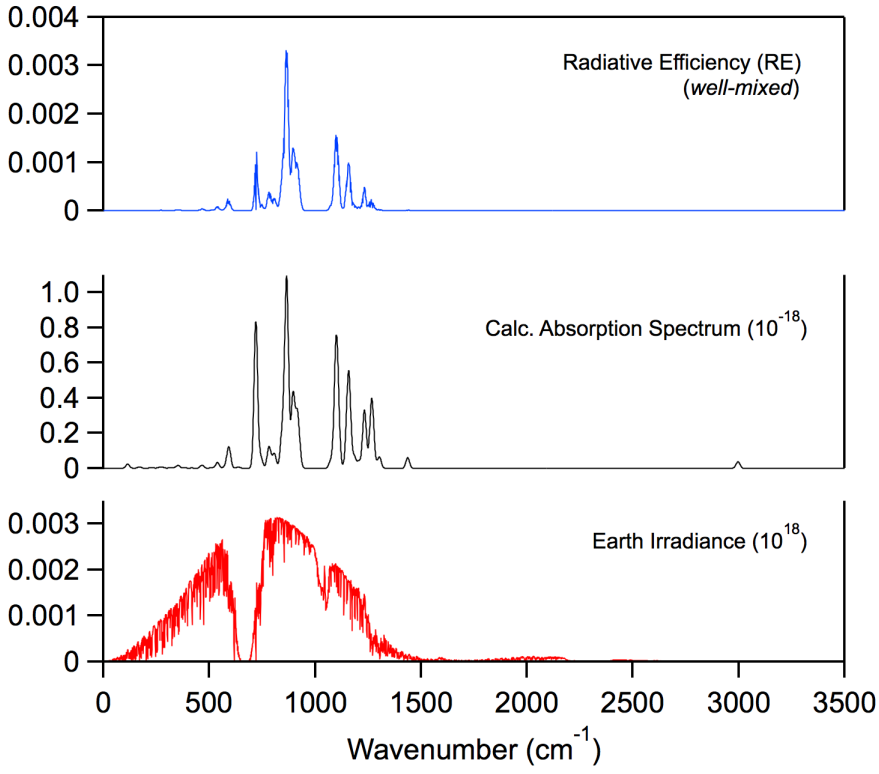
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
34.6644	0.0824
94.7633	0.158
171.0645	0.185
185.9843	0.350
197.5845	0.0294
270.5355	0.237
301.9109	0.305
317.5290	0.224
344.1399	0.0834
384.4596	0.0379
436.4428	1.02
512.4814	0.780
573.4435	8.70
618.1112	1.15
798.2374	12.4
834.4669	21.1
893.7197	17.1
923.1662	11.4
1103.4595	4.91
1160.6451	24.8
1172.5189	12.7
1220.3726	6.11
1296.7393	6.80
1319.1989	2.61
1463.4910	1.94
3106.3645	0.878
3178.5704	0.0113

Infrared Spectrum

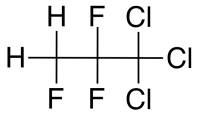


Radiative Efficiency



HCFC-233cc

Molecular Formula:	$CH_2FCF_2CCl_3$
Name:	1,1,1-Trichloro-2,2,3-trifluoropropane
CAS number:	131211-71-7
Molecular Weight:	201.4



Global Atmospheric Lifetime (years):	6.26
Tropospheric Atmospheric Lifetime (years):	7.71
Stratospheric Atmospheric Lifetime (years):	33.2
Ozone Depletion Potential (ODP):	0.100

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.263	0.246
Global Warming Potential (GWP_H):		
GWP_{20}	1766	1651
GWP_{100}	499	466
Global Temperature Potentials (GTP_H)		
GTP_{20}		1016
GTP_{50}		112
GTP_{100}		66

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 7.60 \times 10^{-15}$; $k_{SAR}(272\ K) \approx 4.85 \times 10^{-15}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 7.44$ years

$\tau^{OH}_{Trop} = 7.71$ years

$\tau^{OH}_{Strat} = 212.5$ years

Fractional Atmospheric Loss: 0.841

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: 0.034

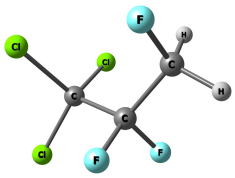
UV Photolysis

UV Spectrum: *No Recommendation*

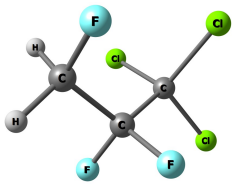
$\tau_{hv} = 50$ years

Fractional Atmospheric Loss: 0.125

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.370



E = 0
Population = 0.370

Optimized Coordinates (Angstroms)

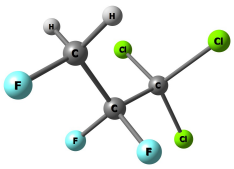
Atom	X	Y	Z
C	-2.022965746633	0.274734395933	-0.548877244491
C	-0.715994690461	0.769843061949	0.084184041621
C	0.541353633863	-0.157335249079	-0.035007063439
H	-1.850504529535	-0.047666780818	-1.578743512694
F	-2.567135889130	-0.743099620812	0.179048895260
H	-2.701914792430	1.134940940435	-0.541819710991
F	-0.924016628822	1.013291857140	1.390791394068
F	-0.412130145346	1.938880670055	-0.524361731750
Cl	1.925547178044	0.663300932806	0.740855004579
Cl	0.239186949675	-1.714850888938	0.770422065429
Cl	0.909087660775	-0.428364318670	-1.767222137593

Atom	X	Y	Z
C	-2.028957954357	0.274030277629	0.531861560720
C	-0.716711915123	0.771654224774	-0.088184127765
C	0.539879035962	-0.155508285903	0.038854410684
H	-2.708125608998	1.134033646704	0.521745827453
F	-2.566424140679	-0.741571888680	-0.204118470709
H	-1.865333718521	-0.051715763135	1.562117045196
F	-0.418553768286	1.938768764669	0.526840714055
F	-0.913464558253	1.019360854718	-1.395736497919
Cl	1.930470380238	0.668139324539	-0.722234873071
Cl	0.892650654634	-0.432156215502	1.773291099346
Cl	0.245264593384	-1.710443939814	-0.774320687990

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
45.3406	0.170
113.7143	0.414
172.4497	0.0909
183.0477	0.216
208.8100	0.167
258.5295	0.0227
263.9800	0.0735
277.3458	0.467
333.7699	0.269
363.5587	0.360
412.5006	0.142
461.5797	1.41
596.4675	4.29
603.6592	8.79
795.6915	16.6
820.1560	23.3
879.0045	6.11
970.1736	5.92
1135.3358	13.8
1166.5138	12.8
1189.0587	5.78
1237.7951	6.73
1303.1895	6.68
1428.1399	0.485
1498.3752	0.979
3053.9476	2.36
3120.3263	1.74

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
45.3420	0.170
113.7155	0.414
172.4503	0.0909
183.0480	0.216
208.8098	0.167
258.5295	0.0227
263.9800	0.0735
277.3459	0.467
333.7699	0.269
363.5586	0.360
412.5008	0.142
461.5792	1.41
596.4676	4.29
603.6589	8.79
795.6922	16.6
820.1564	23.3
879.0045	6.11
970.1729	5.92
1135.3356	13.8
1166.5141	12.8
1189.0583	5.78
1237.7937	6.73
1303.1886	6.68
1428.1384	0.485
1498.3737	0.979
3053.9482	2.36
3120.3271	1.74



$\Delta E = 0.21$ kcal mol^{-1}
Population = 0.259

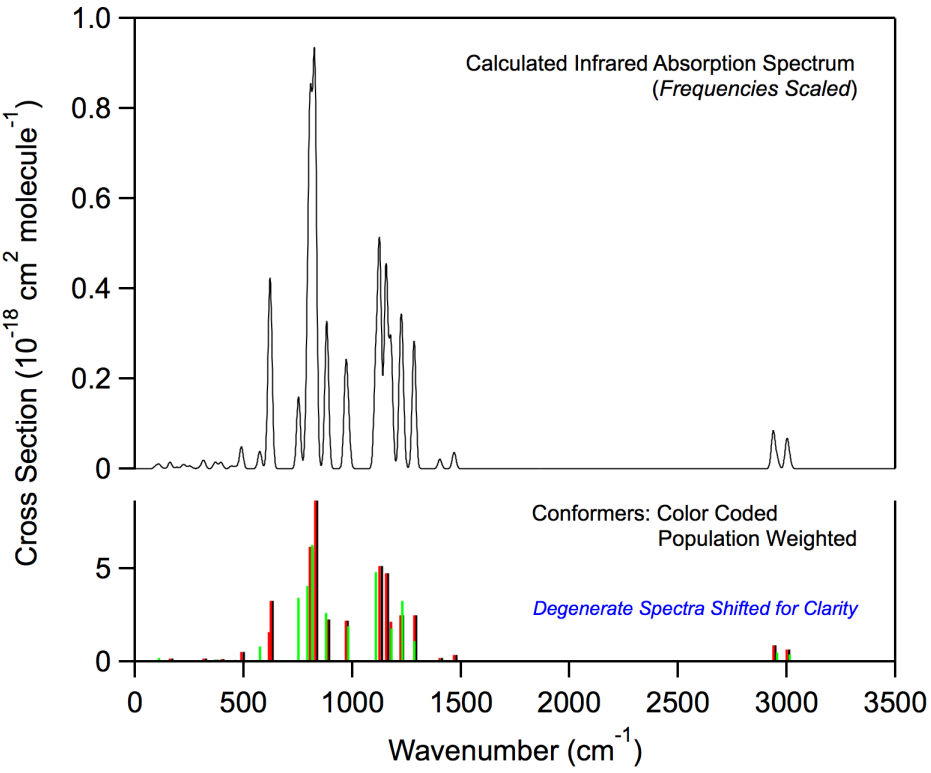
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.863943565229	-0.787660677482	-0.009541846158
C	-0.844848092223	0.357679178213	-0.001165388148
C	0.658991517177	-0.081827463764	-0.001323716142
H	-1.740978188710	-1.405871229128	0.883089358456
F	-3.107007214543	-0.216770832320	-0.008188884508
H	-1.738089412414	-1.395334911149	-0.908979346734
F	-1.047865615807	1.119385704011	1.091820037878
F	-1.044353516356	1.132186198991	-1.085769520299
Cl	1.683446210820	1.375148372307	0.008890345731
Cl	0.996203582634	-1.062284322919	1.456613972631
Cl	1.000921294650	-1.045087016760	-1.469590012707

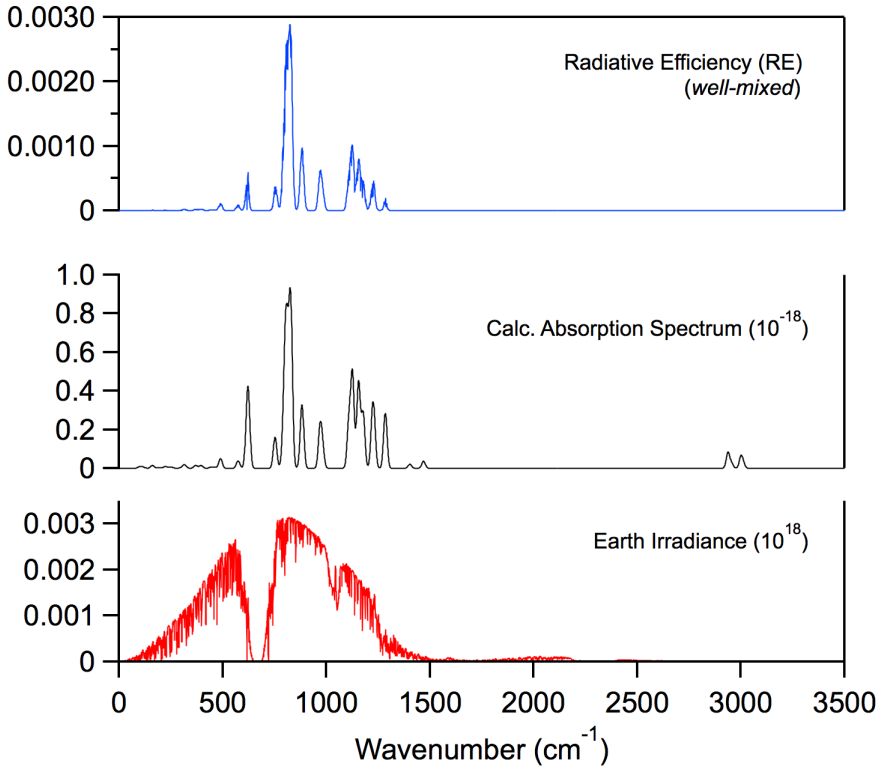
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
61.0505	0.706
82.1096	0.0821
146.6915	0.273
176.6221	0.00990
224.6445	0.0829
249.6397	0.0221
263.7682	0.0230
282.1534	0.180
332.7013	0.358
350.3159	0.350
413.1190	0.0505
432.7923	0.425
551.2354	3.16
740.1537	13.2
783.8936	15.7
805.9894	24.0
875.3902	10.00
983.1760	7.31
1116.7816	18.5
1135.6988	0.307
1192.6318	6.84
1246.7448	12.6
1304.4677	4.21
1431.2564	0.355
1501.2890	0.224
3073.0074	1.85
3133.3077	1.52

Infrared Spectrum

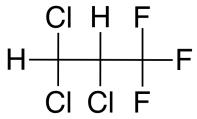


Radiative Efficiency



HCFC-233da

Molecular Formula:	$CHCl_2CHClCF_3$
Name:	2,3,3-Trichloro-1,1,1-trifluoropropane
CAS number:	431-51-6
Molecular Weight:	201.4



Global Atmospheric Lifetime (years):	0.896
Tropospheric Atmospheric Lifetime (years):	0.939
Stratospheric Atmospheric Lifetime (years):	20
Ozone Depletion Potential (ODP):	0.017

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.196	0.142
Global Warming Potential (GWP_H):		
GWP_{20}	196	142
GWP_{100}	53	38
Global Temperature Potentials (GTP_H)		
GTP_{20}		45
GTP_{50}		7
GTP_{100}		5

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 6.24 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 3.98 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

τ^{OH}_{Global} = 0.913 years
τ^{OH}_{Trop} = 0.939 years
τ^{OH}_{Strat} = 31.9 years

Fractional Atmospheric Loss: 0.982

$O(^1D)$ Reactivity

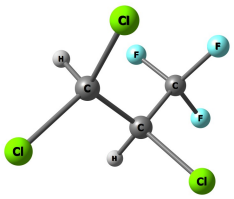
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 2.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)}$ = 185 years
Fractional Atmospheric Loss: 0.005

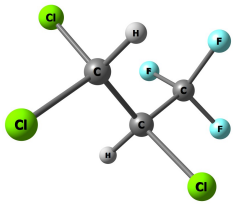
UV Photolysis

UV Spectrum: *No Recommendation*
τ_{hv} = 68 years
Fractional Atmospheric Loss: 0.013

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.631



$\Delta E = 0.69$ kcal mol^{-1}
Population = 0.196

Optimized Coordinates (Angstroms)

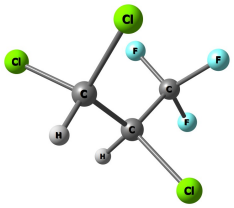
Atom	X	Y	Z
C	-0.940439863591	-0.442217316531	0.516776918400
C	0.237353845538	0.527925747535	0.360290461779
C	1.601706978586	-0.186551300698	0.314245764046
Cl	-2.419928259073	0.454548768114	0.985904147697
Cl	-1.234431503636	-1.455981581305	-0.920766381478
H	-0.721485012420	-1.122038785732	1.337213618023
H	0.256528293658	1.152552410581	1.255483867262
Cl	0.079399741618	1.627932414459	-1.034893390271
F	2.584945171506	0.702543320185	0.453867189874
F	1.674843133692	-1.046523902559	1.346688358080
F	1.806582474122	-0.866513774049	-0.806355553413

Atom	X	Y	Z
C	-1.003212932727	-0.116025155307	-0.378751778416
C	0.232169455733	0.354701808902	0.407506296803
C	1.526911817067	-0.415010257531	0.050751316392
Cl	-1.303992084442	-1.870629205051	-0.162376554243
Cl	-2.458076638320	0.798025523957	0.124983103711
H	-0.866406639567	0.053930762521	-1.443518828021
H	0.061194762657	0.258483705404	1.479813472447
Cl	0.507582028461	2.095740930639	0.052095730898
F	2.601275030377	0.225096561310	0.506945368747
F	1.522491657966	-1.628461341694	0.606610761843
F	1.649344542795	-0.556469333150	-1.272998890163

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
46.6249	0.0357
77.2126	0.0325
145.3408	0.246
167.5609	0.00370
185.0635	0.148
243.6722	0.0939
261.5459	0.129
338.0022	0.0466
358.4443	0.0382
515.5980	1.22
547.6819	1.09
599.9535	1.87
669.7221	9.27
677.7563	6.98
774.8829	6.99
826.0245	5.37
888.5088	3.11
1040.9680	2.35
1150.7740	25.6
1203.8914	25.1
1231.4222	4.56
1247.9127	6.24
1285.7530	32.9
1300.9716	3.63
1352.1823	12.4
3108.6480	0.521
3147.8790	0.276

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
40.4656	0.0348
58.8841	0.0101
156.3283	0.0715
206.8951	0.233
214.8229	0.274
244.6316	0.286
267.3425	0.217
333.8296	0.0155
362.8818	0.0785
414.7011	1.52
542.4620	0.840
556.0841	0.0228
667.0739	9.89
739.2591	16.0
771.6455	7.41
809.8925	1.53
878.2275	0.760
1054.9486	0.0888
1156.4085	20.5
1196.9224	9.10
1221.4229	2.16
1236.2724	24.0
1254.4955	32.5
1297.5120	9.22
1360.5553	9.49
3129.8774	0.288
3161.6420	0.294



$\Delta E = 0.77$ kcal mol^{-1}
Population = 0.173

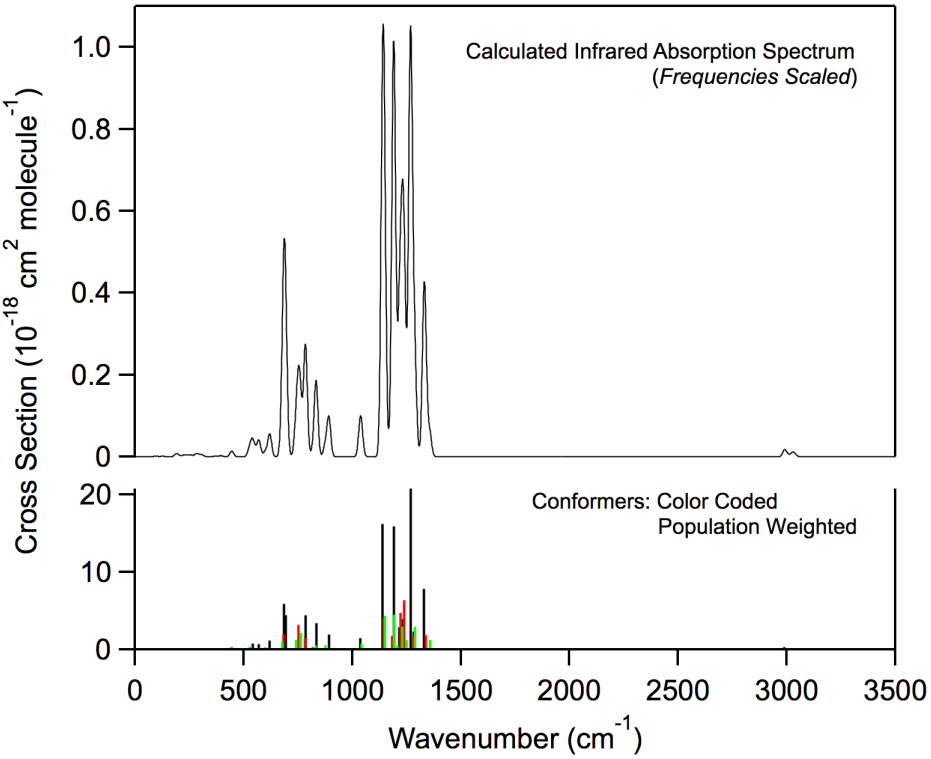
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.088316216281	0.415415805906	0.483038133154
C	0.405379677273	0.132541960050	0.703105310695
C	1.117871390471	-0.794644591453	-0.303281698727
Cl	-1.494203227888	0.959620343368	-1.167692148721
Cl	-2.076003670111	-1.010090911953	0.959431090341
H	-1.385635126312	1.218289507659	1.152085647314
H	0.506437488510	-0.334399308101	1.683669126843
Cl	1.296252670670	1.691051000299	0.787202113742
F	2.316415546821	-1.126033241768	0.188383975961
F	0.419222616425	-1.919430812448	-0.476538653458
F	1.300334850421	-0.227926751561	-1.490666897144

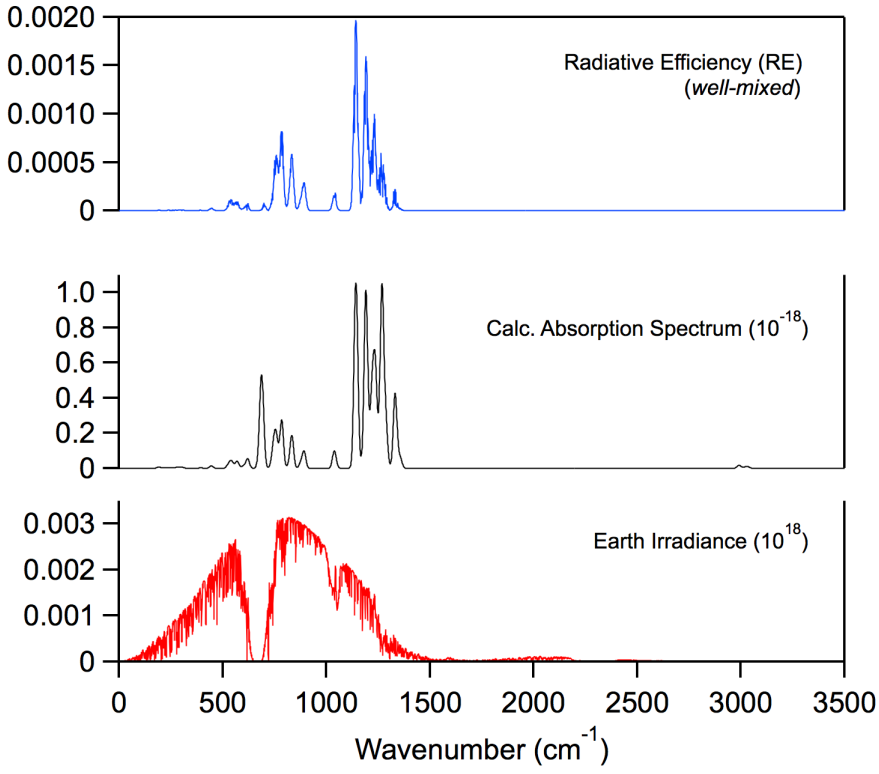
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
38.9952	0.0219
84.0832	0.0266
150.6012	0.0379
165.5184	0.116
200.0768	0.117
235.5986	0.285
276.0249	0.117
320.4163	0.0340
367.3177	0.0846
501.1898	2.34
528.3213	1.37
579.0473	1.70
659.7692	6.05
727.0271	7.28
750.2550	12.5
824.8342	3.03
870.2165	3.12
1047.1866	4.30
1160.3886	25.1
1206.2836	25.8
1222.5397	2.94
1246.1553	17.1
1267.3454	7.29
1308.7926	16.8
1379.7366	7.23
3119.6390	0.438
3155.4917	0.305

Infrared Spectrum

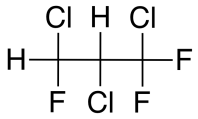


Radiative Efficiency



HCFC-233db

Molecular Formula:	$CHClFCHClCClF_2$
Name:	1,2,3-Trichloro-1,1,3-trifluoropropane
CAS number:	1943659-38-8
Molecular Weight:	201.4



Global Atmospheric Lifetime (years):	2.37
Tropospheric Atmospheric Lifetime (years):	2.52
Stratospheric Atmospheric Lifetime (years):	40.1
Ozone Depletion Potential (ODP):	0.034

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.276	0.238
Global Warming Potential (GWP_H):		
GWP_{20}	731	630
GWP_{100}	198	171
Global Temperature Potentials (GTP_H)		
GTP_{20}		245
GTP_{50}		31
GTP_{100}		24

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 2.33 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 1.48 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 2.44$ years

$\tau^{OH}_{Trop} = 2.52$ years

$\tau^{OH}_{Strat} = 77.6$ years

Fractional Atmospheric Loss: 0.971

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: 0.013

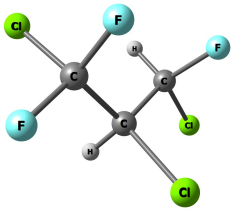
UV Photolysis

UV Spectrum: *No Recommendation*

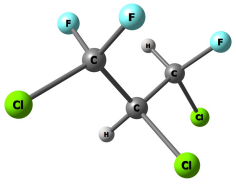
$\tau_{hv} = 150$ years

Fractional Atmospheric Loss: 0.016

Molecular Structure and Infrared Spectrum (12 conformers)



E = 0
Population = 0.335



$\Delta E = 0.43$ kcal mol^{-1}
Population = 0.162

Optimized Coordinates (Angstroms)

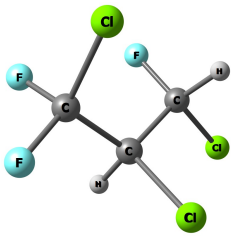
Atom	X	Y	Z
C	-1.000290726513	-0.802849458457	0.180899433536
C	-0.123673205301	0.284120556415	-0.453554310367
C	1.349824530040	0.190794978987	-0.008894709419
Cl	-2.622201055559	-0.840438125235	-0.595348563278
H	-0.565807887327	-1.789747673893	0.013061788867
F	-1.138901349055	-0.591969410644	1.503784409998
Cl	-0.735606818714	1.917871895090	-0.045171988428
H	-0.150008892637	0.181987554670	-1.537619045987
Cl	2.063308026585	-1.381022454610	-0.573563235128
F	2.063334714701	1.171319174293	-0.555505437345
F	1.476650663779	0.256289963383	1.311891657551

Atom	X	Y	Z
C	-1.307656976982	-0.726053698310	-0.114762702796
C	-0.118574615785	0.211733384421	-0.374158932929
C	1.207030345761	-0.512948152257	-0.052763475479
Cl	-2.827829163976	-0.027229826475	-0.769933434641
H	-1.158367348582	-1.671012530168	-0.640105297768
F	-1.449591121880	-0.963820254732	1.203697195860
Cl	-0.255223118514	1.713973734625	0.575073832806
H	-0.105338150219	0.477273771815	-1.430690223423
Cl	2.633755198065	0.430088618320	-0.595142389807
F	1.326143597094	-0.773158497271	1.244352031913
F	1.213677355016	-1.686271549966	-0.713686603736

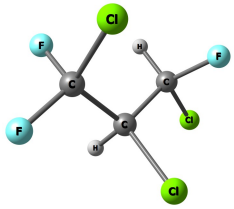
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
47.1010	0.0990
75.8723	0.0477
145.8429	0.278
173.2032	0.117
202.1520	0.0561
256.0856	0.127
286.4967	0.310
297.3535	0.0278
378.7095	0.370
413.5460	0.393
420.9931	0.0888
588.9538	5.25
636.6299	4.90
756.2806	25.4
794.5827	9.30
822.2352	7.72
947.8838	18.2
980.0881	6.53
1143.7604	5.43
1189.9983	23.5
1233.8055	19.0
1256.6413	7.50
1281.2725	4.84
1336.2286	10.1
1377.1150	3.00
3113.8874	0.657
3139.6905	0.576

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
50.5419	0.0575
70.1460	0.0813
139.3622	0.272
177.9768	0.0352
203.0878	0.204
235.5151	0.0581
269.9025	0.0183
325.8047	0.0401
391.0172	0.367
425.0342	0.207
427.5495	0.265
600.1263	3.46
627.0531	9.87
715.3317	21.9
804.7389	2.90
869.3892	2.39
966.0161	7.78
983.0336	22.9
1132.6793	18.0
1153.3881	19.8
1227.6150	19.7
1258.3276	8.79
1283.0499	2.69
1324.4590	8.60
1379.0779	3.26
3111.3856	0.492
3135.5665	0.558



$\Delta E = 0.72$ kcal mol^{-1}
Population = 0.099



$\Delta E = 0.92$ kcal mol^{-1}
Population = 0.071

Optimized Coordinates (Angstroms)

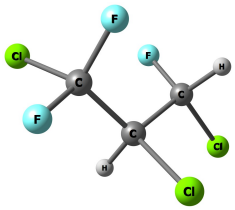
Atom	X	Y	Z
C	-1.133412129020	-0.589246961744	0.345332874544
C	-0.169280447054	0.253645258449	-0.502913441726
C	1.296183650135	-0.236041432188	-0.439930682733
Cl	-2.837630452941	-0.202590074203	-0.075013716901
F	-0.917939673835	-1.901840730851	0.102707469922
H	-1.015335077318	-0.386096976701	1.409961289499
Cl	-0.269848448814	1.965024817081	-0.004408432142
H	-0.458149122244	0.195555087667	-1.554611720424
Cl	1.907836261713	-0.416491935810	1.242579034462
F	1.389346082361	-1.417641052845	-1.054755766493
F	2.085971357016	0.620824001147	-1.086160908009

Atom	X	Y	Z
C	-1.109612604784	-0.775121986682	-0.188800043337
C	-0.171169877186	0.406130050482	-0.464409245101
C	1.307231625124	-0.023558703567	-0.571373110958
Cl	-2.801397688905	-0.346496322942	-0.629872983625
H	-0.836624769850	-1.622857343706	-0.820896593024
F	-1.071309803853	-1.145545529528	1.103952570750
Cl	-0.378344605070	1.718271535697	0.720932456371
H	-0.414255420024	0.812367364544	-1.448264755868
Cl	1.994767699243	-0.720406999831	0.923869193433
F	1.387018161932	-0.951125017012	-1.545000386084
F	2.050677283372	1.018340952547	-0.940726102558

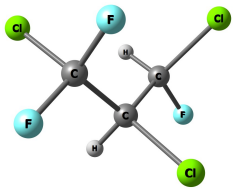
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
54.1306	0.0615
67.3927	0.0260
141.6616	0.120
182.4910	0.0657
199.1739	0.0884
266.5973	0.382
295.5317	0.0478
352.4896	0.104
399.5277	0.859
425.6884	0.673
434.1686	0.112
470.8835	1.89
611.0788	9.63
667.8568	7.06
785.3001	13.7
857.9608	10.3
1031.5034	29.4
1074.2136	5.48
1121.3515	5.86
1175.1128	28.8
1192.6453	19.6
1223.6248	6.58
1273.1971	7.58
1332.1716	5.86
1381.9548	2.18
3105.8666	0.524
3129.6460	0.567

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
48.9315	0.0700
74.1612	0.0744
144.4687	0.234
172.4460	0.195
192.0717	0.0257
227.4777	0.0973
291.3062	0.0955
324.6383	0.0621
397.7572	0.270
424.2129	0.0521
449.1537	0.163
608.6062	8.34
642.9627	4.52
648.0227	9.38
792.8091	13.2
839.0969	3.39
978.8719	3.09
1038.6517	32.6
1154.5806	20.8
1161.0626	20.4
1197.2664	19.4
1253.2900	3.10
1276.8791	1.49
1331.9528	9.54
1379.2799	2.75
3104.3129	0.263
3110.4556	0.885



$\Delta E = 1.05$ kcal mol^{-1}
Population = 0.057



$\Delta E = 1.06$ kcal mol^{-1}
Population = 0.056

Optimized Coordinates (Angstroms)

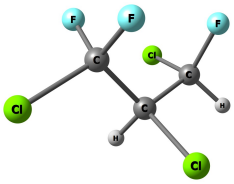
Atom	X	Y	Z
C	-1.072567160656	-0.608575205836	0.445849672754
C	-0.171720411057	0.322765101116	-0.385844614681
C	1.317204307647	0.234808543596	0.029029983533
Cl	-2.721260240670	-0.681974564666	-0.264763659784
F	-0.562902954938	-1.859412997349	0.470768299326
H	-1.181767436848	-0.238354705742	1.465816616120
Cl	-0.739743078705	2.008880307510	-0.140010728966
H	-0.256869968378	0.097629906470	-1.447676784549
Cl	2.094242843604	-1.238477558103	-0.653798525881
F	1.996829544361	1.285542502828	-0.424993223925
F	1.429815555641	0.206186670175	1.361381966054

Atom	X	Y	Z
C	1.082961303357	0.685919397308	-0.656546793490
C	0.100634688219	-0.488923796459	-0.564234318127
C	-1.219629642934	-0.217090754667	0.175880499348
Cl	1.739242213131	1.216908573252	0.922671555555
F	2.105631517443	0.308128833197	-1.456862157419
H	0.588277180847	1.556005155226	-1.090919846455
Cl	0.879068489158	-1.939849344305	0.140523527103
H	-0.165170630029	-0.746984237210	-1.591608184770
Cl	-2.067538593211	1.204473486522	-0.568751662685
F	-2.024475334330	-1.272202941478	0.050106066206
F	-1.048004191652	0.026408628613	1.468156314734

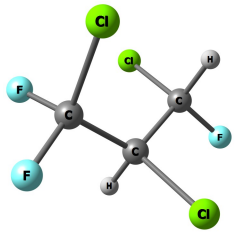
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
45.8146	0.0632
60.0285	0.0222
150.0605	0.0711
180.0042	0.101
220.8353	0.340
251.2044	0.168
284.0271	0.450
349.2071	0.167
361.0382	0.901
423.6874	0.203
435.3423	0.0728
494.4378	1.54
588.6228	4.31
751.8289	26.2
807.5962	15.6
830.7832	2.00
950.2715	18.7
1062.3173	6.20
1128.8218	14.5
1177.9578	20.1
1209.4982	17.7
1222.2404	9.89
1278.6111	4.35
1332.3738	7.14
1384.1252	1.99
3121.6518	0.678
3145.6372	0.416

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
43.1877	0.0691
85.9119	0.0339
146.4623	0.219
174.1439	0.113
189.0765	0.0463
269.5712	0.171
278.0718	0.317
326.3749	0.0322
373.8828	0.426
414.8114	0.450
432.2568	0.352
603.9129	5.79
630.5484	2.07
677.8695	8.54
789.6596	26.8
826.5627	3.21
966.5256	22.3
1045.6756	2.48
1109.9108	16.1
1180.2452	23.0
1238.6232	3.77
1254.0666	15.3
1302.2721	12.8
1326.7080	2.20
1376.4690	2.85
3105.2965	0.278
3116.3137	0.997



$\Delta E = 1.13$ kcal mol^{-1}
Population = 0.050



$\Delta E = 1.15$ kcal mol^{-1}
Population = 0.048

Optimized Coordinates (Angstroms)

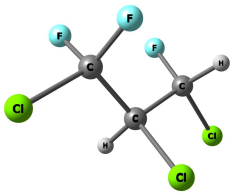
Atom	X	Y	Z
C	-1.501686312799	0.578767430721	-0.172944566893
C	-0.017930281564	0.447999926002	-0.561154335182
C	0.763341339732	-0.588513104431	0.279666559068
Cl	-2.482433007727	-0.759952825379	-0.882563428384
F	-1.653197293557	0.585399711193	1.166066260093
H	-1.912290861624	1.497968915813	-0.592108189299
Cl	0.746134884001	2.064589811000	-0.378099493792
H	0.054172037587	0.173827556611	-1.611594064810
Cl	2.386340322713	-0.900140550024	-0.442442113642
F	0.929393305511	-0.178570887459	1.532322712793
F	0.096578867726	-1.745266984047	0.302846660047

Atom	X	Y	Z
C	-1.324773108118	0.326873883354	0.415910677981
C	-0.108858915580	0.526186014525	-0.499413200606
C	1.000234239884	-0.545644660370	-0.416594757764
Cl	-2.190768918837	-1.206017030335	0.043833554998
H	-1.040507079446	0.285601251726	1.467548461896
F	-2.182992768189	1.349144792330	0.212329668309
Cl	0.592463475449	2.137493024184	-0.130714973515
H	-0.442825912457	0.549203159111	-1.539159011701
Cl	1.529162678157	-0.878997876891	1.271715414240
F	0.569457165522	-1.687392062366	-0.957173763770
F	2.060674143615	-0.146293495268	-1.117863070066

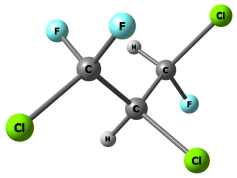
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
43.4521	0.0570
78.4975	0.0634
151.8129	0.0334
167.5808	0.153
203.9517	0.147
248.5691	0.0450
272.5285	0.134
332.8322	0.0441
391.1079	0.254
412.6601	0.343
425.4309	0.371
527.9301	8.69
621.6317	4.68
751.7422	23.9
807.3215	0.765
860.9363	4.55
936.2612	21.4
976.6564	9.16
1152.4005	23.4
1172.7990	21.3
1214.3274	8.48
1251.4445	12.2
1291.6536	6.69
1322.6601	6.89
1393.9617	1.80
3117.9136	0.750
3151.0518	0.440

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
41.6198	0.0315
79.0768	0.0397
146.5823	0.0905
174.9695	0.0848
221.2870	0.269
259.1289	0.181
328.8191	0.0788
330.5260	0.216
393.4283	1.09
409.2788	0.524
435.0102	1.63
462.8169	0.574
639.0156	2.96
674.2225	10.3
757.3046	23.3
836.7814	3.88
1036.5336	26.1
1068.3136	2.99
1128.9621	22.1
1171.7436	12.8
1199.4129	23.9
1216.7693	2.20
1284.8937	8.15
1311.9514	4.56
1390.7807	2.25
3106.6032	0.356
3130.9403	0.553



ΔE = 1.22 kcal mol^{-1}
Population = 0.043



ΔE = 1.43 kcal mol^{-1}
Population = 0.030

Optimized Coordinates (Angstroms)

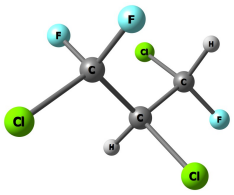
Atom	X	Y	Z
C	-1.350855584992	-0.524497393352	0.310279519118
C	-0.133064378582	0.193672024276	-0.307722318342
C	1.190697146471	-0.494483155324	0.102414504506
Cl	-2.877744924816	0.119090687290	-0.385100031875
F	-1.291562896040	-1.848837579499	0.047848778397
H	-1.398753395772	-0.364689376345	1.388257508256
Cl	-0.147132352825	1.894276352568	0.241273736518
H	-0.200901086834	0.182468974304	-1.395395551558
Cl	2.632592310189	0.385981710872	-0.507529946037
F	1.272625521984	-0.591593635962	1.433147371955
F	1.229946641216	-1.726906608829	-0.409966570938

Atom	X	Y	Z
C	-1.417711057378	-0.209281999994	-0.767992907272
C	-0.054242996200	0.451063175358	-0.505606838235
C	1.038018829643	-0.558432283184	-0.102249843631
Cl	-2.176124283783	-0.925914649392	0.687645977912
F	-2.245459996742	0.725310392759	-1.285110840755
H	-1.298948975270	-1.024065004488	-1.484449048494
Cl	-0.171899400875	1.783760442155	0.670668223320
H	0.248696986713	0.892733635892	-1.457060387142
Cl	2.679986760567	0.153429828978	-0.275036036241
F	0.894084115225	-0.994781933995	1.142170759579
F	0.958561018101	-1.617208604088	-0.929302059041

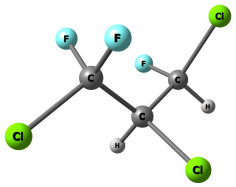
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
44.2567	0.0596
57.8298	0.0438
148.3950	0.0943
186.0942	0.0531
215.7748	0.355
238.2087	0.0636
293.4685	0.0304
354.9674	0.237
390.7098	1.22
419.9304	0.111
439.8079	0.389
466.4729	3.13
602.1891	3.67
702.6463	25.0
823.5296	4.62
872.8804	3.26
959.5749	19.1
1058.2881	15.4
1119.9158	5.93
1161.8922	32.3
1208.5758	4.20
1215.1377	21.7
1275.5888	4.47
1331.5765	6.25
1380.1121	2.58
3118.6760	0.707
3136.0369	0.401

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
47.5208	0.0366
76.5927	0.0650
142.6491	0.196
180.8167	0.162
186.0001	0.0677
226.0779	0.139
306.1927	0.0972
328.8724	0.0246
404.8064	0.495
421.1421	0.167
433.9644	0.666
586.9373	7.45
617.1439	3.63
682.7718	6.66
822.0310	17.1
832.2219	4.35
958.0688	17.8
1047.1072	23.2
1129.0643	15.0
1144.0066	21.1
1239.3346	6.51
1248.8776	14.2
1299.2971	10.7
1323.7314	3.04
1374.4375	2.90
3104.8212	0.236
3112.7024	0.994



ΔE = 1.65 kcal mol^{-1}
Population = 0.021



ΔE = 1.94 kcal mol^{-1}
Population = 0.013

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.497672756501	0.343814910092	0.244858914949
C	-0.085490260724	0.441816689797	-0.369948527483
C	0.895566901145	-0.604054730125	0.204399886022
Cl	-2.359817861818	-1.134149638714	-0.314524776902
H	-1.457978236053	0.300546268894	1.334335316169
F	-2.225811180013	1.409807717466	-0.144400758437
Cl	0.538299938401	2.088826172644	-0.020705008956
H	-0.139166942555	0.327366159493	-1.452159259657
Cl	2.540289313144	-0.441788026583	-0.497777831622
F	0.975801741627	-0.477728305148	1.533426466109
F	0.467884343347	-1.839967217816	-0.064569420192

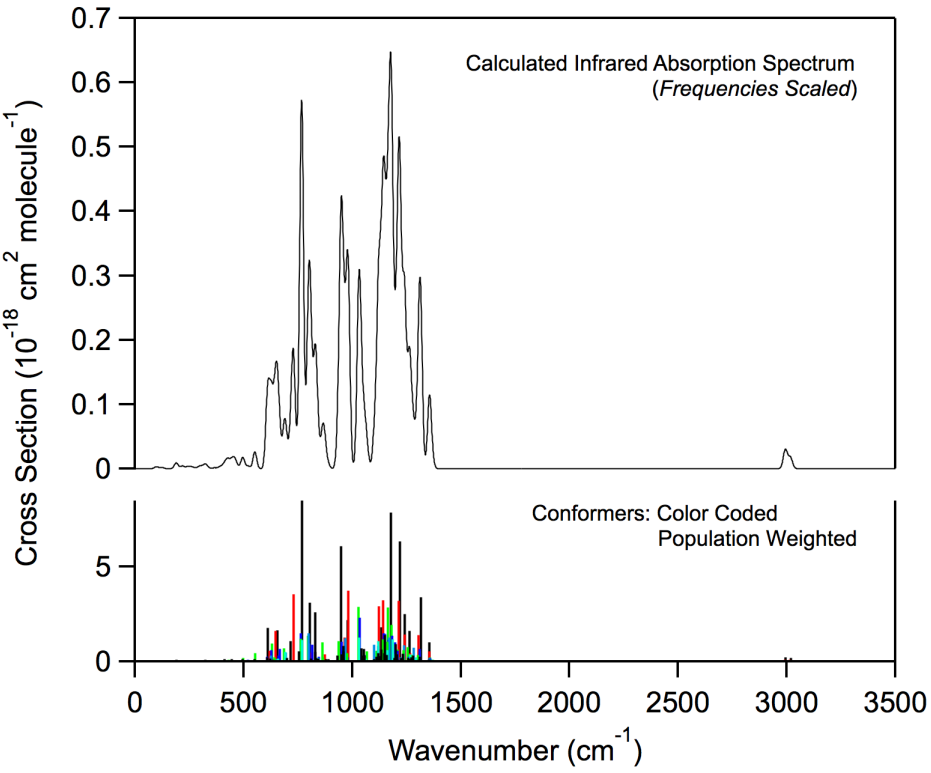
Atom	X	Y	Z
C	-1.492271528405	-0.046714097499	-0.765861957028
C	-0.007826195201	0.357533171813	-0.682271701011
C	0.877415724958	-0.548838182429	0.201394950822
Cl	-2.297815710665	-0.241148371161	0.823880177171
H	-2.043333344240	0.735394363721	-1.291105777008
F	-1.586909136045	-1.205342945257	-1.459110129136
Cl	0.127141758877	2.063902287998	-0.174431485221
H	0.374980564988	0.290981887230	-1.702028913624
Cl	2.622713544550	-0.292024388988	-0.181434202081
F	0.697336781563	-0.322363739266	1.497064405291
F	0.584280539620	-1.828230986162	-0.049194368175

Infrared Absorption Spectrum (unscaled frequencies)

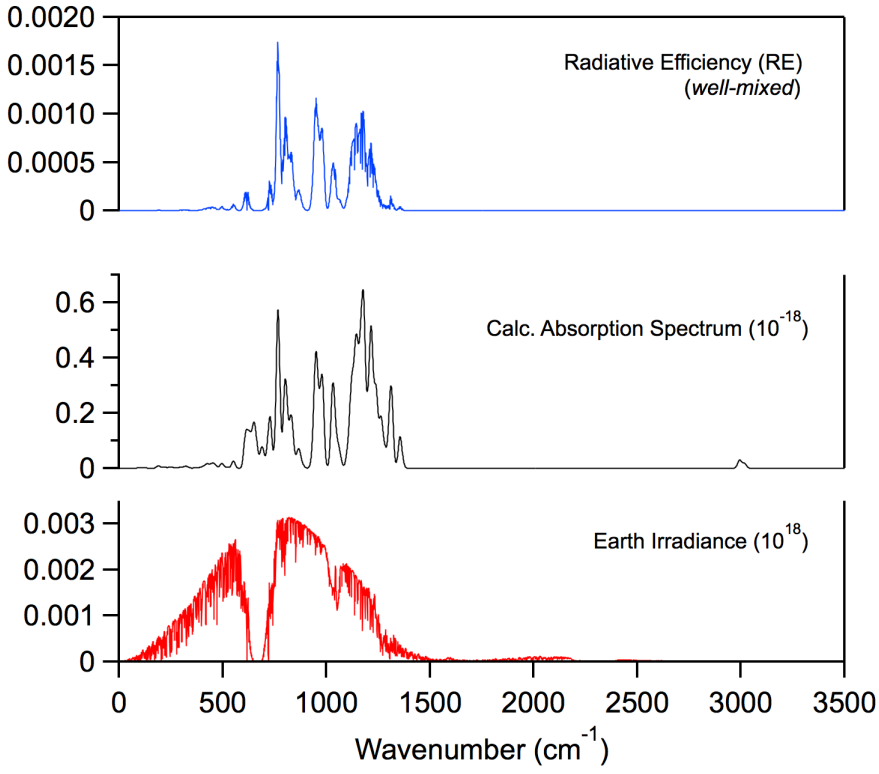
Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
29.9106	0.0408
66.8461	0.0461
152.9029	0.127
185.6206	0.113
206.8460	0.298
260.1504	0.123
303.8826	0.544
340.5922	0.0951
394.4838	1.51
409.4679	0.328
427.4663	0.420
465.4575	1.99
611.7038	1.61
742.0210	25.9
800.4315	7.38
835.6996	7.24
949.2358	18.5
1060.4199	15.8
1137.0911	13.1
1159.0869	21.6
1208.9375	4.96
1220.2762	18.6
1282.0666	5.74
1315.6742	3.19
1392.0420	2.66
3116.6267	0.747
3139.0683	0.274

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
46.4080	0.0261
82.5970	0.0291
144.1448	0.0790
184.1509	0.0488
193.8842	0.104
225.3728	0.0922
305.3914	0.0143
355.0401	0.0398
410.0710	0.163
418.1853	0.256
432.5153	0.718
525.0443	9.94
597.7070	5.40
682.7150	4.13
831.2913	3.94
884.5950	9.36
930.4026	25.1
1049.1059	25.2
1107.6626	9.09
1170.3962	27.3
1221.4593	8.33
1241.7501	5.84
1290.8120	16.4
1355.8505	3.30
1374.5071	1.50
3106.0612	1.27
3114.6368	0.149

Infrared Spectrum

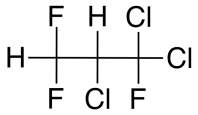


Radiative Efficiency



HCFC-233dc

Molecular Formula: $CHF_2CHClCCl_2F$
Name: 1,1,2-Trichloro-1,3,3-trifluoropropane
CAS number: –
Molecular Weight: 201.4



Global Atmospheric Lifetime (years): 3.55
  Tropospheric Atmospheric Lifetime (years): 3.96
  Stratospheric Atmospheric Lifetime (years): 34.8
Ozone Depletion Potential (ODP): 0.055

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.273	0.245
Global Warming Potential (GWP_H):		
GWP_{20}	1079	969
GWP_{100}	293	263
Global Temperature Potentials (GTP_H)		
GTP_{20}		447
GTP_{50}		50
GTP_{100}		37

* 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) = 1.48×10^{-14}; k_{SAR}(272 K) ≈ 0.946×10^{-14} cm^3 $molecule^{-1}$ s^{-1}

τ^{OH}_{Global} = 3.83 years
τ^{OH}_{Trop} = 3.96 years
τ^{OH}_{Strat} = 116.5 years

Fractional Atmospheric Loss: 0.929

O(^{1}D) Reactivity

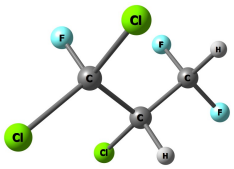
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 2.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)}$ = 185 years
Fractional Atmospheric Loss: 0.019

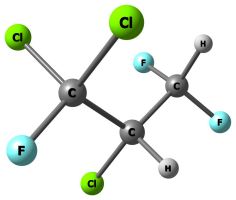
UV Photolysis

UV Spectrum: *No Recommendation*
τ_{hv} = 68 years
Fractional Atmospheric Loss: 0.052

Molecular Structure and Infrared Spectrum (9 conformers)



E = 0
Population = 0.240



$\Delta E = 0.03$ kcal mol^{-1}
Population = 0.227

Optimized Coordinates (Angstroms)

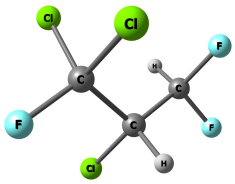
Atom	X	Y	Z
C	1.555258631982	-0.872180863693	-0.199764760499
C	0.480822024043	0.191754482512	-0.496654279478
C	-0.874497639465	-0.104950596266	0.174901201689
F	2.671858742845	-0.551968669078	-0.887559717749
F	1.850625930980	-0.897722349122	1.113615440097
H	1.226057267500	-1.868905260462	-0.510565044661
H	0.326560972835	0.232638817706	-1.574726267960
Cl	1.089925532216	1.792784482883	0.026753313358
Cl	-2.107653941401	1.112391705858	-0.275962793765
Cl	-1.461663926725	-1.730979374583	-0.366574580721
F	-0.758096594809	-0.127480375756	1.500635489688

Atom	X	Y	Z
C	1.262502334266	-1.108037436000	0.111944024023
C	0.537720953728	0.031607975713	-0.621233423752
C	-0.954163470780	0.208610762391	-0.278143615621
F	2.450388991774	-1.306448650162	-0.501946741199
F	1.500094976575	-0.795392281535	1.398563576852
H	0.684044689001	-2.037673072338	0.071035342747
H	0.574395411551	-0.193006914388	-1.688967137450
Cl	1.415095506398	1.573585977210	-0.387815878191
Cl	-1.833481564434	-1.299627615515	-0.763828753211
Cl	-1.267910849947	0.553116482647	1.441060973777
F	-1.453075978132	1.208747771977	-1.009509367974

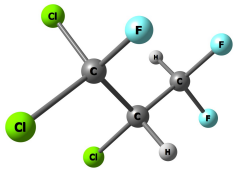
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
47.4552	0.118
80.8433	0.0960
152.2305	0.179
196.6765	0.113
203.8705	0.130
232.0363	0.0111
270.1656	0.363
306.9221	0.122
335.8777	0.132
379.8618	0.303
459.3439	0.330
537.9073	3.52
660.4716	9.97
746.1542	15.7
792.1360	14.0
817.5399	13.3
974.5392	8.35
982.2549	5.23
1143.5482	12.9
1175.2248	14.9
1200.5329	24.2
1255.1040	3.66
1305.8046	4.29
1388.1373	7.17
1411.9281	3.34
3082.5595	2.87
3132.4380	0.549

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
50.7198	0.133
83.5948	0.107
157.1340	0.211
163.3674	0.0945
199.6605	0.0167
240.5007	0.142
275.9608	0.233
304.1472	0.261
353.7334	0.151
384.1275	0.214
478.1055	0.828
570.2422	1.16
644.5383	9.04
669.9184	9.67
771.6763	24.6
831.7062	9.00
988.4195	4.09
1056.2348	8.00
1126.3846	26.6
1174.2613	9.38
1183.3821	19.0
1257.8791	2.92
1303.2958	2.80
1394.8776	6.61
1410.9443	2.86
3073.4947	2.83
3110.6833	0.668



$\Delta E = 0.17$ kcal mol^{-1}
Population = 0.181



$\Delta E = 0.34$ kcal mol^{-1}
Population = 0.135

Optimized Coordinates (Angstroms)

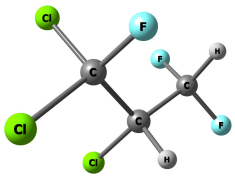
Atom	X	Y	Z
C	1.379776103393	-0.821383095598	0.485104856310
C	0.620381556820	0.086208898458	-0.499189518441
C	-0.900779269917	0.219057124798	-0.269541660658
F	0.830257638802	-2.054262251852	0.506605460499
F	2.648963888966	-0.943386220616	0.043331454321
H	1.386230672866	-0.409854199331	1.498926956607
H	0.765787829546	-0.294709997787	-1.511551184094
Cl	1.382552862414	1.710308140313	-0.431343261607
Cl	-1.735577594919	-1.292204947506	-0.760724287602
Cl	-1.296982339538	0.605397278278	1.438419880409
F	-1.379600348434	1.201232270844	-1.038642695742

Atom	X	Y	Z
C	1.760596763342	-0.435613685362	0.133804882163
C	0.534572507653	0.324179476179	-0.412219868169
C	-0.805805253988	-0.411146238497	-0.191735399007
F	1.803976081417	-1.673742724868	-0.403768046150
F	2.870767915828	0.223714493729	-0.257258770296
H	1.749718833026	-0.512105027268	1.225375482187
H	0.657810605801	0.435591919128	-1.491740455649
Cl	0.529407265699	1.957494050203	0.308201674579
Cl	-1.113147392360	-0.752605255489	1.543292203509
Cl	-2.171647351971	0.525968981200	-0.877171670451
F	-0.755681974447	-1.580159988956	-0.843027032717

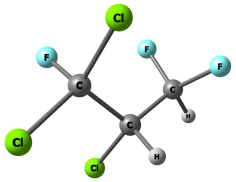
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
44.1959	0.0636
79.6429	0.0718
154.7479	0.105
170.1398	0.0356
220.4514	0.202
227.6953	0.0634
301.9413	0.240
329.9285	0.328
364.3228	0.264
395.4156	0.189
448.2346	3.21
501.7240	1.04
576.7093	1.47
663.1389	9.11
780.9877	29.9
855.4008	11.5
1043.9334	7.61
1075.0126	3.95
1128.3947	26.2
1145.1596	18.5
1174.7468	14.4
1237.0087	1.73
1290.9081	2.63
1397.3642	1.90
1412.6923	6.14
3090.1950	2.53
3118.1391	0.446

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
42.5540	0.0642
78.8558	0.0751
152.0776	0.134
173.8798	0.0298
198.3952	0.0941
242.8212	0.0465
310.6001	0.127
331.7399	0.191
372.6303	0.244
399.2267	0.127
446.9810	5.18
495.0237	0.205
561.8433	3.02
657.6130	7.50
808.1832	29.3
862.6388	7.83
1043.0326	12.7
1086.6306	9.29
1121.3436	4.40
1140.2369	16.9
1158.4056	36.0
1235.9107	2.34
1288.8130	1.33
1395.8946	3.12
1409.1248	6.64
3088.3749	2.65
3109.9707	0.576



$\Delta E = 0.56$ kcal mol^{-1}
Population = 0.093



$\Delta E = 0.99$ kcal mol^{-1}
Population = 0.045

Optimized Coordinates (Angstroms)

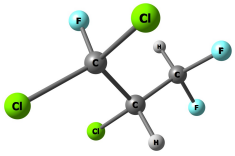
Atom	X	Y	Z
C	1.670196114462	-0.511121941432	-0.598362260058
C	0.485825809539	0.457941695668	-0.429108818216
C	-0.875163233710	-0.267186161933	-0.365925136309
F	2.754207641160	0.209852395228	-0.959812060678
F	1.954180567450	-1.155398144391	0.547412920297
H	1.457239541829	-1.248232262434	-1.381008847318
H	0.453657804591	1.075228188147	-1.329387350705
Cl	0.755058838845	1.548214648148	0.951393265364
Cl	-1.084413163426	-1.279557787890	1.085028678184
Cl	-2.222870171490	0.907205440786	-0.492384810743
F	-0.933689749251	-1.072004069897	-1.449852579817

Atom	X	Y	Z
C	1.820676799511	-0.316332543315	-0.337495470971
C	0.465753181673	0.381681907794	-0.595639675681
C	-0.719568920444	-0.122803715586	0.256582106827
F	2.018578451493	-0.522563677880	0.978338511018
F	1.848843723818	-1.511717449363	-0.968114143167
H	2.634507868906	0.303256010504	-0.729840506322
H	0.214272127721	0.260252601876	-1.648400385661
Cl	0.707580644946	2.139202582567	-0.296177258725
Cl	-2.244453534551	0.675836868185	-0.270612185802
Cl	-0.918357763013	-1.897823562461	0.070692393669
F	-0.528990580060	0.148074977680	1.546465614815

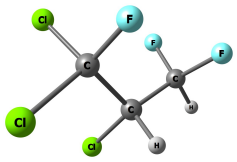
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
49.2956	0.109
79.8137	0.117
151.3399	0.166
167.4994	0.0743
197.4802	0.255
238.6729	0.0306
256.3378	0.132
311.0105	0.196
378.5166	0.127
381.6979	0.0225
494.7297	0.260
543.0155	3.68
655.5511	9.83
676.1498	7.67
783.3498	14.0
849.4288	15.3
986.0776	3.82
1057.2389	19.4
1120.7283	8.02
1141.5201	23.3
1181.4783	19.1
1258.1282	3.01
1299.4195	2.89
1391.8103	7.87
1413.9672	3.00
3069.6607	2.80
3106.0035	0.705

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
45.0215	0.0851
83.5947	0.121
155.4414	0.0348
199.0349	0.150
208.7520	0.188
241.7747	0.117
243.1892	0.0489
327.0439	0.0877
362.9289	0.121
380.6342	0.141
442.3303	1.18
533.5534	5.56
590.1083	6.86
769.4946	29.4
802.5239	5.12
869.2729	4.91
920.2335	4.31
996.3813	5.80
1126.5821	23.6
1177.1732	16.1
1192.9647	14.1
1237.9108	6.17
1319.3231	7.67
1394.1458	4.32
1417.5459	3.61
3071.3924	3.78
3139.7762	0.308



$\Delta E = 1.02$ kcal mol^{-1}
Population = 0.043



$\Delta E = 1.51$ kcal mol^{-1}
Population = 0.019

Optimized Coordinates (Angstroms)

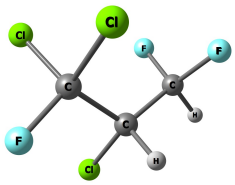
Atom	X	Y	Z
C	1.706404236660	-0.540147255593	0.225655840023
C	0.536728340870	0.272864331730	-0.376935421031
C	-0.841908161710	-0.092963628911	0.216176319975
F	1.579834462251	-1.849529190105	-0.075008291003
F	2.855504982937	-0.109297227925	-0.332533558155
H	1.761088268786	-0.419820033235	1.312635485266
H	0.515358139332	0.135992680237	-1.457682355283
Cl	0.901119161726	2.000646122137	-0.042708774891
Cl	-2.126668689146	1.018216358792	-0.355033521903
Cl	-1.314241824212	-1.763380438837	-0.244158597870
F	-0.782496917494	-0.025980718291	1.554624874872

Atom	X	Y	Z
C	1.873038707271	0.026364666501	-0.429167569361
C	0.424217439239	0.535969856222	-0.577251494959
C	-0.680584743899	-0.459962036599	-0.149994999290
F	2.138698811101	-0.393391952417	0.820601688576
F	2.070854632384	-1.007364458375	-1.278047198168
H	2.567857328276	0.834394389149	-0.687249031926
H	0.266119944382	0.724713916577	-1.640754424479
Cl	0.279734035931	2.106802191230	0.260641484746
Cl	-0.753410211542	-0.755725800711	1.606479804020
Cl	-2.281005484124	0.135404807754	-0.724161122457
F	-0.440614459018	-1.627017579331	-0.765612136701

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
27.9926	0.0673
68.2802	0.0692
164.3466	0.0382
195.8526	0.162
214.9758	0.249
241.6680	0.119
274.0558	0.329
312.6276	0.138
371.7621	0.0831
391.8166	0.141
447.4470	2.19
476.3443	3.30
576.9667	1.32
756.2434	15.1
781.7311	25.7
851.7240	5.38
957.8681	8.11
1071.5208	13.2
1134.6219	18.9
1142.6776	17.2
1171.1071	16.0
1232.4071	2.52
1291.5731	1.67
1396.9375	2.52
1409.8451	7.41
3082.0092	3.05
3139.2524	0.355

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
34.7734	0.0829
95.2533	0.103
159.0450	0.0293
173.3684	0.128
192.5062	0.0720
236.4335	0.0395
264.3028	0.111
341.6326	0.0396
379.8149	0.0805
384.8903	0.269
477.1796	2.48
526.5675	5.67
564.8893	2.63
688.4457	17.0
843.8736	14.0
882.3421	7.72
915.1778	1.80
1078.8139	19.9
1116.4888	9.51
1153.1731	23.2
1186.1753	20.4
1237.8373	3.30
1323.5354	5.43
1394.2032	5.60
1422.5833	2.89
3060.7301	4.32
3110.0514	0.328



$\Delta E = 1.59$ kcal mol^{-1}
Population = 0.016

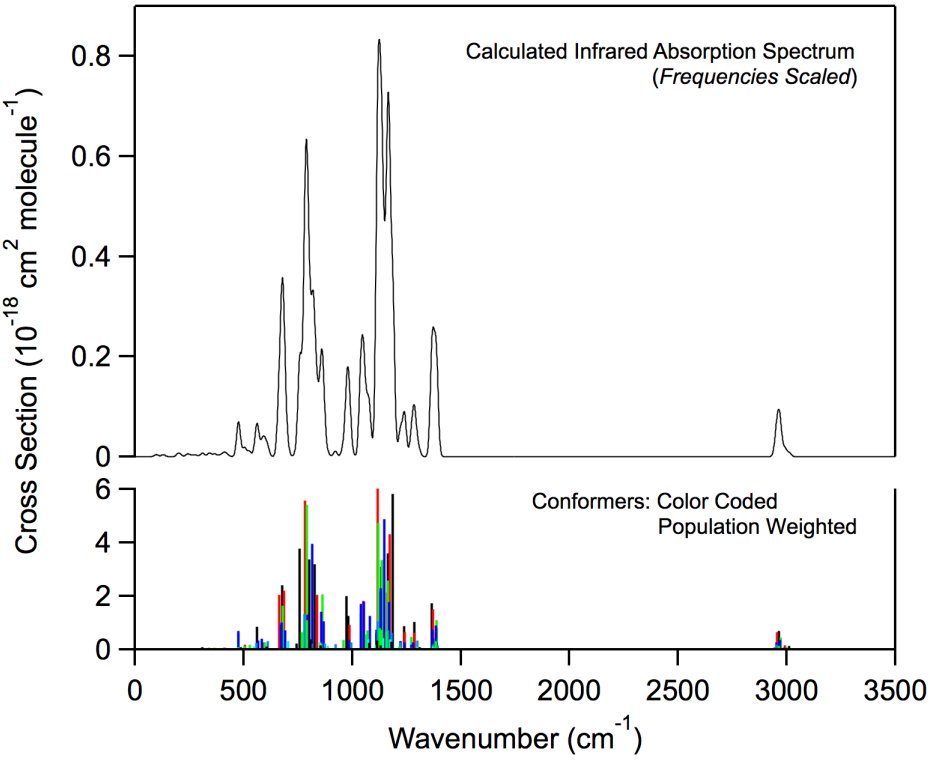
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.239815134152	-1.290694952544	-0.054780540746
C	0.620602360120	-0.036850255383	-0.702046857878
C	-0.748600237000	0.473289689627	-0.199827668544
F	1.337878138257	-1.173090729638	1.281120090606
F	0.486627527955	-2.378037496028	-0.332142149506
H	2.242457980406	-1.443413089300	-0.471035140182
H	0.485880280835	-0.250576993403	-1.764235785031
Cl	1.833389139435	1.286064460562	-0.597939222217
Cl	-2.010713865980	-0.771069151262	-0.505454790256
Cl	-0.768000699395	0.943396427184	1.520138365704
F	-1.074491758784	1.551934090186	-0.927450301950

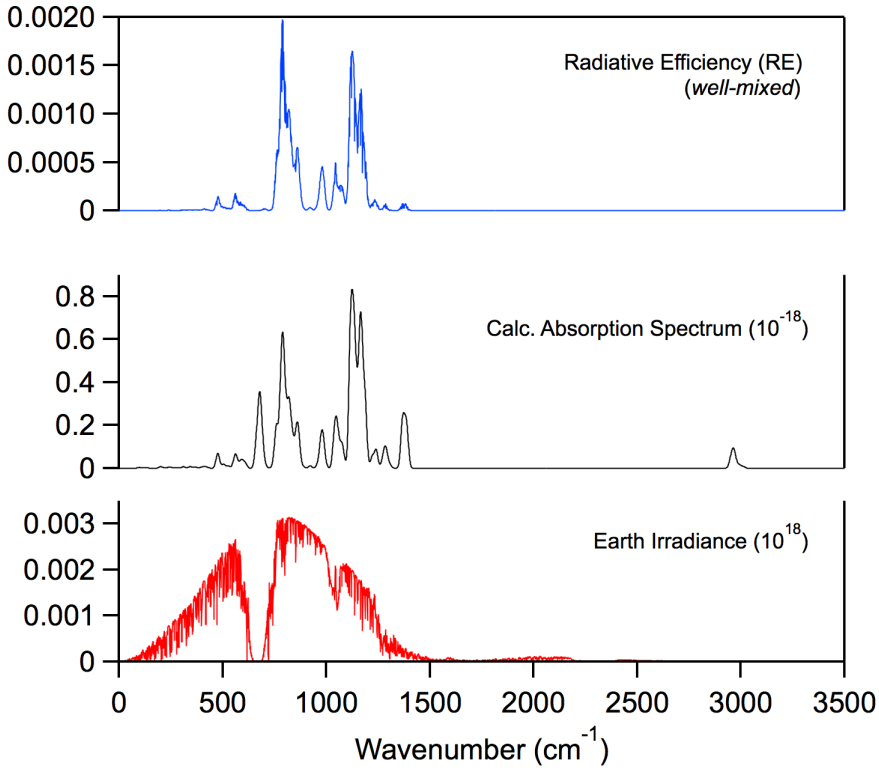
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
26.2388	0.0795
100.1071	0.110
165.3869	0.0733
172.3893	0.120
205.2822	0.0862
231.7167	0.172
270.1006	0.203
325.1197	0.198
370.6717	0.198
386.8236	0.0721
446.0113	1.78
556.7373	1.21
584.5780	6.31
730.0528	13.4
798.2525	23.7
847.5446	8.92
918.6058	1.03
1086.2512	15.2
1124.2889	20.4
1142.0081	9.19
1193.0426	18.4
1237.0973	3.11
1330.7776	6.14
1399.7421	2.94
1425.7250	2.42
3062.4221	4.45
3109.8000	0.270

Infrared Spectrum

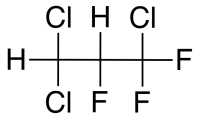


Radiative Efficiency



HCFC-233ea

Molecular Formula:	$CHCl_2CHFCClF_2$
Name:	1,1,3-Trichloro-2,3,3-trifluoropropane
CAS number:	–
Molecular Weight:	201.4



Global Atmospheric Lifetime (years):	0.982
Tropospheric Atmospheric Lifetime (years):	1.03
Stratospheric Atmospheric Lifetime (years):	20.4
Ozone Depletion Potential (ODP):	0.019

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.248	0.183
Global Warming Potential (GWP_H):		
GWP_{20}	272	201
GWP_{100}	74	54
Global Temperature Potentials (GTP_H)		
GTP_{20}		65
GTP_{50}		9
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*

$k_{SAR}(298\ K) = 5.68 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 3.63 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

τ^{OH}_{Global} = 1.00 years
τ^{OH}_{Trop} = 1.03 years
τ^{OH}_{Strat} = 34.7 years

Fractional Atmospheric Loss: 0.980

O(^{1}D) Reactivity

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

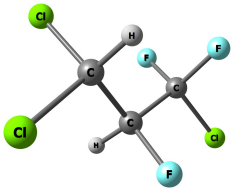
$k_{Est}(T) = 2.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)}$ = 185 years
Fractional Atmospheric Loss: 0.005

UV Photolysis

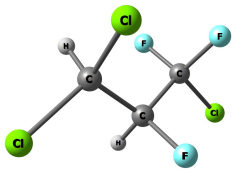
UV Spectrum: *No Recommendation*
τ_{hv} = 68 years
Fractional Atmospheric Loss: 0.015

Papanastasiou et al. (2018)

Molecular Structure and Infrared Spectrum (5 conformers)



E = 0
Population = 0.293



$\Delta E = 0.04$ kcal mol^{-1}
Population = 0.275

Optimized Coordinates (Angstroms)

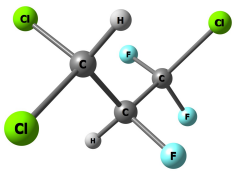
Atom	X	Y	Z
C	1.261220738252	0.014530972885	0.359749279298
C	-0.042110522120	0.507534216351	-0.296310861839
C	-1.287446726771	-0.285462154236	0.167558810084
Cl	1.681518964740	-1.638367710487	-0.169735446753
Cl	2.582341459225	1.156424480433	-0.031004691921
H	1.162769475364	-0.001699701470	1.442371699428
H	0.030592455486	0.448498191200	-1.386041392788
F	-0.226813624236	1.803026496680	0.093626041061
Cl	-2.788110706233	0.551614264122	-0.354220529494
F	-1.294731881165	-1.513271113769	-0.349192527899
F	-1.297597632541	-0.388738941709	1.502402620824

Atom	X	Y	Z
C	1.240307307669	0.050116393487	0.501000804459
C	-0.054934772968	-0.622089732135	0.021224507451
C	-1.311402520152	0.233910870223	0.287221411251
Cl	2.552011169724	-1.175592995132	0.534363795731
Cl	1.704219587777	1.443019358468	-0.510954088746
H	1.119552520479	0.410431944377	1.519563130147
H	-0.174523384697	-1.548660384693	0.592824777917
F	0.007804167948	-0.906200172226	-1.304239928265
Cl	-2.792813740019	-0.717088036935	-0.074396703514
F	-1.329187128195	0.577525237013	1.585168326491
F	-1.335004207567	1.342465517553	-0.443303032922

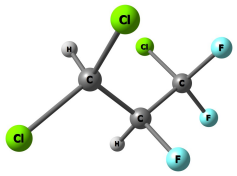
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
28.3788	0.0288
70.1604	0.0337
134.3161	0.116
196.5726	0.149
219.9721	0.380
237.2591	0.243
293.5525	0.114
338.9821	0.149
379.1001	0.237
395.8938	2.01
432.2932	1.35
489.8151	1.21
627.3018	3.75
701.2013	21.4
790.6283	12.5
834.8704	6.00
961.8007	28.9
1070.0222	5.64
1124.4817	6.65
1183.1008	24.6
1226.7249	11.8
1232.5991	9.11
1243.4572	1.71
1359.7629	2.24
1367.2037	0.426
3093.5243	0.604
3157.4826	0.186

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
31.7940	0.0221
76.6207	0.0798
127.6331	0.324
191.4616	0.0749
205.2622	0.153
228.4983	0.0282
254.6292	0.0665
315.1461	0.451
346.7887	0.125
419.8545	0.0730
459.5591	0.804
616.3486	5.06
636.6570	10.9
709.9236	21.9
737.6035	2.94
865.5275	2.95
919.8700	11.2
1021.0373	26.1
1163.9570	29.1
1172.1559	2.86
1228.7635	1.40
1252.5509	17.4
1286.9522	5.52
1347.8834	1.33
1385.2335	0.891
3073.5525	0.701
3155.8090	0.220



$\Delta E = 0.11$ kcal mol^{-1}
Population = 0.241



$\Delta E = 0.34$ kcal mol^{-1}
Population = 0.165

Optimized Coordinates (Angstroms)

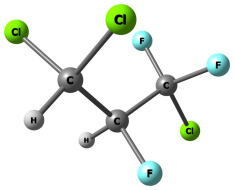
Atom	X	Y	Z
C	1.114476936226	0.031150169257	-0.352495399460
C	0.021306864863	-0.553250339837	0.552127353949
C	-1.391749196794	0.055476549134	0.391096937748
Cl	1.424669622799	1.748512349099	0.024660555358
Cl	2.606845826815	-0.939750413776	-0.157852458556
H	0.832099710340	-0.030391413795	-1.400484215013
H	0.302153350060	-0.429314526425	1.604776052519
F	-0.104696119778	-1.881749760572	0.264196861717
Cl	-1.966858860078	-0.006806820738	-1.313711992646
F	-2.232241228498	-0.660009733808	1.141345414159
F	-1.431763905955	1.316470941463	0.815681890224

Atom	X	Y	Z
C	1.059886241366	-0.189339518142	-0.468695268494
C	-0.000156851992	0.785254704173	0.053313716095
C	-1.427739075386	0.217298497500	0.206524469294
Cl	2.548028100403	0.740629828016	-0.852590237360
Cl	1.415765369809	-1.495494567884	0.692779754769
H	0.733955856374	-0.654515710948	-1.394778615569
H	-0.072688739704	1.616241532218	-0.657037761850
F	0.360891702849	1.266175171609	1.276495521787
Cl	-2.029582990209	-0.417347904055	-1.375304730000
F	-1.501924803128	-0.746102993227	1.115885160579
F	-2.231362810382	1.211981960740	0.588981990748

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
30.0129	0.0235
79.7278	0.0339
142.8885	0.113
178.6834	0.136
231.3706	0.285
233.0182	0.239
311.2937	0.230
334.2075	0.338
359.6526	0.392
410.7124	0.117
439.5111	2.08
508.8680	1.01
631.9120	9.40
666.2660	10.9
766.4532	8.53
792.1438	14.5
1038.9233	21.6
1085.6808	6.79
1133.7443	11.7
1190.1651	17.8
1207.6967	19.1
1230.9476	8.35
1246.5583	4.82
1355.5017	4.91
1371.4260	0.586
3065.0293	0.800
3158.7788	0.264

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
31.8204	0.0397
86.0831	0.0700
133.4028	0.201
185.0491	0.216
205.2541	0.0358
254.3319	0.0527
269.5866	0.236
319.8831	0.240
337.6056	0.505
400.2548	0.191
419.6588	0.800
602.0076	5.12
655.7278	8.95
729.5229	3.71
753.4487	14.7
848.0554	9.85
947.5237	28.2
1001.5102	7.28
1153.3100	4.86
1175.1113	25.5
1226.2581	4.97
1252.5756	21.6
1288.6980	5.12
1351.5963	0.458
1381.6629	2.68
3070.7672	0.623
3164.5409	0.321



$\Delta E = 1.43$ kcal mol^{-1}
Population = 0.026

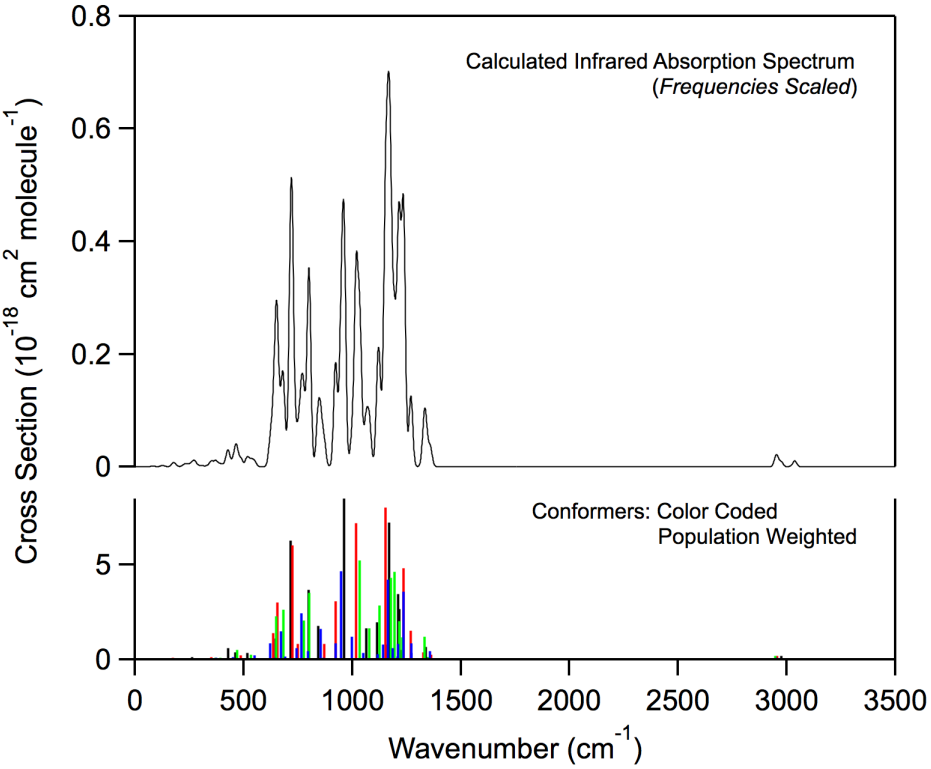
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.357963590254	0.088406364565	-0.619268146527
C	-0.162638173012	0.107686282906	-0.855930694603
C	-1.081188333013	-0.150143423795	0.358196491051
Cl	1.902631337749	1.183583846983	0.680608757444
Cl	1.956581339043	-1.581756136998	-0.380742187175
H	1.819908771692	0.454597313592	-1.534136158918
H	-0.381348312232	-0.654969051220	-1.610340333322
F	-0.482275100577	1.341785347373	-1.348535074462
Cl	-2.784596774344	-0.324075660930	-0.217531732299
F	-0.732424474538	-1.270770747116	0.988603874446
F	-1.040433871021	0.858670864641	1.222087204366

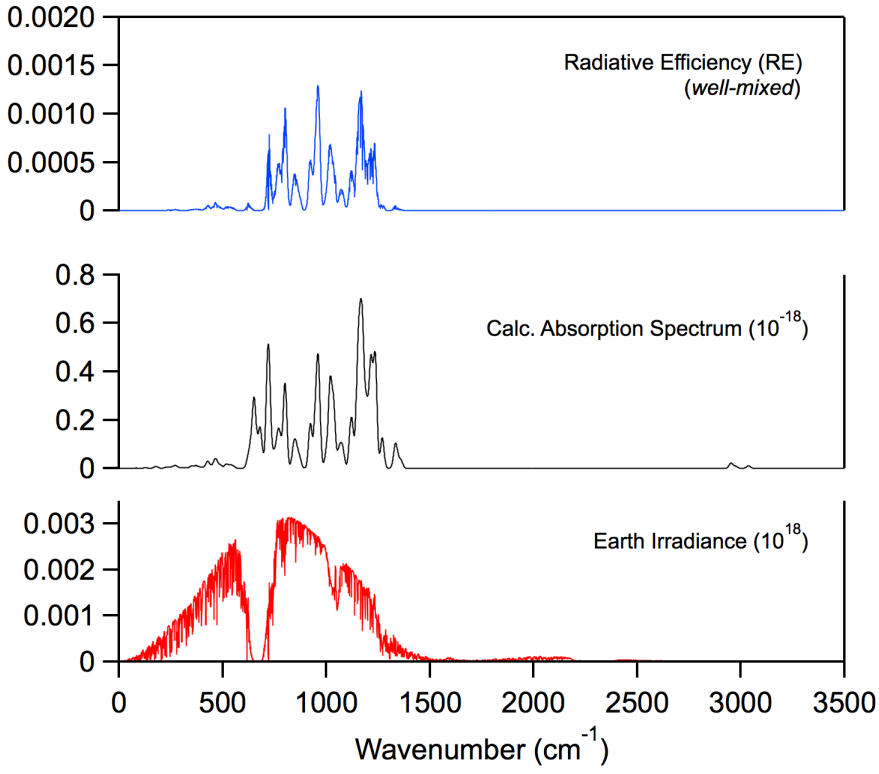
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
26.2053	0.0204
87.5768	0.0351
142.0100	0.0531
181.6736	0.202
193.5197	0.0517
243.8637	0.242
268.1760	0.0297
330.9781	0.0468
380.7917	0.247
412.4374	0.130
461.0363	2.82
525.5694	7.84
625.4988	3.69
674.8919	5.55
785.3270	16.6
861.6642	3.94
922.4868	32.9
1056.6637	13.8
1126.7846	10.8
1199.8752	23.3
1222.4548	5.84
1239.4927	2.67
1289.8763	13.2
1351.7673	1.29
1393.8080	0.442
3077.8451	0.617
3136.7826	0.398

Infrared Spectrum

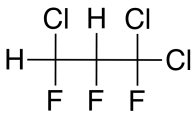


Radiative Efficiency



HCFC-233eb

Molecular Formula:	$CHClFCHFCCl_2F$
Name:	1,1,3-Trichloro-1,2,3-trifluoropropane
CAS number:	54377-32-1
Molecular Weight:	201.4



Global Atmospheric Lifetime (years):	2.32
Tropospheric Atmospheric Lifetime (years):	2.51
Stratospheric Atmospheric Lifetime (years):	30.2
Ozone Depletion Potential (ODP):	0.038

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.257	0.221
Global Warming Potential (GWP_H):		
GWP_{20}	665	571
GWP_{100}	180	155
Global Temperature Potentials (GTP_H)		
GTP_{20}		221
GTP_{50}		28
GTP_{100}		22

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 2.34 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 1.49 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 2.43$ years

$\tau^{OH}_{Trop} = 2.51$ years

$\tau^{OH}_{Strat} = 77.2$ years

Fractional Atmospheric Loss: 0.953

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: 0.013

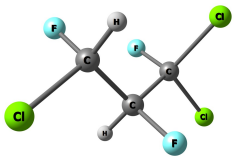
UV Photolysis

UV Spectrum: *No Recommendation*

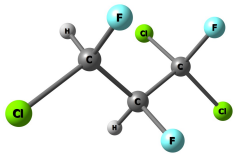
$\tau_{hv} = 68$ years

Fractional Atmospheric Loss: 0.034

Molecular Structure and Infrared Spectrum (8 conformers)



E = 0 kcal mol^{-1}
Population = 0.405



ΔE = 0.64 kcal mol^{-1}
Population = 0.138

Optimized Coordinates (Angstroms)

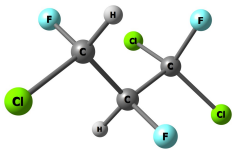
Atom	X	Y	Z
C	-1.473706998256	0.442984219087	0.071011853355
C	-0.312722957189	-0.532335319348	-0.174453845372
C	1.068184270002	0.160916764248	-0.253281403688
Cl	-3.017334758217	-0.477246401693	0.074013462401
H	-1.397668788712	0.929216908533	1.044240804609
F	-1.507010043872	1.368893354747	-0.910695162865
H	-0.466292279258	-1.045063302746	-1.130874481889
F	-0.288516521326	-1.433397211666	0.843518117187
Cl	1.422985948710	1.088995200174	1.240589400447
Cl	2.333138175156	-1.084657343574	-0.500861138482
F	1.088882952963	0.996759132239	-1.294679605703

Atom	X	Y	Z
C	-1.441627226679	0.498758384336	0.063776761910
C	-0.293633926140	-0.438363983443	-0.336713615655
C	1.089336028509	0.058894152836	0.144272136085
Cl	-2.972770006980	-0.112542526754	-0.660922203559
F	-1.567151498685	0.528186002030	1.405546405366
H	-1.299707255732	1.508969508781	-0.320616387065
H	-0.261515060785	-0.531697782187	-1.425486438612
F	-0.512304280475	-1.655733647291	0.235408044205
Cl	2.341422471685	-1.147003401343	-0.283739518742
Cl	1.470347282147	1.631268511942	-0.647908698030
F	1.102164473134	0.231300781093	1.465541514097

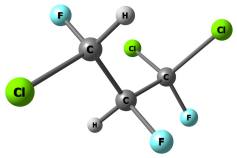
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
32.4227	0.0598
77.9728	0.0432
131.7647	0.153
183.3058	0.107
208.6089	0.142
232.1079	0.117
284.7535	0.0729
340.9290	0.0588
366.8737	0.418
412.3032	0.265
430.3482	4.62
481.1106	0.357
572.5896	0.134
624.3284	18.5
737.8863	26.1
869.2176	19.4
1042.8131	7.02
1102.0038	4.88
1134.8739	3.65
1160.6988	18.1
1177.3253	24.8
1249.1337	3.18
1329.3288	2.06
1348.7392	1.39
1393.6960	0.744
3069.0549	0.680
3125.6245	0.942

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
36.9264	0.0961
81.9108	0.0447
128.5469	0.236
190.0222	0.170
224.4621	0.149
242.0296	0.0743
266.9663	0.0196
302.8606	0.118
344.1403	0.333
385.8865	0.449
400.4007	0.912
460.0099	0.848
675.3024	30.0
757.1385	4.76
829.0710	26.9
866.9138	9.00
899.2825	9.44
983.7121	7.38
1118.6529	9.19
1168.0072	3.59
1209.0905	29.1
1272.7028	1.97
1344.8778	2.33
1360.1801	0.324
1389.7911	1.70
3096.5165	0.445
3126.7632	1.03



$\Delta E = 0.78$ kcal mol^{-1}
Population = 0.109



$\Delta E = 0.88$ kcal mol^{-1}
Population = 0.091

Optimized Coordinates (Angstroms)

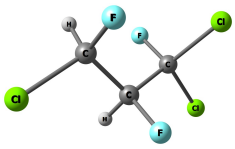
Atom	X	Y	Z
C	-1.473570362837	0.298640826091	0.384876060092
C	-0.317582854639	-0.464731607507	-0.286039209244
C	1.073962262478	0.001445857694	0.211983430882
Cl	-3.033632763612	-0.374861572823	-0.198686995220
H	-1.454288632233	0.158574059850	1.466708341228
F	-1.423740555466	1.612743988172	0.087441448487
H	-0.364037408797	-0.360522723340	-1.373165873872
F	-0.461898423926	-1.775609194727	0.069776227012
Cl	2.317769684180	-1.194346173562	-0.267449974942
Cl	1.498615048350	1.601963297525	-0.461510458942
F	1.064297006502	0.084778242627	1.552597004520

Atom	X	Y	Z
C	-1.318552672916	0.236727006827	0.471774036033
C	-0.364239841611	-0.321840429531	-0.591073770416
C	1.147253647784	-0.144808318668	-0.303167421098
Cl	-3.010340586195	-0.098659714274	-0.037378046319
H	-1.179212827085	-0.257516142083	1.434109583714
F	-1.154467378241	1.568578620504	0.606297387594
H	-0.564806170486	0.149576309616	-1.559673775074
F	-0.582672868865	-1.666555559913	-0.678476835385
Cl	1.645818652070	1.565403856417	-0.430969324263
Cl	1.591018021650	-0.810704228085	1.303580482970
F	1.811028023894	-0.840806400811	-1.234283317755

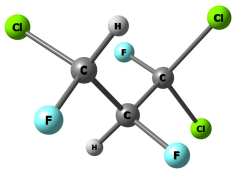
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
29.3917	0.0738
70.8714	0.0420
134.6383	0.0707
197.9854	0.147
222.9036	0.201
233.5851	0.368
281.5664	0.247
322.2980	0.180
369.1865	0.0700
403.6411	0.504
437.0922	4.08
461.1946	1.39
515.6454	0.468
694.5887	29.0
837.8337	1.71
855.4017	35.1
959.5078	9.34
1084.3356	6.87
1123.4353	3.18
1146.2430	22.9
1177.1899	14.6
1246.7282	1.96
1328.1120	2.21
1354.5417	0.971
1391.9073	0.962
3099.0250	0.297
3121.3296	1.04

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
29.3427	0.0638
80.1101	0.0367
141.0941	0.118
180.1904	0.145
200.9015	0.118
252.3675	0.0226
293.7241	0.836
324.3884	0.129
371.9740	0.163
406.7466	0.553
436.0167	2.87
491.3374	1.32
512.4057	0.790
651.9509	15.5
779.8093	24.5
862.1096	25.5
1037.3123	8.81
1099.4554	7.40
1131.9853	6.60
1144.5803	10.7
1164.3374	25.4
1248.8665	4.19
1328.3245	1.67
1349.0508	1.93
1396.9428	0.483
3072.1185	0.545
3123.8699	0.896



$\Delta E = 0.88$ kcal mol^{-1}
Population = 0.091



$\Delta E = 1.06$ kcal mol^{-1}
Population = 0.068

Optimized Coordinates (Angstroms)

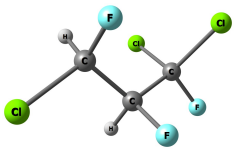
Atom	X	Y	Z
C	-1.469711468998	-0.300614913788	0.459778359524
C	-0.312246763425	0.587221116880	-0.017380280281
C	1.077387292269	0.027197081534	0.366434543336
Cl	-3.014515688175	0.612241406030	0.294179890701
F	-1.547593975190	-1.426167272598	-0.275302227905
H	-1.365928737937	-0.549332614360	1.517135506422
H	-0.397568069523	1.557329254225	0.484401134793
F	-0.378456558756	0.751874568433	-1.361856706593
Cl	1.474105973134	-1.492614353455	-0.471413228910
Cl	2.326700228273	1.261200479935	0.001790476282
F	1.074883768329	-0.193412752834	1.694834532632

Atom	X	Y	Z
C	-1.577393204479	0.394639381485	-0.343738090125
C	-0.233406627708	0.744761106771	0.316578765282
C	0.900717768080	-0.291225778486	0.155144681840
Cl	-2.349914638846	-1.032297645404	0.418950326203
F	-2.384125966307	1.467060884579	-0.180760072920
H	-1.468238320851	0.177951863852	-1.406853521288
H	-0.389743975830	0.897654206886	1.390487250404
F	0.178688172461	1.912123936275	-0.259460894843
Cl	1.189759545205	-0.678340012281	-1.573559416790
Cl	2.400278867417	0.378505691679	0.876440039643
F	0.595909380859	-1.417715635356	0.802207932595

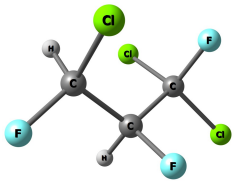
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
32.8966	0.0897
78.3415	0.111
129.5952	0.298
189.2555	0.140
218.4786	0.0859
228.0476	0.0913
248.2124	0.135
282.8953	0.0339
376.1087	0.00575
397.7510	0.396
410.6425	0.564
535.2858	0.518
636.3738	20.8
721.6490	27.2
760.5704	3.31
876.9061	13.4
908.1508	2.73
1074.6427	17.9
1123.9812	18.6
1151.6023	7.54
1195.1534	15.8
1268.9314	2.21
1347.0624	1.96
1362.1349	0.168
1397.4092	2.24
3070.8174	0.687
3116.0463	0.914

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
30.6277	0.0317
90.9192	0.0652
136.7668	0.118
182.3558	0.191
192.0793	0.101
280.2272	0.254
297.6040	0.196
322.6596	0.132
367.7245	0.336
411.5447	0.568
425.6778	3.30
451.8387	1.90
552.0769	0.153
656.9474	12.6
794.7463	33.6
821.4840	15.8
1048.1662	6.17
1104.5969	6.41
1124.8086	10.7
1138.2678	27.3
1175.7185	11.1
1251.6595	4.63
1316.4943	0.896
1354.5607	1.98
1397.3905	1.57
3070.3920	0.445
3126.6830	0.917



$\Delta E = 1.20$ kcal mol^{-1}
Population = 0.053



$\Delta E = 1.52$ kcal mol^{-1}
Population = 0.031

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.298561809350	0.312569534881	0.487623259879
C	-0.349541051646	0.057920585549	-0.686967504838
C	1.160943478401	0.074084970935	-0.354023370593
Cl	-2.972251620444	0.506920505852	-0.153097713738
F	-1.279073686159	-0.724705094587	1.347239202297
H	-1.058938055288	1.237920021606	1.011920206211
H	-0.495283261084	0.844743242051	-1.435568115654
F	-0.630309485598	-1.155440027580	-1.237886309166
Cl	1.607432685841	1.681281826388	0.327113872018
Cl	1.653467989830	-1.231025430501	0.751140853627
F	1.824216815497	-0.082956134595	-1.506895380042

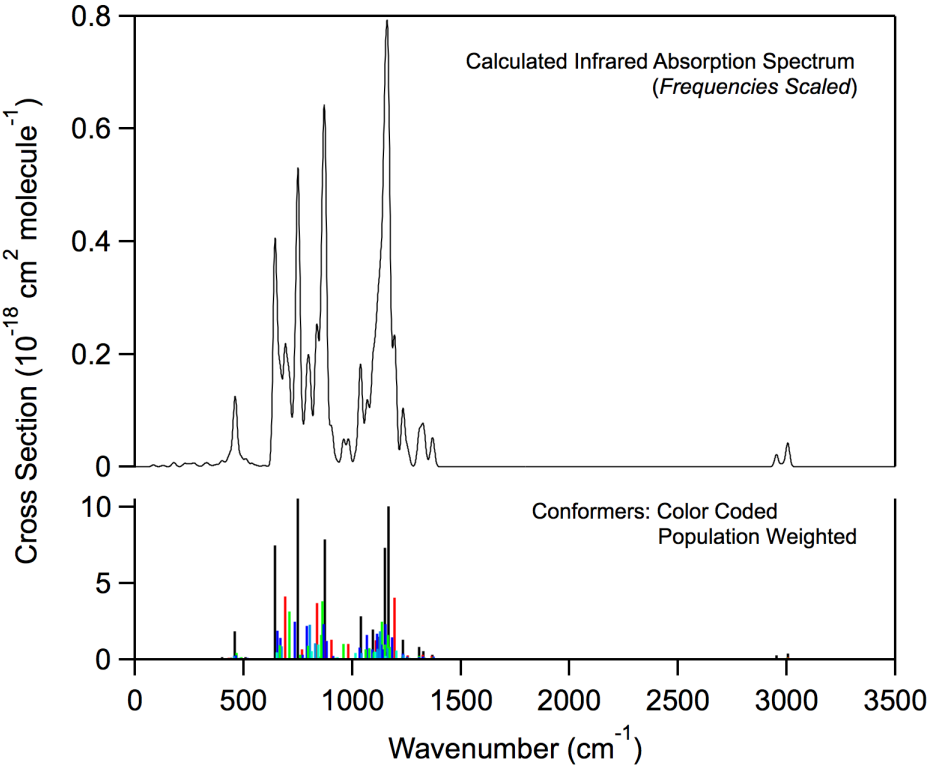
Atom	X	Y	Z
C	-1.527400380880	0.138655070466	-0.619261867525
C	-0.206180915626	-0.641781472419	-0.521138684123
C	0.965499083911	0.121476289291	0.130670703622
Cl	-2.350585873058	0.295056154127	0.962635618178
H	-1.376733019218	1.147291143398	-1.004052700855
F	-2.332646506867	-0.550990480912	-1.464642518299
H	0.090212713238	-0.887781634080	-1.546963388719
F	-0.411311330969	-1.791923879529	0.177668383983
Cl	2.406396000537	-0.940639958984	0.190030019832
Cl	1.339611649809	1.589274615419	-0.844983070803
F	0.672898579123	0.499677153222	1.374065504708

Infrared Absorption Spectrum (unscaled frequencies)

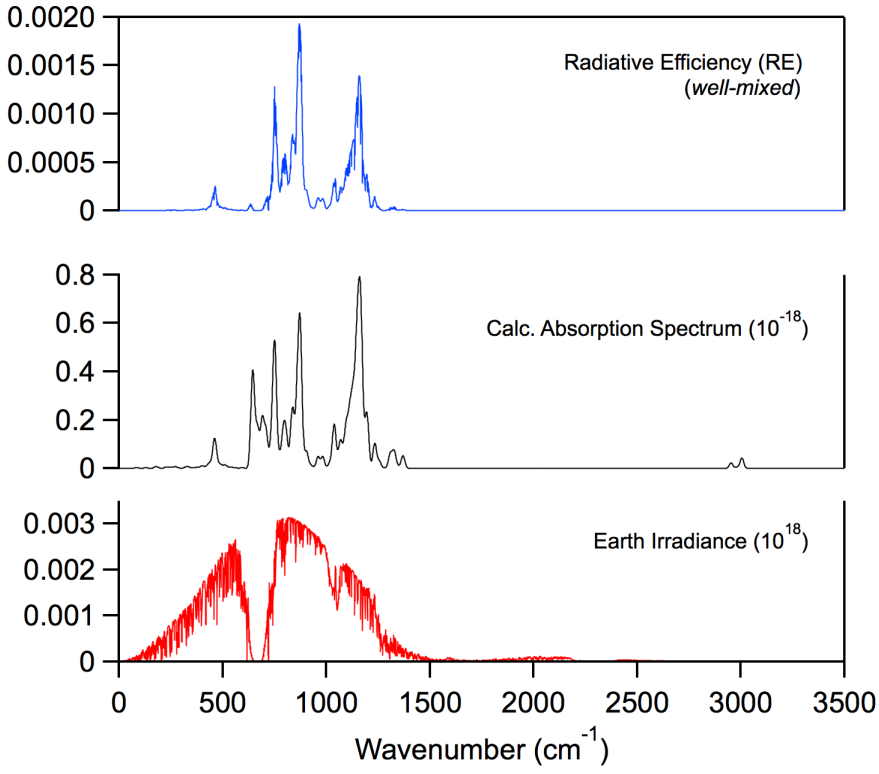
Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
36.0397	0.105
83.7864	0.0897
138.7942	0.232
181.5627	0.172
209.5192	0.134
242.9755	0.0525
262.1598	0.0133
306.2493	0.320
360.2302	0.241
393.4204	0.578
404.6865	0.439
481.4111	1.29
650.1754	17.9
746.9802	6.02
787.2823	17.4
851.5849	30.3
918.7265	2.26
1066.2515	12.6
1108.9180	9.51
1161.3347	18.6
1185.3434	15.4
1268.2164	2.37
1348.3529	1.40
1361.5790	0.0795
1392.4094	2.52
3069.6578	0.591
3126.4895	0.957

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
28.7120	0.0526
83.3524	0.0519
137.3134	0.269
188.3800	0.113
208.4614	0.150
243.3064	0.0506
295.6237	0.160
302.6503	0.159
338.6087	0.384
388.7769	0.543
412.3890	1.31
467.9023	0.462
634.9923	14.9
767.4234	4.21
803.9026	18.3
836.7225	31.0
930.3812	4.58
1018.9305	13.9
1113.0266	16.0
1162.9737	7.81
1215.8933	18.5
1280.0711	3.34
1317.7670	0.237
1372.2034	3.02
1393.9491	0.704
3070.0599	0.604
3127.0921	0.960

Infrared Spectrum

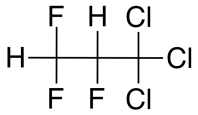


Radiative Efficiency



HCFC-233ec

Molecular Formula:	$CHF_2CHFCCl_3$
Name:	1,1,1-Trichloro-2,3,3-trifluoropropane
CAS number:	54306-56-8
Molecular Weight:	201.4



Global Atmospheric Lifetime (years):	4.13
Tropospheric Atmospheric Lifetime (years):	4.77
Stratospheric Atmospheric Lifetime (years):	30.6
Ozone Depletion Potential (ODP):	0.068

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.259	0.236
Global Warming Potential (GWP_H):		
GWP_{20}	1188	1081
GWP_{100}	324	295
Global Temperature Potentials (GTP_H)		
GTP_{20}		537
GTP_{50}		58
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*

$k_{SAR}(298\ K) = 1.23 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 0.784 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 4.61$ years

$\tau^{OH}_{Trop} = 4.77$ years

$\tau^{OH}_{Strat} = 137.9$ years

Fractional Atmospheric Loss: 0.895

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: 0.022

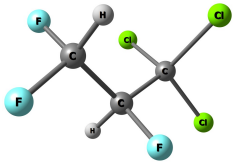
UV Photolysis

UV Spectrum: *No Recommendation*

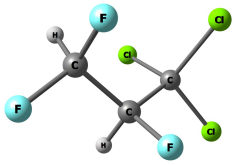
$\tau_{hv} = 50$ years

Fractional Atmospheric Loss: 0.083

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.628



$\Delta E = 0.43$ kcal mol^{-1}
Population = 0.305

Optimized Coordinates (Angstroms)

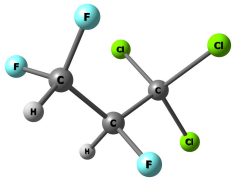
Atom	X	Y	Z
C	1.901421945404	-0.002027502500	0.229557999301
C	0.641397592195	0.536635217232	-0.473072272927
C	-0.712442223685	-0.061239074204	-0.024124888692
F	2.068409290184	-1.317372838053	-0.012535515114
F	2.952348087746	0.660446255033	-0.302454413006
H	1.877812336808	0.173512108901	1.309774901594
H	0.739546142303	0.370216486314	-1.551551337521
F	0.617721833675	1.877944194803	-0.213808870785
Cl	-2.020506014699	0.857293308788	-0.837027469830
Cl	-0.825591711431	-1.776221872613	-0.500384580065
Cl	-0.909852278501	0.096695716301	1.751412447045

Atom	X	Y	Z
C	1.850040259197	-0.354351508936	-0.314470801941
C	0.620892204600	0.558535596928	-0.484388356884
C	-0.739318405791	-0.052563433870	-0.078837899678
F	2.866298567013	0.224024112894	-0.998853888524
F	2.206960864368	-0.425764296186	0.981110330808
H	1.688118428448	-1.363605209107	-0.705137806081
H	0.545547254096	0.819574208244	-1.545903182853
F	0.831649563408	1.686193843899	0.248857952271
Cl	-2.012399557319	1.172569937722	-0.375085820592
Cl	-1.049243551176	-1.483640599629	-1.122348191577
Cl	-0.773245626844	-0.530208651958	1.635627665049

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
29.6987	0.0862
91.1738	0.0777
146.4687	0.0823
178.2560	0.0952
204.3173	0.124
254.9027	0.0576
275.6826	0.217
278.4690	0.237
333.4127	0.136
407.0832	0.0746
452.1555	6.22
485.0034	0.952
573.6671	2.88
653.8017	7.44
767.5562	19.3
822.0013	20.1
1044.0385	3.61
1111.2977	1.74
1131.9290	5.85
1143.5979	24.3
1157.8884	24.4
1296.6821	0.0371
1343.5568	1.79
1398.7631	1.94
1422.1972	4.87
3071.7407	0.131
3088.9801	3.64

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
40.7054	0.139
88.7573	0.0987
141.4107	0.174
177.2497	0.118
223.0378	0.0774
256.0643	0.111
259.9541	0.115
274.5336	0.287
299.3627	0.132
366.3222	0.703
410.6679	0.584
548.8019	3.44
661.2447	10.7
743.9822	18.3
776.9827	10.5
821.5755	14.7
917.8518	5.81
1074.0795	3.58
1131.1246	26.4
1144.1348	1.45
1195.9301	20.6
1313.5790	0.307
1365.4445	2.15
1411.7070	3.55
1417.5580	2.98
3068.8649	0.487
3087.7098	3.72



$\Delta E = 1.32$ kcal mol^{-1}
Population = 0.067

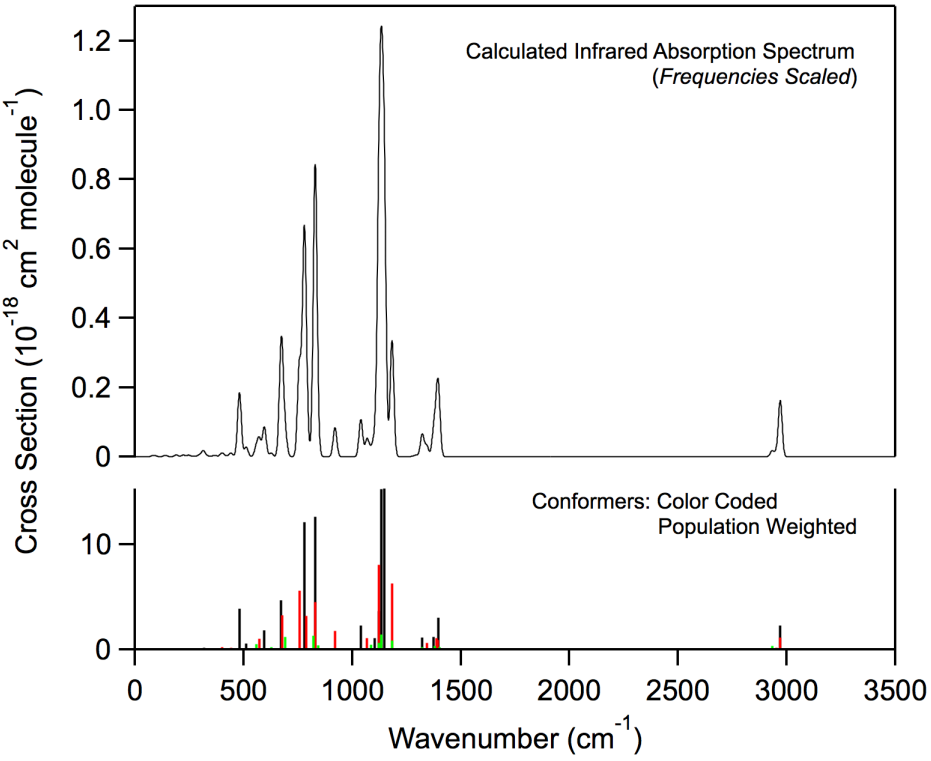
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.945786250483	0.144534496674	-0.487144625299
C	0.485904200846	0.464343931917	-0.872367524730
C	-0.642318643311	-0.050756079975	0.050957192037
F	2.170622962197	0.214802748167	0.837720590888
F	2.266187348988	-1.099168166490	-0.907410971846
H	2.591472724422	0.872432278045	-0.995671507883
H	0.315881623635	0.029177125362	-1.863010423516
F	0.380192005323	1.825986453394	-0.954627101389
Cl	-2.207176863829	0.286301016401	-0.774747981352
Cl	-0.472165519865	-1.813100651446	0.282309051972
Cl	-0.640534088890	0.788525847952	1.622882301117

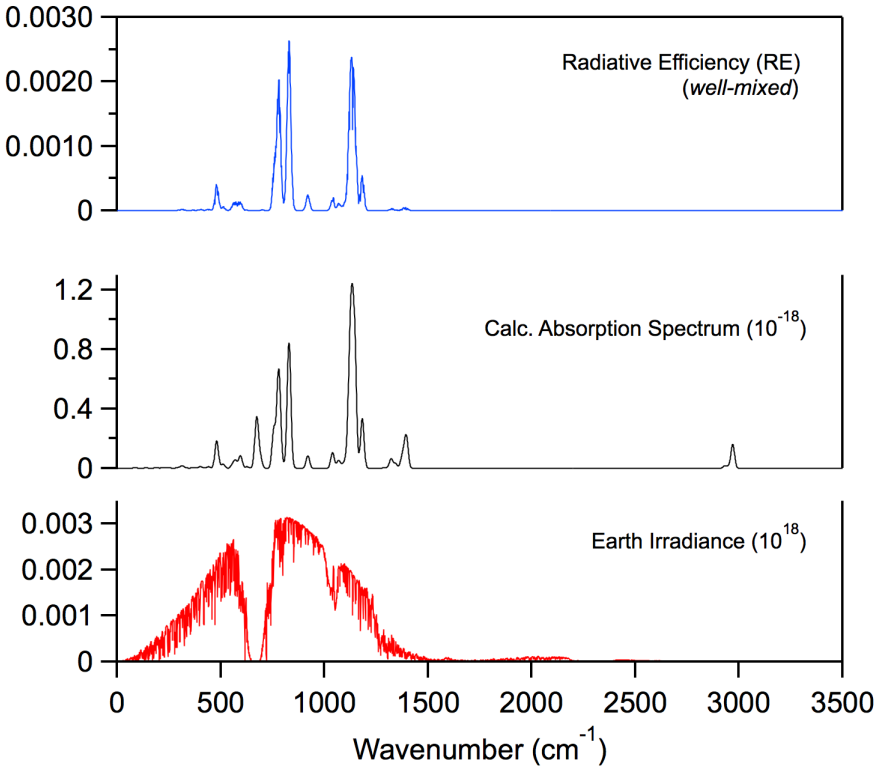
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
39.5517	0.120
97.6038	0.110
146.5551	0.0651
184.7526	0.0599
202.6777	0.254
241.6700	0.221
261.4732	0.0261
289.3906	0.0291
317.4927	0.291
379.9319	0.900
449.9273	0.555
533.7108	7.93
606.4940	3.24
676.5778	17.4
812.0545	19.9
836.9999	5.84
908.2620	0.199
1093.4562	6.73
1131.6702	9.70
1144.2741	21.6
1195.5312	13.0
1331.6621	0.0550
1341.5322	3.70
1402.8693	4.71
1426.4779	3.07
3048.4028	5.34
3073.6852	0.668

Infrared Spectrum

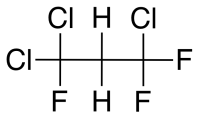


Radiative Efficiency



HCFC-233fa

Molecular Formula:	$CCl_2FCH_2CClF_2$
Name:	1,1,3-Trichloro-1,3,3-trifluoropropane
CAS number:	333-26-6
Molecular Weight:	201.4



Global Atmospheric Lifetime (years):	15.4
Tropospheric Atmospheric Lifetime (years):	23.3
Stratospheric Atmospheric Lifetime (years):	45.7
Ozone Depletion Potential (ODP):	0.207

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.332	0.321
Global Warming Potential (GWP_H):		
GWP_{20}	4156	4017
GWP_{100}	1547	1496
Global Temperature Potentials (GTP_H)		
GTP_{20}		3434
GTP_{50}		942
GTP_{100}		250

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 2.52 \times 10^{-15}$; $k_{SAR}(272\ K) \approx 1.61 \times 10^{-15}$ cm^3 $molecule^{-1}$ s^{-1}

τ^{OH}_{Global} = 22.4 years
τ^{OH}_{Trop} = 23.3 years
τ^{OH}_{Strat} = 575.3 years

Fractional Atmospheric Loss: 0.689

O(^{1}D) Reactivity

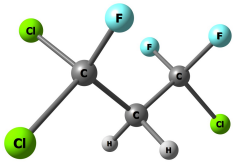
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 2.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)}$ = 185 years
Fractional Atmospheric Loss: 0.083

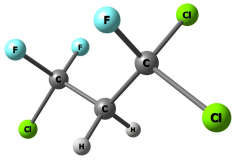
UV Photolysis

UV Spectrum: *No Recommendation*
τ_{hv} = 68 years
Fractional Atmospheric Loss: 0.228

Molecular Structure and Infrared Spectrum (5 conformers)



E = 0
Population = 0.403



E = 0
Population = 0.403

Optimized Coordinates (Angstroms)

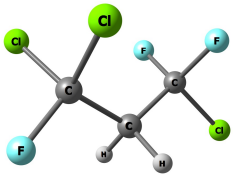
Atom	X	Y	Z
C	-1.163609751666	-0.105051481876	0.196537080689
C	0.180372017247	-0.675478761335	-0.272229026899
C	1.415555159541	0.126608253380	0.143287039830
Cl	-2.451724421315	-1.312718212028	-0.185826980040
F	-1.165963507291	0.090284666121	1.519973995696
Cl	-1.576418507166	1.449510886386	-0.598155715409
H	0.168930135883	-0.771016760529	-1.357477824071
H	0.278692767756	-1.672159215319	0.162406101361
Cl	2.897888993777	-0.746995756999	-0.431877817467
F	1.435766158345	1.350880541413	-0.384764407869
F	1.500597954889	0.248352840787	1.469662554177

Atom	X	Y	Z
C	-1.163621156516	-0.105044472291	-0.190649951258
C	0.180563127332	-0.672252237852	0.281434709395
C	1.415710346889	0.125700519204	-0.142074985847
Cl	-1.574780488049	1.456308183736	0.591490986688
F	-1.167270979104	0.079259147412	-1.515666919544
Cl	-2.451958722913	-1.308800240334	0.203119601948
H	0.277904605270	-1.672575328519	-0.144973047745
H	0.170230639930	-0.758722137897	1.367454267105
Cl	2.898218888298	-0.743836652199	0.438770898462
F	1.499390017420	0.236338469360	-1.469510190773
F	1.437103721443	1.354324749379	0.375724631569

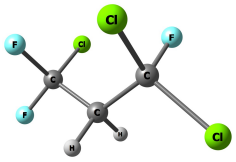
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
20.9116	0.000
113.3212	0.223
133.8654	0.203
205.6559	0.0487
228.0689	0.0465
253.3064	0.0579
314.2222	0.0271
359.6660	0.105
382.6766	0.244
408.4675	0.137
424.4663	0.0163
452.4340	1.11
575.7959	4.28
628.1401	17.1
720.1978	27.2
859.7321	6.21
927.2830	6.50
949.3631	31.9
999.4288	7.97
1148.6205	16.6
1211.6870	32.2
1242.7138	30.6
1314.5486	3.01
1364.1610	8.64
1445.9673	0.894
3100.4711	0.0818
3164.0302	0.0471

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
20.9099	0.0006
113.3241	0.223
133.8696	0.203
205.6567	0.0487
228.0687	0.0465
253.3072	0.0579
314.2230	0.0271
359.6667	0.105
382.6763	0.244
408.4678	0.137
424.4651	0.0163
452.4339	1.11
575.7961	4.28
628.1382	17.1
720.1978	27.2
859.7316	6.21
927.2830	6.50
949.3650	31.9
999.4251	7.97
1148.6164	16.6
1211.6821	32.2
1242.7111	30.6
1314.5440	3.01
1364.1563	8.64
1445.9671	0.894
3100.4762	0.0818
3164.0358	0.0471



ΔE = 1.0 kcal mol^{-1}
Population = 0.075



ΔE = 1.13 kcal mol^{-1}
Population = 0.060

Optimized Coordinates (Angstroms)

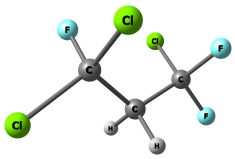
Atom	X	Y	Z
C	-1.227413288845	0.009690239638	0.470135471313
C	0.254125417212	0.032240437827	0.868831204172
C	1.311351692923	-0.003081138147	-0.231880959235
Cl	-1.694286808835	-1.492303291858	-0.392683082346
F	-1.930844956089	0.048559964294	1.616787551227
Cl	-1.709625969688	1.438644523411	-0.501447218711
H	0.417943527919	-0.828700565647	1.520414492044
H	0.408683450101	0.940777112648	1.454740190711
Cl	2.951945641986	0.034368524026	0.545342636298
F	1.240007716121	-1.110301403354	-0.971640125942
F	1.228711577196	1.045435597162	-1.051669159532

Atom	X	Y	Z
C	-1.063989918007	0.115538441996	-0.151548995071
C	0.079421258092	0.564961740426	0.759446940087
C	1.486264719038	0.023229784868	0.485857360634
Cl	-2.550849243703	1.021143964062	0.339429260552
F	-0.818981304306	0.406627458768	-1.432397360782
Cl	-1.398569789783	-1.643085946665	-0.033201426716
H	-0.168794701936	0.282943312247	1.785054103266
H	0.135815243118	1.654093217870	0.707282141552
Cl	2.177226681073	0.580104580545	-1.082004836893
F	2.284245235706	0.482366931068	1.463060712291
F	1.538061820707	-1.309086485186	0.515095101079

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
19.3923	0.00178
112.7052	0.151
140.0546	0.198
199.1613	0.0251
233.9495	0.103
257.8368	0.0612
333.6362	0.0472
347.0164	0.152
390.0743	0.222
409.4281	0.150
425.8918	0.00493
471.2461	1.63
569.2382	8.25
610.9731	4.32
725.9176	26.0
820.3131	14.9
919.5282	21.2
961.4466	1.45
1074.7251	34.1
1129.5030	13.3
1168.9914	36.4
1247.5316	18.9
1309.7369	3.72
1373.8735	7.46
1449.1486	0.944
3088.3310	0.0237
3145.1951	0.00224

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
14.5405	0.00259
115.6849	0.166
140.7908	0.129
203.5036	0.0471
232.9706	0.102
277.7119	0.101
299.7826	0.0678
361.9426	0.0943
384.5866	0.334
396.9069	0.0596
429.4867	0.404
464.0050	0.284
584.7924	7.73
667.4632	12.6
669.1066	13.7
805.6981	22.7
924.8681	6.90
952.6516	1.03
1082.1544	39.3
1155.6906	27.0
1191.3100	24.7
1223.0837	25.6
1298.9315	2.30
1374.7092	7.39
1449.1511	0.822
3088.6104	0.0242
3145.3503	0.00372



$\Delta E = 1.13$ kcal mol^{-1}
Population = 0.060

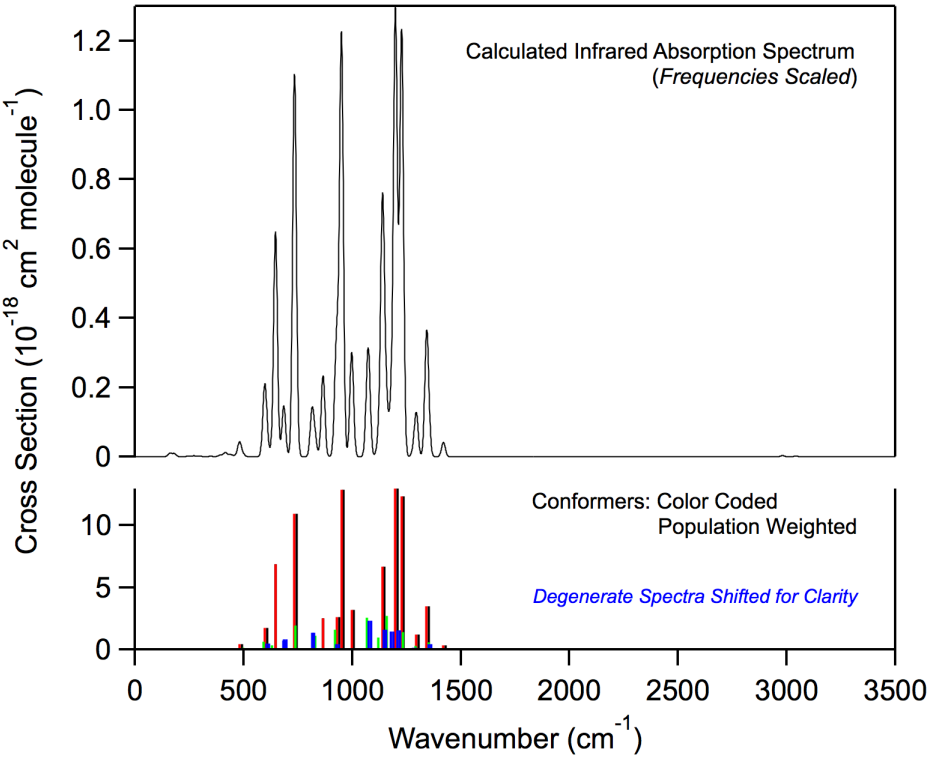
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.063793161235	-0.115772638525	-0.151112693022
C	0.079914123923	-0.563437484948	0.760377264174
C	1.486496320389	-0.021494117041	0.485864609498
Cl	-1.399103907041	1.642873777208	-0.035185103526
F	-0.818809866885	-0.408548433595	-1.431581433909
Cl	-2.550211861033	-1.021320034998	0.341304601182
H	0.136762665566	-1.652616935946	0.709729967761
H	-0.168301378156	-0.280089046908	1.785617879043
Cl	2.177511293493	-0.580272563923	-1.081296783939
F	1.537732886281	1.310883643113	0.513229879955
F	2.284784884697	-0.478924164435	1.463616812784

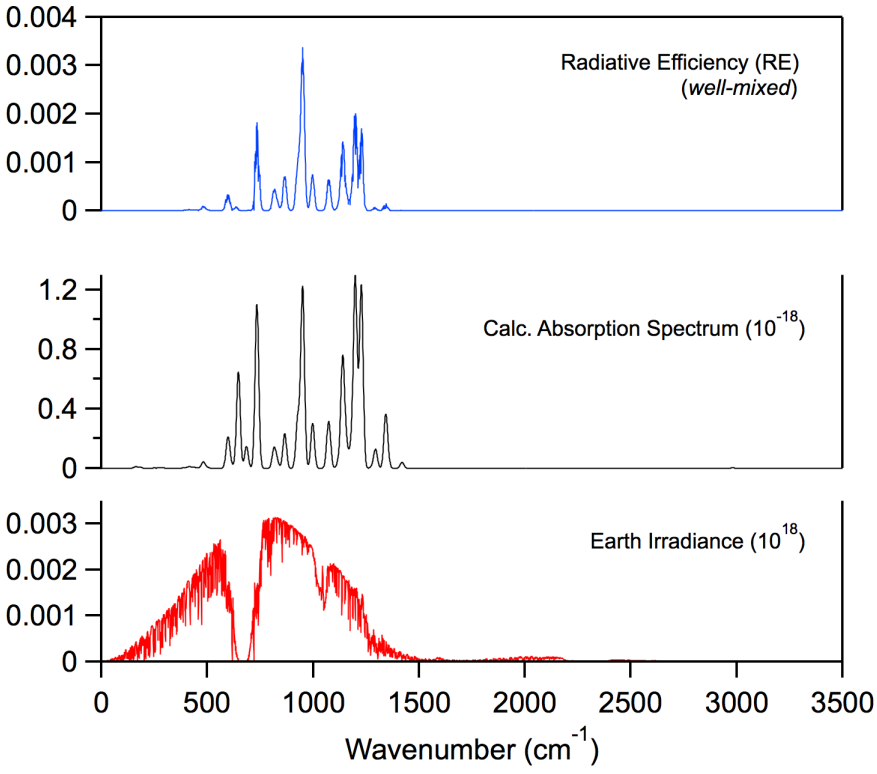
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
14.5405	0.00259
115.6849	0.166
140.7910	0.129
203.5036	0.0471
232.9706	0.102
277.7119	0.101
299.7826	0.0678
361.9426	0.0943
384.5866	0.334
396.9069	0.0596
429.4867	0.404
464.0050	0.284
584.7924	7.73
667.4633	12.6
669.1065	13.7
805.6981	22.7
924.8681	6.90
952.6515	1.03
1082.1544	39.3
1155.6906	27.0
1191.3099	24.7
1223.0836	25.6
1298.9314	2.30
1374.7092	7.39
1449.1512	0.822
3088.6105	0.0242
3145.3504	0.00372

Infrared Spectrum

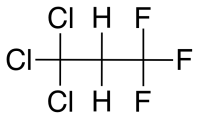


Radiative Efficiency



HCFC-233fb

Molecular Formula:	$CCl_3CH_2CF_3$
Name:	1,1,1-Trichloro-3,3,3-trifluoropropane
CAS number:	7125-84-0
Molecular Weight:	201.4



Global Atmospheric Lifetime (years):	16.4
Tropospheric Atmospheric Lifetime (years):	29.3
Stratospheric Atmospheric Lifetime (years):	37.3
Ozone Depletion Potential (ODP):	0.247

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.211	0.204
Global Warming Potential (GWP_H):		
GWP_{20}	2723	2636
GWP_{100}	1045	1011
Global Temperature Potentials (GTP_H)		
GTP_{20}		2286
GTP_{50}		676
GTP_{100}		176

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 2.00 \times 10^{-15}$; $k_{SAR}(272\ K) \approx 1.28 \times 10^{-15}$ cm^3 $molecule^{-1}$ s^{-1}

τ^{OH}_{Global} = 28.2 years
τ^{OH}_{Trop} = 29.3 years
τ^{OH}_{Strat} = 707.9 years

Fractional Atmospheric Loss: 0.583

O(^{1}D) Reactivity

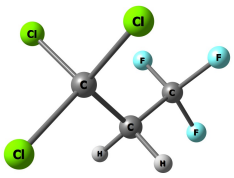
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 2.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)}$ = 185 years
Fractional Atmospheric Loss: 0.089

UV Photolysis

UV Spectrum: *No Recommendation*
τ_{hv} = 50 years
Fractional Atmospheric Loss: 0.328

Molecular Structure and Infrared Spectrum (1 conformer)



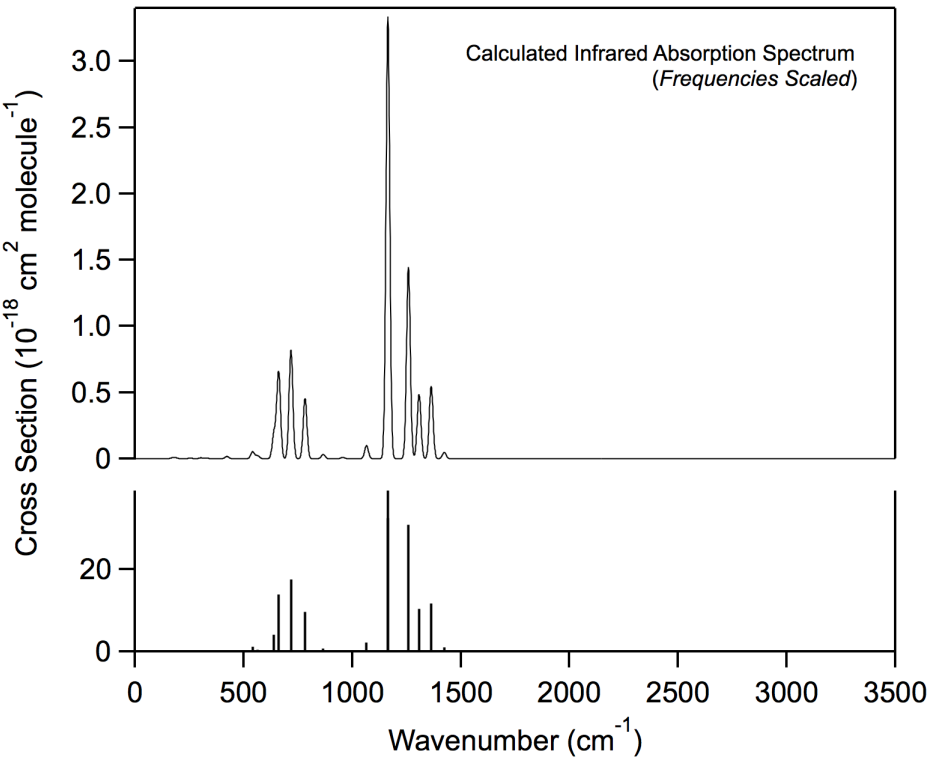
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	0.192439281891	-0.811607872970	0.000000000000
C	0.855453877272	0.570953521174	0.000000000000
C	-0.029165948022	1.819469186377	0.000000000000
Cl	1.525277700947	-2.030954186172	0.000000000000
Cl	-0.809307941452	-1.075447428487	1.459984651470
Cl	-0.809307941452	-1.075447428487	-1.459984651470
H	1.493091703293	0.634047114772	-0.884454772438
H	1.493091703293	0.634047114772	0.884454772438
F	0.784864288753	2.888545666029	0.000000000000
F	-0.809238362363	1.908388656514	-1.079414821775
F	-0.809238362363	1.908388656514	1.079414821775

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
21.5667	0.00244
123.9406	0.140
141.9186	0.147
211.7704	0.0861
213.0866	0.0440
263.7110	0.150
292.7066	0.0599
297.1367	0.0177
390.4886	0.0997
391.6491	0.274
516.3920	1.11
540.3453	0.482
620.9919	4.04
643.2829	13.9
703.3002	17.5
772.0819	9.66
860.5221	0.692
955.9250	0.217
1071.5448	2.12
1174.8282	39.1
1176.9711	32.4
1275.7930	30.8
1327.8033	10.4
1386.7529	11.6
1450.5526	1.02
3086.8901	0.0177
3142.9176	0.00125

Infrared Spectrum



Radiative Efficiency