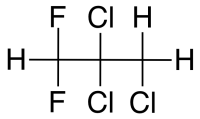
HCFC-242aa

Molecular Formula:	$CHF_2CCl_2CH_2Cl$
Name:	1,2,2-Trichloro-3,3-difluoropropane
CAS number:	–
Molecular Weight:	183.41



Global Atmospheric Lifetime (years):	2.13
Tropospheric Atmospheric Lifetime (years):	2.29
Stratospheric Atmospheric Lifetime (years):	29.3
Ozone Depletion Potential (ODP):	0.039

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.154	0.131
Global Warming Potential (GWP_H):		
GWP_{20}	402	341
GWP_{100}	109	92
Global Temperature Potentials (GTP_H)		
GTP_{20}		128
GTP_{50}		17
GTP_{100}		13

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 2.56 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 1.63 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 2.22$ years

$\tau^{OH}_{Trop} = 2.29$ years

$\tau^{OH}_{Strat} = 71.2$ years

Fractional Atmospheric Loss: 0.958

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

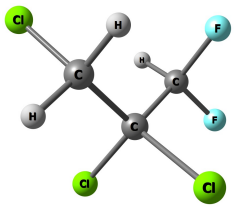
UV Photolysis

UV Spectrum: *No Recommendation*

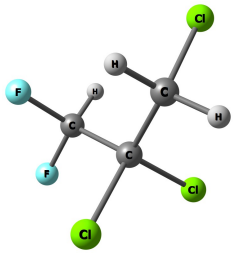
$\tau_{hv} = 68$ years

Fractional Atmospheric Loss: 0.031

Molecular Structure and Infrared Spectrum (5 conformers)



E = 0
Population = 0.379



E = 0
Population = 0.379

Optimized Coordinates (Angstroms)

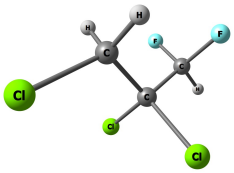
Atom	X	Y	Z
C	-0.530961412859	0.983968635867	0.730506103190
C	-0.180902143422	-0.236031909262	-0.150830273765
C	1.046610442040	-0.000589919348	-1.031704169787
F	-0.639733630179	2.070807883870	-0.067595154728
F	-1.703228797929	0.792385575466	1.354127278471
H	0.255501189458	1.157573969546	1.471394368613
Cl	-1.549178258106	-0.543984187005	-1.280488137656
Cl	0.047972523646	-1.647384744255	0.929154289254
H	1.261188733894	-0.895448261186	-1.611978023709
H	0.848591674196	0.843460511390	-1.690303715007
Cl	2.526174679261	0.402402444919	-0.086296564877

Atom	X	Y	Z
C	-0.523235667804	-0.992496748938	0.720148619755
C	-0.180095198770	0.238957150036	-0.147875268412
C	1.046472158742	0.018710651924	-1.033978878590
F	-1.694940031006	-0.812917696931	1.348383800368
F	-0.629253500150	-2.070560809998	-0.090132712539
H	0.265521746846	-1.171325759450	1.457345299809
Cl	0.045291836353	1.638777514388	0.947739603147
Cl	-1.552064927499	0.554161185306	-1.271035679827
H	0.850508641771	-0.818548914834	-1.701796424957
H	1.256114202749	0.921041727918	-1.604401502370
Cl	2.529716738767	-0.388962299420	-0.096376856384

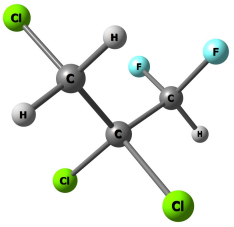
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
75.6501	0.219
107.7756	0.256
142.5839	0.0672
195.0350	0.196
214.6599	0.376
254.0717	0.218
293.9877	0.327
328.1522	0.174
405.1250	0.288
508.9872	2.64
599.3813	2.76
650.1608	10.9
743.0767	8.89
765.0748	5.61
939.8311	9.20
1023.7545	2.35
1105.9996	0.821
1140.3489	19.2
1183.4941	17.4
1239.7657	0.881
1303.4942	2.14
1380.0123	4.77
1395.2853	1.97
1457.9920	1.62
3091.2771	1.90
3115.1317	0.549
3186.7607	0.0469

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
75.6518	0.219
107.7759	0.256
142.5836	0.0672
195.0376	0.197
214.6606	0.376
254.0725	0.218
293.9873	0.327
328.1523	0.174
405.1255	0.288
508.9869	2.64
599.3811	2.76
650.1615	10.9
743.0764	8.89
765.0747	5.61
939.8312	9.20
1023.7550	2.35
1106.0029	0.821
1140.3477	19.2
1183.4924	17.4
1239.7661	0.881
1303.4937	2.14
1380.0114	4.77
1395.2834	1.97
1457.9917	1.62
3091.2801	1.90
3115.1323	0.549
3186.7614	0.0469



$\Delta E = 0.81$ kcal mol^{-1}
Population = 0.096



$\Delta E = 1.14$ kcal mol^{-1}
Population = 0.056

Optimized Coordinates (Angstroms)

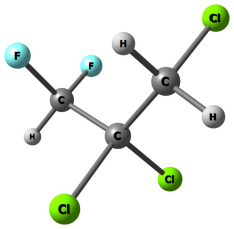
Atom	X	Y	Z
C	-1.698432131899	0.010464403004	0.205381599397
C	-0.197478734146	0.003078620562	-0.181240705104
C	0.660601744041	0.013456147679	1.083934877381
F	-1.964888582512	-1.071843318643	0.968252119228
F	-1.959671474551	1.108804528110	0.946842406171
H	-2.337216104265	0.003273364416	-0.682709875662
Cl	0.094763350134	1.461592652683	-1.183826460755
Cl	0.087741832404	-1.476229646484	-1.154966798501
H	0.425043828430	0.911354671987	1.654409050224
H	0.420784024900	-0.871927615693	1.671925670650
Cl	2.419987247463	0.006249192380	0.778130116972

Atom	X	Y	Z
C	-0.410415296502	1.163833548986	0.683587298640
C	-0.411601810669	-0.219024162717	-0.016243410146
C	0.590788887805	-0.363340541474	-1.164265145074
F	0.710796631563	1.332724491339	1.403763642265
F	-0.447208808251	2.122576389613	-0.269351593912
H	-1.283086109973	1.264356169065	1.337155958756
Cl	-2.046591499999	-0.385401678169	-0.779438660659
Cl	-0.204871698117	-1.483739632037	1.227621637166
H	0.438224568983	-1.323491551428	-1.652866268793
H	0.422258921208	0.448410065504	-1.870455939144
Cl	2.311155213952	-0.284716098681	-0.658362519099

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
88.8638	0.00181
92.7824	0.329
136.7190	0.153
179.2950	0.173
214.8400	0.256
258.2587	0.165
304.1970	0.0834
349.5514	0.269
398.6721	0.677
509.3828	3.83
566.2894	2.23
659.9291	5.50
737.4966	12.7
834.3628	1.59
968.9486	9.44
983.1437	4.35
1124.6746	1.27
1131.4724	17.6
1157.7028	18.5
1215.7156	4.37
1311.2049	2.70
1381.4111	5.92
1383.4441	1.12
1464.6180	0.817
3094.2885	2.51
3103.4207	0.489
3169.3042	0.0158

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
64.9769	0.0698
117.9282	0.197
146.1713	0.0325
189.0287	0.133
233.4226	0.382
269.7177	0.404
276.9222	0.632
358.8780	0.965
391.8430	0.627
428.1970	2.30
570.7033	1.71
703.9016	9.05
746.4964	10.6
837.0746	9.16
881.7617	3.02
990.1865	7.72
1132.4183	10.2
1146.4491	11.5
1170.9722	12.7
1252.2742	1.18
1302.9463	2.93
1386.2719	1.86
1399.6333	3.42
1458.6652	1.83
3082.4871	2.91
3112.1973	0.692
3181.1074	0.0399



$\Delta E = 1.14$ kcal mol^{-1}
Population = 0.056

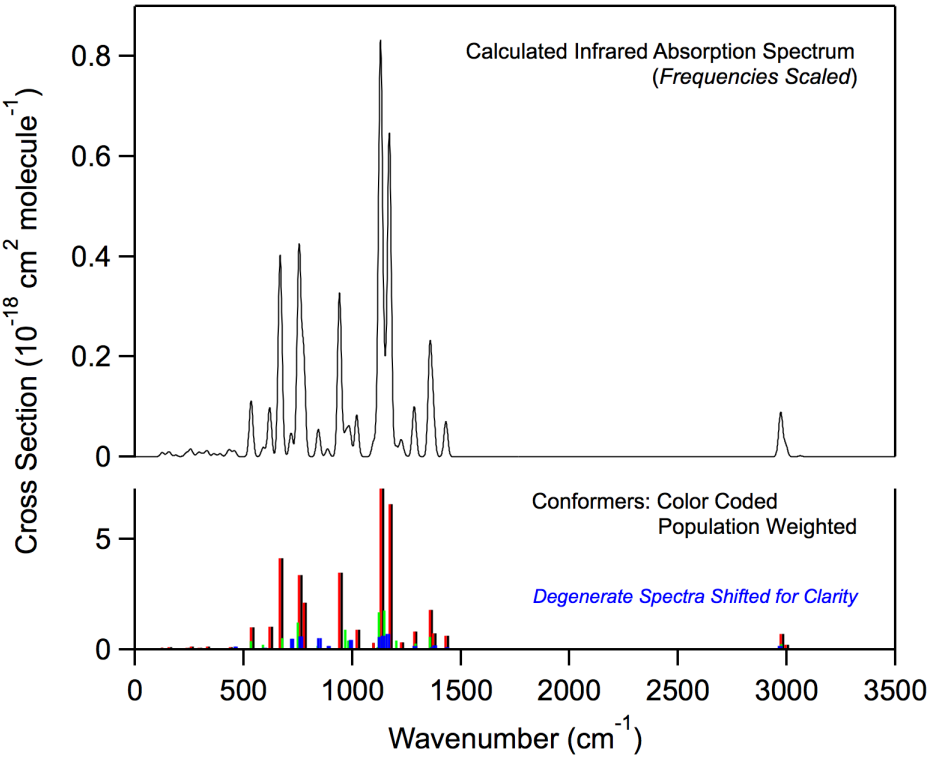
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-0.436211519804	-1.163419549288	0.668575706798
C	-0.406103555681	0.228186334791	-0.013028978195
C	0.596989056746	0.363862496987	-1.161491577049
F	-0.497744623060	-2.108371974395	-0.296780742801
F	0.682207200252	-1.368291112683	1.383740626610
H	-1.309631034053	-1.251863088148	1.322890036814
Cl	-0.166821396788	1.471140392253	1.246832982114
Cl	-2.038305535409	0.443267548464	-0.769995586848
H	0.407772685968	-0.434291207003	-1.877867792483
H	0.466182589905	1.333713234147	-1.637071306626
Cl	2.316079131923	0.237883924875	-0.660854368335

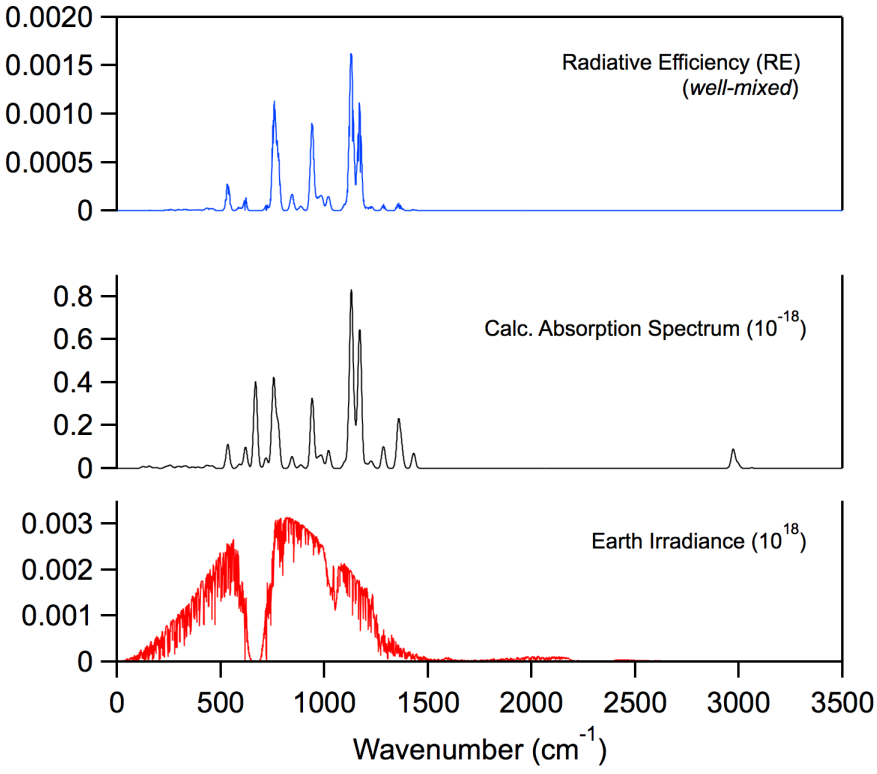
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
64.9766	0.0698
117.9271	0.197
146.1709	0.0325
189.0281	0.133
233.4223	0.382
269.7177	0.404
276.9215	0.632
358.8780	0.965
391.8431	0.627
428.1971	2.30
570.7032	1.71
703.9014	9.05
746.4966	10.6
837.0737	9.16
881.7614	3.02
990.1868	7.72
1132.4175	10.2
1146.4495	11.5
1170.9734	12.7
1252.2754	1.18
1302.9473	2.93
1386.2720	1.86
1399.6343	3.42
1458.6657	1.83
3082.4871	2.91
3112.1969	0.692
3181.1069	0.0399

Infrared Spectrum

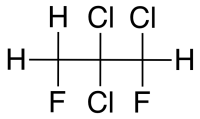


Radiative Efficiency



HCFC-242ab

Molecular Formula: CH_2FCCl_2CHClF
Name: 1,2,2-Trichloro-1,3-difluoropropane
CAS number: –
Molecular Weight: 183.41



Global Atmospheric Lifetime (years): 1.78
  Tropospheric Atmospheric Lifetime (years): 1.91
  Stratospheric Atmospheric Lifetime (years): 27.3
Ozone Depletion Potential (ODP): 0.034

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.159	0.132
Global Warming Potential (GWP_H):		
GWP_{20}	348	288
GWP_{100}	94	78
Global Temperature Potentials (GTP_H)		
GTP_{20}		103
GTP_{50}		14
GTP_{100}		11

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 3.07 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 1.96 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 1.85$ years
$\tau^{OH}_{Trop} = 1.91$ years
$\tau^{OH}_{Strat} = 60.4$ years

Fractional Atmospheric Loss: 0.964

O(^{1}D) Reactivity

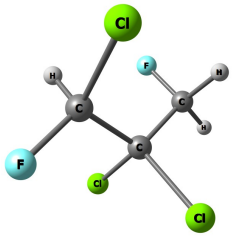
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 2.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)} = 185$ years
Fractional Atmospheric Loss: 0.010

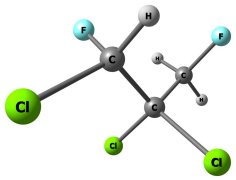
UV Photolysis

UV Spectrum: *No Recommendation*
$\tau_{hv} = 68$ years
Fractional Atmospheric Loss: 0.026

Molecular Structure and Infrared Spectrum (5 conformers)



E = 0
Population = 0.444



$\Delta E = 0.14$ kcal mol^{-1}
Population = 0.352

Optimized Coordinates (Angstroms)

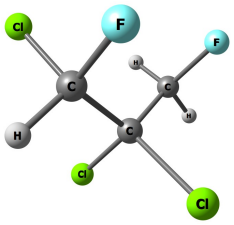
Atom	X	Y	Z
C	-0.649571083693	-1.274937916586	0.941276851689
C	-0.438394095452	0.035261819640	0.179821396797
C	0.731319423713	-0.030550973245	-0.824245722478
F	-0.764020557683	-2.301534070754	0.036703866781
H	0.211041800642	-1.459101829375	1.589885868233
H	-1.563226917922	-1.201697192640	1.536813949201
Cl	-0.191472900304	1.339463007878	1.376998122768
Cl	-1.910120889047	0.379643365212	-0.809610546415
H	0.531598774257	-0.818067406600	-1.551696934789
F	0.884682720783	1.150781001565	-1.444238891879
Cl	2.281487724704	-0.468682805095	-0.017983959907

Atom	X	Y	Z
C	-1.726092201162	0.741019764119	0.347497488836
C	-0.461129926069	-0.108888391249	0.156165102495
C	0.685954171722	0.776388107181	-0.377377033937
F	-2.050216987254	1.339047269603	-0.844951404028
H	-2.548090831679	0.100120782423	0.675572326880
H	-1.523212598140	1.513095882330	1.094746110795
Cl	-0.792876985596	-1.403207990053	-1.037431834541
Cl	-0.055000905460	-0.796905718278	1.757900478180
H	0.402984407686	1.166383754551	-1.356139008162
F	0.858812040487	1.806605773505	0.486246570238
Cl	2.235132815465	-0.085881234131	-0.576170796758

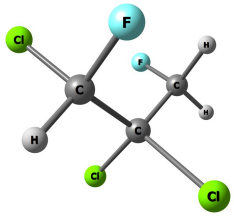
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
71.5504	0.135
110.7611	0.270
155.4617	0.0621
184.4216	0.193
234.1410	0.709
245.8484	0.0636
287.9303	0.434
358.4915	0.220
390.2486	0.137
403.8246	0.426
578.6510	5.08
646.0935	6.72
710.5007	21.4
807.1839	7.26
972.7939	9.98
1068.3455	2.57
1107.4351	8.04
1140.6933	4.99
1171.3406	13.6
1269.5477	3.30
1284.2310	0.560
1364.1450	1.93
1414.1539	0.900
1494.8468	1.38
3068.9816	1.35
3125.9542	0.430
3129.8821	1.16

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
76.0617	0.120
112.4738	0.339
158.0748	0.118
181.8717	0.0590
206.2330	0.382
253.5825	0.151
310.5831	0.714
358.1041	0.145
386.8798	0.232
434.3253	0.566
519.8768	6.87
652.3818	7.05
750.6416	10.1
848.3285	12.8
973.8967	7.48
1059.6836	4.62
1099.5770	11.5
1111.2371	14.9
1150.1364	3.19
1273.8342	2.96
1284.0945	1.44
1360.2279	1.29
1408.5725	1.58
1494.3677	0.919
3068.6925	1.50
3121.3815	0.398
3131.8062	1.02



$\Delta E = 1.06$ kcal mol^{-1}
Population = 0.075



$\Delta E = 1.31$ kcal mol^{-1}
Population = 0.049

Optimized Coordinates (Angstroms)

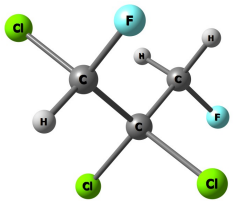
Atom	X	Y	Z
C	-0.521678787428	0.352075582127	1.482516885533
C	-0.446255314056	-0.213175353778	0.060116781553
C	0.752703199389	0.277692544091	-0.788199620433
F	-0.608898089432	1.715060746058	1.439139133880
H	-1.405456696893	-0.061547498693	1.976735568422
H	0.381003720187	0.060515148665	2.027973597219
Cl	-1.927537598345	0.256844599317	-0.849895119062
Cl	-0.364954026747	-2.000711286207	0.194516997669
H	0.777570354721	-0.250561203105	-1.742414419070
F	0.653882898898	1.603132860210	-0.993687445135
Cl	2.327169339706	-0.055130138686	0.023774639425

Atom	X	Y	Z
C	-0.403999508123	-0.486052381722	1.507011093131
C	-0.526249779961	-0.111971299796	0.023093158922
C	0.554056757765	0.867754274817	-0.493400828611
F	0.670280530830	-1.301638753024	1.719219268466
H	-0.284365049499	0.438198287634	2.081885970421
H	-1.318512214494	-1.000710457999	1.813707007558
Cl	-2.098746714697	0.772318414427	-0.134021330216
Cl	-0.553687961865	-1.570700074017	-1.004221241666
H	0.345095491099	1.147959268813	-1.526377844780
F	0.537416187442	1.968351681270	0.295254575703
Cl	2.208262261504	0.178745039597	-0.463028828929

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
62.1894	0.0631
127.0515	0.253
154.3657	0.0282
190.1205	0.102
243.0830	0.0414
266.7066	1.37
294.1405	0.355
341.2951	0.276
385.4541	0.0728
422.3770	1.90
453.5056	1.61
670.5081	15.2
763.0634	10.7
867.2939	16.7
896.0112	3.13
1063.8332	2.93
1108.0126	1.55
1141.2657	22.9
1181.1330	3.04
1276.0341	3.51
1290.6215	0.274
1366.9890	1.05
1423.0572	1.40
1494.9267	1.25
3060.4445	1.54
3117.1003	0.465
3119.1525	1.52

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
67.0144	0.0930
122.8730	0.250
160.1426	0.0278
184.0650	0.219
235.1865	0.359
263.4305	0.755
282.3032	0.687
342.2216	0.395
383.7922	0.166
417.8269	1.57
463.1615	2.33
712.1311	6.92
750.3199	24.9
843.9641	5.84
899.1665	3.55
1069.4301	5.93
1107.6561	14.3
1124.6644	8.36
1175.0128	3.69
1285.1245	4.11
1297.2929	0.774
1357.3237	0.495
1420.9009	1.06
1494.7706	0.856
3057.9951	1.55
3118.4156	0.914
3122.0584	0.930



$\Delta E = 1.35$ kcal mol^{-1}
Population = 0.045

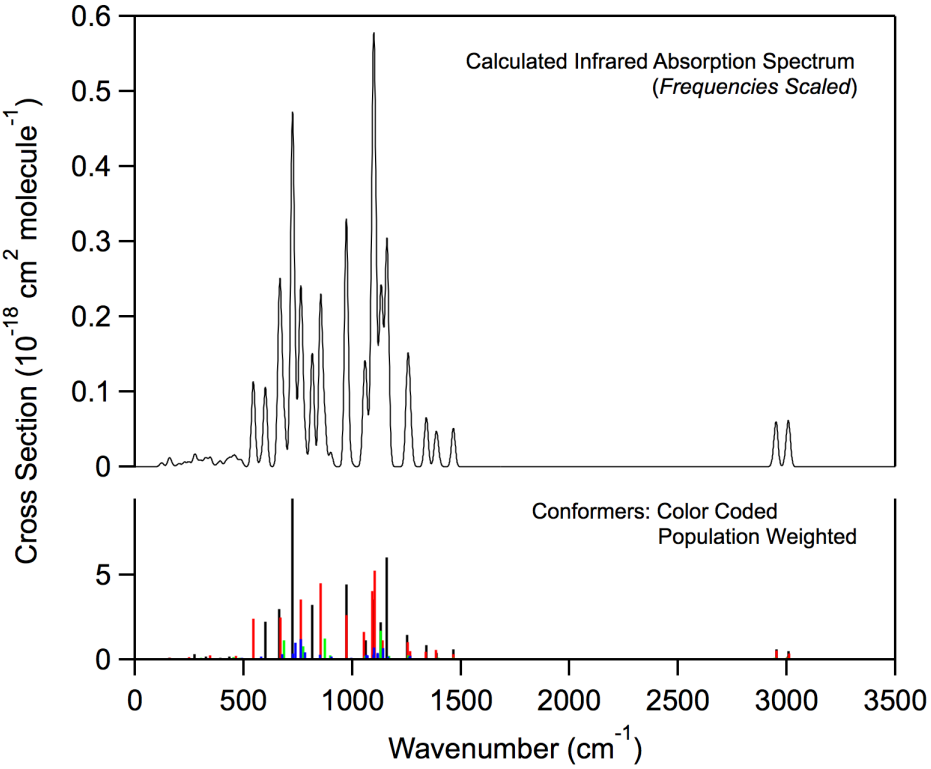
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-0.579226400750	-0.265218940996	1.418434877561
C	-0.350471262102	0.009923307614	-0.070680337431
C	1.025810674120	0.648926348058	-0.357851860701
F	-1.845576593384	-0.728391973440	1.620201357169
H	0.141849922413	-1.014171824722	1.758180350990
H	-0.434673689099	0.670146148476	1.968790686527
Cl	-1.582642883557	1.197525389978	-0.643877531856
Cl	-0.512272725000	-1.499785306736	-1.020850839131
H	1.152047396535	0.822576750153	-1.426741664658
F	1.114981482962	1.816129562113	0.318391683288
Cl	2.389620077862	-0.405051460499	0.165779278242

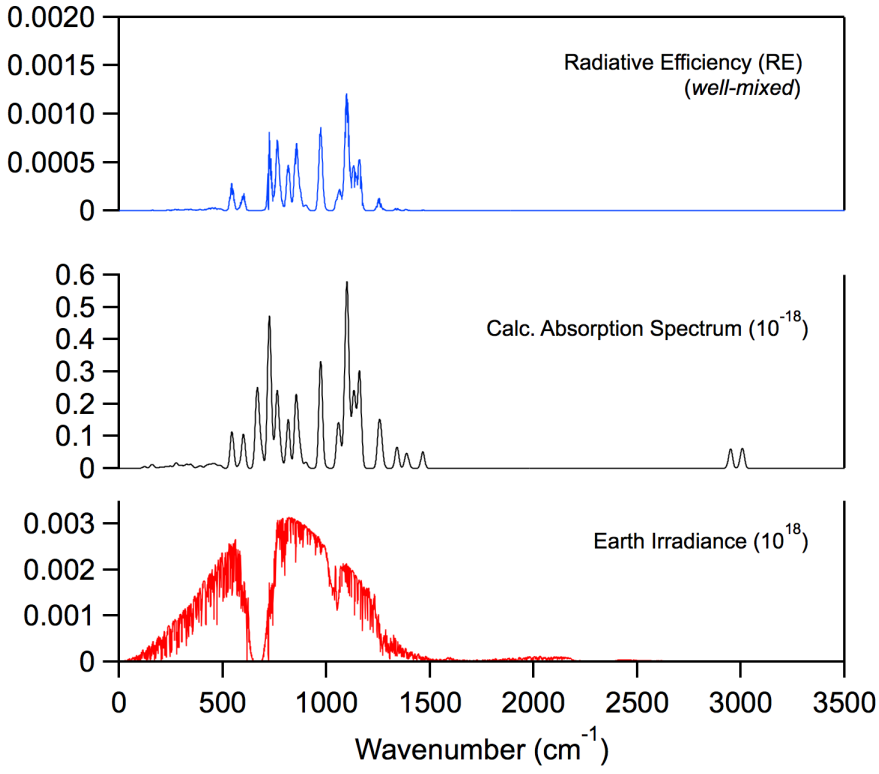
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
77.7943	0.160
104.0439	0.236
155.2425	0.273
166.4254	0.194
238.2941	0.0753
250.1137	0.442
297.1646	0.184
334.2633	0.269
361.6521	0.209
433.1618	0.343
557.6387	4.32
660.7985	7.25
726.3185	22.0
772.4870	9.18
997.2963	2.32
1076.6725	5.57
1105.6714	6.29
1126.6496	7.25
1153.1913	15.1
1280.3675	1.10
1282.2783	3.77
1361.8747	0.590
1418.2205	0.604
1500.7425	0.556
3056.0898	1.70
3115.8406	1.10
3127.2359	0.457

Infrared Spectrum

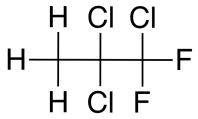


Radiative Efficiency



HCFC-242ac

Molecular Formula:	$CH_3CCl_2CClF_2$
Name:	1,2,2-Trichloro-1,1-difluoropropane
CAS number:	7126-05-8
Molecular Weight:	183.41



Global Atmospheric Lifetime (years):	8.09
Tropospheric Atmospheric Lifetime (years):	10.0
Stratospheric Atmospheric Lifetime (years):	41.9
Ozone Depletion Potential (ODP):	0.125

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.240	0.227
Global Warming Potential (GWP_H):		
GWP_{20}	2178	2061
GWP_{100}	644	610
Global Temperature Potentials (GTP_H)		
GTP_{20}		1426
GTP_{50}		185
GTP_{100}		87

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 5.85 \times 10^{-15}$; $k_{SAR}(272\ K) \approx 3.73 \times 10^{-15}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 9.67$ years

$\tau^{OH}_{Trop} = 10.0$ years

$\tau^{OH}_{Strat} = 269.2$ years

Fractional Atmospheric Loss: 0.837

$O(^1D)$ 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: 0.044

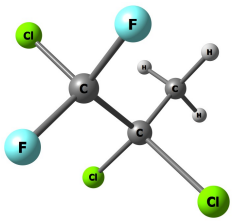
UV Photolysis

UV Spectrum: *No Recommendation*

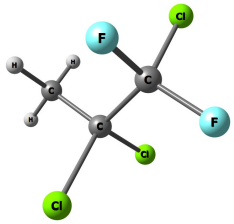
$\tau_{hv} = 68$ years

Fractional Atmospheric Loss: 0.119

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.394



E = 0
Population = 0.394

Optimized Coordinates (Angstroms)

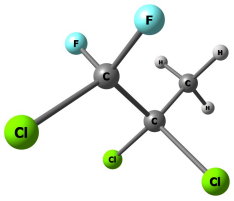
Atom	X	Y	Z
C	0.567307469231	0.345167694015	1.834762530473
C	0.572260677383	0.176922018531	0.323996773927
C	-0.699960935233	-0.545594093078	-0.213869926347
H	1.517156095291	0.776838071507	2.151033409470
H	-0.246725179751	1.006832848935	2.135076502065
H	0.438855266061	-0.630045644011	2.309280230995
Cl	1.972452370138	-0.863832455590	-0.155744811986
Cl	0.726579407298	1.767722251690	-0.491750486959
F	-0.646234889965	-0.699139351063	-1.530494588367
F	-0.783448731207	-1.753550624887	0.351876522381
Cl	-2.208507549245	0.353259283950	0.190596844348

Atom	X	Y	Z
C	0.569784836303	-0.345372559875	1.834606036793
C	0.573104858134	-0.176074880246	0.323953394451
C	-0.699541746513	0.547113525584	-0.212000981759
H	1.519881924040	-0.777485186691	2.149523879041
H	0.442086656984	0.629539747170	2.309945121893
H	-0.244069819181	-1.007056773016	2.135360073669
Cl	0.726146817937	-1.766342211266	-0.493072508302
Cl	1.973009102060	0.864685899442	-0.156612721750
F	-0.782118940492	1.754695674164	0.354677636578
F	-0.647237902263	0.701562236701	-1.528577199642
Cl	-2.207850787009	-0.351667471967	0.193511269028

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
75.7835	0.0203
166.1620	0.0859
205.4338	0.177
239.1249	0.106
265.6813	0.0489
285.5887	0.160
300.0393	0.0954
337.6949	0.119
349.6838	0.139
422.9268	0.106
438.9763	0.459
526.7771	1.52
635.8971	1.66
700.4655	23.1
778.3313	7.93
940.9229	27.2
1085.5217	4.70
1099.9954	7.64
1123.1522	14.2
1205.0252	13.8
1237.6696	14.9
1411.3804	1.83
1479.9684	0.419
1482.8854	1.52
3068.2845	0.289
3152.4962	0.338
3161.5966	0.344

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
75.7835	0.0203
166.1620	0.0859
205.4338	0.177
239.1249	0.106
265.6816	0.0489
285.5888	0.160
300.0393	0.0954
337.6949	0.119
349.6839	0.139
422.9268	0.106
438.9763	0.459
526.7771	1.52
635.8971	1.66
700.4656	23.1
778.3313	7.93
940.9230	27.2
1085.5218	4.70
1099.9954	7.64
1123.1523	14.2
1205.0253	13.8
1237.6697	14.9
1411.3803	1.83
1479.9684	0.419
1482.8854	1.52
3068.2844	0.289
3152.4963	0.338
3161.5965	0.344



$\Delta E = 0.37$ kcal mol^{-1}
Population = 0.212

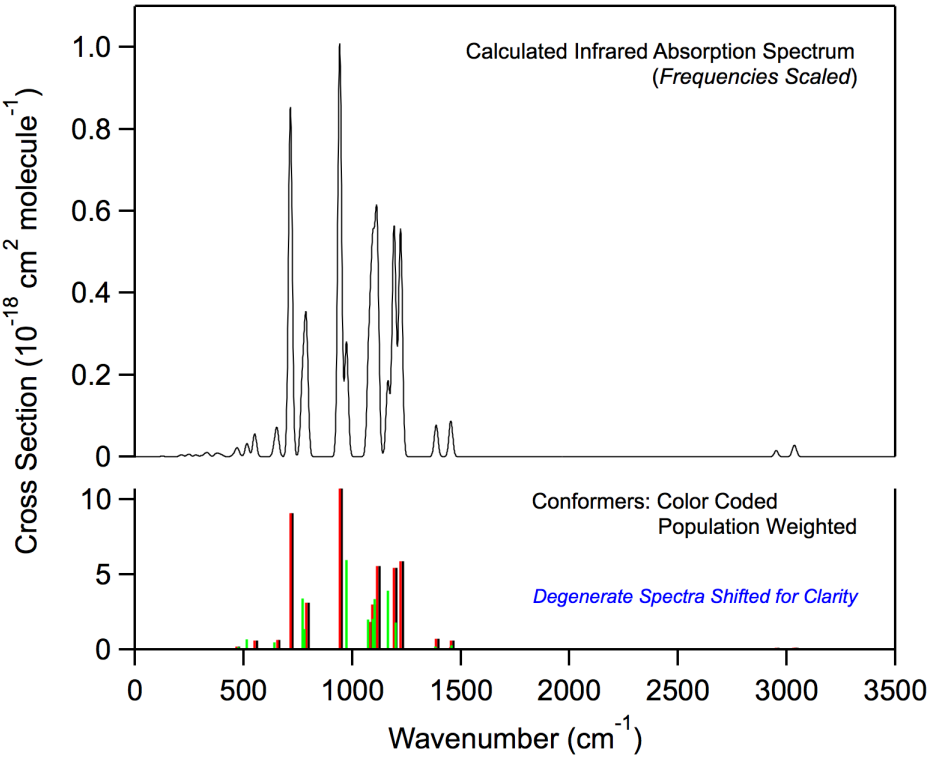
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.443328354522	-0.059643179826	1.569090744980
C	0.706326807147	-0.002195952052	0.234114260296
C	-0.834923775944	-0.030744580489	0.475024656982
H	1.181636105706	-0.980908516099	2.092810360011
H	2.518109976463	-0.039147725290	1.389068511088
H	1.162298709446	0.800096366474	2.180126883328
Cl	1.162360967216	-1.420630380331	-0.767976137626
Cl	1.130460257660	1.516992386351	-0.623956463479
F	-1.141166148032	-1.148457537308	1.143373834568
F	-1.164595815527	1.009327878538	1.249184754507
Cl	-1.821644438658	0.031437240033	-1.011489404655

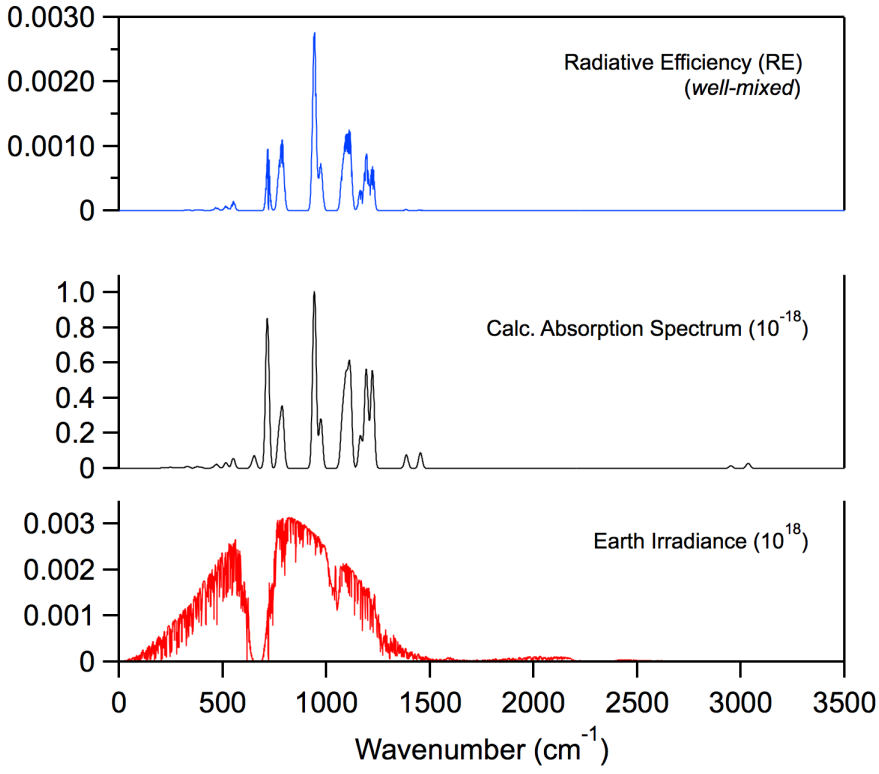
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
75.8209	0.0684
169.4587	0.113
180.9753	0.101
245.6141	0.0382
264.5274	0.00433
297.3574	0.386
312.9161	0.00246
336.4511	0.157
365.1817	0.415
427.0393	0.00744
447.5825	0.698
489.0640	3.28
623.6310	2.28
758.6524	16.0
768.9184	6.38
973.7719	28.1
1080.2486	9.52
1102.2516	9.65
1109.9388	15.9
1175.9472	18.5
1214.6135	8.58
1407.7322	1.02
1480.3033	0.300
1484.8935	1.38
3068.7201	0.428
3153.0313	0.423
3163.4266	0.252

Infrared Spectrum

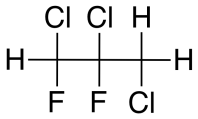


Radiative Efficiency



HCFC-242ba

Molecular Formula:	$CHClFCClFCH_2Cl$
Name:	1,2,3-Trichloro-1,2-difluoropropane
CAS number:	7164-14-9
Molecular Weight:	183.41



Global Atmospheric Lifetime (years):	1.99
Tropospheric Atmospheric Lifetime (years):	2.11
Stratospheric Atmospheric Lifetime (years):	36.7
Ozone Depletion Potential (ODP):	0.033

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.180	0.151
Global Warming Potential (GWP_H):		
GWP_{20}	440	371
GWP_{100}	119	100
Global Temperature Potentials (GTP_H)		
GTP_{20}		137
GTP_{50}		18
GTP_{100}		14

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 2.78 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 1.78 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 2.04$ years

$\tau^{OH}_{Trop} = 2.11$ years

$\tau^{OH}_{Strat} = 66.0$ years

Fractional Atmospheric Loss: 0.976

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

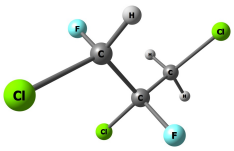
UV Photolysis

UV Spectrum: *No Recommendation*

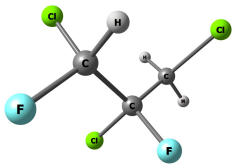
$\tau_{hv} = 150$ years

Fractional Atmospheric Loss: 0.013

Molecular Structure and Infrared Spectrum (8 conformers)



E = 0
Population = 0.478



$\Delta E = 0.58$ kcal mol^{-1}
Population = 0.181

Optimized Coordinates (Angstroms)

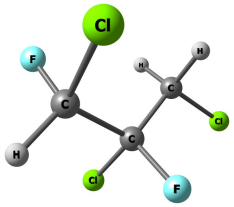
Atom	X	Y	Z
C	0.551331821780	-0.846971822900	-0.285491997392
C	-0.128639557499	0.436312645327	0.231068996267
C	-1.525291167067	0.639325231186	-0.357783735287
Cl	2.171267443368	-1.086672363780	0.422870228227
H	-0.048581980011	-1.711163483121	0.005396855211
F	0.633873964045	-0.784284999272	-1.633418185969
Cl	0.828306288776	1.890907149352	-0.248890997741
F	-0.190451915419	0.373384131849	1.575947431400
H	-1.943970720964	1.567888356578	0.025462158969
H	-1.472110032961	0.662395769833	-1.444003401071
Cl	-2.646066144047	-0.691346615053	0.114997647384

Atom	X	Y	Z
C	0.607733966280	-0.658740329335	0.700100232100
C	-0.072695691864	0.603202246165	0.128916125623
C	-1.236923455552	0.363580757995	-0.824081929161
Cl	1.179129319364	-1.767888587954	-0.586922978693
F	1.643001474540	-0.286887739775	1.473889565036
H	-0.118048240280	-1.214083586541	1.296686929361
Cl	1.132780801639	1.617026976925	-0.751564695523
F	-0.501168434095	1.304006685783	1.208482742416
H	-1.665286644959	1.325807231145	-1.099826242568
H	-0.907212618439	-0.176002897479	-1.708348886694
Cl	-2.542539476632	-0.600951756930	-0.039295861897

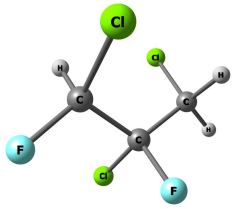
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
63.8981	0.199
98.4320	0.373
154.7162	0.147
178.6138	0.0999
199.7126	0.331
284.8582	0.0689
301.4744	0.610
362.7644	0.0277
405.8228	0.101
495.7555	2.95
563.4199	4.57
641.6095	11.5
739.0062	9.35
823.3157	8.31
903.6816	5.95
965.3810	9.50
1099.1263	7.14
1135.3462	12.0
1184.8032	11.0
1265.0517	3.57
1298.8240	1.26
1301.0836	1.68
1364.6848	1.99
1455.3180	1.40
3114.9321	0.618
3119.3503	0.619
3192.0573	0.0472

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
60.8149	0.161
104.7218	0.272
154.8577	0.144
177.9082	0.264
223.0251	0.537
278.2074	0.0482
318.5503	0.318
362.6709	0.117
408.1305	0.669
438.4920	0.251
587.8872	6.49
656.0227	8.00
740.0370	9.26
818.0393	15.5
889.5033	1.11
974.6792	14.0
1084.7591	1.72
1150.4657	26.1
1190.6210	2.75
1244.5646	4.49
1289.7629	0.371
1304.4739	1.81
1373.3174	2.33
1456.9197	2.41
3116.9350	0.604
3119.8520	0.609
3193.9153	0.0337



$\Delta E = 0.72$ kcal mol^{-1}
Population = 0.141



$\Delta E = 1.33$ kcal mol^{-1}
Population = 0.050

Optimized Coordinates (Angstroms)

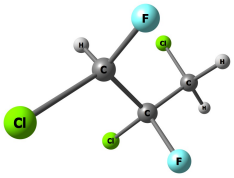
Atom	X	Y	Z
C	1.403495323121	0.471736201787	-0.006412296577
C	-0.088817438610	0.214112677456	0.304305172346
C	-0.725790274013	-0.776252053977	-0.665710872468
Cl	2.382156887006	-1.012249890430	0.278329949615
F	1.535649274404	0.848372716593	-1.294999288147
H	1.801275942074	1.240094580307	0.657418580007
Cl	-0.899680538772	1.829552935986	0.202659221175
F	-0.181245838298	-0.223031724836	1.575851551765
H	-0.690366918982	-0.376933881238	-1.677178116210
H	-0.173865332521	-1.715143394970	-0.616265547777
Cl	-2.426930085409	-1.137624166677	-0.252189353729

Atom	X	Y	Z
C	0.938273400605	0.063785373823	-0.632000495586
C	-0.110823376171	0.437652889598	0.433349201742
C	-1.015021041207	-0.698614585953	0.908477662702
Cl	2.005712826289	-1.251834297387	-0.014077374437
H	0.465734316904	-0.309692812958	-1.539533766651
F	1.697379421255	1.140612650294	-0.901203601846
Cl	-1.100328827756	1.785835249891	-0.254921980922
F	0.530993584844	0.908657951960	1.529446659053
H	-0.401836233796	-1.443752091787	1.414087042350
H	-1.755692626195	-0.291078719588	1.594894316560
Cl	-1.883493444773	-1.522324607894	-0.424818662966

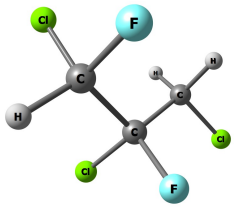
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
74.3154	0.00460
78.5136	0.443
141.7593	0.243
171.4927	0.111
226.3690	0.375
257.1844	0.0268
312.9602	0.172
380.5733	0.108
391.6886	0.314
485.6623	1.87
571.3279	5.22
645.7670	9.65
757.4317	24.4
816.2773	2.71
874.0834	0.522
979.1892	5.97
1114.0617	16.4
1146.0401	1.96
1172.0903	9.25
1244.2884	7.59
1287.9038	3.80
1320.9554	1.11
1363.5090	1.49
1464.2146	1.13
3106.6562	0.727
3124.3989	0.617
3177.5770	0.0280

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
58.7251	0.113
92.0079	0.190
146.0193	0.0478
195.5439	0.569
250.1732	0.151
265.7866	0.210
319.7106	0.381
364.8398	0.167
396.7385	0.537
431.1018	0.547
577.0489	3.08
701.3400	23.5
763.5705	5.41
795.2270	5.71
851.6915	5.68
986.7184	8.89
1124.5968	16.7
1140.9174	8.23
1168.4151	10.7
1231.3741	3.09
1281.3201	1.42
1312.4780	0.330
1379.3055	0.752
1464.7864	2.23
3107.5871	0.705
3140.6345	0.493
3175.5031	0.00958



$\Delta E = 1.40$ kcal mol^{-1}
Population = 0.045



$\Delta E = 1.53$ kcal mol^{-1}
Population = 0.036

Optimized Coordinates (Angstroms)

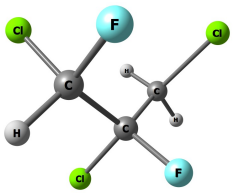
Atom	X	Y	Z
C	0.733703833531	-0.718308099018	-0.338271335979
C	-0.092838017321	0.273392921345	0.506622579142
C	-1.489759559791	-0.258622351697	0.844149097773
Cl	2.452178640398	-0.241841470045	-0.424772769503
F	0.642965247810	-1.935481864980	0.256654385104
H	0.352649113743	-0.776885176244	-1.356958690011
Cl	-0.192010975932	1.847646369791	-0.353184900654
F	0.522921340251	0.465444597149	1.699229120850
H	-1.370842901334	-1.168275761776	1.431365968235
H	-2.025643882820	0.496974836320	1.416174285901
Cl	-2.468879838534	-0.667051000844	-0.599346740858

Atom	X	Y	Z
C	1.394192543805	-0.266938712583	0.529215764574
C	-0.118486678196	0.050403349053	0.447687867755
C	-0.825530293265	-0.741427620821	-0.648098255529
Cl	2.264587275318	0.076706378651	-0.998628172208
H	1.857571625765	0.333143528966	1.313740893209
F	1.521417801380	-1.582304441290	0.822220137812
Cl	-0.330708302369	1.823845261781	0.247828302402
F	-0.613473360253	-0.298962439701	1.661259048306
H	-0.514290267772	-0.392829821753	-1.629927386980
H	-0.567078268139	-1.793889356208	-0.525433249618
Cl	-2.604795076273	-0.603800126094	-0.539437949722

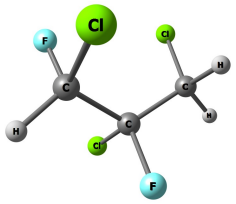
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
62.6769	0.115
85.1776	0.221
142.8850	0.0796
186.7879	0.335
231.3522	0.0952
292.3782	0.657
326.0625	0.232
362.2570	0.0650
413.7240	0.811
451.8293	0.491
517.5221	6.34
735.6529	9.54
765.5718	0.246
815.4015	15.2
877.2908	8.05
994.4235	14.4
1094.9597	14.8
1117.2066	2.56
1154.4216	15.0
1231.6954	1.85
1291.2738	1.11
1310.0875	2.05
1366.7718	0.532
1461.6297	1.13
3108.5367	0.766
3140.3607	0.564
3178.7527	0.0104

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
75.6365	0.0492
82.7372	0.315
140.4122	0.279
173.8397	0.0848
211.3767	0.289
300.9845	0.305
314.4073	0.0857
382.1341	0.0339
404.0207	0.773
437.4555	0.788
558.1267	6.87
665.6119	4.91
798.2871	12.0
818.1887	6.29
883.0710	7.80
990.6815	14.9
1090.1738	2.15
1131.8300	19.9
1158.6440	4.61
1231.2271	7.19
1284.4175	2.42
1319.4740	0.826
1363.3624	2.14
1463.4446	1.09
3105.3757	0.753
3119.9334	0.704
3181.3840	0.104



$\Delta E = 1.77$ kcal mol^{-1}
Population = 0.024



$\Delta E = 1.96$ kcal mol^{-1}
Population = 0.017

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	0.654564113573	-0.721373613206	0.725328663370
C	0.077602012889	0.644477681138	0.277124581502
C	-0.910252504796	0.671104739645	-0.884145875261
Cl	1.291330886981	-1.675026146187	-0.654118560960
H	1.488795549140	-0.553475494176	1.408839227842
F	-0.307119741947	-1.425249368887	1.351297090106
Cl	1.477373388155	1.691981514876	-0.209772961158
F	-0.484163500051	1.187002493531	1.381174242878
H	-1.180055516536	1.707869353515	-1.079117572519
H	-0.463432820002	0.225877535172	-1.769970590653
Cl	-2.428726867405	-0.217069695423	-0.518414245147

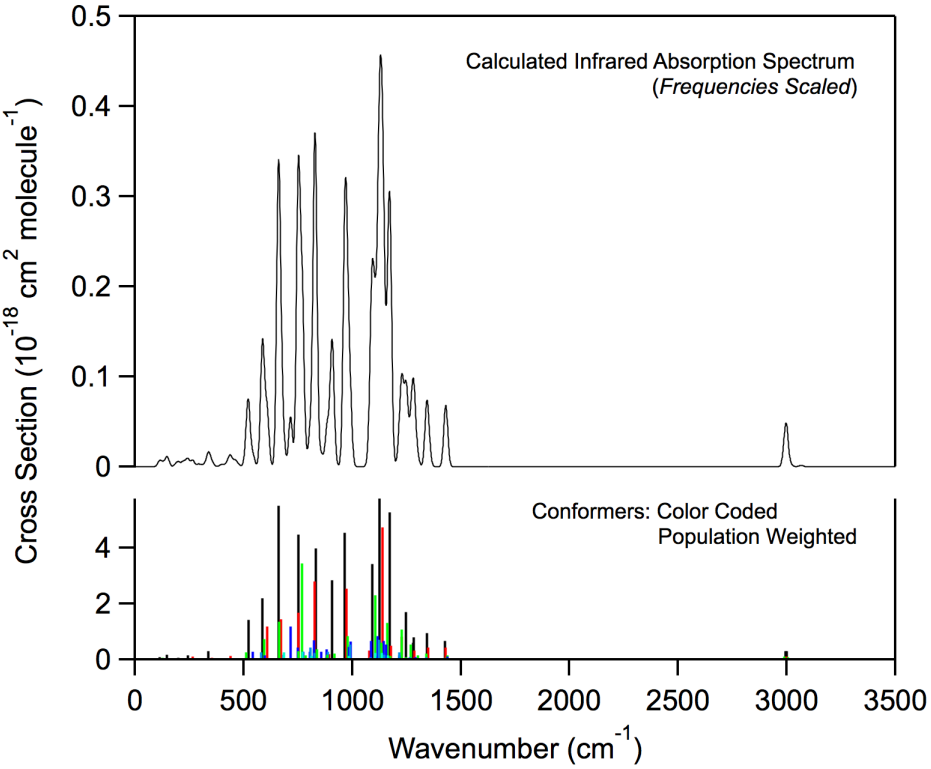
Atom	X	Y	Z
C	0.997489059626	0.351343272368	-0.641979700955
C	-0.137459125605	0.619421892551	0.370081200645
C	-0.737601708869	-0.572547589834	1.115580001507
Cl	2.347670242643	-0.539484993259	0.154190395655
F	0.562945958962	-0.351349634479	-1.698432714101
H	1.411762424544	1.307830014206	-0.966605140206
Cl	-1.410038880366	1.548848567279	-0.507958243025
F	0.387811125906	1.434543692466	1.324208954700
H	0.062233000263	-1.072240148645	1.661652574410
H	-1.479871148600	-0.189330247017	1.814819179175
Cl	-1.529861948502	-1.788839825636	0.073775492195

Infrared Absorption Spectrum (unscaled frequencies)

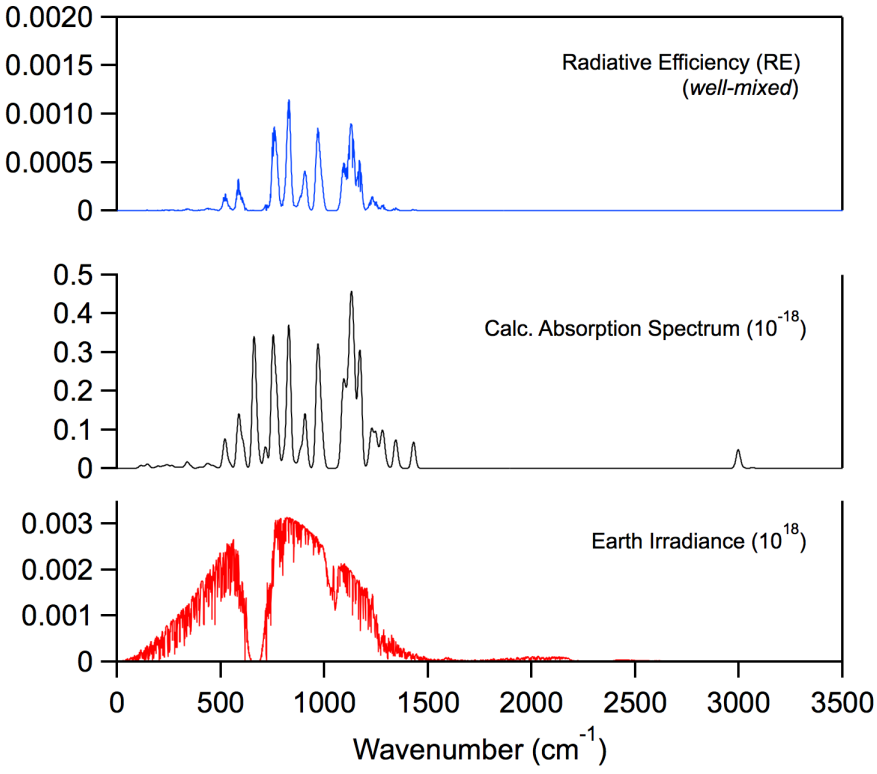
Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
50.1209	0.0475
114.8237	0.242
158.1359	0.106
173.1968	0.0157
252.2518	1.32
272.0257	0.265
308.4419	0.186
370.7113	0.0601
409.8681	0.578
427.2140	1.69
484.0777	3.00
739.5423	12.1
773.8122	6.58
828.9763	14.7
879.1412	7.14
916.0217	9.23
1093.6194	1.68
1143.4298	24.6
1188.8170	4.92
1264.5002	3.99
1290.4766	0.0600
1311.7090	1.95
1383.0894	1.93
1457.6132	2.38
3112.1609	0.706
3116.8755	0.871
3187.8251	0.0158

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
48.4782	0.0654
108.3349	0.165
150.1328	0.0412
181.6360	0.0955
252.3929	0.900
268.8704	0.531
329.8130	0.00286
373.2094	0.523
398.6194	1.07
425.4975	2.29
545.5570	0.0472
669.3522	14.4
760.3033	16.0
803.3160	7.14
877.2205	1.57
985.3239	7.40
1115.5476	13.5
1146.7566	14.1
1176.2532	8.44
1255.4281	2.54
1280.7634	1.22
1312.1147	1.67
1379.7718	0.709
1464.4504	2.03
3103.1541	0.764
3110.7607	1.01
3168.6155	0.0155

Infrared Spectrum

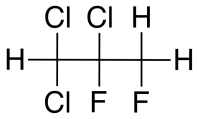


Radiative Efficiency



HCFC-242bb

Molecular Formula: $CHCl_2CClFCH_2F$
Name: 1,1,2-Trichloro-2,3-difluoropropane
CAS number: –
Molecular Weight: 183.41



Global Atmospheric Lifetime (years): 1.03
  Tropospheric Atmospheric Lifetime (years): 1.09
  Stratospheric Atmospheric Lifetime (years): 21.0
Ozone Depletion Potential (ODP): 0.021

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.178	0.133
Global Warming Potential (GWP_H):		
GWP_{20}	226	169
GWP_{100}	61	46
Global Temperature Potentials (GTP_H)		
GTP_{20}		55
GTP_{50}		8
GTP_{100}		6

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 5.39 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 3.44 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 1.06$ years
$\tau^{OH}_{Trop} = 1.09$ years
$\tau^{OH}_{Strat} = 36.4$ years

Fractional Atmospheric Loss: 0.979

O(^{1}D) Reactivity

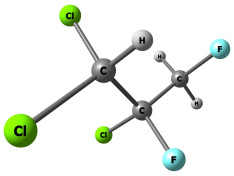
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 2.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)} = 185$ years
Fractional Atmospheric Loss: 0.006

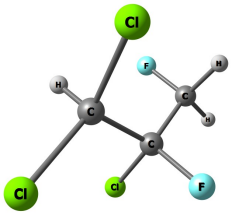
UV Photolysis

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

Molecular Structure and Infrared Spectrum (5 conformers)



E = 0
Population = 0.584



$\Delta E = 0.55$ kcal mol^{-1}
Population = 0.233

Optimized Coordinates (Angstroms)

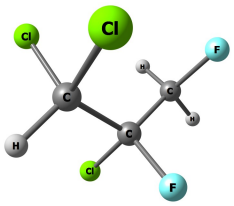
Atom	X	Y	Z
C	0.598780698756	-0.444934223589	0.466088287808
C	-0.665346076021	0.358902038741	0.092255458166
C	-1.896554633701	-0.528692237431	-0.098826817319
Cl	1.035288377067	-1.630535956223	-0.795975682419
Cl	1.964796917510	0.625001618169	0.863328042156
H	0.361587010113	-1.012915119183	1.363057399050
Cl	-0.453755763376	1.332798485196	-1.401119253132
F	-0.904524827259	1.199849396172	1.129965263978
H	-2.772508725019	0.119556803694	-0.195482743285
H	-1.787519287309	-1.155101669285	-0.986063975254
F	-2.033579690761	-1.322417136262	1.016393020251

Atom	X	Y	Z
C	0.683186388036	0.031338579279	0.463797618877
C	-0.592672563765	0.016022282340	-0.403769921623
C	-1.415171569533	1.304695137475	-0.294552421124
Cl	1.632971754999	-1.463130305568	0.280228866597
Cl	1.696869955845	1.455970995911	0.040824076634
H	0.408966287506	0.138236267526	1.509251497118
Cl	-1.626600273168	-1.362380713179	0.149188480166
F	-0.280297654908	-0.165485401898	-1.703211282017
H	-0.845205144934	2.129984452039	-0.730113298975
H	-2.353703755805	1.167191912682	-0.838918448021
F	-1.671392424274	1.569110793393	1.025113832368

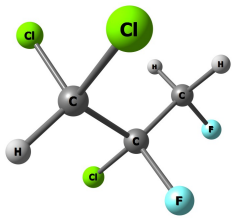
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
62.1774	0.101
109.3379	0.390
166.4128	0.0454
179.7960	0.203
200.1790	0.420
263.2515	0.335
330.1452	0.400
349.3985	0.110
381.5641	0.318
447.8151	0.638
543.6708	6.42
636.6521	6.14
799.8621	16.6
813.9781	5.05
943.1123	14.1
985.2987	10.7
1091.0348	6.81
1163.3437	2.69
1178.9803	10.4
1238.8046	2.11
1266.8991	1.18
1300.1092	2.12
1413.3631	0.778
1491.3692	1.13
3070.6281	1.49
3139.0297	1.24
3150.8131	0.433

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
53.5609	0.0764
89.9614	0.324
165.3189	0.0971
198.6731	0.461
213.7814	0.0240
257.5779	0.126
311.4503	0.787
332.4119	0.152
386.4290	0.312
475.1299	1.06
552.1610	6.28
693.1726	20.8
738.9994	1.29
779.1254	9.55
875.0885	4.17
1075.8409	6.11
1115.5616	16.8
1142.6214	0.0461
1193.6197	8.93
1226.0809	2.19
1262.9517	1.69
1295.4685	0.760
1417.4178	0.854
1501.0816	1.43
3065.2686	2.08
3124.5489	1.60
3171.8709	0.499



$\Delta E = 1.36$ kcal mol^{-1}
Population = 0.059



$\Delta E = 1.47$ kcal mol^{-1}
Population = 0.049

Optimized Coordinates (Angstroms)

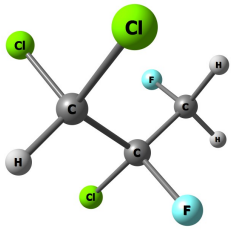
Atom	X	Y	Z
C	0.527764981495	0.548768097598	0.521098688040
C	-0.637978935990	-0.427394439581	0.225968818712
C	-0.669844814191	-1.115850103850	-1.138484109631
Cl	2.062509082322	-0.331125780684	0.776287392833
Cl	0.701823499182	1.784404129559	-0.758194769215
H	0.313159771150	1.075613972842	1.447525031802
Cl	-2.186091787191	0.508312501103	0.369943734558
F	-0.629444600716	-1.361789269882	1.203258002448
H	-1.560711463174	-1.751310298551	-1.167627798847
H	-0.720606258001	-0.367864945926	-1.933160544397
F	0.447456525114	-1.889649862628	-1.296790446303

Atom	X	Y	Z
C	0.922462877426	-0.192616669834	-0.451548126774
C	-0.553176221786	0.225565551020	-0.258185005875
C	-0.915839802611	0.733363676437	1.136986895700
Cl	1.992026780239	1.244368060013	-0.332255217696
Cl	1.431184362559	-1.456923908654	0.701386102856
H	1.047535938149	-0.593427746952	-1.454345916482
Cl	-1.593678391241	-1.189097621148	-0.688092922213
F	-0.810234635177	1.200180309660	-1.163394496151
H	-0.743141014136	-0.047838088100	1.880676656065
H	-0.293776226863	1.606949369562	1.360141213430
F	-2.230876666557	1.102625067996	1.141595817139

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
49.2370	0.0675
114.3255	0.312
169.5875	0.0382
179.2610	0.203
232.0236	0.00435
259.1497	1.40
316.2062	0.307
333.4005	0.240
376.5420	0.255
433.7311	2.12
470.9615	1.91
722.7059	9.64
775.8107	18.9
824.2197	9.65
887.7825	10.2
970.0662	5.21
1113.1485	8.02
1167.0318	12.1
1193.3882	1.21
1230.1429	1.25
1291.3746	1.47
1316.2404	1.85
1428.2193	0.845
1491.6112	0.998
3063.1906	1.69
3127.4312	1.36
3152.7150	0.430

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
68.2923	0.192
91.0728	0.374
160.8912	0.378
166.5130	0.0526
235.0455	0.0480
245.1482	0.285
305.9301	0.227
335.2224	0.287
382.2489	0.0462
425.3920	0.761
589.3580	4.30
656.7012	9.80
733.3243	14.5
794.5471	12.8
899.4759	8.59
1056.2659	4.98
1121.1321	10.8
1147.9540	3.89
1161.8180	9.93
1225.0797	1.80
1287.3244	2.17
1305.3127	0.890
1427.2580	0.286
1499.3788	0.456
3057.9900	1.89
3124.8555	1.25
3155.8467	0.425



$\Delta E = 1.50$ kcal mol^{-1}
Population = 0.046

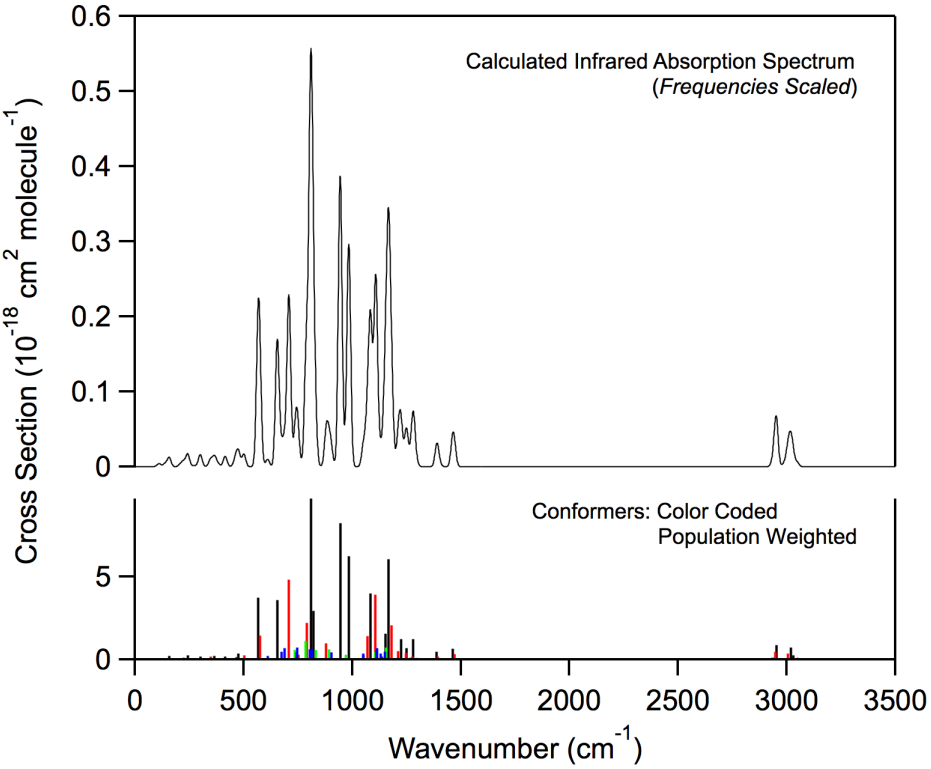
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	0.725676313162	-0.073530783215	-0.626670027261
C	-0.584747227455	0.572260786675	-0.118421703876
C	-0.781208574653	0.678486636925	1.397746143308
Cl	2.126695787042	0.945409281105	-0.146633678332
Cl	0.942894433709	-1.747550139006	-0.066633836357
H	0.711715322679	-0.085924193685	-1.713850599878
Cl	-1.969030392448	-0.312304400549	-0.860295810436
F	-0.601167079534	1.844461075632	-0.596913386310
H	0.125330041375	1.105366853380	1.840408319876
H	-1.625338318651	1.355880864878	1.563132515162
F	-1.041478305225	-0.534308982141	1.962981064104

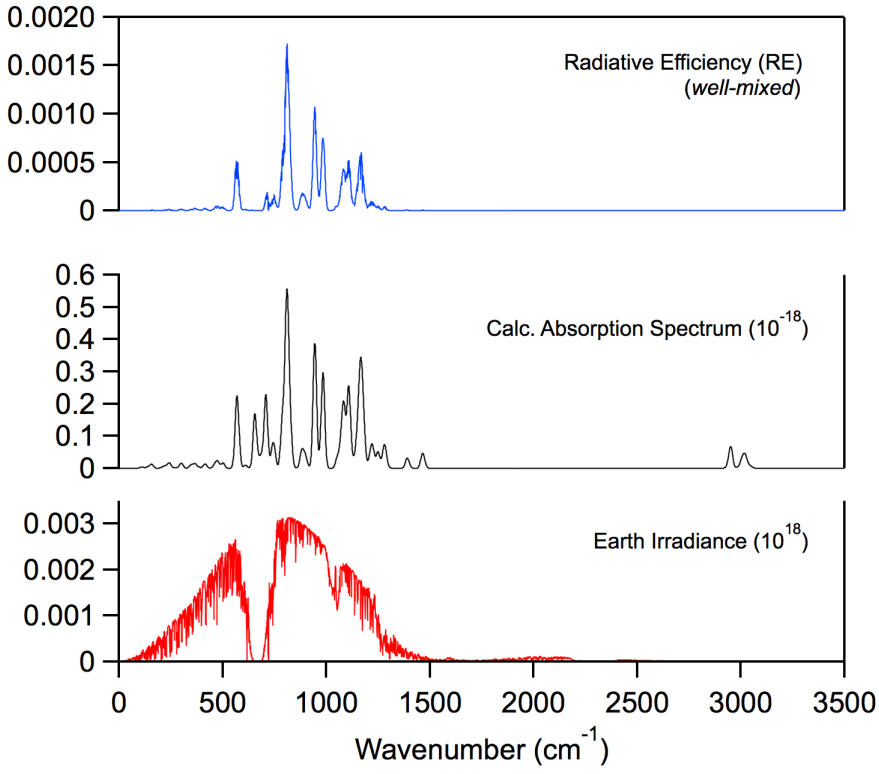
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
56.0524	0.119
111.6365	0.319
165.1216	0.0458
181.3552	0.152
226.9805	0.557
260.3091	0.873
307.8586	0.115
348.6863	0.244
382.4343	0.564
436.8928	2.81
530.2887	0.295
672.1295	14.8
730.6520	9.50
806.5129	14.1
893.7503	1.21
1057.2179	8.18
1121.8519	15.2
1141.5419	7.61
1195.0686	1.82
1224.9981	2.48
1280.0658	1.68
1302.2733	0.560
1425.4941	0.457
1499.9733	1.03
3049.7155	2.14
3106.4452	1.83
3152.1658	0.408

Infrared Spectrum

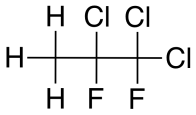


Radiative Efficiency



HCFC-242bc

Molecular Formula:	$CH_3CClFCCl_2F$
Name:	1,1,2-Trichloro-1,2-difluoropropane
CAS number:	7126-04-7
Molecular Weight:	183.41



Global Atmospheric Lifetime (years):	8.09
Tropospheric Atmospheric Lifetime (years):	10.0
Stratospheric Atmospheric Lifetime (years):	41.9
Ozone Depletion Potential (ODP):	0.125

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.258	0.244
Global Warming Potential (GWP_H):		
GWP_{20}	2347	2221
GWP_{100}	694	657
Global Temperature Potentials (GTP_H)		
GTP_{20}		1537
GTP_{50}		199
GTP_{100}		93

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 5.85 \times 10^{-15}$; $k_{SAR}(272\ K) \approx 3.73 \times 10^{-15}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 9.67$ years

$\tau^{OH}_{Trop} = 10.0$ years

$\tau^{OH}_{Strat} = 269.2$ years

Fractional Atmospheric Loss: 0.837

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: 0.044

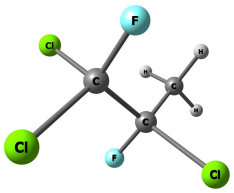
UV Photolysis

UV Spectrum: *No Recommendation*

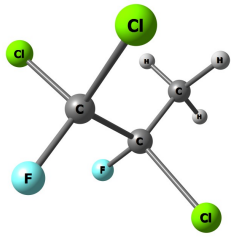
$\tau_{hv} = 68$ years

Fractional Atmospheric Loss: 0.119

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.510



$\Delta E = 0.30$ kcal mol^{-1}
Population = 0.306

Optimized Coordinates (Angstroms)

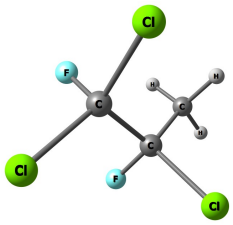
Atom	X	Y	Z
C	-1.002920072007	-1.923270277102	0.251947630744
C	-0.737484039124	-0.518637270486	-0.262192453510
C	0.560371554645	0.123251114145	0.325411651781
H	-1.043102783436	-1.925890399560	1.341602337177
H	-1.960979328425	-2.262209477905	-0.144449369666
H	-0.213131691434	-2.595355876377	-0.087436803588
Cl	-2.134951070601	0.543982049215	0.190839776135
F	-0.625429130461	-0.518021518931	-1.606915150632
F	0.454195032957	0.175751456760	1.656234985236
Cl	1.979108720737	-0.908462925239	-0.084480625748
Cl	0.845986807151	1.763460125480	-0.310086977930

Atom	X	Y	Z
C	-0.801950580084	-0.824020472704	1.688843727314
C	-0.733772064458	-0.547311590910	0.201738151051
C	0.568447090099	0.157595966952	-0.303052465666
H	-1.728020153936	-1.364647165630	1.891466957337
H	0.047159984964	-1.443525657712	1.985627008066
H	-0.795286222682	0.104075007491	2.259169857255
Cl	-2.143404128632	0.469931812720	-0.308998683885
F	-0.809842733276	-1.710310223013	-0.491904967637
F	0.475881359980	0.364652867751	-1.615207529694
Cl	0.843567885899	1.723552443127	0.513570477294
Cl	1.978114562127	-0.924620988072	-0.018510531434

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
68.3588	0.134
171.5463	0.0990
197.6840	0.141
217.8319	0.00178
251.8985	0.00870
282.9444	0.146
304.3209	0.288
327.3482	0.130
379.4772	0.0483
391.1355	0.130
437.2265	0.295
514.6509	2.96
582.6642	1.72
700.9288	24.2
823.0787	29.4
919.2720	3.39
989.0678	10.8
1105.0542	5.65
1146.2758	15.6
1201.7435	14.1
1228.8874	4.64
1408.6612	2.14
1478.2648	0.273
1484.5212	0.776
3073.5479	0.263
3157.8358	0.500
3165.9855	0.265

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
74.4130	0.0561
166.1012	0.0495
211.2421	0.181
222.7120	0.0107
237.5105	0.0683
284.6623	0.222
311.9177	0.182
331.1811	0.183
374.9764	0.0863
391.1295	0.0179
439.0917	0.649
472.8417	0.556
597.2245	2.12
709.0092	27.6
840.0414	25.5
929.2052	13.8
955.2558	4.83
1111.9626	9.90
1151.3712	18.1
1200.9298	6.01
1220.9373	6.98
1412.9993	3.37
1478.8439	0.406
1483.6442	0.702
3071.6261	0.226
3150.9402	0.514
3171.9655	0.270



$\Delta E = 0.60$ kcal mol^{-1}
Population = 0.185

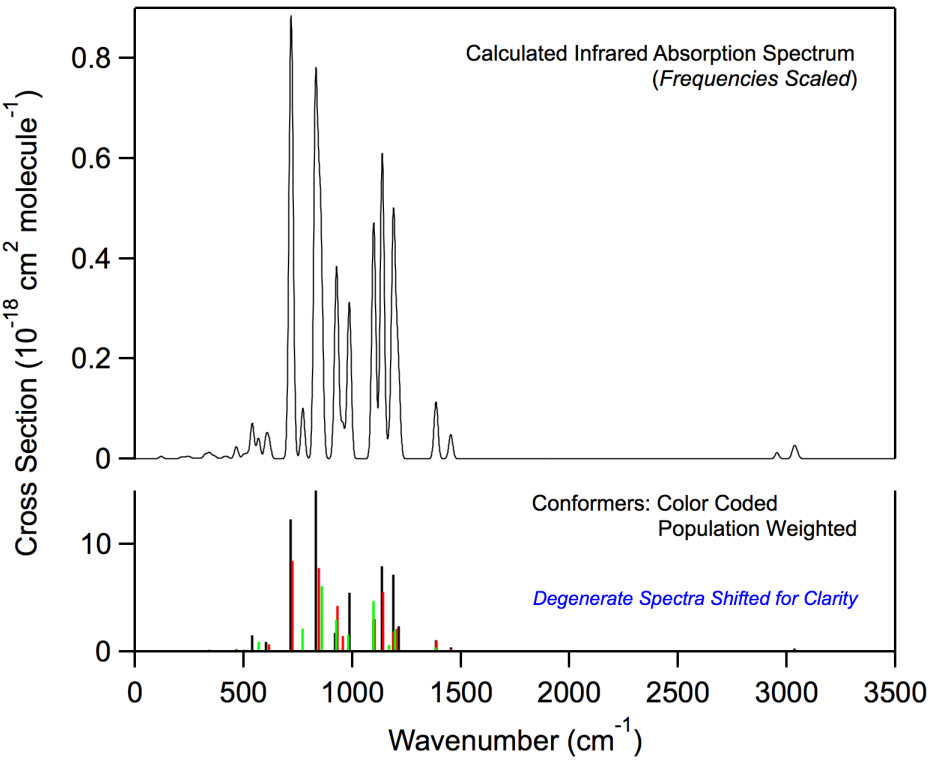
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.507611266830	-1.371303318023	-0.844447195044
C	-0.907837563175	-0.063227302948	-0.358195091757
C	0.656063441302	-0.094757902388	-0.298423045144
H	-2.583383129665	-1.230490100022	-0.960192600219
H	-1.069888160158	-1.626602496159	-1.811903293200
H	-1.322886189958	-2.176319840130	-0.134306791679
Cl	-1.592157032646	0.389891423306	1.243191849253
F	-1.215059447471	0.921033573295	-1.240831562682
F	1.079064833454	-0.429944736450	-1.529362145586
Cl	1.334228945922	1.505233360964	0.098644834847
Cl	1.256993569223	-1.327656661446	0.849033041211

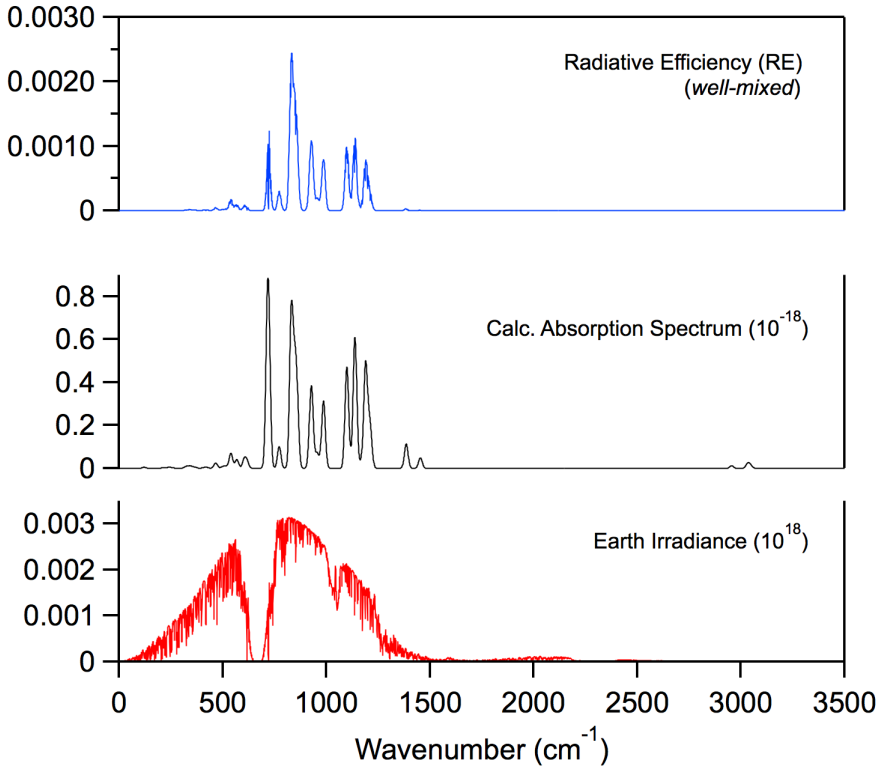
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
74.4176	0.104
168.6993	0.0541
185.5794	0.144
227.7706	0.00219
255.6022	0.0649
292.2503	0.320
308.4636	0.271
347.0782	0.0717
376.1510	0.105
394.9444	0.0787
434.1756	0.937
490.5394	0.985
544.8764	4.72
761.2764	11.6
852.3352	32.9
923.8044	16.2
981.2828	8.53
1104.7875	25.5
1118.9236	0.665
1180.8508	3.32
1210.5343	10.8
1407.6406	2.11
1478.8060	0.413
1484.6567	0.676
3071.4992	0.337
3152.6560	0.435
3172.8161	0.307

Infrared Spectrum

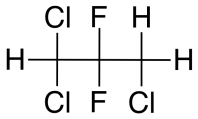


Radiative Efficiency



HCFC-242ca

Molecular Formula: $CHCl_2CF_2CH_2Cl$
Name: 1,1,3-Trichloro-2,2-difluoropropane
CAS number: –
Molecular Weight: 183.41



Global Atmospheric Lifetime (years): 1.09
  Tropospheric Atmospheric Lifetime (years): 1.15
  Stratospheric Atmospheric Lifetime (years): 21.6
Ozone Depletion Potential (ODP): 0.022

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.190	0.144
Global Warming Potential (GWP_H):		
GWP_{20}	255	193
GWP_{100}	69	52
Global Temperature Potentials (GTP_H)		
GTP_{20}		63
GTP_{50}		9
GTP_{100}		7

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 5.10 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 3.26 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

τ^{OH}_{Global} = 1.12 years
τ^{OH}_{Trop} = 1.15 years
τ^{OH}_{Strat} = 38.2 years

Fractional Atmospheric Loss: 0.978

O(^{1}D) Reactivity

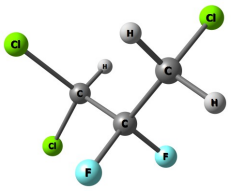
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 2.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)}$ = 185 years
Fractional Atmospheric Loss: 0.006

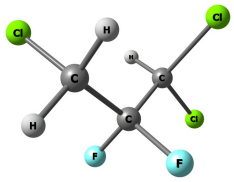
UV Photolysis

UV Spectrum: *No Recommendation*
τ_{hv} = 68 years
Fractional Atmospheric Loss: 0.016

Molecular Structure and Infrared Spectrum (5 conformers)



E = 0
Population = 0.363



E = 0
Population = 0.363

Optimized Coordinates (Angstroms)

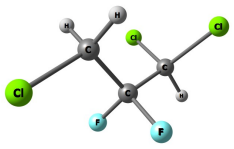
Atom	X	Y	Z
C	0.689680987210	0.230064610979	0.439615187273
C	-0.233358848109	-0.612472066592	-0.466443695277
C	-1.604178048171	-0.002978272371	-0.763561459984
Cl	2.218197349428	-0.636977414933	0.734420989878
Cl	0.985047930230	1.838988602850	-0.285234193516
H	0.211587013335	0.391434685565	1.401981925567
F	-0.400335473977	-1.813712225762	0.130571128797
F	0.365352578049	-0.823421410110	-1.660753830206
H	-1.494860329067	0.944531862665	-1.286024957194
H	-2.153986748994	-0.714876969704	-1.378978360786
Cl	-2.554960409934	0.285993597412	0.729936265448

Atom	X	Y	Z
C	0.688542608745	-0.209064232692	0.447303864760
C	-0.249032234086	0.574105642146	-0.496314286884
C	-1.608171623844	-0.073420990288	-0.765308501067
Cl	1.014074789285	-1.843687774545	-0.203326334387
Cl	2.200602381961	0.698510766132	0.702289350975
H	0.212645973173	-0.335111041967	1.416013711627
F	0.346729016696	0.741259847883	-1.699003330221
F	-0.438552377899	1.798085109952	0.045202869804
H	-2.170429037306	0.599393781082	-1.412621312150
H	-1.481023159069	-1.041640213976	-1.243930033684
Cl	-2.554775337654	-0.311293893726	0.739812001229

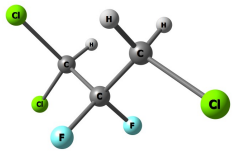
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
47.6695	0.109
85.5672	0.288
163.0429	0.209
195.0865	0.428
212.3435	0.0502
272.7016	0.310
334.8706	0.132
347.8090	0.0713
407.8930	0.945
552.1098	2.24
578.5648	5.63
733.7697	0.947
790.8590	12.7
792.8448	12.0
845.4676	3.16
902.7728	4.44
1073.6068	10.4
1150.0177	13.8
1199.7106	10.5
1232.4533	2.75
1256.3120	3.32
1310.3544	6.22
1323.4047	0.572
1462.3249	2.17
3111.0610	0.820
3164.4654	0.387
3185.1810	0.00832

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
47.6688	0.109
85.5674	0.288
163.0442	0.209
195.0859	0.428
212.3423	0.0502
272.7014	0.310
334.8693	0.132
347.8087	0.0712
407.8942	0.945
552.1076	2.24
578.5654	5.63
733.7692	0.946
790.8583	12.7
792.8452	12.0
845.4667	3.16
902.7730	4.44
1073.6066	10.4
1150.0162	13.8
1199.7102	10.5
1232.4532	2.75
1256.3149	3.32
1310.3532	6.22
1323.4048	0.572
1462.3253	2.17
3111.0620	0.820
3164.4639	0.387
3185.1825	0.00830



$\Delta E = 0.36$ kcal mol^{-1}
Population = 0.199



$\Delta E = 1.34$ kcal mol^{-1}
Population = 0.038

Optimized Coordinates (Angstroms)

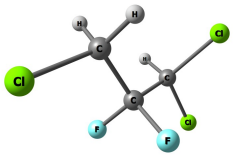
Atom	X	Y	Z
C	1.212771952648	0.001715840460	-0.428615177416
C	-0.334090302521	-0.008905721600	-0.528615758619
C	-1.071017592618	0.039672962363	0.804101608545
Cl	1.805694902062	1.511974229423	0.317705964882
Cl	1.818559526997	-1.440905953556	0.432369530340
H	1.609051522961	-0.035883541378	-1.441356385126
F	-0.666516281099	-1.127258039200	-1.212253571772
F	-0.675997174420	1.050089408653	-1.296864997138
H	-0.807970920336	-0.829087054033	1.404788075109
H	-0.815699364929	0.954656458584	1.335496216163
Cl	-2.843402268746	0.022115410283	0.549852495032

Atom	X	Y	Z
C	1.088065957284	0.096058745269	0.518616901659
C	-0.318192362345	-0.313311947940	0.013653343760
C	-1.412164394118	0.653862073008	0.469759913677
Cl	2.302505014771	-1.094444513238	-0.009549873519
Cl	1.516390416408	1.745712882191	-0.028455672746
H	1.097303690287	0.104693375447	1.606502913482
F	-0.562990808326	-1.544235399511	0.520652459637
F	-0.310316749367	-0.407579425141	-1.327722406420
H	-1.388876456235	0.759317186452	1.554879384355
H	-1.274554522594	1.623844197199	-0.002205486937
Cl	-3.032299785766	0.043396826263	0.014065523050

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
63.6001	0.170
72.0810	0.412
135.7845	0.243
187.8036	0.0527
206.6116	0.157
258.0293	0.137
324.5651	0.354
368.3634	0.105
430.4148	0.174
522.3490	3.67
573.4179	3.51
738.0156	3.05
797.2741	21.1
799.5345	6.95
841.8546	1.83
905.5173	2.72
1100.6740	10.9
1136.3895	12.7
1163.4167	6.91
1224.1880	4.31
1267.9434	4.93
1313.0056	1.34
1340.8504	4.44
1465.1737	1.74
3116.2867	0.965
3145.8063	0.441
3183.2527	0.001

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
59.9479	0.159
70.7239	0.430
123.5087	0.157
198.6576	0.122
232.3417	0.0443
245.4559	0.0934
307.3887	0.0599
342.8785	0.173
403.7448	0.239
532.3848	1.84
663.1018	13.2
730.0430	5.67
762.7716	5.74
821.4335	13.1
847.0487	2.20
906.6886	1.62
1069.7269	10.1
1119.1166	8.32
1218.2628	8.03
1235.5911	8.67
1246.7293	1.28
1322.2245	1.66
1326.2387	2.81
1462.2945	1.09
3103.5003	1.48
3143.7981	0.372
3180.6139	0.0632



$\Delta E = 1.34$ kcal mol^{-1}
Population = 0.038

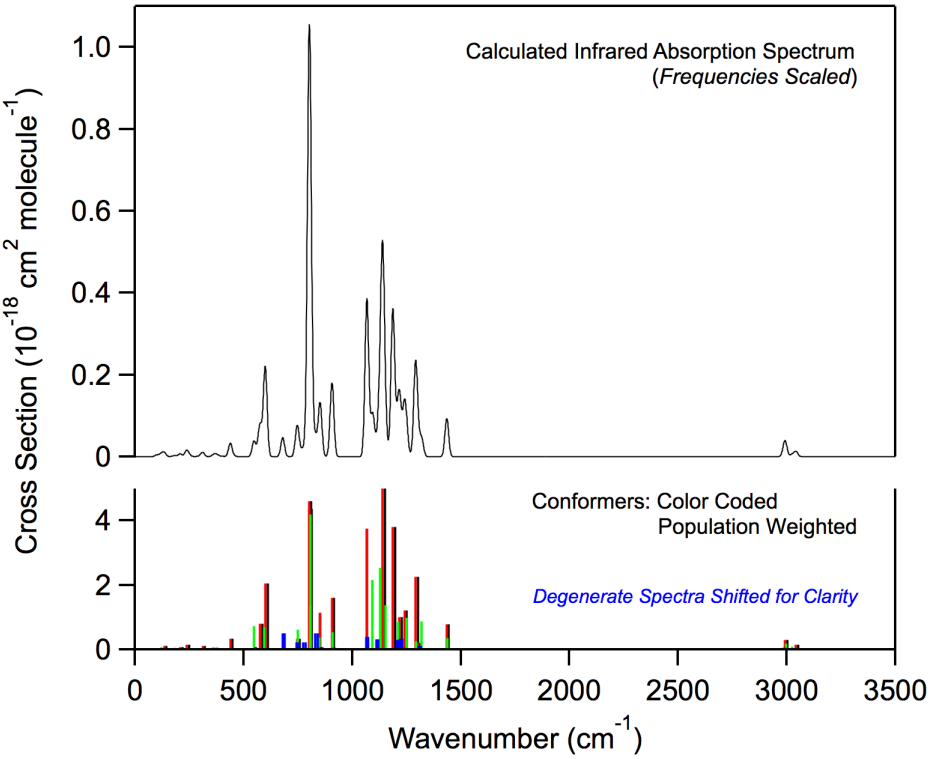
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.088045315591	-0.086485687400	0.524976554431
C	-0.317655666772	0.313869623681	0.011308003497
C	-1.416343755513	-0.627266217262	0.508681465564
Cl	1.501818946229	-1.758762439915	0.038775697631
Cl	2.308458731782	1.074198971218	-0.053402250403
H	1.102485852321	-0.054050268248	1.612356610707
F	-0.315598419387	0.357291816204	-1.332696375142
F	-0.551124361494	1.564856411053	0.472471185803
H	-1.288012591171	-1.615389331897	0.073139010937
H	-1.388560908339	-0.691786413378	1.596896788064
Cl	-3.034226143248	-0.022521464057	0.037613308911

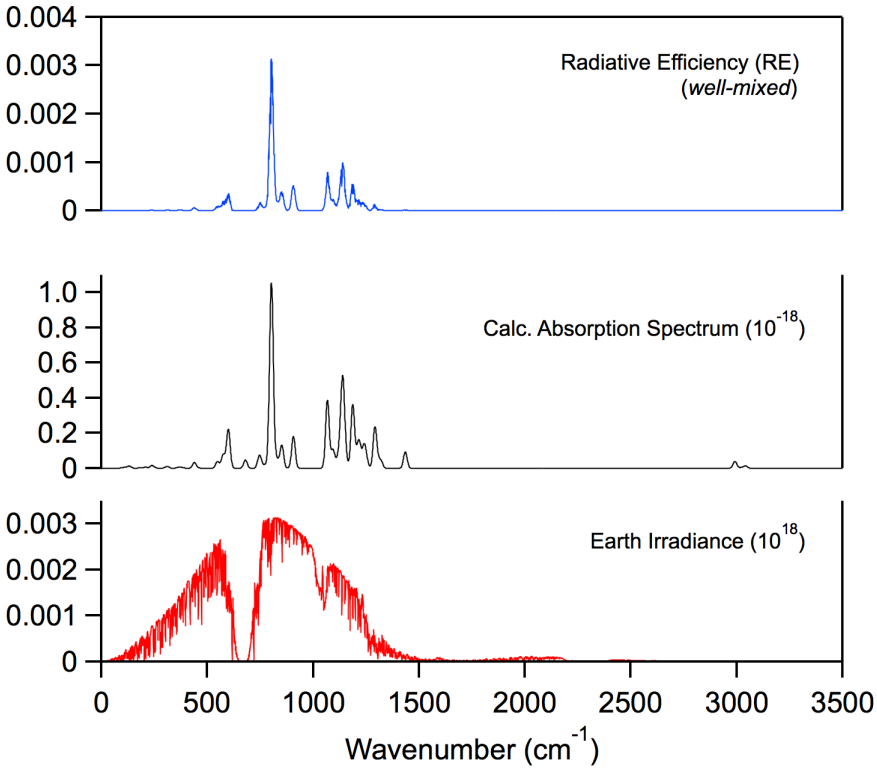
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
59.9485	0.159
70.7256	0.430
123.5093	0.157
198.6578	0.122
232.3417	0.0443
245.4559	0.0934
307.3888	0.0599
342.8784	0.173
403.7450	0.239
532.3855	1.84
663.1016	13.2
730.0428	5.67
762.7714	5.74
821.4334	13.1
847.0487	2.20
906.6885	1.62
1069.7266	10.1
1119.1160	8.31
1218.2623	8.03
1235.5911	8.67
1246.7288	1.28
1322.2240	1.66
1326.2385	2.81
1462.2941	1.09
3103.5002	1.48
3143.7976	0.372
3180.6132	0.0632

Infrared Spectrum

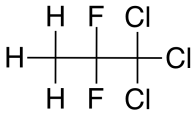


Radiative Efficiency



HCFC-242cb

Molecular Formula:	$CH_3CF_2CCl_3$
Name:	1,1,1-Trichloro-2,2-difluoropropane
CAS number:	1112-05-6
Molecular Weight:	183.41



Global Atmospheric Lifetime (years):	12.3
Tropospheric Atmospheric Lifetime (years):	18.7
Stratospheric Atmospheric Lifetime (years):	36.3
Ozone Depletion Potential (ODP):	0.206

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.261	0.251
Global Warming Potential (GWP_H):		
GWP_{20}	3168	3043
GWP_{100}	1069	1027
Global Temperature Potentials (GTP_H)		
GTP_{20}		2450
GTP_{50}		508
GTP_{100}		155

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 3.14 \times 10^{-15}$; $k_{SAR}(272\ K) \approx 2.00 \times 10^{-15}$ cm^3 $molecule^{-1}$ s^{-1}

τ^{OH}_{Global} = 18.0 years
τ^{OH}_{Trop} = 18.7 years
τ^{OH}_{Strat} = 471.3 years

Fractional Atmospheric Loss: 0.687

O(^{1}D) Reactivity

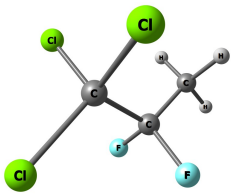
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 2.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)}$ = 185 years
Fractional Atmospheric Loss: 0.067

UV Photolysis

UV Spectrum: *No Recommendation*
τ_{hv} = 50 years
Fractional Atmospheric Loss: 0.246

Molecular Structure and Infrared Spectrum (1 conformer)



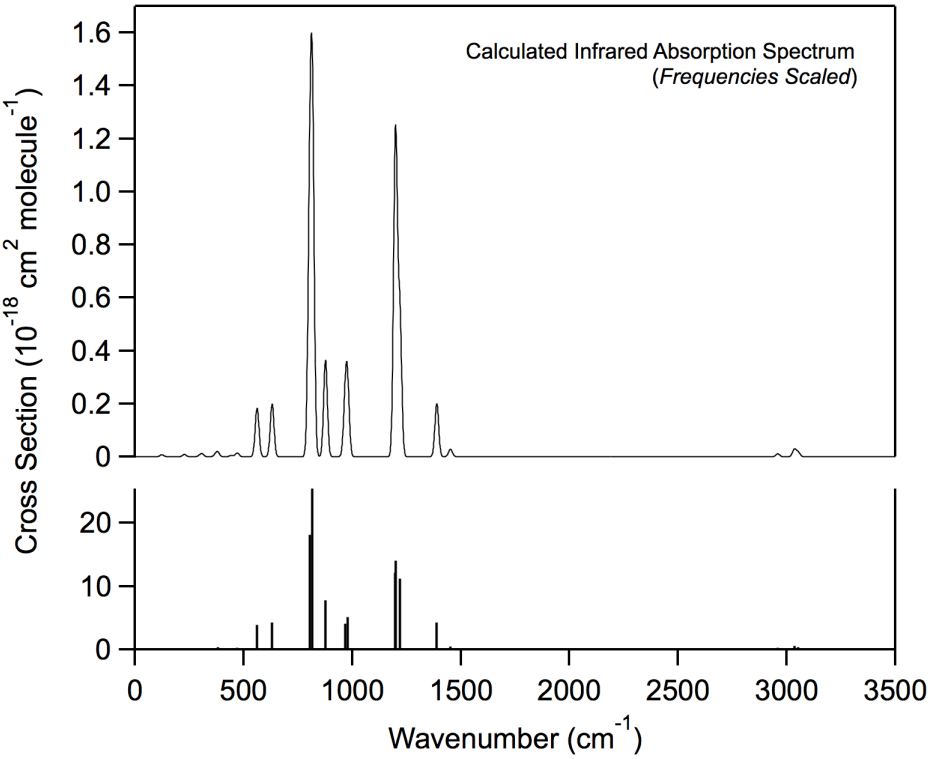
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	2.114153544077	0.887935414073	0.000000000000
C	0.604348846282	1.015641528864	0.000000000000
C	-0.203642229955	-0.332256209530	0.000000000000
H	2.522660445012	1.900978698152	0.000000000000
H	2.456859257277	0.362817229755	0.891221034157
H	2.456859257277	0.362817229755	-0.891221034157
F	0.203786751824	1.710586747479	-1.090036357535
F	0.203786751824	1.710586747479	1.090036357535
Cl	-1.949284716276	0.034061368872	0.000000000000
Cl	0.204755046294	-1.277095877679	-1.462819361153
Cl	0.204755046294	-1.277095877679	1.462819361153

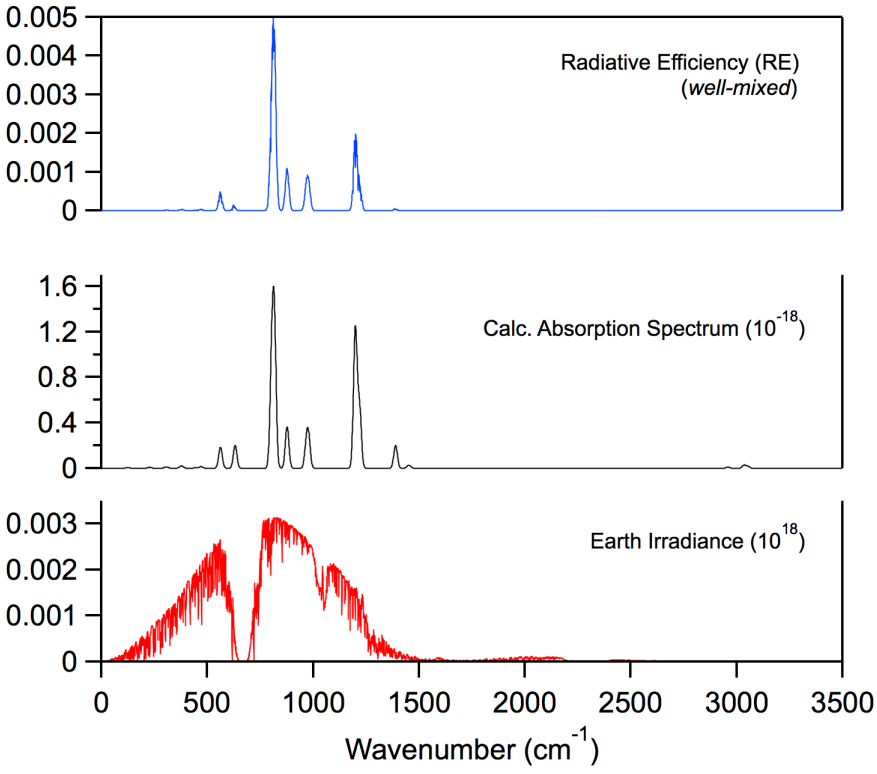
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
73.8924	0.167
179.7572	0.0208
184.0854	0.163
193.1651	0.000
256.7249	0.0636
266.9375	0.0115
269.5213	0.230
336.2594	0.133
345.9804	0.343
411.9234	0.0986
441.4453	0.304
538.2888	3.91
611.6655	4.24
794.9140	18.1
807.8961	25.5
871.6623	7.75
968.0906	4.06
979.0870	5.15
1211.3249	12.2
1213.9817	14.1
1234.0379	11.2
1414.0975	4.26
1479.5966	0.514
1486.0400	0.112
3075.9749	0.239
3156.8247	0.580
3175.5578	0.372

Infrared Spectrum

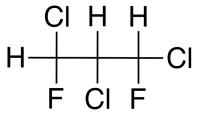


Radiative Efficiency



HCFC-242da

Molecular Formula: CHClFCHClCHClF
Name: 1,2,3-Trichloro-1,3-difluoropropane
CAS number: –
Molecular Weight: 183.41



Global Atmospheric Lifetime (years): 1.32
  Tropospheric Atmospheric Lifetime (years): 1.38
  Stratospheric Atmospheric Lifetime (years): 29.2
Ozone Depletion Potential (ODP): 0.024

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.187	0.147
Global Warming Potential (GWP_H):		
GWP_{20}	302	237
GWP_{100}	82	64
Global Temperature Potentials (GTP_H)		
GTP_{20}		80
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*

$k_{SAR}(298\ K) = 4.25 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 2.71 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

τ^{OH}_{Global} = 1.34 years
τ^{OH}_{Trop} = 1.38 years
τ^{OH}_{Strat} = 45.1 years

Fractional Atmospheric Loss: 0.984

O(^{1}D) Reactivity

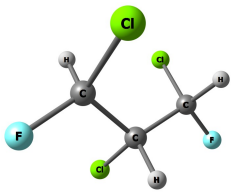
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 2.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)}$ = 185 years
Fractional Atmospheric Loss: 0.007

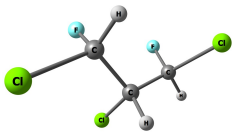
UV Photolysis

UV Spectrum: *No Recommendation*
τ_{hv} = 150 years
Fractional Atmospheric Loss: 0.009

Molecular Structure and Infrared Spectrum (10 conformers)



E = 0
Population = 0.211



$\Delta E = 0.06$ kcal mol^{-1}
Population = 0.190

Optimized Coordinates (Angstroms)

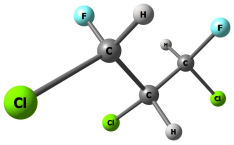
Atom	X	Y	Z
C	-1.246486816279	0.239341441128	0.387670039470
C	-0.015897199255	0.484677252065	-0.484555549871
C	0.936080720405	-0.707134337656	-0.605850891980
Cl	-2.182990334241	-1.171760143274	-0.258681727509
H	-0.987539428995	-0.004197792546	1.418149678619
F	-2.045862571818	1.322643877893	0.354615547119
Cl	0.847232186474	1.930729711643	0.144473367015
H	-0.348549044743	0.738264300806	-1.494197881794
H	0.421121587540	-1.561321125762	-1.047749657602
F	1.982460742257	-0.361561485701	-1.383526512016
Cl	1.547622158654	-1.272471698595	0.991703588550

Atom	X	Y	Z
C	-0.712971775232	-0.776190883873	0.274891228408
C	-0.009005647154	0.320318550064	-0.531915999874
C	1.466820758494	0.485810268207	-0.153676005342
Cl	-2.314812940445	-1.171569864009	-0.448481413482
H	-0.132229372695	-1.700332459566	0.238785853230
F	-0.883435023707	-0.401282604724	1.556212737511
Cl	-0.817431162955	1.910322644732	-0.296965677970
H	-0.070846137611	0.081273461034	-1.592523869744
H	1.913901013766	1.330267384028	-0.679582160106
F	1.619928124354	0.640528931318	1.173631186880
Cl	2.397700163186	-0.979325427210	-0.685264879510

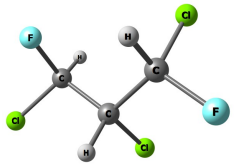
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
57.7609	0.138
83.1576	0.128
141.4439	0.117
176.5836	0.320
205.8462	0.210
282.1523	0.313
329.4297	0.166
388.1138	0.452
421.7762	2.10
469.3559	0.459
612.8108	6.82
671.0418	9.03
742.5451	19.8
826.9033	5.01
1038.1171	4.78
1072.9642	3.44
1123.5264	18.2
1156.0450	16.3
1213.1934	3.95
1253.3286	1.96
1296.9676	4.55
1306.4236	4.46
1369.4144	0.781
1397.4493	2.43
3097.1410	0.216
3118.6244	0.788
3133.4405	0.514

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
51.7803	0.230
81.1281	0.0556
154.4888	0.283
166.1792	0.147
202.9927	0.0747
261.6114	0.0871
294.0020	0.177
373.9950	0.595
391.7232	0.401
543.7217	7.54
641.6291	8.35
743.3456	20.5
788.9789	3.94
835.8484	6.68
931.7365	2.73
989.2341	2.46
1153.9126	13.1
1156.4075	19.2
1232.4937	5.02
1263.2790	0.947
1283.6357	2.20
1324.8547	6.12
1376.6794	2.57
1395.8142	2.10
3105.2981	0.662
3119.0966	0.917
3140.1092	0.334



$\Delta E = 0.11$ kcal mol^{-1}
Population = 0.176



$\Delta E = 0.38$ kcal mol^{-1}
Population = 0.111

Optimized Coordinates (Angstroms)

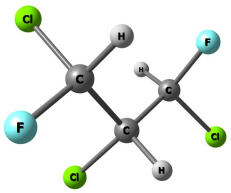
Atom	X	Y	Z
C	-1.213581748024	-0.743094600241	0.031241977777
C	0.016235510248	0.105542749083	-0.308567403222
C	1.277180167150	-0.583590454542	0.236538207610
Cl	-2.709261384464	-0.071022331964	-0.695342967056
H	-1.096148504806	-1.744914113767	-0.384410901625
F	-1.358860416554	-0.832424200642	1.373687664799
Cl	-0.110942385228	1.746249321586	0.393889968904
H	0.092039667659	0.207786919483	-1.391425503658
H	1.325577810150	-0.538351873180	1.324919442669
F	1.258090119342	-1.885263753194	-0.161961694030
Cl	2.769610164527	0.180895337376	-0.394718792169

Atom	X	Y	Z
C	-1.053608464792	-0.659140213722	0.133451739623
C	-0.039451658434	0.285949690333	-0.516828377123
C	1.338331440595	-0.370317980783	-0.664539789678
Cl	-2.730385441008	-0.053458978522	-0.061667913533
F	-0.956646258033	-1.869397018043	-0.481795610866
H	-0.877498570427	-0.778515329046	1.202433107844
Cl	0.061244081445	1.821630386292	0.393448980801
H	-0.375959893726	0.536616064440	-1.525844742996
H	1.250316660224	-1.283734392765	-1.254914052929
F	2.179698069014	0.485806232830	-1.278295112247
Cl	2.047202035142	-0.868749461014	0.914079771105

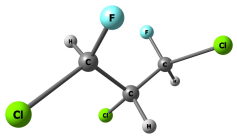
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
59.0401	0.103
69.0709	0.204
137.5735	0.252
179.4031	0.0500
209.6195	0.388
238.5555	0.0320
344.6377	0.0801
389.8310	0.633
413.2370	1.44
460.1313	1.97
632.8617	7.96
712.0307	20.7
816.8871	4.28
853.1908	3.84
962.6175	6.06
1055.7055	9.48
1101.8931	14.7
1136.5342	14.9
1207.0353	3.17
1265.5356	1.03
1285.1869	1.17
1326.1874	7.27
1369.6207	0.868
1378.9441	3.72
3115.3673	0.425
3121.0663	0.430
3132.8601	0.658

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
62.1826	0.109
71.7397	0.156
138.5096	0.133
182.4206	0.299
189.8934	0.0693
266.4734	0.561
343.9589	0.0545
395.7466	1.05
431.9667	0.126
468.3172	1.94
600.2920	8.67
680.3080	6.23
781.4125	14.7
841.0821	9.73
1023.7924	7.31
1076.7347	11.1
1106.6864	7.54
1139.6973	17.6
1215.7905	2.37
1247.4019	2.82
1299.8164	9.54
1324.5273	1.86
1366.2243	1.46
1379.8473	2.63
3095.4094	0.342
3115.6263	0.713
3133.5867	0.583



$\Delta E = 0.38$ kcal mol^{-1}
Population = 0.111



$\Delta E = 0.75$ kcal mol^{-1}
Population = 0.059

Optimized Coordinates (Angstroms)

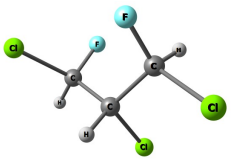
Atom	X	Y	Z
C	-1.328159810053	-0.384403180803	-0.661619058288
C	0.046874638011	0.277488287989	-0.513403087053
C	1.058509848636	-0.655372077975	0.158142516384
Cl	-2.047502621787	-0.861402740893	0.918883196955
F	-2.167043927177	0.460452862453	-1.294100465553
H	-1.233525280736	-1.306166299526	-1.237827853839
Cl	-0.064334045636	1.826105440263	0.373435046525
H	0.390236904762	0.514185729217	-1.523481903067
H	0.874775194931	-0.759527627520	1.227431544569
F	0.969094467089	-1.874762283319	-0.439976126097
Cl	2.735201631960	-0.048318109887	-0.033445810537

Atom	X	Y	Z
C	-0.791479751491	-0.610911847798	0.474793729671
C	-0.074632415815	0.376238141127	-0.459138166892
C	1.403362206060	0.578787166401	-0.091468176449
Cl	-2.443395397703	-0.979524192791	-0.133930232990
F	-0.091445017696	-1.764672335327	0.539669063878
H	-0.908536919968	-0.196452592811	1.476251107181
Cl	-0.887658841995	1.982571861217	-0.328758673272
H	-0.158640977129	0.055838469814	-1.496288464449
H	1.787462595424	1.497055277930	-0.535979428668
F	1.543899631071	0.637979049113	1.253130180590
Cl	2.432193889240	-0.749282996875	-0.743704938600

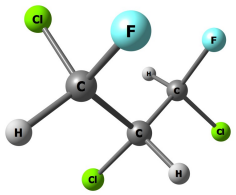
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
62.1810	0.109
71.7397	0.156
138.5092	0.133
182.4188	0.299
189.8910	0.0693
266.4702	0.561
343.9560	0.0545
395.7457	1.05
431.9634	0.126
468.3125	1.94
600.2907	8.67
680.3076	6.23
781.4098	14.7
841.0819	9.73
1023.7929	7.31
1076.7264	11.1
1106.6735	7.55
1139.6957	17.6
1215.7903	2.37
1247.4017	2.82
1299.8167	9.54
1324.5259	1.86
1366.2259	1.46
1379.8452	2.63
3095.4201	0.342
3115.6201	0.713
3133.5880	0.583

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
49.4649	0.0732
72.0015	0.100
147.1910	0.0144
176.0998	0.205
216.8883	0.424
253.0921	0.0734
349.7709	0.0720
367.4899	3.29
391.2506	0.305
443.7439	0.675
599.4519	7.95
750.9975	26.1
814.5549	3.90
834.6970	5.06
919.6326	2.81
1075.1793	11.7
1129.7108	14.0
1143.8839	14.6
1204.8613	1.51
1254.1148	1.38
1286.6932	4.26
1323.3884	6.08
1367.7316	1.11
1401.3912	0.954
3122.0508	0.792
3125.7802	0.583
3145.4575	0.282



$\Delta E = 0.75$ kcal mol^{-1}
Population = 0.059



$\Delta E = 1.06$ kcal mol^{-1}
Population = 0.035

Optimized Coordinates (Angstroms)

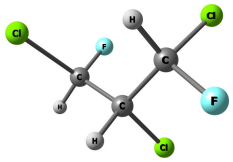
Atom	X	Y	Z
C	-1.403697557538	0.578429381736	-0.119110122256
C	0.076853880005	0.372445330263	-0.474379676865
C	0.783400308175	-0.616797936854	0.465171435815
Cl	-2.430189758973	-0.746908688354	-0.780526843158
F	-1.555434391687	0.637453794509	1.224277594118
H	-1.781818635462	1.497788959978	-0.566482814280
Cl	0.892635405316	1.976754935991	-0.336501234366
H	0.168836834017	0.052241316855	-1.510912807869
H	0.892976881135	-0.203020024356	1.467755956937
F	0.080065342910	-1.768892651054	0.523642530440
Cl	2.439515692102	-0.989147418716	-0.129709018514

Atom	X	Y	Z
C	-1.424497126188	-0.138010752005	-0.668528365272
C	0.066805853296	0.234961562901	-0.624334262482
C	0.882581790968	-0.564258252958	0.398706719612
Cl	-2.188791204508	-0.168629469243	0.963181527132
H	-1.980278254699	0.602561141622	-1.245786728152
F	-1.560159908883	-1.353125411250	-1.243002385812
Cl	0.224658282236	1.991078381478	-0.302385818619
H	0.463498202665	0.050554400582	-1.625109279382
H	0.670298323283	-0.254713305793	1.421973599831
F	0.600915519787	-1.878559753886	0.248758259075
Cl	2.645885522042	-0.320616541447	0.136899734069

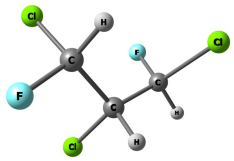
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
49.4647	0.0732
72.0026	0.100
147.1933	0.0144
176.1012	0.205
216.8879	0.424
253.0914	0.0734
349.7714	0.0720
367.4888	3.29
391.2510	0.305
443.7424	0.675
599.4506	7.95
750.9971	26.1
814.5549	3.90
834.6982	5.06
919.6313	2.81
1075.1786	11.7
1129.7085	14.0
1143.8831	14.6
1204.8597	1.51
1254.1127	1.38
1286.6907	4.26
1323.3863	6.08
1367.7308	1.11
1401.3896	0.954
3122.0504	0.792
3125.7841	0.583
3145.4647	0.282

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
57.6949	0.0858
76.4759	0.0383
142.0028	0.0920
181.0598	0.0421
202.1345	0.221
287.2314	0.513
358.3761	0.320
374.7182	2.15
428.9843	0.540
444.3539	0.507
545.3767	9.57
695.8015	5.09
819.9007	16.3
856.7912	7.70
971.8761	4.86
1095.0383	9.26
1121.6191	10.2
1131.1394	21.7
1210.3206	0.951
1241.6808	1.54
1287.7647	10.5
1339.0835	0.844
1365.1120	2.74
1394.0011	1.34
3102.4238	0.623
3112.5149	0.756
3132.6068	0.600



$\Delta E = 1.34$ kcal mol^{-1}
Population = 0.022



$\Delta E = 1.34$ kcal mol^{-1}
Population = 0.022

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.274469860553	0.649856507616	0.208277588228
C	0.054085749336	0.606591046374	-0.547847836531
C	0.739145565057	-0.759204977872	-0.658873640815
Cl	-2.486591978000	-0.412609744626	-0.628881412571
F	-1.154139135611	0.254171322247	1.485678692210
H	-1.693672219966	1.656632698948	0.176326606148
Cl	1.150517619757	1.846108700107	0.156335793096
H	-0.142808742667	0.926304447406	-1.573514547944
H	0.033607487228	-1.494387577799	-1.050767625609
F	1.781410222513	-0.639782969129	-1.514795868950
Cl	1.336395292908	-1.416430453271	0.896057252738

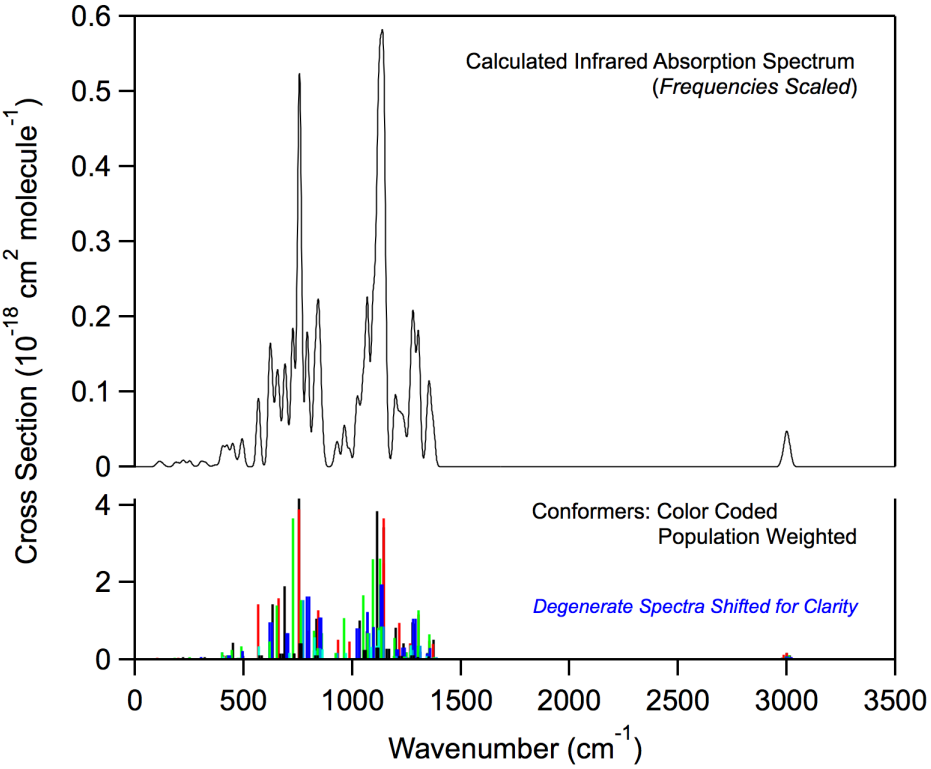
Atom	X	Y	Z
C	-0.746169890781	-0.732297291932	-0.685118621873
C	-0.041083539552	0.617188832678	-0.515494647620
C	1.277643865983	0.611275607865	0.258832063008
Cl	-1.374740908109	-1.435626190809	0.836949156745
F	-1.774742470749	-0.564884557929	-1.549520816196
H	-0.047156019498	-1.464223992474	-1.094412434257
Cl	-1.127131738582	1.848118814652	0.219182785973
H	0.174714734300	0.970621344665	-1.526183807791
H	1.713161678179	1.611560175601	0.269061167914
F	1.133785776643	0.171536622165	1.519282306580
Cl	2.483966512167	-0.439801364482	-0.600780152484

Infrared Absorption Spectrum (unscaled frequencies)

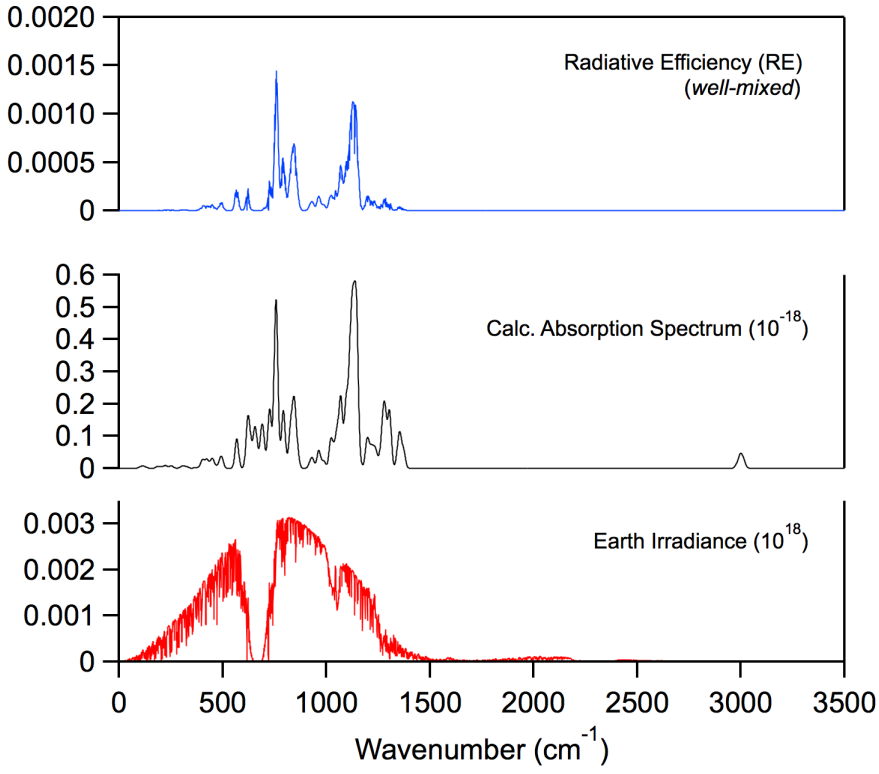
Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
43.2022	0.184
95.1429	0.0293
152.1374	0.418
171.4163	0.0451
183.5802	0.104
282.2707	0.214
293.7247	0.267
384.3506	0.687
391.3073	0.474
549.5280	4.86
653.1836	7.24
719.8177	7.21
744.3049	19.0
822.9129	4.94
936.2298	0.660
1057.6676	11.3
1118.9036	14.3
1170.9668	13.0
1232.2969	4.61
1275.7859	2.44
1290.3501	4.81
1321.3801	2.96
1375.8873	3.62
1404.5442	0.339
3100.4350	0.399
3109.1996	1.04
3115.5645	0.683

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
43.2030	0.184
95.1435	0.0293
152.1380	0.418
171.4165	0.0451
183.5809	0.104
282.2704	0.214
293.7241	0.267
384.3507	0.687
391.3076	0.474
549.5286	4.86
653.1846	7.24
719.8165	7.21
744.3048	19.0
822.9126	4.94
936.2298	0.660
1057.6674	11.3
1118.9037	14.3
1170.9660	13.0
1232.2961	4.61
1275.7848	2.44
1290.3488	4.81
1321.3784	2.96
1375.8856	3.62
1404.5424	0.339
3100.4359	0.399
3109.1991	1.04
3115.5654	0.683

Infrared Spectrum

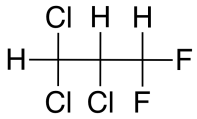


Radiative Efficiency



HCFC-242db

Molecular Formula:	$CHCl_2CHClCHF_2$
Name:	1,1,2-Trichloro-3,3-difluoropropane
CAS number:	1980063-50-0
Molecular Weight:	183.41



Global Atmospheric Lifetime (years): 0.729
- Tropospheric Atmospheric Lifetime (years): 0.761
- Stratospheric Atmospheric Lifetime (years): 20

Ozone Depletion Potential (ODP): 0.015

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.174	0.119
Global Warming Potential (GWP_H):		
GWP_{20}	155	106
GWP_{100}	42	29
Global Temperature Potentials (GTP_H)		
GTP_{20}		33
GTP_{50}		5
GTP_{100}		4

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 7.71 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 4.92 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 0.739$ years

$\tau^{OH}_{Trop} = 0.761$ years

$\tau^{OH}_{Strat} = 26.4$ years

Fractional Atmospheric Loss: 0.985

$O(^1D)$ 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: 0.004

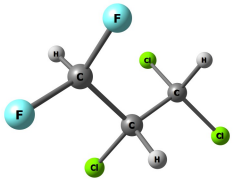
UV Photolysis

UV Spectrum: *No Recommendation*

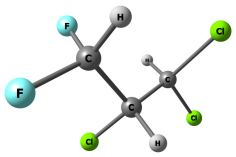
$\tau_{hv} = 68$ years

Fractional Atmospheric Loss: 0.011

Molecular Structure and Infrared Spectrum (6 conformers)



E = 0
Population = 0.444



$\Delta E = 0.34$ kcal mol^{-1}
Population = 0.252

Optimized Coordinates (Angstroms)

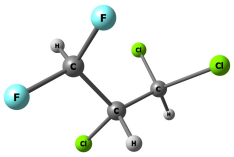
Atom	X	Y	Z
C	-0.810091745260	-0.500269236697	0.416947532105
C	0.445679796011	0.370104810113	0.364101366124
C	1.703006669551	-0.454050615451	0.052850856720
Cl	-2.216777815666	0.422105621577	1.022254867230
Cl	-1.175369415933	-1.280895866699	-1.154879778071
H	-0.638963222576	-1.308504912386	1.124219814715
H	0.581498710197	0.816504931663	1.351970089372
Cl	0.327947388399	1.718494770769	-0.806402843311
H	1.720348119681	-0.835926142684	-0.972075370070
F	2.794692934182	0.304133326252	0.268631797349
F	1.743229581413	-1.501683686456	0.919956667837

Atom	X	Y	Z
C	-0.909556406107	-0.105447210449	-0.333240596493
C	0.393870413383	0.170155730130	0.423120633984
C	1.473335232730	-0.882951978858	0.126242751829
Cl	-1.504722605058	-1.764971020063	0.055715743235
Cl	-2.175835400303	1.088271126315	0.064458782744
H	-0.752398601145	-0.074616849993	-1.408215542059
H	0.206192522698	0.194223316050	1.497461923443
Cl	1.026105138125	1.786585336523	-0.047219705967
H	1.169370184687	-1.874450465447	0.476008281920
F	1.700356896149	-0.942238150265	-1.206597053495
F	2.620759624840	-0.539603833942	0.743777780859

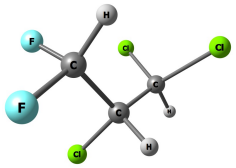
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
61.4585	0.102
78.1361	0.179
141.9696	0.164
166.6374	0.0212
188.5052	0.252
248.8017	0.185
332.6743	0.0590
381.6741	0.239
449.8729	4.28
554.4975	2.25
593.6377	2.41
672.4635	4.34
773.0949	15.7
830.3060	6.34
1033.7339	4.70
1074.5953	3.71
1114.0463	19.3
1148.8424	20.9
1229.6496	0.438
1234.0297	3.54
1282.7085	1.97
1296.5112	2.95
1389.3350	2.67
1413.8399	6.22
3091.5887	1.95
3105.2194	1.15
3151.0919	0.288

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
53.2300	0.0945
73.5470	0.264
153.2194	0.156
204.3287	0.0833
209.1054	0.468
245.9726	0.326
291.7903	0.295
336.4173	0.156
445.1760	1.17
536.8636	2.27
655.5213	10.4
720.8596	10.2
759.8707	11.5
804.4254	1.72
965.8151	2.79
1067.4246	0.124
1140.4668	19.0
1171.2304	17.5
1201.4683	1.72
1227.6991	3.27
1270.1396	3.90
1335.9642	1.19
1387.6692	7.06
1411.7696	2.59
3085.2982	2.75
3119.6944	0.511
3163.9486	0.251



$\Delta E = 0.81$ kcal mol^{-1}
Population = 0.113



$\Delta E = 0.97$ kcal mol^{-1}
Population = 0.086

Optimized Coordinates (Angstroms)

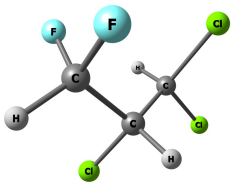
Atom	X	Y	Z
C	-0.914476943306	0.431812215054	0.463382135078
C	0.552109343953	-0.004447710017	0.554786851461
C	1.083174563160	-0.865544417079	-0.600426252639
Cl	-1.342587941897	1.093937583411	-1.148515316277
Cl	-2.011187658986	-0.913831218238	0.918413180689
H	-1.102050520074	1.229081924870	1.176933235891
H	0.687515275652	-0.557705579169	1.485555717923
Cl	1.588462527761	1.466714723915	0.674398059727
H	1.113706487698	-0.318019556575	-1.546968966410
F	2.328715689829	-1.281087968570	-0.285535884723
F	0.302236176211	-1.959180997601	-0.741616760721

Atom	X	Y	Z
C	-0.999180091475	0.276500385828	0.534792016810
C	0.466253164080	-0.152777170737	0.654046414485
C	1.005467790649	-1.030171360480	-0.483800152821
Cl	-1.388994280637	1.149309853085	-0.970709332460
Cl	-2.051423642968	-1.181256876424	0.719390782580
H	-1.256411122467	0.938885680842	1.356718595313
H	0.552781165973	-0.735334807905	1.573031370128
Cl	1.505577241590	1.295798979747	0.876146444826
H	0.297757020165	-1.832356171227	-0.725020338908
F	1.249254827712	-0.311798475527	-1.594739749541
F	2.170452927379	-1.584562037200	-0.075885050412

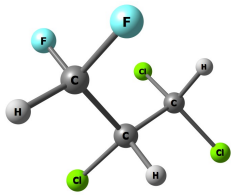
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
48.8155	0.0880
80.0912	0.0601
151.0227	0.0414
166.3650	0.0907
219.4461	0.341
238.2938	0.386
326.8001	0.163
374.3836	0.267
408.4599	3.50
535.9804	2.62
615.0860	1.45
689.5349	3.31
745.7626	21.0
829.3881	5.24
987.6995	4.53
1110.6393	1.38
1135.0065	19.0
1139.8726	21.8
1219.0364	1.43
1242.0147	4.47
1267.4470	0.567
1314.9508	0.638
1397.7751	1.63
1420.8098	5.68
3092.3745	2.48
3117.7904	0.473
3159.4427	0.239

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
53.7113	0.214
82.9927	0.0883
154.8160	0.212
162.3255	0.176
198.1919	0.0348
247.5283	0.301
288.4425	0.233
337.8944	0.0846
490.9322	2.73
629.7234	3.58
642.2857	5.40
680.0543	7.81
726.2881	13.5
810.6432	2.34
968.2236	1.83
1052.8391	7.26
1129.3762	18.6
1178.7923	14.3
1217.2099	1.35
1255.9815	6.24
1263.1240	0.0955
1339.0327	1.36
1398.8105	6.29
1411.9877	2.88
3063.1506	2.95
3109.5012	0.541
3158.6633	0.221



$\Delta E = 1.25$ kcal mol^{-1}
Population = 0.054



$\Delta E = 1.39$ kcal mol^{-1}
Population = 0.043

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-0.737732952247	-0.143667363676	-0.384428982888
C	0.388435768399	0.376241961107	0.516932364631
C	1.761511198185	-0.275177105267	0.251464372026
Cl	-0.934628989143	-1.916977228084	-0.197069165434
Cl	-2.290172921677	0.671945646817	-0.018599134176
H	-0.513048694841	0.042026396154	-1.430931574691
H	0.128715419536	0.245099095339	1.567453035847
Cl	0.601931108765	2.148369876861	0.235676807464
H	2.567349925130	0.354369370827	0.643086943034
F	1.831520776076	-1.484545473635	0.847369120843
F	1.944311361819	-0.443322176442	-1.078479786657

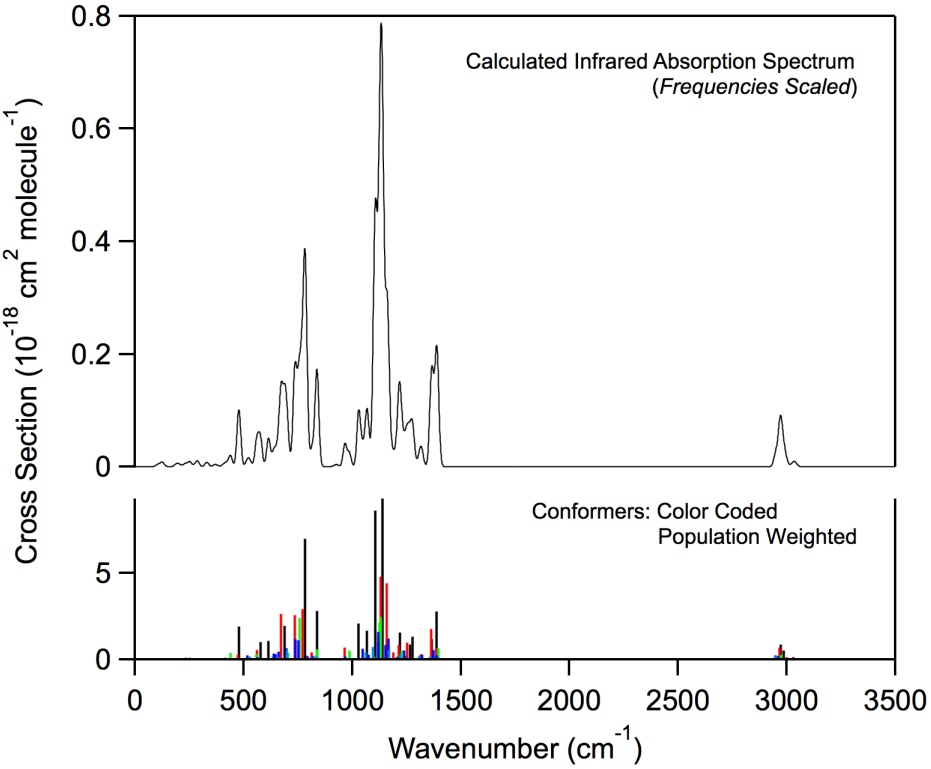
Atom	X	Y	Z
C	-0.654228041780	-0.522080577379	0.458063915254
C	0.347274900305	0.637530179931	0.441189774140
C	1.813303408644	0.178150305976	0.438686661395
Cl	-2.277047252598	0.063733418494	0.957263776202
Cl	-0.751527742476	-1.426629680575	-1.074838044958
H	-0.337432776458	-1.231157134656	1.220194164163
H	0.198723359804	1.192703377592	1.369786538927
Cl	0.088057833908	1.802096701337	-0.891972804202
H	2.488305272327	1.034928635153	0.545295327076
F	1.986395225088	-0.652179869102	1.503792041641
F	2.139005813236	-0.498249356772	-0.675095349639

Infrared Absorption Spectrum (unscaled frequencies)

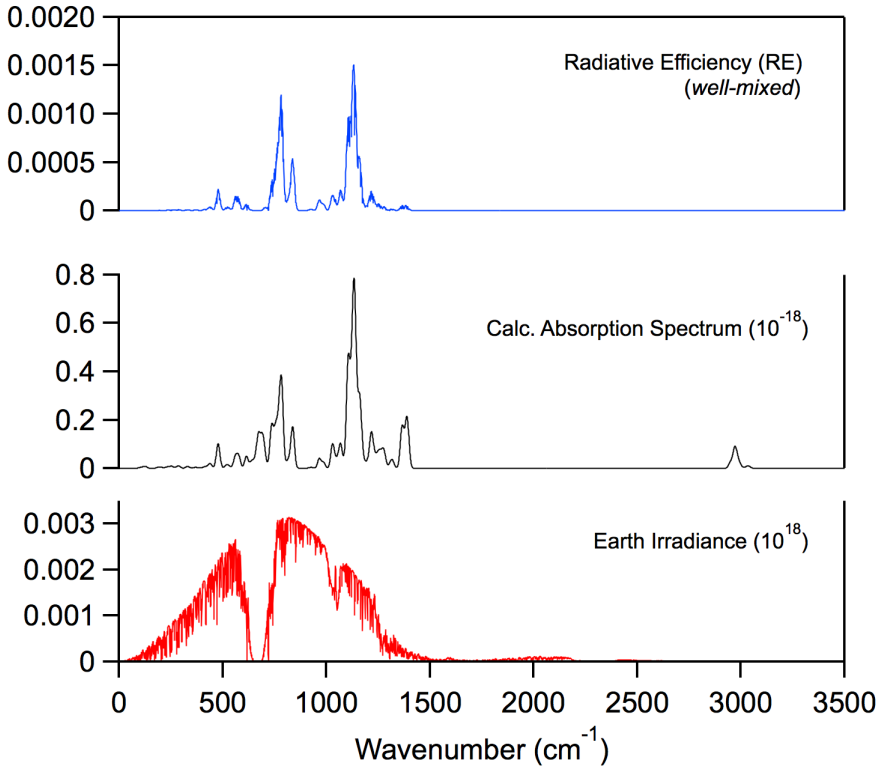
Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
45.5013	0.0662
76.1863	0.178
156.1663	0.0576
203.6116	0.141
211.7481	0.410
254.4192	0.175
297.2656	1.01
352.4699	0.398
395.4059	1.52
539.4506	2.31
620.1190	6.37
738.5770	20.4
784.4949	3.77
837.2035	0.843
914.2243	0.526
1082.2675	5.09
1128.0561	18.2
1165.5444	15.6
1203.9711	0.873
1223.5059	2.37
1256.6246	3.87
1342.6492	4.94
1395.3536	4.24
1414.5691	2.41
3076.8566	3.81
3129.0916	0.220
3167.5828	0.229

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
47.6210	0.157
92.2404	0.0607
152.1135	0.208
168.9609	0.0999
181.4807	0.103
250.1675	0.0170
291.2620	0.601
369.8377	0.102
502.8354	4.34
547.7312	1.87
643.3519	3.15
684.2617	13.4
815.0676	4.79
829.0368	4.03
926.2930	1.69
1067.9643	9.53
1103.3486	17.4
1182.2929	12.9
1228.3921	0.712
1237.4098	7.31
1294.6271	2.15
1328.8648	5.04
1381.0695	4.00
1423.0106	3.48
3067.9553	4.68
3102.2795	0.418
3144.4679	0.251

Infrared Spectrum

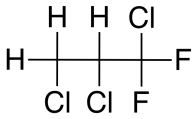


Radiative Efficiency



HCFC-242dc

Molecular Formula:	$CH_2ClCHClCClF_2$
Name:	1,2,3-Trichloro-1,1-difluoropropane
CAS number:	431-24-3
Molecular Weight:	183.41



Global Atmospheric Lifetime (years):	1.20
Tropospheric Atmospheric Lifetime (years):	1.25
Stratospheric Atmospheric Lifetime (years):	27.6
Ozone Depletion Potential (ODP):	0.023

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.221	0.170
Global Warming Potential (GWP_H):		
GWP_{20}	325	251
GWP_{100}	88	68
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) = 4.68×10^{-14}; k_{SAR}(272 K) ≈ 2.99×10^{-14} cm^3 $molecule^{-1}$ s^{-1}

τ^{OH}_{Global} = 1.22 years
τ^{OH}_{Trop} = 1.25 years
τ^{OH}_{Strat} = 41.4 years

Fractional Atmospheric Loss: 0.986

O(^{1}D) Reactivity

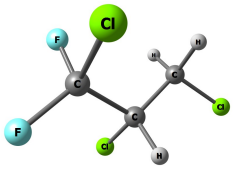
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 2.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)}$ = 185 years
Fractional Atmospheric Loss: 0.006

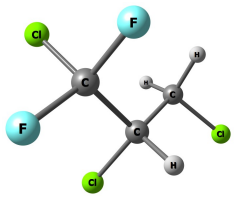
UV Photolysis

UV Spectrum: *No Recommendation*
τ_{hv} = 150 years
Fractional Atmospheric Loss: 0.008

Molecular Structure and Infrared Spectrum (7 conformers)



E = 0
Population = 0.405



$\Delta E = 0.45$ kcal mol^{-1}
Population = 0.188

Optimized Coordinates (Angstroms)

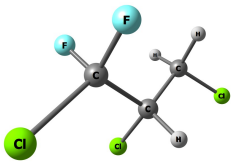
Atom	X	Y	Z
C	1.040240018291	-0.840283666694	0.450744659681
C	0.235974285093	0.173659217287	-0.355702580845
C	-1.250305189076	0.171367824481	0.044066720315
Cl	2.699348349000	-1.039604560005	-0.206200845617
H	1.129694185287	-0.525030326779	1.489195012931
H	0.562947261659	-1.818581066465	0.400571889872
H	0.300222109120	-0.032135787680	-1.423630661547
Cl	0.877284287062	1.840127765755	-0.109479397211
F	-1.395185905464	0.316175787139	1.362997063386
F	-1.918467038474	1.145360543044	-0.564507836675
Cl	-2.018468362496	-1.400064730083	-0.439175024290

Atom	X	Y	Z
C	1.130627905038	-0.889963594164	0.200237622863
C	0.263599958441	0.161942258693	-0.479757466393
C	-1.226677816475	-0.225249612794	-0.467486639480
Cl	2.865107480256	-0.685068614550	-0.221683636861
H	1.046307320360	-0.831637781892	1.283810782963
H	0.833971263422	-1.881676280000	-0.142428545553
H	0.529983843002	0.243891943908	-1.536122584150
Cl	0.494217070837	1.789492833978	0.231565197413
F	-1.957787920137	0.697753823583	-1.086144888560
F	-1.361052937477	-1.378639623309	-1.144767292578
Cl	-1.890410167269	-0.471052353453	1.185764450336

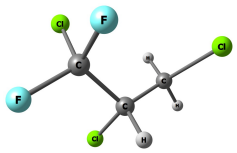
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
61.0213	0.0166
74.1360	0.410
162.6690	0.646
176.0022	0.132
252.0920	0.0663
263.3076	0.285
310.4706	0.0455
369.2690	0.356
414.6585	0.418
479.3876	0.821
593.6422	2.84
688.5624	9.80
755.3842	11.3
811.3058	10.9
913.4479	19.5
967.5480	8.26
1062.4266	0.848
1170.1415	6.64
1183.4748	12.5
1235.1307	18.2
1281.0479	3.82
1293.4397	6.59
1352.6812	5.39
1469.7311	0.938
3104.5700	0.908
3133.8137	0.328
3171.9809	0.0179

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
64.7684	0.00872
80.2260	0.435
142.7134	0.306
184.8839	0.274
219.0075	0.223
293.6437	0.125
318.3865	0.0506
405.6701	0.336
429.5370	0.680
462.8921	0.538
610.1489	7.02
647.2365	6.83
744.9927	6.45
773.0059	5.10
948.4278	5.23
1029.6614	32.1
1069.6488	0.963
1161.3871	19.8
1173.3061	5.45
1211.2456	13.6
1279.6830	6.00
1290.3191	5.64
1350.0033	4.51
1468.3459	0.769
3099.4177	1.04
3103.3869	0.365
3173.0360	0.0314



$\Delta E = 0.66$ kcal mol^{-1}
Population = 0.134



$\Delta E = 0.78$ kcal mol^{-1}
Population = 0.108

Optimized Coordinates (Angstroms)

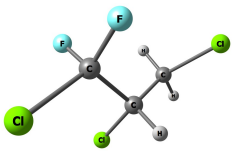
Atom	X	Y	Z
C	1.373851197206	-0.827503387982	0.237152558556
C	0.253218114200	0.063773719964	-0.298480893308
C	-1.112233259764	-0.536754016112	0.089409288925
Cl	2.965980317543	-0.380406580853	-0.460397578584
H	1.451220800944	-0.747198193119	1.320483789084
H	1.182714763989	-1.862348958767	-0.045345338087
H	0.296117389633	0.124106079676	-1.385795940543
Cl	0.400268220258	1.734698934893	0.332291327750
F	-1.172229869999	-1.792822116376	-0.388939137631
F	-1.248941085450	-0.600931846738	1.415654980168
Cl	-2.493806588558	0.374646365414	-0.596958056329

Atom	X	Y	Z
C	1.233646328939	0.944994611147	0.466660100288
C	0.038837453448	0.725339837907	-0.456262561237
C	-0.607716837958	-0.674589716265	-0.419276013213
Cl	2.695314231164	0.037258950492	-0.071814319682
H	1.500134092540	1.999883767318	0.453323245419
H	1.006804101919	0.636210969411	1.485991639829
H	0.320339266655	0.894249172438	-1.497838847793
Cl	-1.201601765388	1.967586528360	-0.050560141381
F	-1.690515823190	-0.693249326334	-1.197972410050
F	0.254308279021	-1.573568782925	-0.902271316328
Cl	-1.091617327150	-1.191950011548	1.236221624149

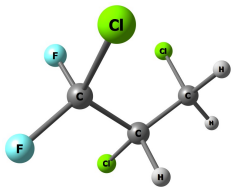
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
56.4735	0.0134
79.8749	0.497
144.0348	0.444
178.4816	0.115
250.7064	0.0959
264.1041	0.303
323.6995	0.0354
389.0777	0.830
423.0430	0.132
452.9589	1.77
599.7855	2.69
712.6012	13.5
726.2285	5.59
840.3519	0.404
944.6107	6.99
967.5870	23.3
1060.9298	7.82
1132.2860	21.9
1176.9767	2.38
1221.2451	18.4
1283.9598	5.15
1288.4482	1.70
1346.6762	4.64
1470.9348	0.750
3103.7542	0.756
3128.9806	0.328
3171.2327	0.0217

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
38.9347	0.0958
109.9910	0.316
164.0775	0.139
195.5418	0.292
221.4068	0.489
268.2835	0.0455
334.4682	0.0508
396.1659	0.945
416.4093	0.191
478.7126	1.19
556.3625	5.39
658.2308	2.94
737.8031	12.0
828.3913	4.75
874.6184	14.5
1035.8646	13.8
1084.1697	7.78
1172.1777	17.2
1185.2251	10.7
1206.4412	14.2
1231.8307	3.11
1314.9945	4.09
1364.2105	3.30
1475.3333	1.82
3105.3450	0.0960
3114.3357	0.700
3179.4533	0.00510



$\Delta E = 0.84$ kcal mol^{-1}
Population = 0.098



$\Delta E = 1.29$ kcal mol^{-1}
Population = 0.046

Optimized Coordinates (Angstroms)

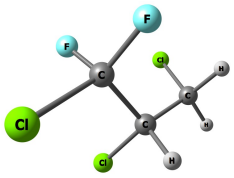
Atom	X	Y	Z
C	1.535058403587	0.832324052069	0.134671995333
C	0.132677758869	0.583242224168	-0.431600189202
C	-0.578963145031	-0.607270312480	0.240210631408
Cl	2.757530988587	-0.316410255363	-0.524614026460
H	1.863523674107	1.828983587110	-0.150635541751
H	1.539594831602	0.742192596678	1.220496582281
H	0.167211448371	0.410308394211	-1.506266588267
Cl	-0.831028555763	2.081760861669	-0.160813740807
F	0.158911974081	-1.711481679384	0.089612855379
F	-0.725452667770	-0.389789288566	1.550445660002
Cl	-2.195854710640	-0.926589180111	-0.478085637915

Atom	X	Y	Z
C	1.085839800202	-0.718565114049	-1.024311919204
C	0.191473773125	0.475940853530	-0.714976794363
C	-0.989083786677	0.236049936942	0.242633699392
Cl	1.948692385141	-1.411678971159	0.389646206992
H	0.486551862454	-1.519095378448	-1.457752027782
H	1.847229914810	-0.406489688207	-1.738136743187
H	-0.249066727091	0.806476973251	-1.658591000470
Cl	1.146412441710	1.873305361292	-0.096561285823
F	-0.605566573417	-0.077168227281	1.472634838362
F	-1.746953951227	1.332455074352	0.306120317049
Cl	-2.033842139031	-1.106346820223	-0.392748290965

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
42.6301	0.0975
101.9218	0.416
165.9551	0.184
176.0920	0.280
227.8227	0.0820
272.5283	0.0159
338.8863	0.0478
375.4285	2.77
414.6619	0.189
435.1315	1.90
581.4020	1.73
712.9803	8.46
741.8175	7.31
821.7686	3.45
936.2125	19.9
960.5500	15.3
1060.4922	7.30
1158.0378	20.7
1175.8696	6.74
1215.8198	7.63
1247.7442	9.10
1312.9797	3.57
1358.9890	1.61
1476.5530	0.976
3111.2400	0.491
3139.2631	0.287
3179.6773	0.0288

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
46.2998	0.100
95.9973	0.0440
157.5073	0.0420
188.0948	0.267
255.6051	0.269
272.4475	0.219
322.0753	0.128
383.8598	0.336
414.3777	0.472
509.6619	2.67
638.2187	2.54
670.9137	3.53
711.9596	13.2
813.2361	1.33
897.7963	29.2
977.1584	5.93
1038.4641	4.17
1162.3682	17.3
1195.5818	11.2
1244.1351	1.19
1272.2550	9.27
1316.1224	11.9
1361.3377	1.26
1463.5492	2.39
3095.0668	0.517
3105.2287	0.819
3162.9145	0.0780



$\Delta E = 1.74$ kcal mol^{-1}
Population = 0.021

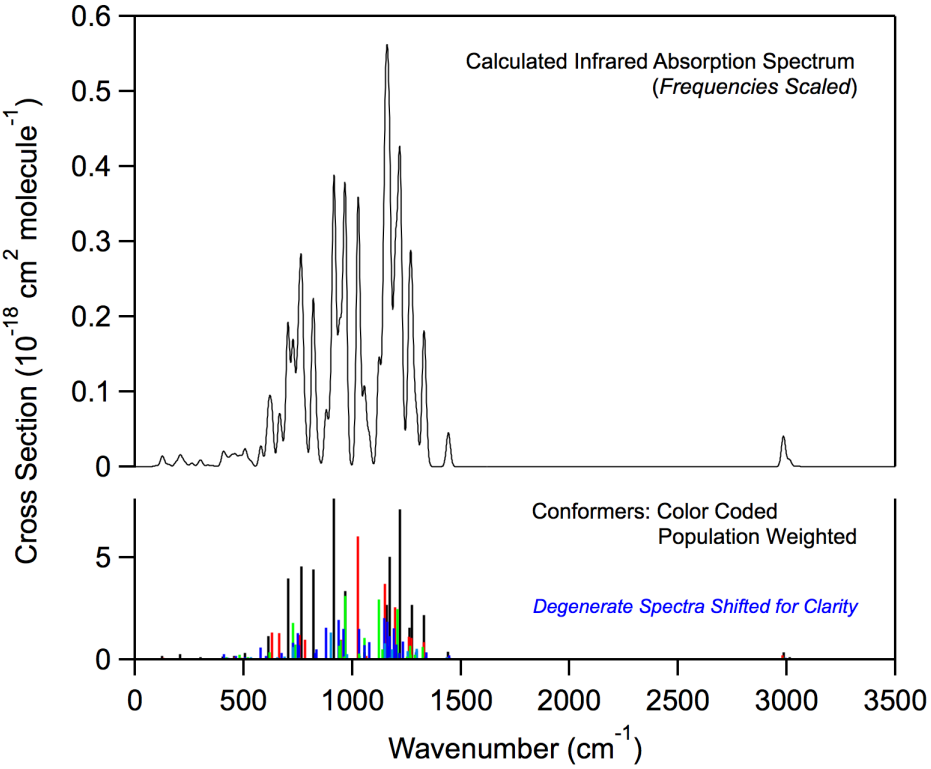
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.505882268264	-0.117677245926	-1.053351811996
C	0.121629177064	0.432331909358	-0.713605861079
C	-0.793515922345	-0.587553604776	-0.005558441049
Cl	2.514639873996	-0.570071479337	0.361628795521
H	1.391758323753	-1.013332708896	-1.664330579403
H	2.058529243149	0.638140685654	-1.609939991235
H	-0.360770720750	0.681111885177	-1.661453239060
Cl	0.212189715654	1.954848604999	0.224796600825
F	-0.701836542900	-1.759258205595	-0.657326809641
F	-0.451659022480	-0.789317661255	1.260099076152
Cl	-2.518856393404	-0.067620179402	-0.056206739036

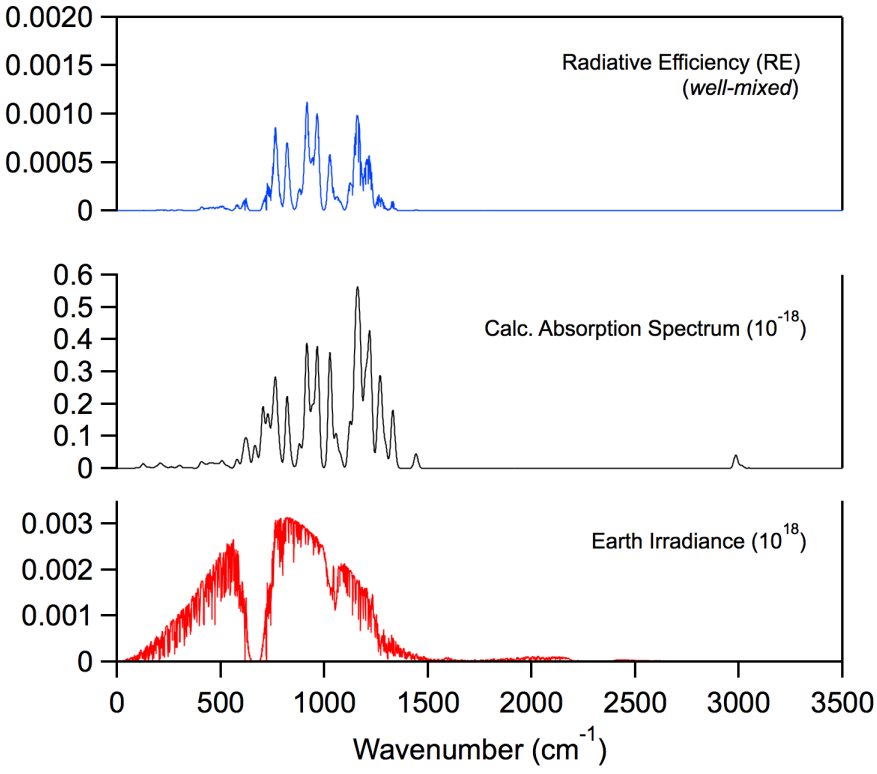
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
50.1859	0.0651
90.3959	0.108
148.2411	0.0472
186.7544	0.126
231.2739	0.0616
296.5763	0.733
325.0742	0.0230
414.3587	0.0562
425.0467	0.231
494.9192	6.04
594.1641	2.83
671.6365	2.72
745.4563	3.85
819.4337	1.77
938.6126	31.2
960.6269	6.81
1036.0520	13.5
1148.3088	23.2
1185.0828	4.78
1244.0739	2.64
1269.7413	7.27
1307.3568	10.8
1355.2988	2.19
1462.1845	1.35
3094.6144	0.682
3104.6839	0.834
3162.5463	0.0400

Infrared Spectrum

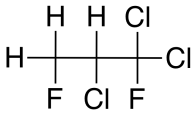


Radiative Efficiency



HCFC-242dd

Molecular Formula: $CH_2FCHClCCl_2F$
Name: 1,1,2-Trichloro-1,3-difluoropropane
CAS number: –
Molecular Weight: 183.41



Global Atmospheric Lifetime (years): 0.832
  Tropospheric Atmospheric Lifetime (years): 0.871
  Stratospheric Atmospheric Lifetime (years): 20
Ozone Depletion Potential (ODP): 0.017

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.224	0.159
Global Warming Potential (GWP_H):		
GWP_{20}	229	162
GWP_{100}	62	44
Global Temperature Potentials (GTP_H)		
GTP_{20}		52
GTP_{50}		8
GTP_{100}		6

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 6.73 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 4.30 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

τ^{OH}_{Global} = 0.846 years
τ^{OH}_{Trop} = 0.871 years
τ^{OH}_{Strat} = 29.8 years

Fractional Atmospheric Loss: 0.984

O(^{1}D) Reactivity

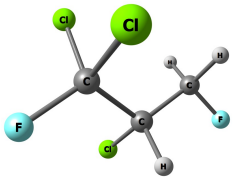
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 2.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)}$ = 185 years
Fractional Atmospheric Loss: 0.004

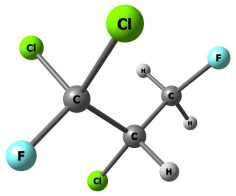
UV Photolysis

UV Spectrum: *No Recommendation*
τ_{hv} = 68 years
Fractional Atmospheric Loss: 0.012

Molecular Structure and Infrared Spectrum (9 conformers)



E = 0
Population = 0.263



$\Delta E = 0.35$ kcal mol^{-1}
Population = 0.147

Optimized Coordinates (Angstroms)

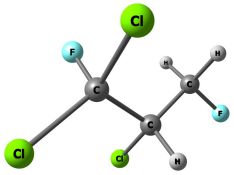
Atom	X	Y	Z
C	-1.199813887722	1.197177197135	0.631078543758
C	-0.678695185284	0.224383569754	-0.423118611770
C	0.798927092948	-0.170488962116	-0.264868727753
F	-2.442178613957	1.628444950961	0.243335714555
H	-1.273923205900	0.705921685223	1.605144489360
H	-0.529534383833	2.060291737066	0.703697707092
H	-0.776352608350	0.675815088895	-1.412396444144
Cl	-1.701972719908	-1.256889719981	-0.451612941823
F	1.131746761650	-1.083909269254	-1.177450245569
Cl	1.827005866667	1.287143737112	-0.564122597358
Cl	1.169121883691	-0.834383014796	1.358495113651

Atom	X	Y	Z
C	-0.739242337843	1.689863413225	0.496043767410
C	-0.683760490520	0.512457532500	-0.480941440548
C	0.425396772192	-0.534643334016	-0.252058750955
F	0.351777301655	2.505628154993	0.333526079793
H	-1.646400321497	2.263140451132	0.282822086984
H	-0.775661353243	1.327916682173	1.527840429740
H	-0.555517595076	0.876227705655	-1.502244240806
Cl	-2.289741774841	-0.304136035153	-0.421833026515
F	0.259878083687	-1.548992628646	-1.108227622972
Cl	2.030053592775	0.197655193582	-0.593056678226
Cl	0.413479122711	-1.203518135445	1.412893396094

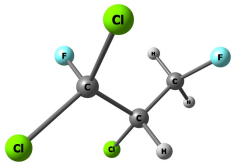
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
68.4535	0.0658
92.9969	0.538
158.8220	0.145
180.3825	0.306
242.2610	0.144
249.1109	0.415
304.6865	0.160
358.0694	0.0867
382.7289	0.187
448.0115	2.04
505.4083	0.197
651.1120	10.1
699.1402	13.8
803.7639	27.8
1004.4680	4.54
1054.5133	8.26
1086.6835	6.24
1116.1657	13.9
1180.8143	9.91
1247.0403	0.781
1289.5498	4.25
1305.7482	1.72
1428.9900	1.12
1504.7322	0.594
3053.8743	2.52
3104.4880	0.387
3118.8454	1.56

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
42.5101	0.104
123.8007	0.543
168.0779	0.0203
202.0333	0.251
227.0619	0.443
240.3042	0.157
305.8901	0.389
373.6007	0.0268
383.7236	0.0847
433.2131	1.57
509.7378	1.90
589.2700	5.98
771.5607	30.6
840.0676	12.8
920.5680	5.59
1083.4311	12.0
1087.7415	3.01
1122.3325	7.53
1163.4905	15.3
1223.5543	0.623
1271.4452	0.888
1353.5893	1.59
1427.5494	1.13
1507.1675	0.875
3058.8125	2.07
3104.9334	1.37
3120.1104	1.07



$\Delta E = 0.53$ kcal mol^{-1}
Population = 0.108



$\Delta E = 0.60$ kcal mol^{-1}
Population = 0.095

Optimized Coordinates (Angstroms)

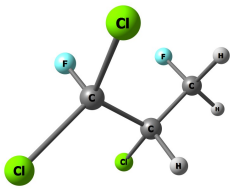
Atom	X	Y	Z
C	-1.547070731985	1.172387577381	0.177731472267
C	-0.680250065565	0.032591569103	-0.368506005259
C	0.747876461177	0.055259745590	0.203068874069
F	-2.774906609237	1.115923040689	-0.426372377004
H	-1.666435504621	1.068196556416	1.260471452609
H	-1.084685194776	2.136940270476	-0.051426100508
H	-0.623598075200	0.087304326348	-1.455332371823
Cl	-1.475524831995	-1.532831082195	0.033368703972
F	0.713382359808	0.008069818988	1.539838937701
Cl	1.745481757987	-1.302250242447	-0.394238358839
Cl	1.556531434409	1.602886419652	-0.276468227185

Atom	X	Y	Z
C	-1.602680775465	1.250103448413	0.027932775340
C	-0.797996630555	0.036229727414	-0.465312487593
C	0.556397880918	-0.149835685344	0.246662715683
F	-1.110507004461	2.408192366634	-0.517889692682
H	-2.640807157379	1.125707524981	-0.291258156537
H	-1.563726037668	1.310893817262	1.120255528032
H	-0.626656707289	0.105643512513	-1.538947627848
Cl	-1.821989152178	-1.419428865033	-0.168155637167
F	0.365808667906	-0.291002204905	1.564532775834
Cl	1.430557638934	-1.594334337708	-0.360343604676
Cl	1.595082277239	1.293685695773	-0.013216588386

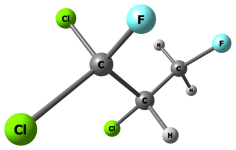
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
56.7466	0.0915
96.5992	0.713
159.6619	0.269
191.2880	0.216
234.3607	0.104
280.0984	0.324
294.6249	0.287
314.1659	0.174
379.7363	0.198
447.8644	0.986
475.7022	1.96
695.7744	12.4
756.7018	10.0
807.9740	28.6
962.0149	12.3
1003.0716	1.62
1091.9633	5.70
1119.6699	9.35
1183.5484	14.3
1244.4991	0.689
1289.9707	1.83
1309.3250	2.58
1425.3572	1.43
1508.4541	0.374
3056.8558	2.52
3111.9223	1.45
3135.4310	0.707

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
42.7990	0.0954
118.3004	0.815
164.7909	0.0325
204.2865	0.275
231.2521	0.0439
242.4652	0.0852
295.2239	0.256
368.7639	0.447
377.0934	0.148
429.9678	4.34
448.9775	0.817
678.8959	5.73
777.4544	29.3
843.0854	8.52
932.7041	8.90
1010.0672	5.10
1085.0838	5.67
1104.9799	17.4
1182.6372	10.1
1218.1938	1.64
1272.0530	1.10
1349.4315	0.740
1422.0708	1.52
1507.5281	0.624
3058.5450	2.13
3114.1852	2.09
3138.8335	0.152



$\Delta E = 0.61$ kcal mol^{-1}
Population = 0.095



$\Delta E = 0.63$ kcal mol^{-1}
Population = 0.091

Optimized Coordinates (Angstroms)

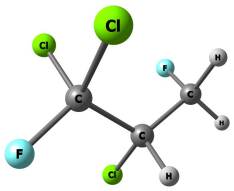
Atom	X	Y	Z
C	-1.515205384700	1.230897924627	-0.596360419401
C	-0.659123363236	-0.033600812900	-0.667197530501
C	0.627738291775	0.022674042585	0.182930012647
F	-1.909951292847	1.484393057673	0.688853548654
H	-0.944143337530	2.086055630926	-0.971920873438
H	-2.399765019472	1.081746281959	-1.224610275944
H	-0.368529225344	-0.210222626097	-1.703367747707
Cl	-1.653426655201	-1.444488570976	-0.146684133219
F	0.348125123231	0.155281288367	1.476094342410
Cl	1.625876556376	-1.452703538823	-0.040113760583
Cl	1.617418306949	1.449601322658	-0.329925162918

Atom	X	Y	Z
C	-2.053219027587	0.122627121628	-0.005181699571
C	-0.709436498809	-0.443570419234	-0.479518678991
C	0.502891589825	0.453292430229	-0.146850982285
F	-2.335126201430	1.281814363157	-0.683289430311
H	-2.830970763455	-0.617099516474	-0.218874433222
H	-2.030218625485	0.322417845308	1.070417639112
H	-0.720389210403	-0.545298926547	-1.566728344035
Cl	-0.530739898045	-2.087652875796	0.207834064676
F	0.292468750358	1.652027282511	-0.707070236620
Cl	0.719430343741	0.697660951566	1.617021411021
Cl	2.011294541288	-0.218115256347	-0.852265309774

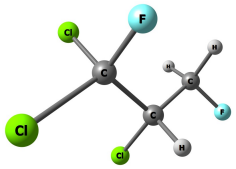
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
48.4141	0.133
102.4873	0.192
168.2104	0.0859
204.0925	0.215
237.1664	0.0384
259.3738	0.180
318.9213	0.385
335.0948	0.425
379.3318	0.231
434.8230	0.903
542.6906	6.63
687.9408	14.1
787.3505	10.8
821.3151	17.7
929.3816	6.25
973.8047	6.07
1049.1502	1.94
1132.7913	14.7
1204.6036	12.5
1241.9376	2.70
1285.4000	2.39
1329.6450	2.40
1426.4585	1.99
1501.3044	1.61
3049.6791	3.04
3101.0711	2.31
3123.0471	0.372

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
44.7697	0.0905
126.1358	0.480
168.8355	0.0471
192.4006	0.172
204.5731	0.255
261.4314	0.0818
342.6141	0.0141
366.9160	0.580
384.1465	0.252
440.4330	4.54
488.6533	0.693
557.0516	4.98
800.9042	30.5
851.9863	7.71
942.7622	5.85
1082.1615	15.6
1087.5471	2.01
1103.7937	9.91
1154.7897	18.6
1222.8539	0.817
1265.6166	0.628
1350.2469	0.711
1421.8087	2.04
1506.8331	0.932
3055.8070	2.13
3101.2414	1.22
3116.8437	1.29



$\Delta E = 0.66$ kcal mol^{-1}
Population = 0.086



$\Delta E = 0.68$ kcal mol^{-1}
Population = 0.083

Optimized Coordinates (Angstroms)

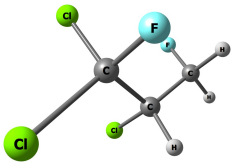
Atom	X	Y	Z
C	-1.014136938477	1.541437850602	-0.582241698443
C	-0.644781732555	0.073201862256	-0.773453958761
C	0.661882276572	-0.409822313249	-0.111367232022
F	-1.368513541388	1.814910850950	0.709804034696
H	-0.164319949988	2.172363838347	-0.864877798848
H	-1.862941043731	1.765318395857	-1.237294712838
H	-0.510285234089	-0.108065727536	-1.842616422889
Cl	-2.007178033807	-0.982134417080	-0.252750579605
F	0.848987554778	-1.702219351986	-0.398379836468
Cl	2.043462328443	0.503055646008	-0.850234550716
Cl	0.700364314243	-0.214781634170	1.658283755894

Atom	X	Y	Z
C	-1.710346152825	0.973392312395	-0.265613065292
C	-0.701727678104	-0.164268697990	-0.436283585301
C	0.752568274710	0.323581724628	-0.301047753781
F	-2.944630550091	0.522602377343	-0.654403130843
H	-1.754403391565	1.300374712881	0.776883303905
H	-1.417760098899	1.813530522045	-0.904633999999
H	-0.795914800128	-0.570442890978	-1.445798598209
Cl	-1.077117585383	-1.505100228333	0.688657478100
F	0.930096053711	1.298680621003	-1.215503148867
Cl	1.098674960862	1.020779038685	1.314137422203
Cl	1.924557967711	-0.977598491679	-0.665555921917

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
56.9982	0.222
113.0873	0.228
169.4533	0.205
183.1203	0.00981
226.2985	0.229
275.5113	0.273
288.3005	0.379
360.5709	0.0674
382.9586	0.145
443.6815	1.34
576.4014	3.95
651.2444	8.13
738.1621	22.8
827.1974	13.9
918.1835	3.55
997.2358	7.33
1120.5521	7.40
1133.8202	8.50
1163.0223	16.4
1241.2215	1.06
1294.2251	0.999
1336.5817	3.07
1429.8976	1.01
1500.7623	1.24
3045.3327	2.91
3095.5444	2.59
3098.3665	0.414

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
66.8669	0.0373
95.3291	0.644
152.5522	0.291
166.7872	0.0637
242.9605	0.269
254.3708	0.332
316.0162	0.192
364.7856	0.230
382.2859	0.0310
444.8874	2.69
494.0177	0.262
638.6990	9.18
746.9012	5.79
815.0488	32.0
1011.3267	4.95
1041.4258	14.6
1097.2856	8.47
1115.9866	10.3
1129.7007	11.1
1247.8161	0.817
1282.4454	1.94
1310.0214	2.47
1425.5900	1.52
1507.5660	0.381
3052.2024	2.50
3099.7557	0.240
3117.2040	1.84



$\Delta E = 1.24$ kcal mol^{-1}
Population = 0.032

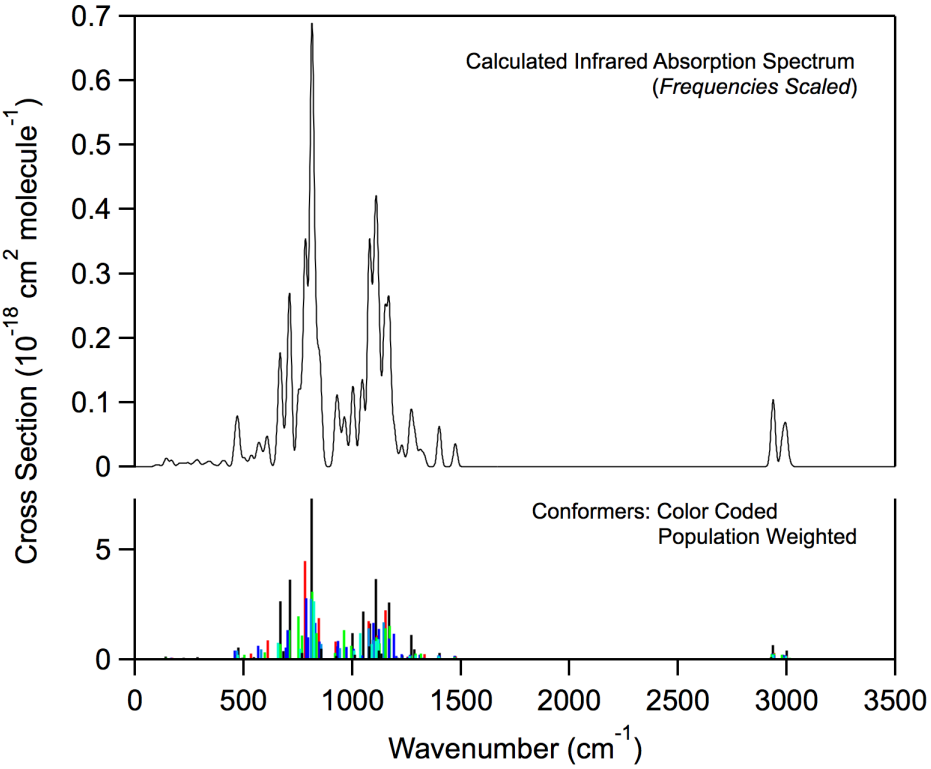
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.842856080681	0.343335130489	-0.951950190770
C	-0.607471676279	-0.503035143980	-0.643328363339
C	0.649771768275	0.330325406234	-0.307953664822
F	-2.331989835006	0.966137384016	0.162169967195
H	-1.577102295177	1.097803617930	-1.701058761616
H	-2.616426417422	-0.316135958811	-1.359869294520
H	-0.353975751670	-1.057283987178	-1.550702517481
Cl	-0.968474177788	-1.716705921012	0.620556212793
F	0.804514568371	1.219373972505	-1.311440873611
Cl	0.530823459572	1.236913173308	1.220696571187
Cl	2.113971437806	-0.710857673501	-0.286663085015

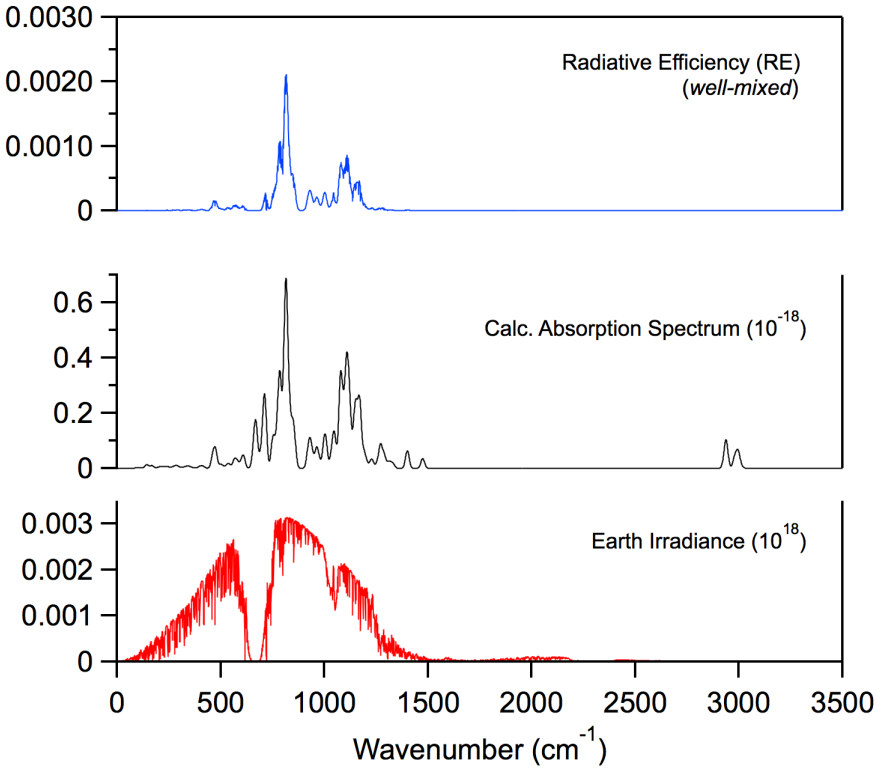
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
55.3865	0.183
110.7860	0.294
162.4103	0.0290
174.2660	0.126
234.0023	0.0846
259.9741	0.186
306.4734	0.692
378.5153	0.0390
381.8713	0.0586
468.7341	2.46
521.8033	3.67
665.4220	12.1
758.1672	9.43
849.7418	15.0
925.3077	5.24
1014.8943	6.68
1084.6932	18.9
1130.8924	12.5
1143.4989	8.50
1241.7496	1.02
1295.7136	1.36
1328.0693	1.95
1426.7205	1.63
1501.4775	1.03
3042.6730	3.23
3092.0876	1.46
3095.1011	1.42

Infrared Spectrum

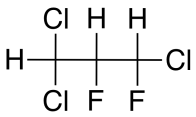


Radiative Efficiency



HCFC-242ea

Molecular Formula:	$CHCl_2CHFCHClF$
Name:	1,1,3-Trichloro-2,3-difluoropropane
CAS number:	2106760-91-0
Molecular Weight:	183.41



Global Atmospheric Lifetime (years):	0.724
Tropospheric Atmospheric Lifetime (years):	0.756
Stratospheric Atmospheric Lifetime (years):	20
Ozone Depletion Potential (ODP):	0.015

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.174	0.119
Global Warming Potential (GWP_H):		
GWP_{20}	155	106
GWP_{100}	42	29
Global Temperature Potentials (GTP_H)		
GTP_{20}		33
GTP_{50}		5
GTP_{100}		4

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 7.76 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 4.95 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 0.735$ years

$\tau^{OH}_{Trop} = 0.756$ years

$\tau^{OH}_{Strat} = 26.2$ years

Fractional Atmospheric Loss: 0.985

$O(^1D)$ 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: 0.004

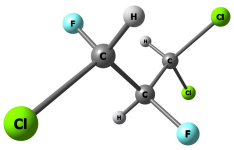
UV Photolysis

UV Spectrum: *No Recommendation*

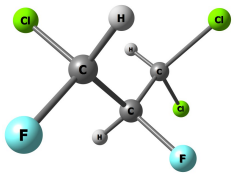
$\tau_{hv} = 68$ years

Fractional Atmospheric Loss: 0.011

Molecular Structure and Infrared Spectrum (7 conformers)



E = 0
Population = 0.367



$\Delta E = 0.33$ kcal mol^{-1}
Population = 0.210

Optimized Coordinates (Angstroms)

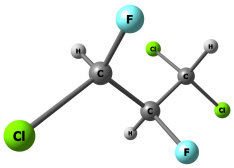
Atom	X	Y	Z
C	-1.121105833500	0.124533466351	0.460045209018
C	0.197407121189	-0.533231170275	0.039431370281
C	1.378067154114	0.435487825913	0.172702049398
Cl	-1.536697950439	1.501995723352	-0.610055753887
Cl	-2.430990018990	-1.094128134894	0.469806267388
H	-1.037583242162	0.519169676253	1.469263389331
F	0.125164073625	-0.961671469280	-1.250947626181
H	0.368338913529	-1.390520402756	0.701401718234
H	1.317975935255	1.259957394816	-0.538281248664
F	1.392072955955	0.919825848622	1.441551678207
Cl	2.917106891424	-0.423512758102	-0.154781053124

Atom	X	Y	Z
C	-0.906421809954	-0.322105472118	-0.344333289393
C	0.165006804440	0.740675295707	-0.099824837292
C	1.512821489973	0.190653378659	0.380461632658
Cl	-1.264141676363	-1.242917498038	1.152901247801
Cl	-2.387123463934	0.458078522455	-0.980097824675
H	-0.578689415786	-1.041054706521	-1.089681865041
F	-0.262261238817	1.618108752455	0.858376721042
H	0.329658732585	1.285814026782	-1.036946324674
F	2.357977184353	1.230225927630	0.535390865591
H	1.430020304954	-0.360671420591	1.317565737159
Cl	2.195453088549	-0.944893806420	-0.844388063176

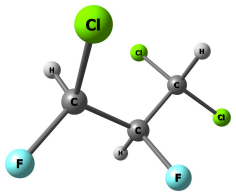
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
50.0267	0.0781
72.5763	0.161
123.0917	0.278
188.0123	0.164
208.6422	0.180
232.3198	0.0333
313.2378	0.415
374.1639	0.170
430.4971	3.84
486.1529	0.600
625.2138	11.1
721.4407	21.4
732.2287	1.16
842.4528	9.99
960.5602	2.15
1088.6167	10.4
1118.5813	8.88
1159.2334	11.3
1221.9632	1.66
1257.4895	4.31
1273.6801	0.0214
1334.1735	1.81
1357.3062	2.05
1396.3488	0.235
3059.3620	0.837
3128.7623	0.887
3160.2905	0.230

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
46.8985	0.0772
86.9916	0.224
127.2494	0.126
185.8253	0.340
204.6772	0.0430
273.2784	0.317
317.6091	0.159
374.0104	0.515
414.5777	0.524
440.3752	3.97
643.5884	7.42
722.2508	2.47
765.7146	17.9
799.5059	16.3
970.7106	2.73
1085.3163	1.31
1135.1328	6.04
1140.6323	27.2
1223.6548	2.29
1248.8378	2.98
1276.9889	0.300
1316.3141	1.29
1367.7360	1.25
1403.5906	1.70
3060.3232	0.641
3128.8875	0.845
3167.2744	0.313



$\Delta E = 0.33$ kcal mol^{-1}
Population = 0.210



$\Delta E = 0.64$ kcal mol^{-1}
Population = 0.125

Optimized Coordinates (Angstroms)

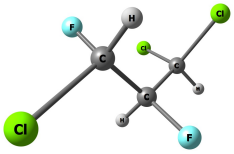
Atom	X	Y	Z
C	-1.152979860966	0.054520452715	-0.328030391191
C	0.173580492390	-0.427499143919	0.279028190171
C	1.335072528204	0.492393760170	-0.111456561763
Cl	-2.450826762958	-1.119582365473	0.019687414777
Cl	-1.567948082592	1.678960044057	0.313624873734
H	-1.074553743248	0.143720307118	-1.408611312936
F	0.423220121440	-1.675493105080	-0.219893059037
H	0.089681864307	-0.473636796269	1.369355380371
F	1.400460934188	0.578977073368	-1.463403175696
H	1.227029722714	1.489875755587	0.313818690106
Cl	2.880329786522	-0.170750982273	0.516747951464

Atom	X	Y	Z
C	-0.985669380496	0.117535244798	-0.292821691856
C	0.119979430548	-0.575434313212	0.509115204030
C	1.445729416501	0.193168828375	0.550541957731
Cl	-2.444159958730	-0.912603316424	-0.333783821700
Cl	-1.350699409133	1.719412039469	0.430453780967
H	-0.684256028802	0.289041140381	-1.323190651772
F	0.352017628775	-1.802746736813	-0.043821235681
H	-0.211994658225	-0.707796698766	1.546595871252
H	1.327899293922	1.198201222964	0.954978813252
F	2.308778529433	-0.510001668773	1.316767294258
Cl	2.146137136206	0.379812258000	-1.098941520479

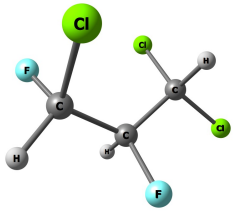
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
51.4664	0.143
72.3260	0.134
125.5285	0.227
198.4623	0.300
220.0171	0.284
249.1646	0.0476
310.5898	0.168
378.6549	0.558
392.3186	0.453
422.1234	3.20
687.2665	20.3
753.3636	6.13
788.0298	12.0
836.9338	9.49
902.7832	5.50
1071.5838	0.764
1088.7974	11.5
1159.0133	13.9
1224.6932	0.203
1235.5281	2.90
1280.1541	1.76
1354.2742	0.713
1368.1329	0.527
1386.8223	1.47
3081.6934	0.788
3131.0906	1.00
3160.4497	0.183

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
45.9101	0.0853
79.4857	0.162
136.4869	0.222
184.5772	0.212
231.7267	0.236
253.8400	0.291
314.0681	0.205
372.9988	0.507
402.7189	1.52
450.1025	1.10
634.0293	12.9
744.9010	5.59
772.5311	15.4
793.9766	10.0
959.5467	5.44
1093.6794	1.90
1120.7584	14.5
1147.0358	13.8
1225.1367	1.07
1234.8968	3.86
1283.7166	4.08
1336.8106	0.374
1370.9873	2.91
1395.5346	0.798
3052.4639	0.965
3131.0176	0.963
3159.4065	0.244



$\Delta E = 1.44$ kcal mol^{-1}
Population = 0.032



$\Delta E = 1.60$ kcal mol^{-1}
Population = 0.025

Optimized Coordinates (Angstroms)

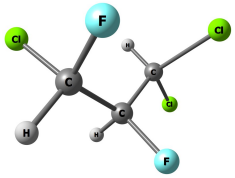
Atom	X	Y	Z
C	-1.250632895881	-0.198208058693	0.544677162224
C	0.274335331101	-0.246105633560	0.736589715124
C	1.112163400691	0.175738974600	-0.474872376285
Cl	-1.877958210407	1.473263567915	0.591051970321
Cl	-1.771526547942	-1.063075296615	-0.938533977395
H	-1.707510202352	-0.730384295741	1.376280332485
F	0.590623701488	-1.548261662166	1.027847369888
H	0.526243394254	0.389709200023	1.592732071204
H	0.958720860184	-0.492187275388	-1.322984129268
F	0.815433875942	1.444509774438	-0.824981445796
Cl	2.858276292922	0.070279705188	-0.051420692502

Atom	X	Y	Z
C	-0.884143494324	-0.024056397407	-0.364457677971
C	0.059533000057	-0.533370003653	0.729672146348
C	1.514172019529	-0.035817370237	0.675684048843
Cl	-2.470045333709	-0.843199738253	-0.205887341730
Cl	-1.069544553216	1.749677402462	-0.266050761216
H	-0.504526757889	-0.259801049801	-1.354964197059
F	0.127482017990	-1.899944482267	0.631896906593
H	-0.343268748037	-0.259266030728	1.712348686280
F	1.609474668354	1.245902567589	1.079598855522
H	2.115166005906	-0.672848504546	1.328607748049
Cl	2.235065175340	-0.208697393159	-0.966875413660

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
34.1083	0.0903
80.1876	0.0299
139.5384	0.0466
183.4714	0.191
201.0985	0.216
263.8095	0.116
336.3179	0.387
371.8208	3.64
399.8722	0.589
512.2100	0.125
541.5207	7.84
679.0136	5.49
788.7764	20.4
826.1953	12.2
980.7451	3.30
1107.0655	7.89
1122.2428	4.75
1146.2901	17.6
1229.6513	2.54
1232.4810	0.552
1280.3824	5.17
1335.2643	1.34
1349.5665	0.678
1412.2271	0.312
3067.8229	0.721
3127.4119	0.930
3142.7073	0.306

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
38.1505	0.0913
86.0245	0.0452
147.3078	0.117
178.9134	0.139
224.9348	0.234
264.7684	0.530
341.6927	1.25
347.1784	0.644
401.6650	1.46
512.7897	0.525
558.2619	9.64
690.2546	7.89
789.1594	13.6
807.7073	9.46
978.4511	2.93
1106.2153	5.81
1120.2165	6.05
1149.0623	18.8
1229.3934	2.64
1232.6683	0.970
1291.7519	4.58
1326.0640	1.37
1371.7642	3.42
1398.3009	1.11
3057.1635	1.05
3099.7446	1.61
3164.2599	0.235



$\Delta E = 1.88$ kcal mol^{-1}
Population = 0.015

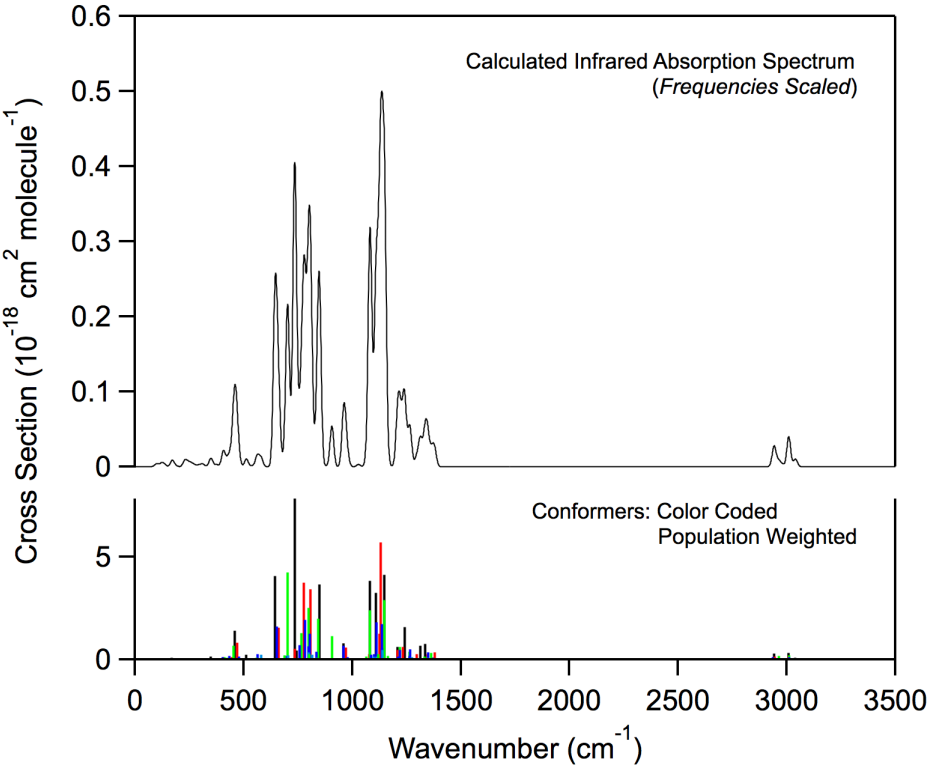
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-0.816434742079	-0.127239546201	0.454552500533
C	0.103036260438	-0.592440208376	-0.679612945455
C	1.562384119901	-0.125310400785	-0.594036432283
Cl	-1.176466039878	1.617679433841	0.371525042731
Cl	-2.337893158492	-1.085672376796	0.404051921858
H	-0.358242005719	-0.322046816081	1.420844700709
F	-0.382014115423	-0.168248471360	-1.886835790655
H	0.114747011447	-1.688033206631	-0.665804661420
H	2.111765760983	-0.502119502215	-1.460042750403
F	1.673690716117	1.213353887077	-0.546396420914
Cl	2.350949192707	-0.848987792474	0.862471835299

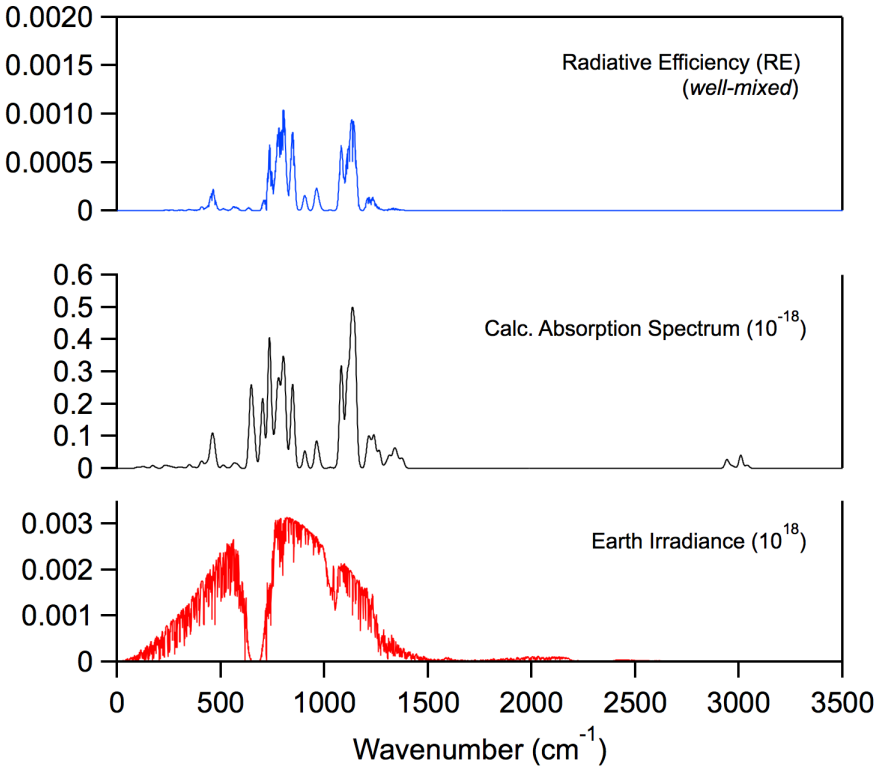
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
31.1501	0.131
85.9304	0.111
150.7123	0.297
184.0814	0.225
208.4847	0.0100
252.8383	0.0585
295.2416	0.534
332.9144	0.405
402.0068	0.578
533.7408	6.29
673.1206	14.2
728.1130	2.65
791.2379	16.8
826.0078	5.64
882.0749	0.979
1032.2265	4.17
1129.5705	17.7
1174.4317	11.0
1223.7490	2.45
1259.2594	4.79
1278.8565	0.142
1346.2808	2.04
1376.9927	0.661
1408.5859	2.18
3065.2220	0.921
3099.1499	1.53
3157.3598	0.254

Infrared Spectrum

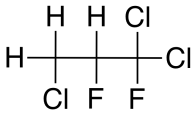


Radiative Efficiency



HCFC-242eb

Molecular Formula: $CH_2ClCHFCCl_2F$
Name: 1,1,3-Trichloro-1,2-difluoropropane
CAS number: –
Molecular Weight: 183.41



Global Atmospheric Lifetime (years): 1.24
  Tropospheric Atmospheric Lifetime (years): 1.31
  Stratospheric Atmospheric Lifetime (years): 23.0
Ozone Depletion Potential (ODP): 0.025

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.215	0.167
Global Warming Potential (GWP_H):		
GWP_{20}	326	253
GWP_{100}	88	68
Global Temperature Potentials (GTP_H)		
GTP_{20}		84
GTP_{50}		12
GTP_{100}		10

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 4.49 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 2.87 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 1.27$ years
$\tau^{OH}_{Trop} = 1.31$ years
$\tau^{OH}_{Strat} = 42.9$ years

Fractional Atmospheric Loss: 0.975

O(^{1}D) Reactivity

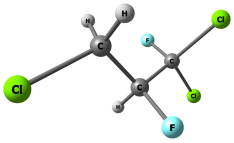
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 2.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)} = 185$ years
Fractional Atmospheric Loss: 0.007

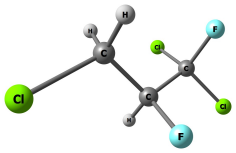
UV Photolysis

UV Spectrum: *No Recommendation*
$\tau_{hv} = 68$ years
Fractional Atmospheric Loss: 0.018

Molecular Structure and Infrared Spectrum (5 conformers)



E = 0
Population = 0.420



$\Delta E = 0.27$ kcal mol^{-1}
Population = 0.267

Optimized Coordinates (Angstroms)

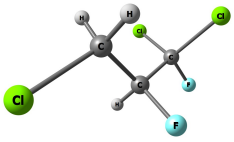
Atom	X	Y	Z
C	-1.544180851037	0.536181308482	-0.364413191248
C	-0.461627975234	-0.477314629610	-0.018052869078
C	0.950029818830	0.046519928067	-0.361669692645
Cl	-3.169429866184	-0.223725889443	-0.238375639785
H	-1.521823818279	1.375309356374	0.329129360379
H	-1.423448524630	0.890462917642	-1.387150075893
H	-0.599921843242	-1.393624024414	-0.603789443992
F	-0.505803739302	-0.784200757636	1.308739058440
F	0.987535786256	0.329016194702	-1.674634057687
Cl	1.348242266122	1.535367595223	0.553813088908
Cl	2.171089746700	-1.215015999389	-0.017978537398

Atom	X	Y	Z
C	-1.529642428050	0.531321553287	0.364540114552
C	-0.456534581787	-0.342599301760	-0.274987829066
C	0.958687054078	0.056596858458	0.201310588454
Cl	-3.148293060953	0.093686207493	-0.282451520917
H	-1.549933880259	0.368356379099	1.441470221026
H	-1.364691250103	1.584728155797	0.147369021728
H	-0.485909354652	-0.275550532360	-1.366096181730
F	-0.660206017888	-1.641818123376	0.104043809634
F	0.997501667778	0.095043971161	1.540481201962
Cl	2.168253610011	-1.130194287649	-0.365460685097
Cl	1.376344241826	1.690616119850	-0.426800740546

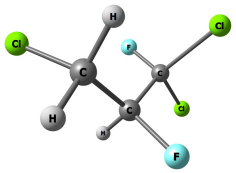
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
69.7189	0.550
71.0505	0.0406
128.1933	0.438
193.6335	0.0679
228.3375	0.190
257.2655	0.305
285.1303	0.0285
373.1637	0.0502
404.9845	0.519
471.1182	2.25
549.3055	0.331
629.1504	15.2
737.1439	17.6
857.2514	19.4
871.1859	1.53
1028.0036	3.52
1079.9051	15.1
1145.4292	6.01
1155.7127	12.2
1224.7163	1.64
1273.7710	3.94
1355.2045	0.830
1386.5828	1.31
1465.4867	0.867
3061.7891	1.08
3109.3521	0.883
3178.0977	0.0310

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
66.5379	0.336
70.3108	0.252
137.2775	0.536
200.1288	0.125
240.6543	0.190
256.3729	0.0169
312.6114	0.0843
332.7442	0.486
393.1769	0.652
458.0868	0.691
488.6890	2.67
703.3343	19.2
815.2618	7.61
842.8659	21.4
879.3421	10.3
957.4281	12.4
1053.0117	2.64
1124.7610	5.12
1180.6084	13.3
1220.3944	1.82
1277.2544	2.79
1357.7319	1.01
1382.4506	0.660
1467.0882	1.00
3090.9629	0.817
3111.2799	0.822
3180.1705	0.0684



$\Delta E = 0.34$ kcal mol^{-1}
Population = 0.237



$\Delta E = 1.17$ kcal mol^{-1}
Population = 0.058

Optimized Coordinates (Angstroms)

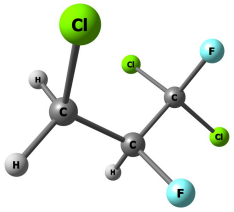
Atom	X	Y	Z
C	-1.350373328212	0.334927786431	0.600377401949
C	-0.478901782021	-0.103126753621	-0.564898694355
C	1.040118204325	-0.025561092685	-0.294430899718
Cl	-3.076980269499	0.374507787525	0.095358708424
H	-1.269504505948	-0.372598614735	1.424412615793
H	-1.085502398221	1.335500717057	0.936771508918
H	-0.663872141312	0.522290154374	-1.446127770453
F	-0.751758528385	-1.404913237870	-0.885360847710
F	1.682931828542	-0.484165860534	-1.372243107213
Cl	1.534456690414	1.684050844924	-0.035098552472
Cl	1.521557230317	-1.030079730866	1.108998636836

Atom	X	Y	Z
C	-1.654077200968	-0.731732211441	0.489672616798
C	-0.279756020787	-0.981925343328	-0.134235178503
C	0.660783153368	0.241743777208	-0.155762651108
Cl	-2.779045979317	0.094235855608	-0.641508437898
H	-2.086108858332	-1.703801966696	0.726724243056
H	-1.586386883439	-0.131770122971	1.396126650265
H	-0.389571324035	-1.318485384562	-1.170967286197
F	0.330845080098	-1.965934650995	0.597756299409
F	0.088124408119	1.236803716125	-0.838215349550
Cl	1.017758988257	0.818256813805	1.506731338765
Cl	2.195829637036	-0.199719482752	-0.973703245037

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
64.3966	0.478
76.8935	0.0638
145.4433	0.481
189.8135	0.124
218.3660	0.183
260.5908	0.0434
308.2301	0.363
371.5554	0.00968
394.6228	0.549
465.4868	1.37
509.0280	1.01
646.7790	15.0
766.9457	9.01
835.4833	25.2
880.2980	9.31
1031.9287	4.97
1065.6322	7.63
1136.6985	6.58
1161.8798	15.8
1227.3605	3.39
1273.4126	4.30
1357.8223	0.869
1381.5432	1.26
1466.1703	1.13
3062.3784	0.987
3112.3179	1.02
3180.9183	0.0268

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
37.2198	0.120
99.0892	0.267
178.5035	0.232
185.7485	0.356
204.3407	0.164
281.4524	0.0965
322.5721	0.234
367.5597	0.244
415.6409	2.42
431.6332	2.08
551.6589	0.119
575.3401	7.63
773.9575	17.9
803.9412	18.5
912.3630	12.3
1028.6158	3.48
1110.0279	4.38
1118.3485	14.0
1173.5611	13.7
1189.1039	3.06
1283.3964	2.02
1364.8195	0.894
1373.0378	1.67
1478.2119	1.50
3069.3843	0.719
3103.1721	0.932
3168.8766	0.0503



$\Delta E = 1.92$ kcal mol^{-1}
Population = 0.016

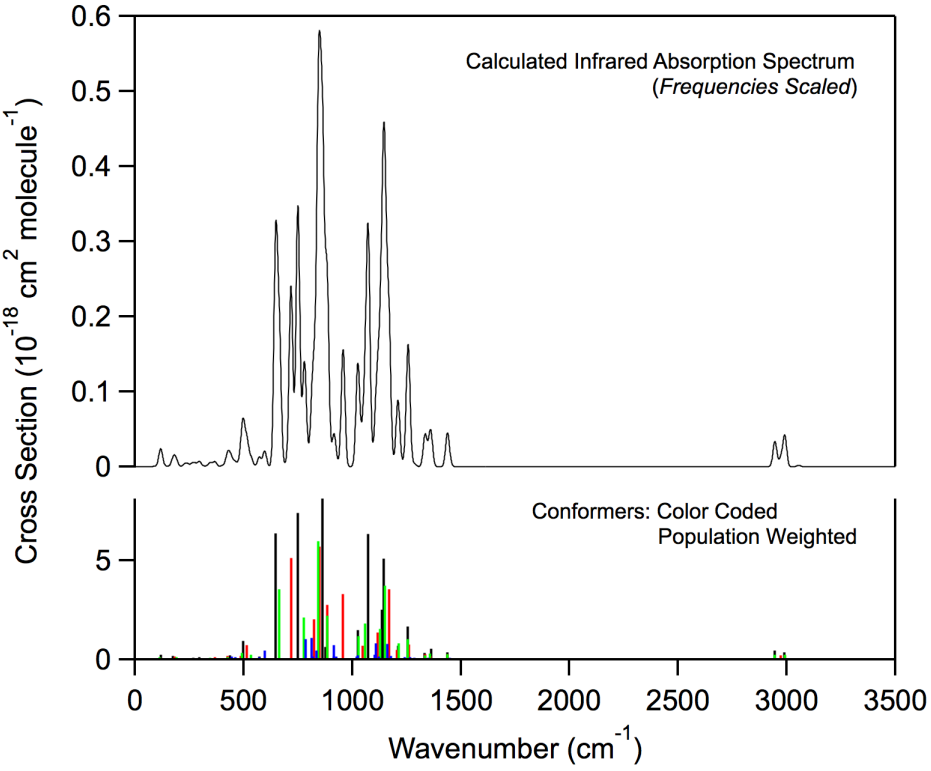
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.620080292484	0.094689518022	-0.986031395584
C	-0.261949951995	-0.580253928892	-0.820516837153
C	0.727929946097	0.091229059185	0.157797775846
Cl	-2.644080421247	0.051825305623	0.489327596392
H	-1.502209240769	1.135104510798	-1.283982839918
H	-2.167172180932	-0.445554453931	-1.759198797290
H	0.226362025328	-0.586450606021	-1.803047018918
F	-0.439388957282	-1.869419563415	-0.400951123138
F	0.250695210143	0.121463445466	1.399187883331
Cl	2.266688590604	-0.836243845866	0.174265388169
Cl	1.057245272536	1.779074559031	-0.378097631738

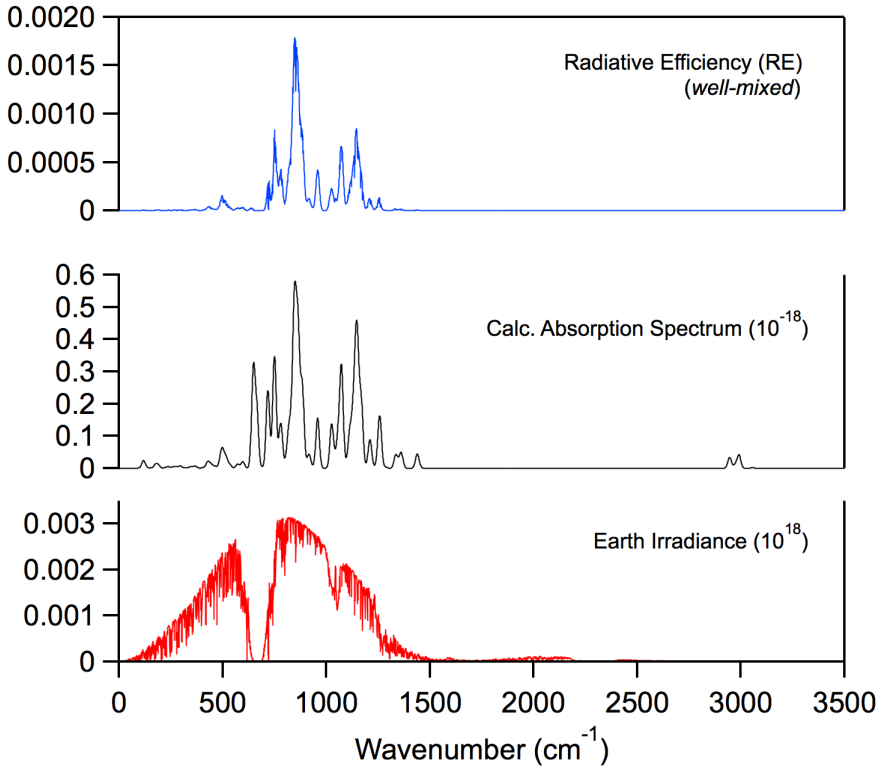
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
34.6785	0.154
100.8012	0.0519
179.4544	0.184
185.7128	0.222
219.3422	0.105
282.9010	0.120
315.9974	0.397
341.7532	0.262
394.3943	0.667
444.5529	1.21
548.6882	7.85
675.7239	3.68
810.6486	9.24
827.2853	27.6
910.8849	8.58
922.8732	8.84
1024.0027	9.45
1130.9330	8.94
1184.4807	5.18
1257.3008	7.82
1304.6994	4.78
1358.7776	2.77
1378.4641	0.519
1461.8893	1.89
3049.2921	0.874
3101.9110	1.36
3167.8623	0.0992

Infrared Spectrum

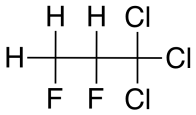


Radiative Efficiency



HCFC-242ec

Molecular Formula: $CH_2FCHFCCl_3$
Name: 1,1,1-Trichloro-2,3-difluoropropane
CAS number: –
Molecular Weight: 183.41



Global Atmospheric Lifetime (years): 1.70
  Tropospheric Atmospheric Lifetime (years): 1.84
  Stratospheric Atmospheric Lifetime (years): 23.5
Ozone Depletion Potential (ODP): 0.034

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.211	0.174
Global Warming Potential (GWP_H):		
GWP_{20}	441	363
GWP_{100}	120	98
Global Temperature Potentials (GTP_H)		
GTP_{20}		129
GTP_{50}		17
GTP_{100}		14

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 3.19 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 2.04 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

τ^{OH}_{Global} = 1.78 years
τ^{OH}_{Trop} = 1.84 years
τ^{OH}_{Strat} = 58.3 years

Fractional Atmospheric Loss: 0.957

O(^{1}D) Reactivity

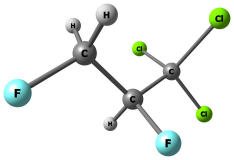
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 2.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)}$ = 185 years
Fractional Atmospheric Loss: 0.009

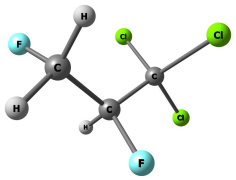
UV Photolysis

UV Spectrum: *No Recommendation*
τ_{hv} = 50 years
Fractional Atmospheric Loss: 0.034

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.596



$\Delta E = 0.40$ kcal mol^{-1}
Population = 0.306

Optimized Coordinates (Angstroms)

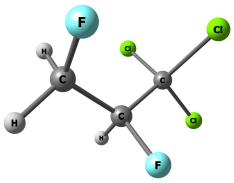
Atom	X	Y	Z
C	-1.981332956326	0.530607687450	0.192219656355
C	-0.884534171997	-0.309048177627	-0.455734942648
C	0.555879112471	0.072151214837	-0.047641302361
F	-3.157584771328	0.241807934172	-0.457220061206
H	-2.079001114971	0.261522894785	1.248056790846
H	-1.770304202634	1.599418172351	0.099568866744
H	-0.947404295251	-0.207659383672	-1.545324875499
F	-1.089445618818	-1.620825293360	-0.123371458322
Cl	1.700706377174	-1.074096215201	-0.805102042211
Cl	0.911560083202	1.729978968582	-0.635740489036
Cl	0.753071558479	0.005943197682	1.731548857339

Atom	X	Y	Z
C	-2.069563187000	-0.611982810279	-0.060356495618
C	-0.662431893930	-0.752178695213	-0.651844805076
C	0.447570562837	0.082261467134	0.026415796231
F	-2.690813054519	0.499692907991	-0.569583629547
H	-2.624911732903	-1.507363120230	-0.361128867082
H	-2.047381920030	-0.551422110617	1.031718901158
H	-0.687805680130	-0.457566404966	-1.707108162446
F	-0.302784135003	-2.071542438009	-0.554875232887
Cl	1.991672839053	-0.206368138631	-0.838573953893
Cl	0.031595874884	1.816129492746	-0.062809223399
Cl	0.643326326740	-0.409896149925	1.738886672559

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
71.2579	0.578
84.3074	0.124
150.9691	0.349
182.9501	0.0963
247.3854	0.297
258.3312	0.0447
273.6304	0.254
303.9036	0.216
369.4384	0.854
409.6863	0.402
495.8165	2.88
646.1289	10.3
774.3812	20.9
804.1691	20.5
914.1472	6.27
1048.7789	2.57
1105.8608	15.2
1119.2383	1.38
1151.0402	6.11
1279.8329	0.331
1303.2974	0.820
1380.1981	1.41
1432.5153	0.742
1500.8809	0.419
3060.6170	1.24
3066.4158	1.59
3121.7241	2.24

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
52.2903	0.195
115.2790	0.607
167.2216	0.201
184.2911	0.0854
220.8625	0.236
260.5775	0.0333
274.8631	0.161
315.5556	0.259
391.1775	0.690
440.9910	4.98
476.4531	0.386
590.4022	6.86
764.2918	19.2
816.5508	22.9
925.6900	1.26
1081.5356	3.14
1107.1059	8.24
1116.9991	10.7
1134.7545	4.14
1257.2827	0.452
1326.1431	0.126
1367.4980	1.84
1427.1084	0.760
1510.2477	0.840
3048.9040	2.73
3065.9749	1.03
3108.5230	2.51



$\Delta E = 1.07$ kcal mol^{-1}
Population = 0.098

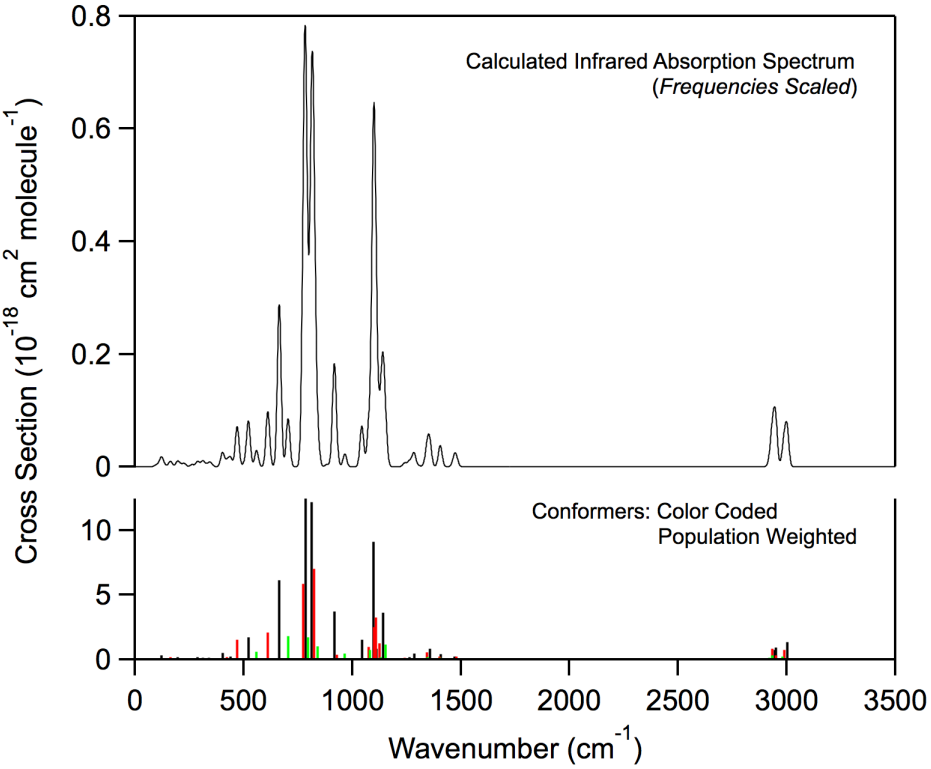
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-2.009915321346	0.219229219624	-0.828423948608
C	-0.677676344821	-0.523942184619	-0.846204577421
C	0.482272451794	0.073568317409	-0.011793737383
F	-2.572727567447	0.230669099004	0.418752288563
H	-1.879836881463	1.245372639854	-1.185194734593
H	-2.681058560261	-0.315837150103	-1.511527213348
H	-0.320853006014	-0.544375253969	-1.884141556947
F	-0.882428995410	-1.807004748590	-0.416678538259
Cl	1.945492876780	-0.931606214415	-0.293431505214
Cl	0.809551856074	1.742894697070	-0.591346533383
Cl	0.121774492115	0.092182578735	1.729650056593

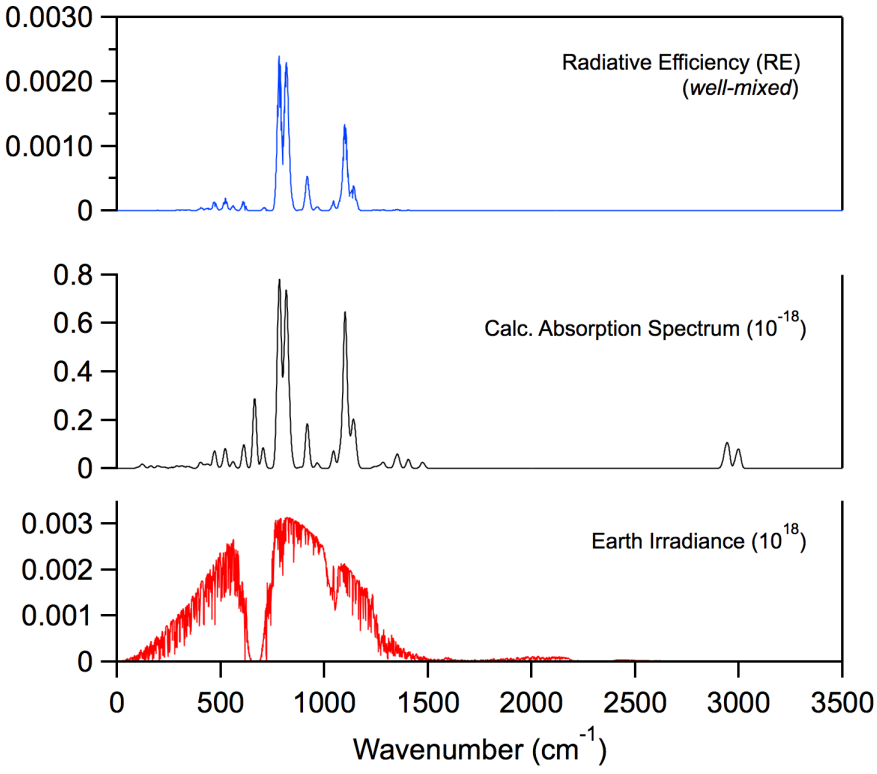
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
43.7524	0.312
119.7513	0.252
175.9331	0.0765
185.0765	0.278
224.2264	0.0899
259.9061	0.0502
286.0341	0.416
293.8308	0.0936
371.1126	0.237
404.1088	1.14
535.4589	6.20
689.3847	18.6
785.3656	17.4
833.8135	10.5
879.4665	0.944
965.9255	4.91
1087.1750	7.65
1139.9594	2.06
1164.9012	12.0
1293.1106	0.798
1354.8807	0.625
1368.3976	1.74
1431.7258	1.46
1497.1231	1.18
3035.6606	1.58
3048.4639	3.53
3100.7623	2.60

Infrared Spectrum

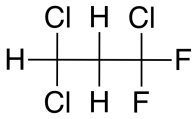


Radiative Efficiency



HCFC-242fa

Molecular Formula:	$CHCl_2CH_2CClF_2$
Name:	1,3,3-Trichloro-1,1-difluoropropane
CAS number:	460-63-9
Molecular Weight:	183.41



Global Atmospheric Lifetime (years): 0.735
- Tropospheric Atmospheric Lifetime (years): 0.768
- Stratospheric Atmospheric Lifetime (years): 20

Ozone Depletion Potential (ODP): 0.015

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.223	0.153
Global Warming Potential (GWP_H):		
GWP_{20}	201	138
GWP_{100}	54	37
Global Temperature Potentials (GTP_H)		
GTP_{20}		43
GTP_{50}		6
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*

$k_{SAR}(298\ K) = 7.64 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 4.87 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 0.746$ years

$\tau^{OH}_{Trop} = 0.768$ years

$\tau^{OH}_{Strat} = 26.6$ years

Fractional Atmospheric Loss: 0.985

$O(^1D)$ 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: 0.004

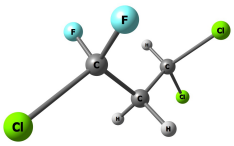
UV Photolysis

UV Spectrum: *No Recommendation*

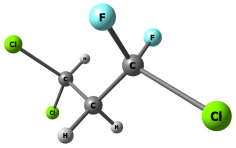
$\tau_{hv} = 68$ years

Fractional Atmospheric Loss: 0.011

Molecular Structure and Infrared Spectrum (4 conformers)



E = 0
Population = 0.314



E = 0
Population = 0.314

Optimized Coordinates (Angstroms)

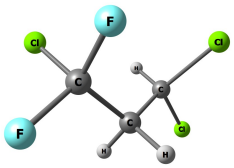
Atom	X	Y	Z
C	1.234800674563	0.116556205735	0.370379589817
C	-0.058703323824	0.663379937639	-0.234524093337
C	-1.301331367733	-0.111657400561	0.196357670739
Cl	1.713057211428	-1.459588617274	-0.336397578792
Cl	2.548217620763	1.324737598417	0.142266857701
H	1.145263404049	-0.039999319738	1.442084988275
H	-0.000695645601	0.671674677959	-1.324046628301
H	-0.182447259570	1.691573835083	0.111253038661
F	-1.349271078971	-1.340205720908	-0.319511304598
F	-1.343239910002	-0.229686600849	1.533413719310
Cl	-2.792546325102	0.767118404497	-0.332428259475

Atom	X	Y	Z
C	1.234739558967	-0.111719142222	0.387461661893
C	-0.057471703963	-0.673147814894	-0.206732440163
C	-1.299948142041	0.117668781390	0.194924345434
Cl	2.545909850136	-1.329574461062	0.201821658375
Cl	1.720470254283	1.441249097352	-0.364105108029
H	1.140747117574	0.077192220625	1.453555943622
H	-0.185567386418	-1.690169431241	0.169186823424
H	0.005471730356	-0.714317023489	-1.295234217497
F	-1.347624806551	0.275909052252	1.527625979339
F	-1.342214655164	1.330288421869	-0.357811484402
Cl	-2.791111817180	-0.772760700579	-0.314143161996

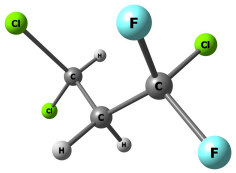
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
32.0947	0.0222
101.7010	0.374
128.5739	0.416
200.9583	0.0219
243.7620	0.0310
311.7770	0.426
331.4084	0.223
397.3734	0.228
421.9221	0.257
438.5923	2.56
572.9601	3.19
667.2040	9.88
701.1223	19.4
832.3472	1.84
915.9062	7.17
960.0885	27.4
1056.9649	12.3
1130.8384	12.7
1226.6231	18.8
1236.9322	1.70
1264.4406	18.4
1325.7722	1.34
1369.5187	6.06
1454.8478	1.05
3092.7667	0.0451
3146.1759	0.0309
3161.6189	0.0396

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
32.0949	0.0222
101.7009	0.374
128.5740	0.416
200.9583	0.0219
243.7619	0.0310
311.7770	0.426
331.4084	0.223
397.3731	0.228
421.9218	0.257
438.5919	2.56
572.9601	3.19
667.2034	9.88
701.1222	19.4
832.3472	1.84
915.9065	7.17
960.0879	27.4
1056.9640	12.3
1130.8383	12.7
1226.6230	18.8
1236.9329	1.70
1264.4408	18.4
1325.7719	1.34
1369.5184	6.06
1454.8477	1.05
3092.7677	0.0451
3146.1765	0.0309
3161.6187	0.0396



$\Delta E = 0.33$ kcal mol^{-1}
Population = 0.181



$\Delta E = 0.33$ kcal mol^{-1}
Population = 0.181

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.094336774602	0.142060644562	0.313952022212
C	0.012840487854	0.653345215773	-0.630448585433
C	-1.392236584392	0.095491388108	-0.416508749738
Cl	1.480956850709	-1.586954791697	0.043916356665
Cl	2.572501782543	1.149024319995	0.105732514920
H	0.807235006205	0.235439000718	1.357795340264
H	0.289647086987	0.437670525750	-1.666583191154
H	-0.059370460886	1.737018902409	-0.514253207023
F	-2.231106391654	0.719528615032	-1.253484489925
F	-1.474907862413	-1.211818185390	-0.660498493886
Cl	-1.988176689555	0.385665364740	1.272981483097

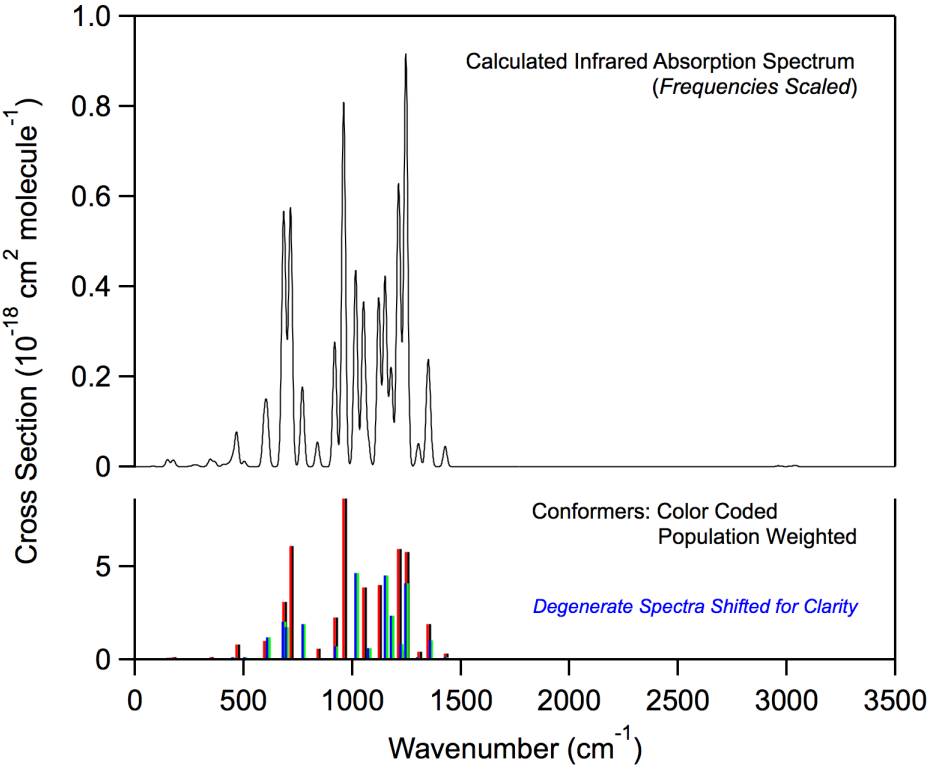
Atom	X	Y	Z
C	1.095106005094	-0.138068807469	0.332687677300
C	0.017561365648	-0.686307574415	-0.595358040925
C	-1.387855329689	-0.118780385832	-0.411158764022
Cl	2.573039902904	-1.154173399578	0.172857683401
Cl	1.485114234848	1.578118531835	-0.005667895831
H	0.802858871244	-0.188553956073	1.378057818087
H	-0.056518741683	-1.764274630917	-0.435472241041
H	0.299622626362	-0.513300336769	-1.638057565353
F	-1.467768250205	1.177588147718	-0.708591940267
F	-2.223434382666	-0.775544864725	-1.226095285761
Cl	-1.992284301856	-0.339287723775	1.285828554413

Infrared Absorption Spectrum (unscaled frequencies)

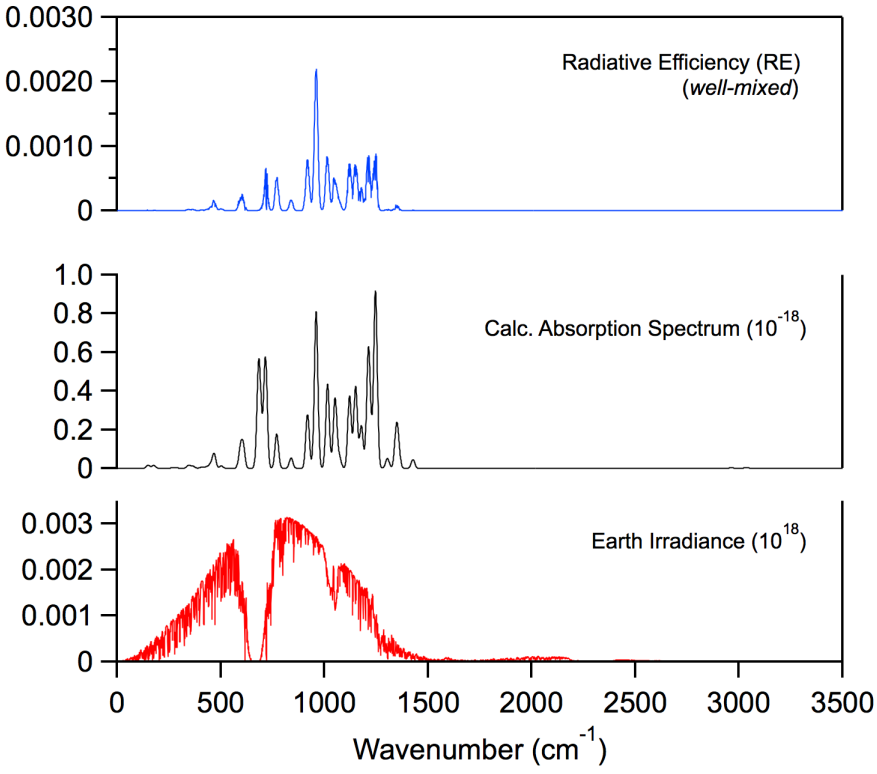
Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
30.2063	0.0385
101.9368	0.294
135.0612	0.199
228.8499	0.208
246.3526	0.135
303.1880	0.302
332.5957	0.221
373.3352	0.295
417.0162	0.744
475.6558	0.720
587.3101	6.55
664.4857	11.3
677.0723	9.65
758.8139	10.4
917.5030	3.87
1018.5671	25.6
1079.2142	3.40
1161.8356	24.8
1191.2617	12.9
1236.8965	4.66
1261.7259	22.6
1320.0459	0.820
1380.0420	5.78
1455.0419	0.829
3075.3077	0.103
3131.6049	0.0420
3161.6503	0.114

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
30.2060	0.0385
101.9371	0.294
135.0617	0.199
228.8502	0.208
246.3526	0.135
303.1880	0.302
332.5957	0.221
373.3353	0.295
417.0160	0.744
475.6559	0.720
587.3099	6.55
664.4855	11.3
677.0719	9.65
758.8141	10.4
917.5029	3.87
1018.5668	25.6
1079.2152	3.40
1161.8353	24.8
1191.2616	12.9
1236.8965	4.66
1261.7256	22.6
1320.0456	0.820
1380.0421	5.78
1455.0423	0.829
3075.3080	0.103
3131.6054	0.0420
3161.6502	0.114

Infrared Spectrum

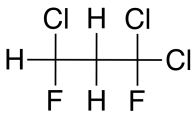


Radiative Efficiency



HCFC-242fb

Molecular Formula:	$CHClFCH_2CCl_2F$
Name:	1,1,3-Trichloro-1,3-difluoropropane
CAS number:	175897-95-7
Molecular Weight:	183.41



Global Atmospheric Lifetime (years):	1.61
Tropospheric Atmospheric Lifetime (years):	1.71
Stratospheric Atmospheric Lifetime (years):	26.1
Ozone Depletion Potential (ODP):	0.031

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.249	0.203
Global Warming Potential (GWP_H):		
GWP_{20}	491	400
GWP_{100}	133	108
Global Temperature Potentials (GTP_H)		
GTP_{20}		140
GTP_{50}		19
GTP_{100}		15

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 3.42 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 2.18 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 1.66$ years

$\tau^{OH}_{Trop} = 1.71$ years

$\tau^{OH}_{Strat} = 54.8$ years

Fractional Atmospheric Loss: 0.968

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: 0.009

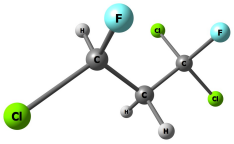
UV Photolysis

UV Spectrum: *No Recommendation*

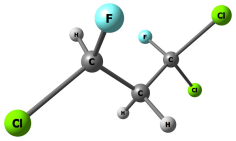
$\tau_{hv} = 68$ years

Fractional Atmospheric Loss: 0.023

Molecular Structure and Infrared Spectrum (4 conformers)



E = 0
Population = 0.557



$\Delta E = 0.52$ kcal mol^{-1}
Population = 0.231

Optimized Coordinates (Angstroms)

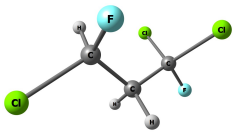
Atom	X	Y	Z
C	-1.495934214481	-0.328832637036	-0.027687671374
C	-0.331206094072	0.625592606013	0.210808654199
C	1.028486331052	0.038590815316	-0.168684622978
Cl	-3.021788662106	0.450403034389	0.554625017996
F	-1.623687260765	-0.603163289238	-1.345376853504
H	-1.407915328425	-1.263785060850	0.526866330111
H	-0.305379211591	0.916096805806	1.260998530773
H	-0.483482723648	1.522868697723	-0.395434728142
F	1.064262622843	-0.311487236062	-1.457715848139
Cl	2.311514923970	1.272724768066	0.107659995240
Cl	1.409854617223	-1.430169504128	0.811445195819

Atom	X	Y	Z
C	-1.510329543699	-0.155047085934	0.362653903516
C	-0.341710236141	0.623137731935	-0.235032673943
C	1.023921364746	0.136562239025	0.253678543380
Cl	-3.048276833466	0.732597238679	0.013084513084
F	-1.601969615570	-1.393687740708	-0.168966099178
H	-1.449779765503	-0.234096262039	1.449086968200
H	-0.431535086664	1.667392411032	0.071713756283
H	-0.383884916907	0.576323369108	-1.324110894897
F	1.038283804471	0.102082224565	1.599160161733
Cl	1.441251410973	-1.502555178848	-0.341085873045
Cl	2.297119417762	1.295313053187	-0.280414305133

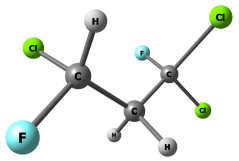
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
37.2873	0.0660
103.3128	0.362
129.1121	0.226
210.2693	0.0229
252.5061	0.0383
289.6714	0.320
332.4079	0.223
384.4432	0.407
391.1581	0.613
449.4674	0.687
490.3541	3.24
617.0128	13.6
724.4722	26.4
859.7642	19.3
887.9026	3.92
985.6307	10.1
1069.2738	7.51
1134.2710	9.65
1191.0428	27.2
1244.1764	6.72
1289.4684	1.19
1356.6058	6.18
1399.1138	3.11
1447.9000	0.776
3084.6249	0.0363
3120.3123	1.00
3155.3161	0.0545

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
32.8997	0.0646
103.0235	0.375
131.3709	0.403
212.2561	0.0421
236.6198	0.0909
272.9506	0.0596
365.9539	0.153
377.2788	0.410
396.3428	0.536
446.9901	0.704
487.2041	2.98
633.7197	15.5
722.4451	23.2
840.9511	14.3
915.7782	5.26
957.3789	8.07
1084.2156	15.0
1139.5573	25.4
1168.1611	14.8
1239.8463	2.64
1284.6806	1.10
1357.8384	6.07
1400.8510	2.84
1450.1765	0.808
3091.7996	0.0385
3115.1062	1.00
3153.3444	0.0422



$\Delta E = 0.82$ kcal mol^{-1}
Population = 0.139



$\Delta E = 1.20$ kcal mol^{-1}
Population = 0.073

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.369346218196	-0.035203864766	-0.390574667646
C	-0.391654308269	-0.288951312798	0.747253588384
C	1.095028484304	-0.181546753419	0.402413301272
Cl	-3.037278886496	-0.469912402343	0.165744058225
F	-1.367697012526	1.265433530869	-0.756974805593
H	-1.176831059802	-0.655750746643	-1.266571587990
H	-0.544424915753	-1.303200225361	1.123425910267
H	-0.595389575632	0.415419121717	1.558525282846
F	1.798907534679	-0.533202746567	1.489925763669
Cl	1.542021958423	-1.326191205529	-0.922533784740
Cl	1.594745999268	1.477650604840	-0.053561058694

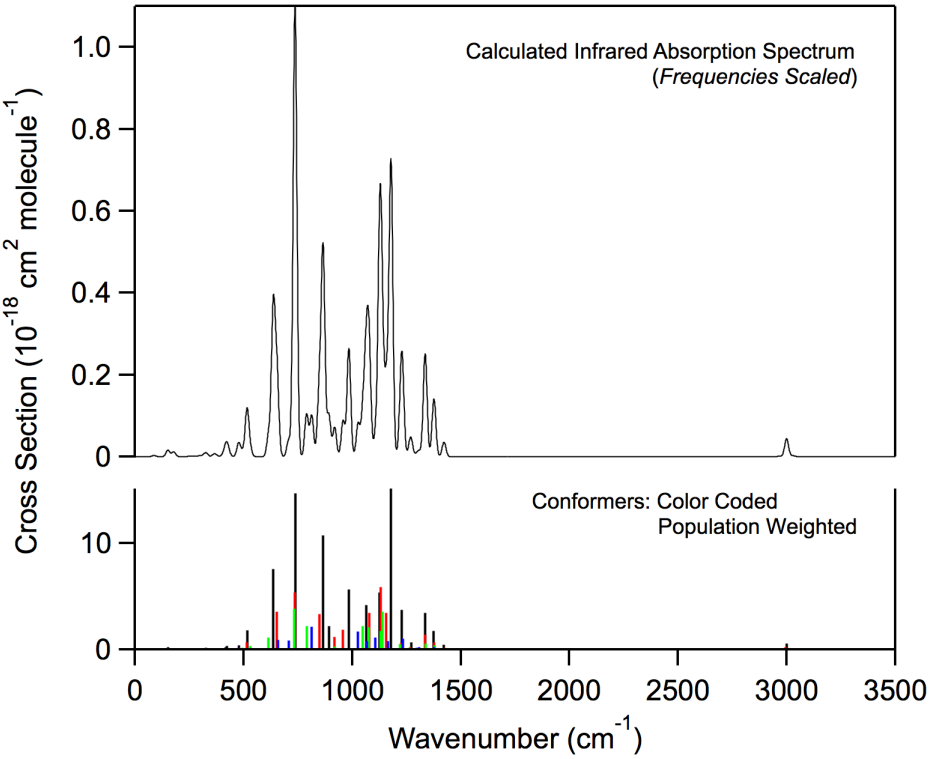
Atom	X	Y	Z
C	-1.560141207490	0.183318182341	-0.606967710958
C	-0.228302710432	0.882275291123	-0.341846869831
C	0.913926861285	-0.006436215814	0.138696906960
Cl	-2.393274321924	-0.310348619504	0.913357033378
F	-2.359139378614	1.061831171014	-1.263792931333
H	-1.457803882009	-0.723753207269	-1.203538449766
H	-0.375786753778	1.671373556818	0.400148947567
H	0.080058345988	1.346981586170	-1.281396454636
F	0.643072548367	-0.575486873360	1.315868785100
Cl	1.263041459662	-1.328193018341	-1.042966273520
Cl	2.398356038946	0.996474146821	0.341956017039

Infrared Absorption Spectrum (unscaled frequencies)

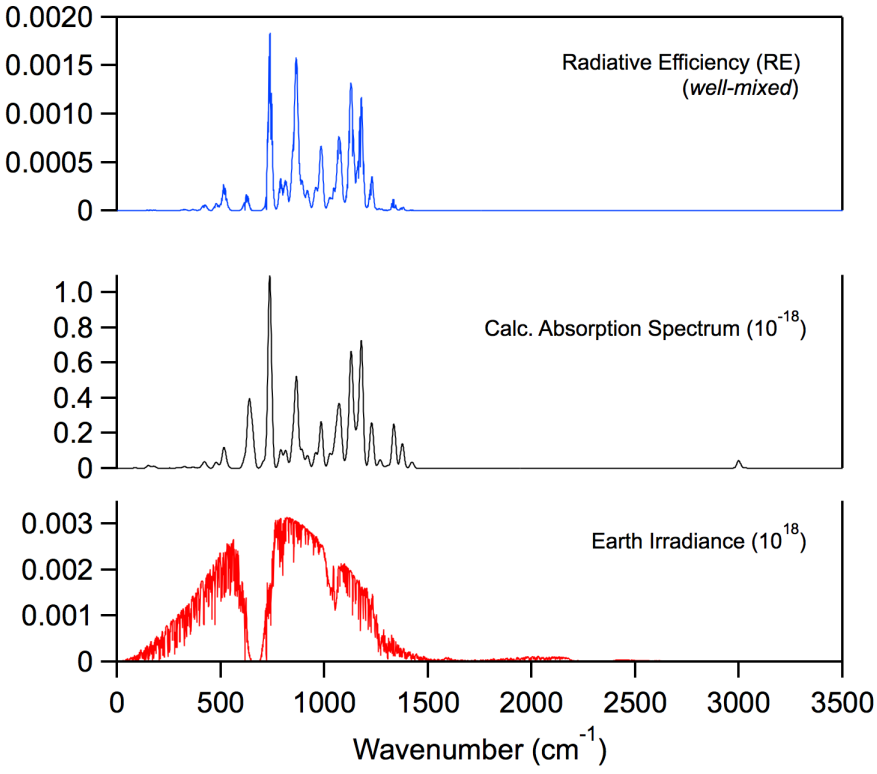
Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
34.9174	0.0783
100.0692	0.270
138.9837	0.241
214.0090	0.0933
254.4428	0.136
275.1174	0.317
344.3147	0.123
388.5741	0.436
398.9813	0.273
466.7396	1.30
505.7459	2.27
594.5742	8.23
719.0888	27.7
779.4683	15.8
917.6225	2.23
1053.7656	15.8
1083.2275	15.1
1139.3102	12.6
1149.1404	25.5
1233.3457	3.82
1280.4839	1.34
1361.2899	4.19
1404.0185	3.04
1451.5382	0.693
3076.7110	0.0214
3118.3205	0.747
3137.1077	0.240

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
30.0489	0.0358
106.8603	0.287
133.5840	0.243
202.3100	0.0332
280.5240	0.191
302.0152	0.163
323.1316	0.541
385.6468	0.498
402.7088	0.819
448.4060	2.44
474.3962	1.05
639.0632	12.3
691.4825	11.3
804.6328	29.3
925.1989	0.112
1030.4521	23.4
1073.5127	11.1
1115.7280	15.3
1176.2276	10.8
1247.8072	14.3
1317.6466	2.05
1328.9659	3.23
1401.8388	3.51
1454.1336	0.891
3077.9725	0.0269
3118.8525	0.837
3136.3613	0.239

Infrared Spectrum

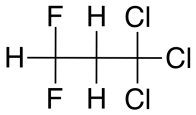


Radiative Efficiency



HCFC-242fc

Molecular Formula:	$CHF_2CH_2CCl_3$
Name:	1,1,1-Trichloro-3,3-difluoropropane
CAS number:	213248-60-3
Molecular Weight:	183.41



Global Atmospheric Lifetime (years):	4.14
Tropospheric Atmospheric Lifetime (years):	4.78
Stratospheric Atmospheric Lifetime (years):	30.6
Ozone Depletion Potential (ODP):	0.075

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.217	0.198
Global Warming Potential (GWP_H):		
GWP_{20}	1096	997
GWP_{100}	299	272
Global Temperature Potentials (GTP_H)		
GTP_{20}		496
GTP_{50}		54
GTP_{100}		38

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 1.23 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 0.782 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 4.62$ years

$\tau^{OH}_{Trop} = 4.78$ years

$\tau^{OH}_{Strat} = 138.2$ years

Fractional Atmospheric Loss: 0.895

$O(^1D)$ 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: 0.022

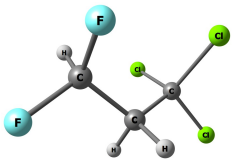
UV Photolysis

UV Spectrum: *No Recommendation*

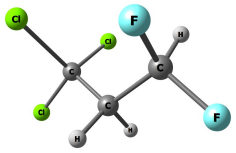
$\tau_{hv} = 50$ years

Fractional Atmospheric Loss: 0.083

Molecular Structure and Infrared Spectrum (2 conformers)



E = 0
Population = 0.493



E = 0
Population = 0.493

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.937999007275	-0.278612361003	0.145200795475
C	0.655875173522	-0.638469682831	-0.603699349206
C	-0.650718439108	-0.079871077579	-0.039739832147
F	2.928826753417	-1.058488187070	-0.359692957721
F	2.282452624175	1.011104814148	-0.072220856205
H	1.877458004892	-0.447174593259	1.225600462730
H	0.570441756030	-1.727708958700	-0.605381036940
H	0.759925952927	-0.298422719176	-1.637528681706
Cl	-2.009976014114	-0.695879521345	-1.047114187290
Cl	-0.897724660628	-0.647874059276	1.653406553122
Cl	-0.688067158387	1.708236346090	-0.062476910113

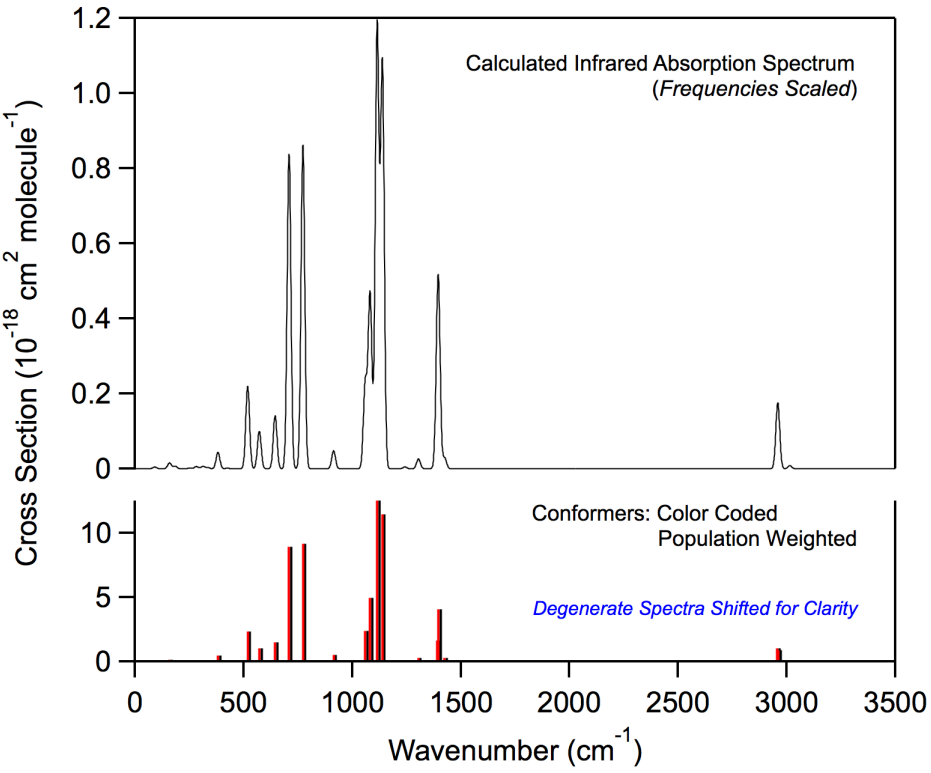
Atom	X	Y	Z
C	1.938936173178	0.280909634603	0.152881823667
C	0.654912533465	0.667536739704	-0.579234290151
C	-0.650066770799	0.087399794605	-0.033579144474
F	2.283686284269	-0.999569945316	-0.113222214056
F	2.928150660723	1.079747434276	-0.324795564340
H	1.880720396742	0.409046966331	1.238945095788
H	0.756846564215	0.366324955016	-1.625247004627
H	0.568808855466	1.756022390965	-0.540131415917
Cl	-2.011964202313	0.739568716322	-1.014273769339
Cl	-0.686362743514	-1.698644400934	-0.122850957688
Cl	-0.893617751429	0.591743714429	1.680102441137

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
39.5081	0.0933
111.3715	0.333
138.6366	0.150
211.5581	0.0469
242.1366	0.124
274.1295	0.133
297.0110	0.0721
347.5290	0.942
394.1751	0.0302
492.2645	4.75
548.9952	2.16
626.1482	3.05
693.9457	18.1
761.5753	18.6
911.1183	1.03
1065.3878	4.88
1088.7550	10.1
1123.2832	25.4
1148.9641	23.2
1258.9657	0.100
1324.7370	0.574
1417.1333	3.34
1422.2742	8.25
1452.4053	0.621
3074.0347	2.16
3078.9599	1.81
3134.8175	0.176

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
39.5087	0.0933
111.3727	0.333
138.6374	0.150
211.5582	0.0469
242.1366	0.124
274.1295	0.133
297.0110	0.0721
347.5292	0.942
394.1748	0.0302
492.2648	4.75
548.9949	2.16
626.1481	3.05
693.9457	18.1
761.5755	18.6
911.1180	1.03
1065.3879	4.88
1088.7542	10.1
1123.2840	25.4
1148.9629	23.2
1258.9646	0.100
1324.7363	0.574
1417.1329	3.34
1422.2734	8.25
1452.4048	0.621
3074.0350	2.16
3078.9602	1.81
3134.8174	0.176

Infrared Spectrum



Radiative Efficiency