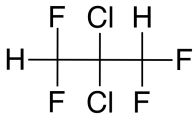
HCFC-234aa

Molecular Formula:	$CHF_2CCl_2CHF_2$
Name:	2,2-Dichloro-1,1,3,3-tetrafluoropropane
CAS number:	17705-30-5
Molecular Weight:	184.95



Global Atmospheric Lifetime (years):	6.51
Tropospheric Atmospheric Lifetime (years):	7.54
Stratospheric Atmospheric Lifetime (years):	47.4
Ozone Depletion Potential (ODP):	0.062

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.212	0.198
Global Warming Potential (GWP_H):		
GWP_{20}	1601	1499
GWP_{100}	455	426
Global Temperature Potentials (GTP_H)		
GTP_{20}		940
GTP_{50}		105
GTP_{100}		60

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 7.77 \times 10^{-15}$; $k_{SAR}(272\ K) \approx 4.69 \times 10^{-15}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 7.28$ years

$\tau^{OH}_{Trop} = 7.54$ years

$\tau^{OH}_{Strat} = 208.3$ years

Fractional Atmospheric Loss: 0.894

$O(^1D)$ Reactivity

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

$k_{Est}(T) = 1.4 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 265$ years

Fractional Atmospheric Loss: 0.025

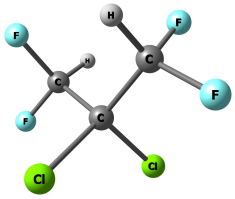
UV Photolysis

UV Spectrum: *No Recommendation*

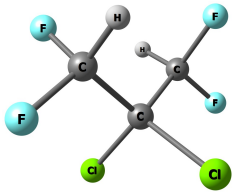
$\tau_{hv} = 80$ years

Fractional Atmospheric Loss: 0.081

Molecular Structure and Infrared Spectrum (5 conformers)



E = 0
Population = 0.352



E = 0
Population = 0.352

Optimized Coordinates (Angstroms)

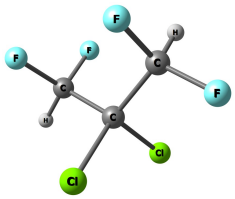
Atom	X	Y	Z
C	1.183008050714	0.758827076616	0.437001888066
C	-0.002354200537	-0.131753641102	0.002739922295
C	-1.183437450248	0.748513750819	-0.463079276398
F	2.258690959135	0.010408568664	0.714938416147
F	1.488670471274	1.591578833667	-0.586591422647
H	0.908035008623	1.352902041706	1.314297423773
Cl	-0.499055341028	-1.114047728461	1.409075370905
Cl	0.489490800856	-1.165905087834	-1.367667621190
H	-0.905663979200	1.309624220169	-1.360953863398
F	-2.262747599015	-0.004120497287	-0.714286684685
F	-1.484993720574	1.618667463043	0.530168847132

Atom	X	Y	Z
C	1.181580534379	0.753798518468	-0.451130563822
C	-0.001128605539	-0.132389629447	-0.000936861772
C	-1.182443077820	0.752538778743	0.455360153202
F	1.488575731960	1.601671722630	0.559568350898
F	2.257770280734	0.003224874314	-0.721181799572
H	0.903274496393	1.334756532269	-1.336125270266
Cl	0.496088902506	-1.145938618750	1.382858417736
Cl	-0.499930193199	-1.135597728625	-1.391679439081
H	-0.903227919622	1.326940785137	1.344338855152
F	-1.488094986949	1.607843604371	-0.549466801952
F	-2.259817162843	0.001819160891	0.720234959476

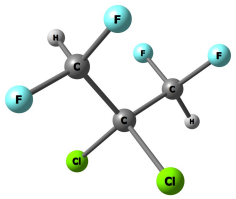
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
79.7222	0.238
87.9076	0.210
148.2286	0.00754
177.8436	0.0776
211.7380	0.354
223.2713	0.313
258.1382	0.0928
338.0453	0.129
368.9433	0.122
425.6123	0.000
549.5908	2.53
582.7808	0.440
645.6374	11.6
692.9864	8.06
891.9113	16.3
1051.9292	2.16
1055.8609	0.897
1128.7582	17.6
1148.9818	14.1
1185.7871	32.9
1200.3527	8.55
1373.5621	4.55
1379.7955	6.85
1395.8374	0.405
1396.8256	5.11
3088.0050	0.851
3088.7139	3.21

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
79.7227	0.238
87.9074	0.210
148.2281	0.00754
177.8441	0.0776
211.7382	0.354
223.2717	0.313
258.1378	0.0928
338.0454	0.129
368.9432	0.122
425.6124	0.000
549.5906	2.53
582.7807	0.440
645.6372	11.6
692.9869	8.06
891.9112	16.3
1051.9289	2.16
1055.8628	0.897
1128.7582	17.6
1148.9823	14.1
1185.7870	32.9
1200.3519	8.55
1373.5622	4.55
1379.7953	6.85
1395.8366	0.405
1396.8248	5.11
3088.0060	0.851
3088.7149	3.21



$\Delta E = 0.60$ kcal mol^{-1}
Population = 0.128



$\Delta E = 0.60$ kcal mol^{-1}
Population = 0.128

Optimized Coordinates (Angstroms)

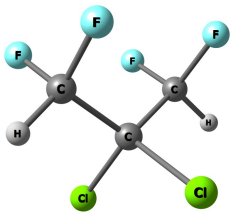
Atom	X	Y	Z
C	0.574491454845	0.668157554981	-1.013766205179
C	0.079968949403	-0.218166360711	0.154132146627
C	-1.465544067914	-0.259013756579	0.244283727419
F	0.161693396739	1.934696848781	-0.815679715453
F	1.916599460003	0.658774600728	-1.061101032769
H	0.170219068013	0.296444614311	-1.961063807855
Cl	0.728596136142	0.382030498219	1.700827882791
Cl	0.634762477323	-1.894940346342	-0.161417201559
H	-1.789298177618	-0.997615112739	0.984656196071
F	-1.949008070906	0.951425215583	0.567771803545
F	-1.953790626031	-0.593631756232	-0.973567793638

Atom	X	Y	Z
C	0.578956432698	-0.657281667861	-1.018027067013
C	0.076862699445	0.217871586877	0.155053319419
C	-1.468956311228	0.245451631926	0.244987935615
F	1.920953416318	-0.636563750913	-1.064904728365
F	0.176553000701	-1.928349680505	-0.827712360080
H	0.171871746038	-0.283195852357	-1.963183812855
Cl	0.617911753157	1.901030697072	-0.150199954020
Cl	0.730022617740	-0.386297423160	1.698291280362
H	-1.798964261067	0.976875620230	0.989711892943
F	-1.959637496759	0.583393317019	-0.970965855845
F	-1.942519597042	-0.970858478327	0.561013349839

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
65.5633	0.173
100.7452	0.0937
159.6162	0.0512
171.0300	0.0786
213.5318	0.260
244.8328	0.192
255.5977	0.211
333.8302	0.238
391.4554	0.243
402.3067	0.508
529.8260	3.56
571.0668	1.47
653.2288	6.56
716.4709	7.60
874.4179	18.7
1003.0379	4.29
1115.0786	0.860
1130.6060	15.7
1151.1055	1.40
1179.9994	26.7
1189.1219	30.3
1368.7961	4.91
1386.2067	1.38
1394.9127	2.55
1404.0695	6.61
3083.3205	2.04
3084.9562	2.82

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
65.5633	0.173
100.7453	0.0937
159.6161	0.0512
171.0300	0.0786
213.5319	0.260
244.8328	0.192
255.5978	0.211
333.8303	0.238
391.4554	0.243
402.3068	0.508
529.8260	3.56
571.0668	1.47
653.2288	6.56
716.4710	7.60
874.4180	18.7
1003.0380	4.29
1115.0789	0.860
1130.6060	15.7
1151.1055	1.40
1179.9993	26.7
1189.1218	30.3
1368.7959	4.91
1386.2065	1.38
1394.9125	2.55
1404.0693	6.61
3083.3205	2.04
3084.9563	2.82



$\Delta E = 1.41$ kcal mol^{-1}
Population = 0.032

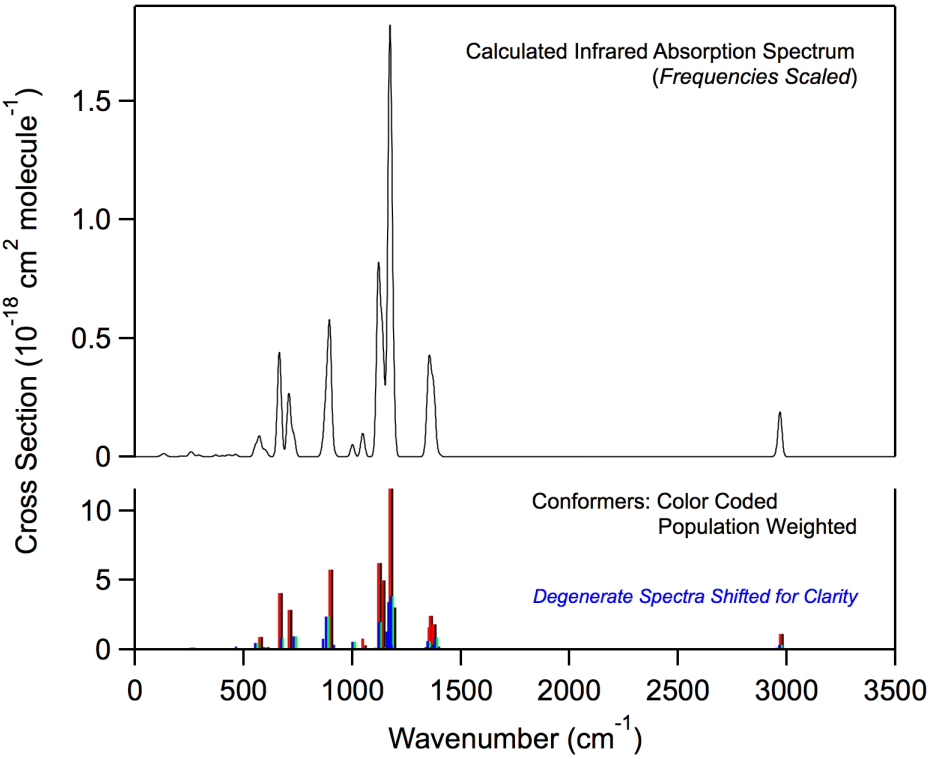
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-0.456764132481	-0.015659865438	-1.309313506955
C	0.375118600153	0.002921755345	-0.000222207933
C	-0.455370024287	0.011890688643	1.309855111475
F	-1.237157953096	-1.111530902429	-1.337086366963
F	-1.249799699949	1.070270196700	-1.360018031355
H	0.213820567355	-0.020883920877	-2.175974934167
Cl	1.389382933520	1.477966107196	-0.016279319831
Cl	1.406388618357	-1.460297516594	0.014621995444
H	0.216137421493	0.024870800566	2.175720377660
F	-1.248347743893	1.098666078338	1.338563524647
F	-1.235736587173	-1.083135421451	1.361491357977

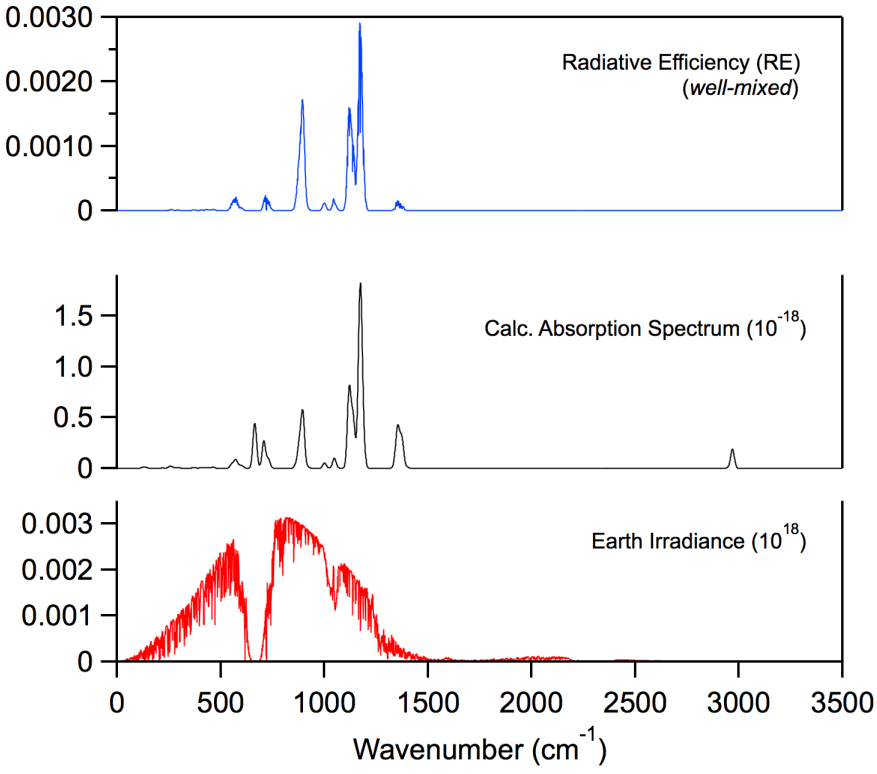
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
44.3002	0.000
121.7511	0.303
161.6109	0.0
176.4757	0.00485
214.1704	0.0727
251.1191	0.00101
270.3291	0.152
363.5130	0.0
399.7724	0.0381
406.9760	0.703
433.6739	6.64
573.4459	2.25
584.5594	0.469
858.7845	23.4
873.4996	0.969
913.4467	11.0
1116.5087	0.0272
1139.4311	0.0
1168.8405	39.7
1182.5397	26.0
1192.6998	9.35
1360.1627	5.10
1387.4885	0.0
1397.1011	3.19
1425.0768	6.89
3069.4304	3.35
3073.3628	2.87

Infrared Spectrum

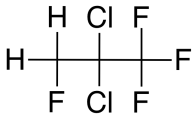


Radiative Efficiency



HCFC-234ab

Molecular Formula:	$CH_2FCCl_2CF_3$
Name:	2,2-Dichloro-1,1,1,3-tetrafluoropropane
CAS number:	149329-24-8
Molecular Weight:	184.95



Global Atmospheric Lifetime (years):	3.76
Tropospheric Atmospheric Lifetime (years):	4.14
Stratospheric Atmospheric Lifetime (years):	40.8
Ozone Depletion Potential (ODP):	0.039

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.238	0.215
Global Warming Potential (GWP_H):		
GWP_{20}	1085	979
GWP_{100}	295	267
Global Temperature Potentials (GTP_H)		
GTP_{20}		464
GTP_{50}		51
GTP_{100}		37

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

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

OH Reactivity

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

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

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

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

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

Fractional Atmospheric Loss: 0.939

$O(^1D)$ Reactivity

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

$k_{Est}(T) = 1.4 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 265$ years

Fractional Atmospheric Loss: 0.014

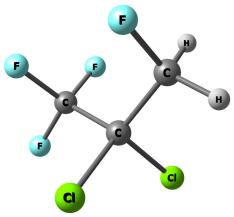
UV Photolysis

UV Spectrum: *No Recommendation*

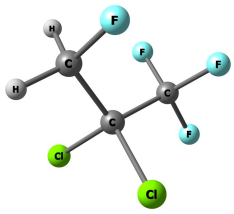
$\tau_{hv} = 80$ years

Fractional Atmospheric Loss: 0.047

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.448



E = 0
Population = 0.448

Optimized Coordinates (Angstroms)

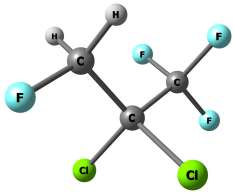
Atom	X	Y	Z
C	-0.990837141420	0.677310333854	1.232580100830
C	-0.387712875974	-0.151303517115	0.090093374013
C	1.122306176470	0.146092001728	-0.124446174843
H	-0.425462981390	0.474290164405	2.147645735521
F	-0.920455488042	2.009719018664	0.938397859613
H	-2.034976347236	0.380510011568	1.364059910190
Cl	-1.250790865385	0.180357816232	-1.438256856330
Cl	-0.557870963881	-1.875030587735	0.556306390383
F	1.653973346859	-0.663774522104	-1.031961794893
F	1.299284702450	1.402911698777	-0.519706712145
F	1.773999437549	-0.023750418274	1.031815167660

Atom	X	Y	Z
C	-0.952607187645	0.731075769208	-1.232444381067
C	-0.396009063147	-0.129052904514	-0.089635593389
C	1.127563396564	0.086851115385	0.126576643789
H	-2.011020641839	0.490744002805	-1.365130271818
F	-0.811177699652	2.057698065842	-0.937690069504
H	-0.397959422986	0.498312976390	-2.146992188248
Cl	-0.657896201710	-1.841025275323	-0.556657323994
Cl	-1.241670449137	0.247954456703	1.437936753561
F	1.614068514228	-0.750640533287	1.034353282489
F	1.770428505056	-0.117353753756	-1.029068376537
F	1.371285250267	1.332250080547	0.522468524717

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
62.2935	0.0479
123.5130	0.304
166.0179	0.0151
194.8609	0.217
228.2584	0.388
259.1322	0.179
290.7926	0.406
331.8126	0.0394
368.9574	0.152
409.1316	0.0852
519.6772	3.01
555.1684	1.18
601.3860	2.92
711.9295	6.24
822.3612	8.75
884.5648	13.7
1070.3150	4.82
1091.4321	6.08
1127.3331	8.03
1216.2111	25.6
1244.5063	27.1
1258.3398	26.5
1304.2205	8.18
1417.9819	2.70
1494.6526	0.981
3059.4184	1.58
3120.2914	1.24

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
62.2914	0.0479
123.5142	0.304
166.0177	0.0151
194.8604	0.217
228.2582	0.388
259.1319	0.179
290.7919	0.406
331.8129	0.0394
368.9572	0.152
409.1316	0.0852
519.6774	3.01
555.1684	1.18
601.3863	2.92
711.9293	6.24
822.3615	8.75
884.5641	13.7
1070.3158	4.82
1091.4322	6.08
1127.3331	8.03
1216.2104	25.6
1244.5045	27.1
1258.3393	26.5
1304.2191	8.17
1417.9818	2.70
1494.6538	0.981
3059.4185	1.58
3120.2913	1.24



$\Delta E = 0.87$ kcal mol^{-1}
Population = 0.103

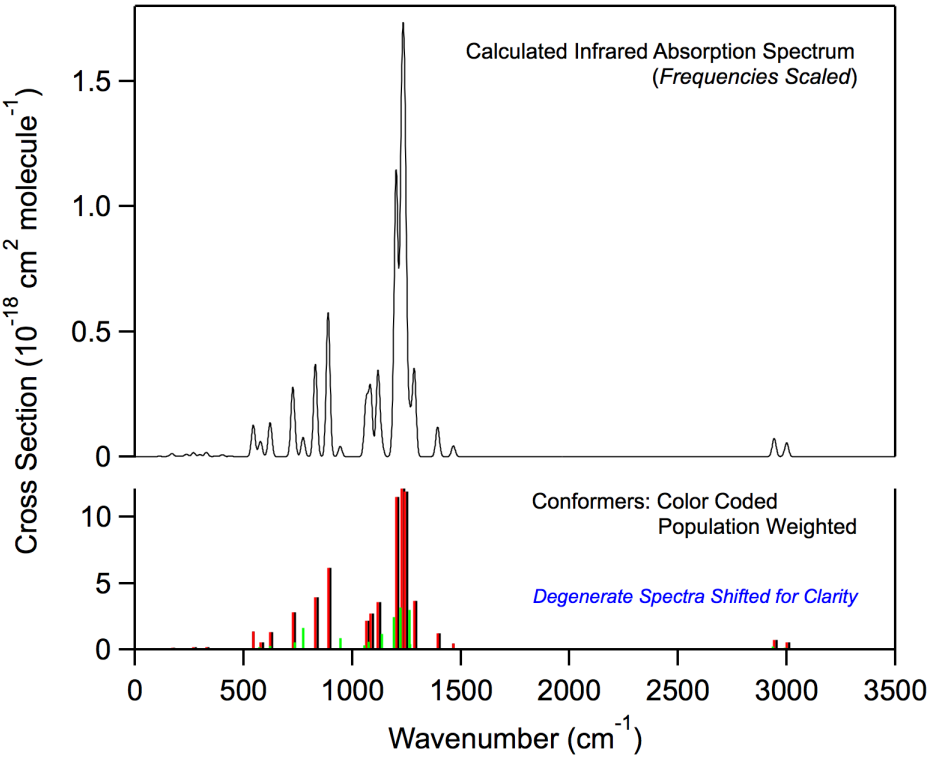
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-0.999281702752	-0.000717936326	1.342870453259
C	-0.268283449701	0.000254188111	-0.006225176474
C	1.266034025564	-0.000517513529	0.217928493037
H	-0.708341609842	0.895493287242	1.900200835976
F	-2.346118719986	-0.000051178033	1.143184749582
H	-0.708986532047	-0.898155941001	1.898560933220
Cl	-0.705695190617	1.469046592611	-0.931938732942
Cl	-0.706774194062	-1.466508425732	-0.934641360127
F	1.937587085141	0.000293396672	-0.922522036413
F	1.617884807483	1.078987445878	0.924451156575
F	1.617090480818	-1.081589915893	0.922446684306

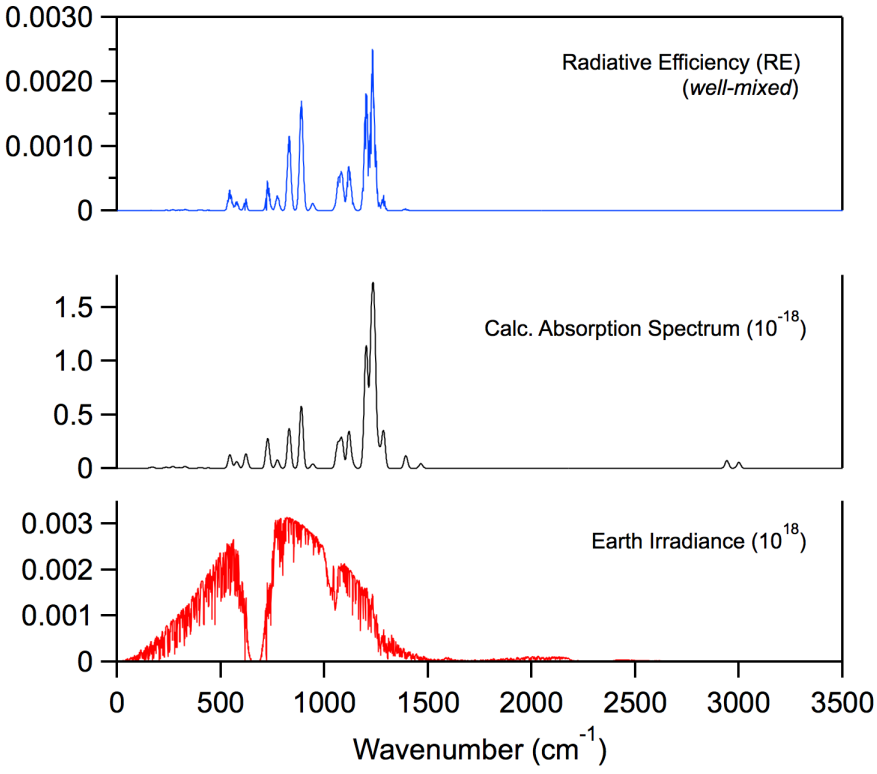
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
68.9949	0.0333
106.0656	0.339
156.6624	0.299
180.9924	0.279
216.8893	0.00609
261.4130	0.180
306.0874	0.0637
348.5681	0.0935
367.0538	0.288
376.7916	0.138
547.9464	1.59
553.3457	1.24
603.0628	2.78
720.7499	5.28
762.4769	15.9
943.1724	8.46
1062.6202	3.27
1081.5798	5.63
1145.0937	11.3
1205.0808	23.5
1237.9535	30.6
1281.8447	28.8
1283.1535	4.16
1419.9138	1.06
1502.5889	0.542
3051.5663	1.98
3110.0732	1.32

Infrared Spectrum

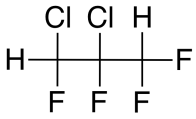


Radiative Efficiency



HCFC-234ba

Molecular Formula:	$CHClFCClFCHF_2$
Name:	1,2-Dichloro-1,2,3,3-tetrafluoropropane
CAS number:	425-94-5
Molecular Weight:	184.95



Global Atmospheric Lifetime (years):	3.39
Tropospheric Atmospheric Lifetime (years):	3.61
Stratospheric Atmospheric Lifetime (years):	56.9
Ozone Depletion Potential (ODP):	0.028

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.240	0.215
Global Warming Potential (GWP_H):		
GWP_{20}	987	883
GWP_{100}	268	240
Global Temperature Potentials (GTP_H)		
GTP_{20}		398
GTP_{50}		45
GTP_{100}		34

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 1.63 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 1.04 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 3.49$ years

$\tau^{OH}_{Trop} = 3.61$ years

$\tau^{OH}_{Strat} = 107.1$ years

Fractional Atmospheric Loss: 0.972

O(^{1}D) Reactivity

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

$k_{Est}(T) = 1.4 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 265$ years

Fractional Atmospheric Loss: 0.013

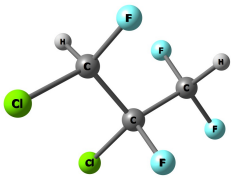
UV Photolysis

UV Spectrum: *No Recommendation*

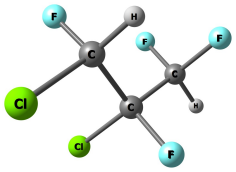
$\tau_{hv} = 225$ years

Fractional Atmospheric Loss: 0.015

Molecular Structure and Infrared Spectrum (14 conformers)



E = 0
Population = 0.185



$\Delta E = 0.06$ kcal mol^{-1}
Population = 0.166

Optimized Coordinates (Angstroms)

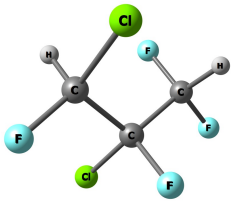
Atom	X	Y	Z
C	0.960010440206	-0.582297835518	-0.433721358255
C	-0.235986737914	0.086645545797	0.271043140162
C	-1.522749085398	-0.741895434691	0.049067053711
Cl	2.509294429713	0.157141513129	0.045334517486
F	0.963084114883	-1.893979927796	-0.073276789168
H	0.866462431890	-0.500647566018	-1.516191112311
Cl	-0.460249741459	1.740720232788	-0.367605001603
F	-0.022890360745	0.132263856449	1.602759558480
H	-1.421922635796	-1.717586166517	0.535798135970
F	-2.576765161801	-0.092713594280	0.564468269113
F	-1.714544693578	-0.914846623342	-1.276753413583

Atom	X	Y	Z
C	-0.685774349405	0.823596198418	-0.167628425850
C	0.245293781447	-0.279907015870	0.374019868854
C	1.738628349617	0.088705978621	0.207982699212
F	-0.549514840085	0.914738555703	-1.503773119141
Cl	-2.392415674873	0.507566064890	0.258691087690
H	-0.413844438531	1.772629378781	0.298806313922
Cl	-0.045827310410	-1.846098580456	-0.431287358676
F	0.033714537969	-0.403280426640	1.704431678267
H	2.366887585799	-0.659958489775	0.703271006194
F	2.071645166956	0.189327946490	-1.086962733725
F	1.932994191515	1.294280389838	0.796128983254

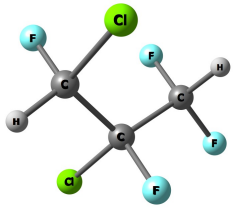
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
65.0198	0.0910
74.9025	0.272
139.0900	0.0561
193.2610	0.101
210.9957	0.562
231.6939	0.0919
303.7043	0.295
325.4646	0.103
374.4618	0.131
436.1284	0.239
484.5081	0.548
567.6937	3.95
668.7545	12.0
774.5913	11.6
797.3268	11.4
1000.4800	12.8
1082.2915	8.46
1096.7019	6.21
1158.2809	23.8
1197.2823	19.1
1208.6472	11.1
1287.5875	1.98
1362.9445	1.06
1380.3245	6.94
1400.0498	3.01
3084.3438	2.57
3136.0897	0.543

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
53.2686	0.154
90.4216	0.106
149.0810	0.0919
181.0757	0.0251
202.8899	0.247
226.8179	0.195
317.4449	0.141
345.3558	0.0872
400.6595	0.395
425.7597	0.524
540.4206	1.68
555.0013	10.3
612.7277	2.67
669.0763	9.45
850.8873	8.78
1000.5617	13.2
1117.2161	5.04
1135.7593	5.86
1171.9549	41.2
1176.2418	1.36
1192.1365	17.2
1294.4077	3.73
1359.5757	1.71
1384.4427	1.98
1399.5898	7.29
3076.3727	3.27
3110.6985	0.556



$\Delta E = 0.11$ kcal mol^{-1}
Population = 0.154



$\Delta E = 0.19$ kcal mol^{-1}
Population = 0.134

Optimized Coordinates (Angstroms)

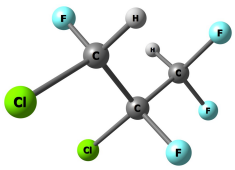
Atom	X	Y	Z
C	-1.062109864478	-0.392131337007	-0.502381292177
C	0.252031842665	-0.198260366327	0.276299836611
C	0.912655144374	1.171933015147	0.019625535849
F	-1.587676809828	-1.590972609168	-0.200146033816
Cl	-2.248541074817	0.888484526309	-0.046605062234
H	-0.894548715557	-0.303126018116	-1.575360645581
Cl	1.372368226411	-1.506336818485	-0.236540071659
F	0.018847517185	-0.306690680839	1.600010341253
H	0.302812687989	1.972437013134	0.451170751451
F	2.134253311928	1.197806463907	0.573148498554
F	1.026061734129	1.359126811443	-1.314040858250

Atom	X	Y	Z
C	1.070238353749	0.730615231278	-0.076726649973
C	-0.276271696903	0.168229556757	0.421516364670
C	-0.701753418856	-1.176451893241	-0.206705534885
Cl	2.404374944622	-0.429966826470	0.281162731599
F	1.029550164458	0.966374367420	-1.397309819162
H	1.303684830441	1.646398581754	0.469443422558
Cl	-1.528651053592	1.411707297437	0.096089994294
F	-0.176630406384	-0.018279824661	1.756774747552
H	0.039647993083	-1.949875716224	0.022094576040
F	-1.890168227936	-1.537328062257	0.308926053689
F	-0.820193482682	-1.043175711793	-1.539080886384

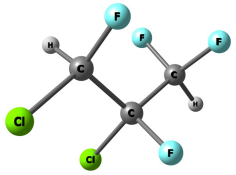
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
61.2473	0.164
77.8640	0.201
142.6000	0.0522
197.4172	0.176
203.3713	0.494
255.6030	0.111
270.7330	0.0227
340.6330	0.134
375.3830	0.208
416.1526	0.524
484.6677	0.339
578.1050	1.91
657.7573	15.1
755.3768	22.2
781.8429	4.28
986.1568	7.55
1084.7855	8.49
1137.1268	16.8
1170.4151	16.0
1198.3643	16.9
1216.8620	12.7
1277.7257	1.97
1373.9987	0.231
1385.1578	3.95
1403.1072	3.25
3085.5306	2.52
3136.2895	0.487

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
48.8289	0.196
92.1536	0.0786
152.6626	0.178
181.9568	0.0596
197.8128	0.164
265.5465	0.0777
276.6224	0.590
351.9941	0.0804
379.4144	0.201
417.6643	0.270
508.2889	3.14
598.8692	1.47
640.6912	7.09
679.4140	12.5
761.8369	18.4
1011.3715	3.84
1128.0478	3.24
1154.7044	9.73
1168.2592	10.4
1179.4468	39.9
1202.9269	10.6
1288.2221	1.31
1361.5046	2.68
1398.4392	2.64
1401.2697	3.48
3078.5193	2.68
3112.9286	0.772



$\Delta E = 0.26$ kcal mol^{-1}
Population = 0.119



$\Delta E = 0.71$ kcal mol^{-1}
Population = 0.056

Optimized Coordinates (Angstroms)

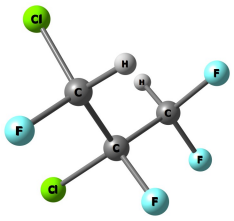
Atom	X	Y	Z
C	-0.902377220574	0.773419310061	-0.208041616621
C	0.269587153452	-0.133917131633	0.208799940900
C	1.603468770511	0.426843735874	-0.339049456272
F	-0.949351487118	0.826610457467	-1.559311513078
Cl	-2.459778322863	0.208988034340	0.447273608855
H	-0.731521704095	1.774155777572	0.192788708589
Cl	0.070061875532	-1.796935880264	-0.418084375494
F	0.336377252608	-0.152208397496	1.554894382949
H	1.637638378428	0.391125636839	-1.431644468629
F	1.711935455595	1.714355687105	0.074234378468
F	2.623852848524	-0.270759229864	0.179836410332

Atom	X	Y	Z
C	0.704742431196	-0.585579980210	-0.540836048530
C	-0.238704346567	0.255991867220	0.342927247835
C	-1.734374482239	-0.075434462054	0.105512015779
Cl	2.418492240141	-0.300020649166	-0.116738293894
F	0.416236487888	-1.891899359082	-0.347702387384
H	0.574712480997	-0.327385193886	-1.591638610163
Cl	-0.014834152848	1.997255019038	-0.041914373926
F	0.020680428709	0.042796671278	1.645887003785
H	-2.370865805817	0.662716523198	0.605553984535
F	-1.980705296175	-0.063550736043	-1.222671988249
F	-2.007700985286	-1.299639700293	0.586670450211

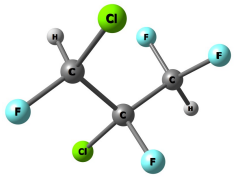
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
68.4202	0.191
73.1573	0.165
137.3975	0.0821
182.2341	0.0136
205.1456	0.510
250.3545	0.177
285.4608	0.113
342.2551	0.367
368.5971	0.0630
423.3839	0.244
512.3835	1.46
561.8799	2.37
632.3765	8.17
782.4697	25.5
835.9212	2.30
966.9573	13.4
1103.4557	6.17
1123.1718	14.8
1138.3002	18.6
1178.9854	9.87
1227.5378	21.2
1293.5584	2.17
1359.9029	2.84
1388.7801	3.24
1404.6163	3.42
3097.3421	2.54
3114.9605	0.606

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
54.8102	0.0622
84.3043	0.154
149.7529	0.0395
196.2151	0.0833
211.1695	0.445
230.6605	0.0685
310.6937	0.0513
322.0061	0.110
389.5390	0.434
436.0527	0.763
474.2364	0.636
559.0434	8.01
608.1296	8.30
788.9543	5.26
863.0981	4.20
921.7300	24.3
1106.0106	3.59
1122.5142	11.9
1149.7676	18.2
1187.0748	15.1
1215.6767	21.5
1289.7472	3.59
1367.3867	1.21
1388.1200	2.34
1402.5554	6.36
3077.0289	3.18
3132.4818	0.549



$\Delta E = 0.88$ kcal mol^{-1}
Population = 0.042



$\Delta E = 1.05$ kcal mol^{-1}
Population = 0.031

Optimized Coordinates (Angstroms)

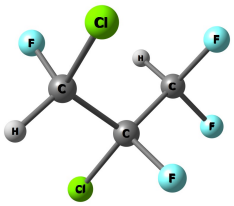
Atom	X	Y	Z
C	1.044553154896	-0.311271512202	0.668423085459
C	-0.323367845252	0.277039195251	0.272498246543
C	-1.257115288064	-0.748404771069	-0.403698463154
Cl	1.902437422757	-1.028049235491	-0.734060929271
F	1.800095943175	0.652055737586	1.221447210290
H	0.882607209763	-1.116476635797	1.387427017110
Cl	-0.139258389839	1.698091609580	-0.795506757548
F	-0.907024762593	0.668045170405	1.431877508755
H	-0.919283400066	-1.016327461432	-1.407818088782
F	-1.281020464406	-1.857317687760	0.377342759286
F	-2.496782580372	-0.237944409071	-0.454192588688

Atom	X	Y	Z
C	-0.659512438030	-0.721553246954	-0.553002826396
C	0.433289297266	-0.127247054036	0.358434397582
C	0.729041096188	1.375059783139	0.138091275394
F	-0.729016062038	-2.051508715731	-0.348157864998
Cl	-2.262759076892	-0.004408702599	-0.190868308398
H	-0.437061859787	-0.508513550608	-1.598263604796
Cl	1.967379358108	-1.010059491232	-0.009805993298
F	0.122996769475	-0.315099776760	1.653078871565
H	1.665570773232	1.652999600824	0.633288613399
F	0.828844087986	1.608757374168	-1.189204359826
F	-0.272446945508	2.120822779791	0.634599799771

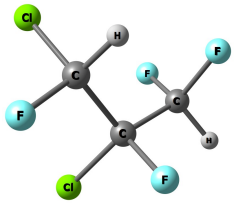
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
64.5439	0.168
81.4365	0.176
138.7658	0.0244
179.9162	0.245
203.5367	0.336
266.4918	0.0960
300.0914	0.202
346.2742	0.418
361.7551	0.0905
426.4387	0.911
456.4171	0.358
568.9866	1.66
635.4181	8.76
783.2310	8.27
842.8985	19.3
983.6678	19.2
1082.3566	9.84
1116.8564	8.43
1162.2569	10.1
1178.2950	19.9
1211.3344	21.0
1278.3294	1.50
1369.6387	2.82
1390.4823	2.09
1405.7418	3.03
3107.5987	2.21
3114.8191	0.694

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
45.4779	0.102
88.4348	0.108
152.5022	0.0752
195.3950	0.0604
208.3851	0.458
254.4877	0.0897
293.5709	0.453
314.0081	0.100
392.8114	0.561
408.2104	0.616
467.1743	0.883
576.7190	1.34
659.0604	12.6
779.6161	18.5
799.4376	9.71
913.4631	10.4
1124.0607	6.51
1130.9788	13.4
1150.5412	14.6
1202.6895	15.6
1215.9757	18.7
1285.1756	1.37
1378.0289	2.06
1391.0347	1.36
1404.1905	3.17
3079.4277	3.19
3133.9711	0.494



ΔE = 1.11 kcal mol^{-1}
Population = 0.028



ΔE = 1.22 kcal mol^{-1}
Population = 0.024

Optimized Coordinates (Angstroms)

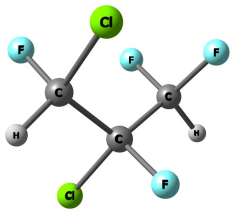
Atom	X	Y	Z
C	0.935461260171	0.877697115188	0.021915733112
C	-0.387005758486	0.145275412890	0.336024355180
C	-0.729313525247	-1.012896102213	-0.629892725884
Cl	2.371621480290	-0.100887050995	0.448990381663
F	0.958826465485	1.166714938095	-1.300208723348
H	0.998503758840	1.796575863420	0.606092336838
Cl	-1.698002275149	1.379804051065	0.185407135580
F	-0.360095825481	-0.313231753430	1.598414809843
H	-0.755709840361	-0.666023164733	-1.666986131981
F	0.197486832467	-1.982136586845	-0.496534781601
F	-1.924023572530	-1.525067722442	-0.285140389402

Atom	X	Y	Z
C	0.878280719480	-0.127872420193	0.796557929617
C	-0.372267302191	0.525639366820	0.173058762864
C	-1.544628335151	-0.437924402002	-0.112237633138
Cl	1.640736504125	-1.343233886503	-0.264891607428
F	1.765618660565	0.842162100973	1.089824377214
H	0.578256701833	-0.641834847676	1.711535597913
Cl	0.018470156493	1.450509944277	-1.300272707520
F	-0.837942611541	1.388513421047	1.118932728477
H	-2.454729375729	0.147195869442	-0.287749455781
F	-1.303510377146	-1.233503713012	-1.162306150785
F	-1.717227740738	-1.212956433174	0.986830158567

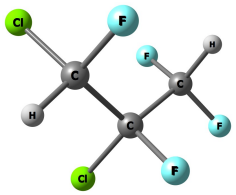
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
44.7240	0.134
82.9617	0.0745
155.0792	0.0429
177.6521	0.0732
218.4814	0.484
255.0478	0.0985
271.9247	0.326
335.5512	0.471
380.5470	0.236
402.7449	0.339
503.7203	1.66
541.4585	2.98
661.3913	2.63
770.2799	30.9
831.7196	9.72
912.8137	6.73
1116.9255	20.0
1138.7180	5.13
1152.0957	17.2
1179.3763	3.81
1220.2623	20.4
1298.5988	5.94
1363.7483	0.390
1399.5247	1.99
1409.4271	3.27
3095.2825	2.48
3119.5159	0.716

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
53.8410	0.144
94.4859	0.0870
149.5211	0.0859
172.9988	0.144
194.7408	0.165
278.9631	0.662
314.5359	0.291
318.9964	0.0431
400.7338	1.07
407.9289	0.144
492.3262	1.15
581.8989	1.98
625.7936	7.30
709.2593	8.67
829.1164	15.1
1006.2223	16.1
1102.8887	6.83
1136.8262	13.4
1145.2149	22.4
1173.5985	10.3
1211.1947	15.1
1278.1344	3.21
1368.9124	2.66
1388.4254	2.51
1401.3489	3.40
3071.8073	3.62
3114.2980	0.635



$\Delta E = 1.35$ kcal mol^{-1}
Population = 0.019



$\Delta E = 1.46$ kcal mol^{-1}
Population = 0.016

Optimized Coordinates (Angstroms)

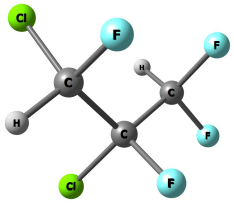
Atom	X	Y	Z
C	0.609860077098	1.004609088186	-0.176222062443
C	-0.457115957059	0.095642529991	0.472617925292
C	-0.563691152062	-1.367015484929	-0.021132311949
Cl	2.275475399013	0.474100375535	0.228769767818
F	0.451674227411	1.020712189558	-1.511888682041
H	0.503465190488	2.013237530393	0.227989417347
Cl	-2.057753320985	0.874062231484	0.169602857825
F	-0.240065944665	0.061293289028	1.803650897808
H	-1.403920890634	-1.855815980023	0.486713205768
F	-0.752292241123	-1.401531749707	-1.350488009821
F	0.572825612517	-2.025657019515	0.274087994397

Atom	X	Y	Z
C	-1.136720059157	0.168853551433	-0.703784388879
C	0.385330390371	0.220230519419	-0.450113037979
C	0.974741987580	-1.055251723251	0.192312713528
F	-1.373048450313	-0.935598040818	-1.457826462737
Cl	-2.130195075546	0.092690415932	0.774163703997
H	-1.435092184890	1.060750708770	-1.257854949977
Cl	0.821276879080	1.671299697520	0.488495569681
F	0.943529863296	0.311307784382	-1.687204026837
H	0.648807904682	-1.935553855178	-0.373715308924
F	2.316357217708	-0.971027679812	0.153510747256
F	0.582863527190	-1.169225378399	1.472023440870

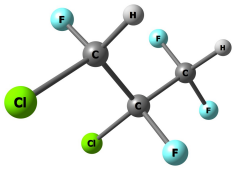
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
26.7386	0.00306
108.3277	0.286
159.1831	0.0205
180.1654	0.0255
200.6264	0.0662
253.1716	0.0313
313.3027	0.114
353.6019	0.113
398.3977	0.604
420.1336	0.994
433.5385	6.90
543.5161	0.710
607.7161	0.661
757.8881	26.0
855.6880	8.95
901.2514	5.63
1133.0637	5.21
1146.1000	7.32
1178.1337	33.5
1180.2409	20.4
1228.9706	2.32
1293.1566	4.77
1351.7604	2.80
1394.3337	2.14
1424.5279	2.82
3062.7041	3.75
3105.9706	1.000

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
50.4374	0.182
88.4087	0.0670
154.4127	0.111
165.8303	0.0398
196.0588	0.214
267.9273	0.704
311.3125	0.190
338.3831	0.0455
379.6813	0.224
434.8309	0.190
490.0984	2.32
570.5180	2.77
648.2187	4.51
695.2425	9.81
829.4332	15.6
1027.8995	15.1
1093.7858	3.65
1125.7992	13.3
1144.2620	10.9
1172.1008	27.5
1197.3471	13.8
1287.8587	2.25
1357.0004	2.07
1397.3882	2.92
1401.3891	4.35
3072.0252	2.67
3111.9959	0.848



$\Delta E = 1.57$ kcal mol^{-1}
Population = 0.013



$\Delta E = 1.95$ kcal mol^{-1}
Population = 0.007

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.129834854040	0.138969650170	0.657569505327
C	0.358912032581	-0.181298777281	0.394283772068
C	1.006549677015	0.578462394740	-0.784560801344
F	-1.229741180401	1.406899286182	1.098185192360
Cl	-2.134053635908	-0.061237187938	-0.817267454007
H	-1.522682959649	-0.547607206776	1.409855299935
Cl	0.536887970160	-1.944722079055	0.111797093659
F	1.021582420092	0.151906143783	1.524485576427
H	0.571597965176	0.287427776144	-1.744382051834
F	0.829436431426	1.900710851990	-0.585705590732
F	2.326279133546	0.319712148041	-0.782810541860

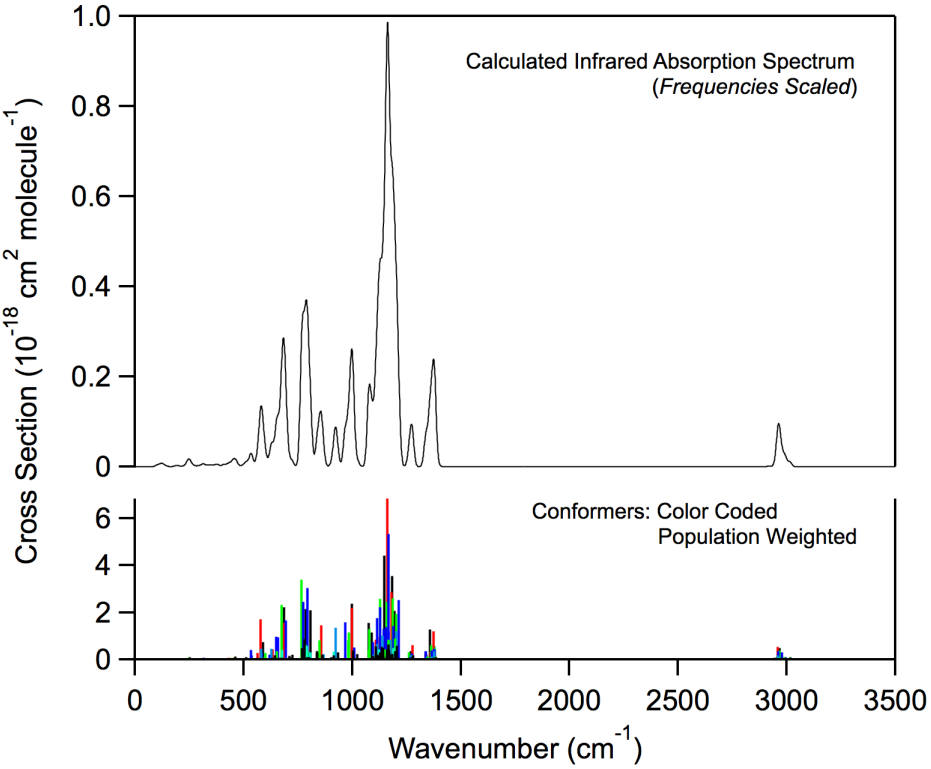
Atom	X	Y	Z
C	-0.960205781673	-0.719346016261	-0.362069794286
C	0.231980273744	0.259439687297	-0.281957020219
C	1.571656576999	-0.458238001069	-0.576076914173
F	-0.908180487118	-1.597377271441	0.654755804597
Cl	-2.520765435961	0.152271219808	-0.342726768786
H	-0.923292821254	-1.257204340330	-1.314765475956
Cl	0.305101494280	1.054918011884	1.309574005955
F	0.081255158409	1.184246666160	-1.259821095050
H	1.545537339008	-0.881467146789	-1.590167494243
F	2.575900366956	0.428973052280	-0.502448203065
F	1.784666316610	-1.442232861539	0.314098955228

Infrared Absorption Spectrum (unscaled frequencies)

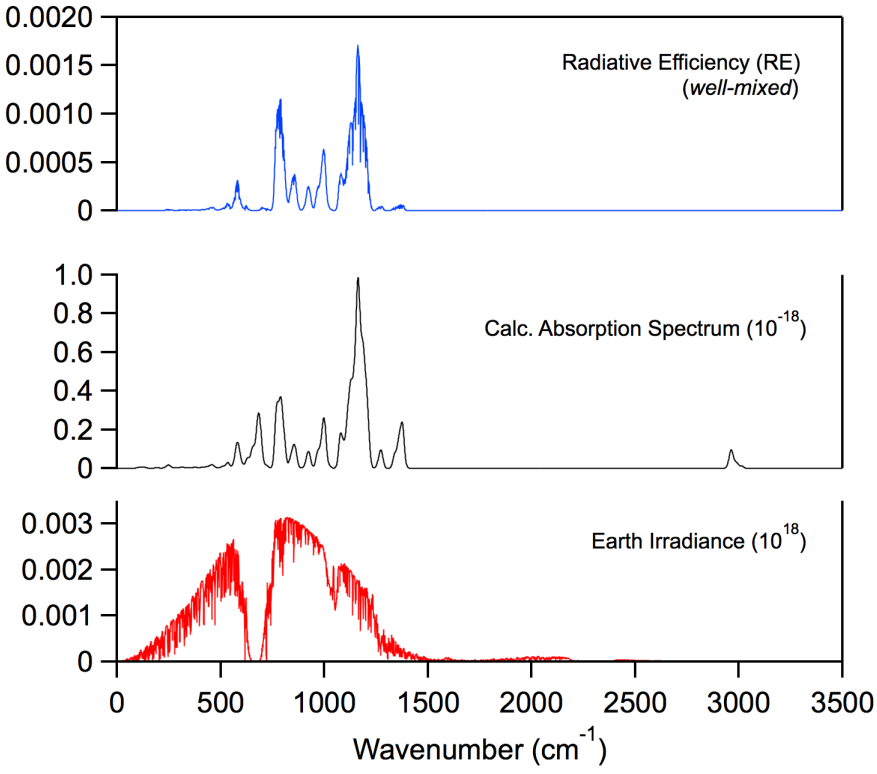
Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
52.1401	0.119
87.9778	0.0607
150.5490	0.0887
180.0851	0.0285
213.6279	0.420
269.5727	0.185
308.9753	0.198
335.4990	0.437
376.4642	0.124
413.4062	0.559
445.7939	1.25
538.5216	3.61
661.8610	3.85
784.7686	8.64
855.5160	16.5
931.6531	24.3
1107.7319	1.97
1138.6267	4.24
1151.4755	13.2
1174.1368	32.0
1197.5230	17.4
1291.2407	2.38
1368.3666	2.17
1400.2352	2.20
1408.1542	3.23
3102.2007	2.51
3111.3271	0.807

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
51.0099	0.0572
79.8017	0.109
147.1137	0.109
187.3085	0.0782
212.1709	0.364
228.1130	0.120
301.6403	0.263
344.2154	0.0152
367.2988	0.422
438.3216	0.0920
539.2615	2.36
601.2678	2.28
611.0244	10.2
702.1881	9.67
791.5335	14.1
1062.3140	2.58
1084.1627	3.60
1148.1783	6.83
1170.6068	19.0
1183.8879	31.8
1198.9582	10.0
1296.8539	5.91
1355.4721	1.62
1387.7119	6.63
1405.3297	4.28
3033.2597	4.40
3073.7970	2.60

Infrared Spectrum

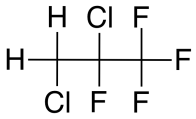


Radiative Efficiency



HCFC-234bb

Molecular Formula:	$CH_2ClCClFCF_3$
Name:	2,3-Dichloro-1,1,1,2-tetrafluoropropane
CAS number:	149329-25-9
Molecular Weight:	184.95



Global Atmospheric Lifetime (years):	4.84
Tropospheric Atmospheric Lifetime (years):	5.21
Stratospheric Atmospheric Lifetime (years):	67.0
Ozone Depletion Potential (ODP):	0.035

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.237	0.218
Global Warming Potential (GWP_H):		
GWP_{20}	1374	1264
GWP_{100}	378	348
Global Temperature Potentials (GTP_H)		
GTP_{20}		682
GTP_{50}		73
GTP_{100}		49

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

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

OH Reactivity

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

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

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

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

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

Fractional Atmospheric Loss: 0.960

$O(^1D)$ Reactivity

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

$k_{Est}(T) = 1.4 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 265$ years

Fractional Atmospheric Loss: 0.018

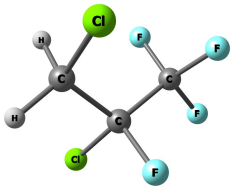
UV Photolysis

UV Spectrum: *No Recommendation*

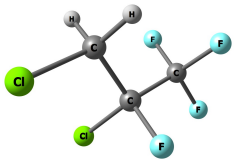
$\tau_{hv} = 225$ years

Fractional Atmospheric Loss: 0.022

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.527



$\Delta E = 0.21$ kcal mol^{-1}
Population = 0.373

Optimized Coordinates (Angstroms)

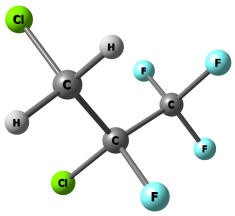
Atom	X	Y	Z
C	1.005647300866	1.021204271635	-0.485452327210
C	-0.195242783499	0.460619103645	0.274567420573
C	-0.587016688025	-0.997710673421	-0.091275883440
Cl	2.550871213155	0.219087259915	-0.045246014212
H	0.851721847906	0.902002377388	-1.556169773346
H	1.107260694896	2.076145295088	-0.236969450763
Cl	-1.596885639542	1.525656176595	-0.137569674102
F	0.006774818645	0.500141261196	1.604799797942
F	-1.744294709718	-1.330460947961	0.469544013690
F	-0.695300564537	-1.120889013056	-1.416360064120
F	0.342639509852	-1.844996111024	0.341518954989

Atom	X	Y	Z
C	1.001801787080	-0.837562553768	-0.491123173960
C	0.014545114328	0.072972556363	0.236288856307
C	-1.445749300214	-0.336836760347	-0.098756524218
Cl	2.691635984488	-0.529801178265	-0.002151828907
H	0.768243589160	-1.871224452708	-0.233663298239
H	0.918993758028	-0.693504985451	-1.566729992609
Cl	0.239353025383	1.793443634443	-0.216013621719
F	0.150956236006	-0.053023291334	1.573468252750
F	-2.319761993483	0.434464291768	0.529486539473
F	-1.662623110543	-0.266985880612	-1.412987613097
F	-1.640932090233	-1.602270380088	0.291836404219

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
46.1740	0.0681
106.2419	0.276
159.0384	0.118
193.2794	0.118
229.1607	0.592
270.4544	0.0314
312.3533	0.180
326.2777	0.273
384.0822	0.0706
442.5940	0.578
536.8499	1.82
581.2649	0.810
609.5241	3.47
749.7028	15.0
762.9726	2.31
867.8642	3.44
923.6949	13.0
1058.0266	10.4
1183.2927	10.2
1218.4825	22.0
1231.7479	33.0
1254.1954	19.3
1304.0312	3.13
1344.1996	11.2
1458.2909	1.84
3115.3219	0.725
3184.3756	0.0267

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
63.6984	0.0197
81.8615	0.374
138.5651	0.226
185.9702	0.174
225.5830	0.166
292.0004	0.0183
311.8518	0.254
326.7721	0.0586
391.7544	0.0831
435.6114	0.580
546.9479	1.51
575.5163	0.393
641.1512	3.95
715.9758	10.2
789.1851	4.16
869.6277	5.37
972.7911	11.8
1037.0464	10.2
1173.6694	13.6
1209.8871	16.6
1244.0998	27.6
1256.7511	15.9
1292.2545	22.2
1325.3098	10.0
1464.0172	0.904
3102.8254	0.781
3173.6614	0.0372



$\Delta E = 0.98$ kcal mol^{-1}
Population = 0.100

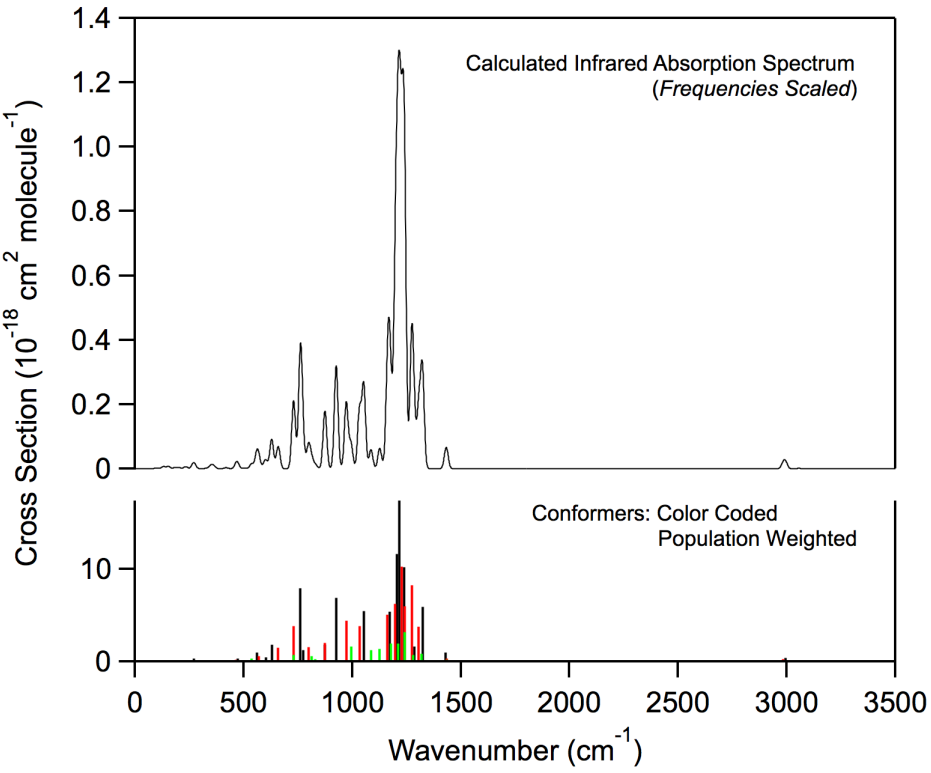
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.184643938569	0.048246668974	1.027953884949
C	-0.166425652911	0.462518727044	0.441011773779
C	-0.986570508532	-0.693071280522	-0.193222199675
Cl	2.376115495979	-0.543747764125	-0.163566850756
H	1.608460318162	0.916804874905	1.530558456752
H	1.006927181064	-0.749240067459	1.749502971052
Cl	-0.013169668799	1.794992818204	-0.741137618633
F	-0.905341404097	0.899662199318	1.496601295992
F	-2.230002854734	-0.291453298086	-0.432556240317
F	-0.448137175180	-1.127479834672	-1.324685968732
F	-1.032327669519	-1.710761043581	0.676756495589

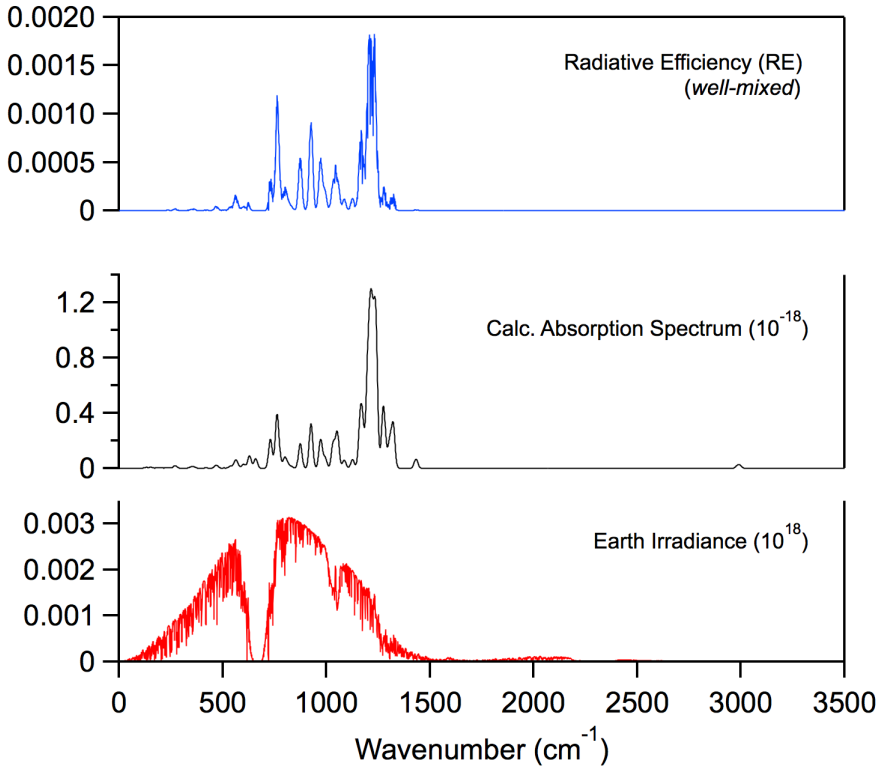
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
50.9186	0.0650
95.7531	0.145
149.2176	0.0240
194.6337	0.191
236.0127	0.624
295.4316	0.234
319.8490	0.218
334.9151	0.117
385.6985	0.0433
478.8039	0.495
511.2971	3.20
573.1277	0.696
605.5576	1.22
717.3770	7.13
804.2223	6.15
822.9609	2.68
995.8049	16.4
1093.2682	12.5
1135.8745	13.5
1190.6420	19.7
1224.4509	19.4
1257.1593	31.5
1299.1654	7.22
1338.3839	8.56
1464.0558	1.79
3101.6920	0.890
3168.9109	0.0111

Infrared Spectrum

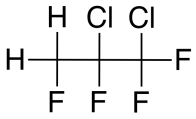


Radiative Efficiency



HCFC-234bc

Molecular Formula:	$CH_2FCClFCClF_2$
Name:	1,2-Dichloro-1,1,2,3-tetrafluoropropane
CAS number:	149329-26-0
Molecular Weight:	184.95



Global Atmospheric Lifetime (years): 7.01
- Tropospheric Atmospheric Lifetime (years): 7.71
- Stratospheric Atmospheric Lifetime (years): 77.3

Ozone Depletion Potential (ODP): 0.045

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.297	0.279
Global Warming Potential (GWP_H):		
GWP_{20}	2387	2244
GWP_{100}	686	645
Global Temperature Potentials (GTP_H)		
GTP_{20}		1457
GTP_{50}		170
GTP_{100}		91

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

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

OH Reactivity

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

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

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

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

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

Fractional Atmospheric Loss: 0.942

O(^{1}D) Reactivity

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

$k_{Est}(T) = 1.4 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 265$ years

Fractional Atmospheric Loss: 0.027

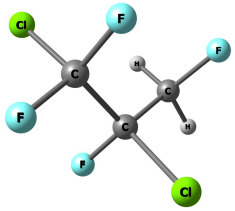
UV Photolysis

UV Spectrum: *No Recommendation*

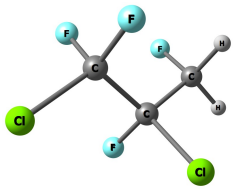
$\tau_{hv} = 225$ years

Fractional Atmospheric Loss: 0.031

Molecular Structure and Infrared Spectrum (9 conformers)



E = 0
Population = 0.200



$\Delta E = 0.04$ kcal mol^{-1}
Population = 0.187

Optimized Coordinates (Angstroms)

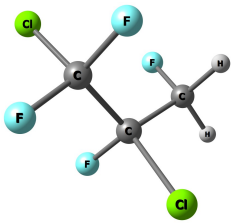
Atom	X	Y	Z
C	-0.829180160826	-1.496935486971	-0.527808809361
C	-0.516896880981	0.001125617362	-0.491132974669
C	0.723165275920	0.399934712061	0.358222262599
H	0.041065603994	-2.030672445093	-0.923253095381
F	-1.125945077100	-1.960088765644	0.720202113942
H	-1.684229229786	-1.637622348481	-1.196909441159
Cl	-1.928893311808	0.899774662625	0.166022366181
F	-0.290097875977	0.403206455693	-1.761657641562
Cl	2.210150459210	-0.382927406648	-0.298063416762
F	0.899487909718	1.716480106315	0.315262500794
F	0.564300287635	0.023048898782	1.621031135377

Atom	X	Y	Z
C	-1.936711298240	-0.083681826957	0.286562403570
C	-0.558275817365	0.324955544326	-0.249237557676
C	0.591901992801	-0.578509492716	0.281614476369
H	-2.669358125758	0.634865116220	-0.093491608537
F	-2.255111779187	-1.337719060902	-0.155585118513
H	-1.925815522885	-0.061856375745	1.379978758876
Cl	-0.284316660797	2.023361564063	0.267874824756
F	-0.551336519472	0.249266745995	-1.593682375152
Cl	2.188718124163	-0.103693421736	-0.367192534954
F	0.617673475536	-0.521489502559	1.615712072071
F	0.349705131205	-1.838525289989	-0.079922340809

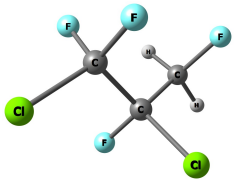
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
48.4941	0.0799
107.4254	0.274
166.8500	0.0172
193.3625	0.169
247.4929	0.686
257.3953	0.160
311.4679	0.362
339.3617	0.0868
382.9763	0.200
415.0894	0.217
420.5398	0.161
523.6832	2.67
608.3373	3.29
667.8160	1.64
734.1608	31.0
938.0188	20.4
1080.3977	4.73
1125.6172	6.95
1146.7638	19.7
1179.8834	15.0
1230.5319	24.1
1241.5344	6.72
1295.3879	3.92
1423.8191	0.813
1500.0175	1.42
3053.7211	2.10
3110.6871	1.81

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
47.7126	0.0588
123.8760	0.525
168.6431	0.217
190.9646	0.0230
209.5086	0.311
299.4923	0.449
304.6849	0.297
320.4218	0.0955
358.7855	0.129
424.9363	0.0309
431.2614	0.475
498.5319	1.12
578.8720	10.9
662.4045	3.35
876.7062	10.5
940.4240	23.2
999.6798	23.4
1100.1372	3.14
1134.9000	19.9
1196.0534	10.6
1212.2380	26.8
1234.5200	9.23
1316.6303	2.65
1418.1846	1.82
1490.7869	0.796
3060.5756	1.58
3121.2491	1.39



$\Delta E = 0.08$ kcal mol^{-1}
Population = 0.173



$\Delta E = 0.13$ kcal mol^{-1}
Population = 0.159

Optimized Coordinates (Angstroms)

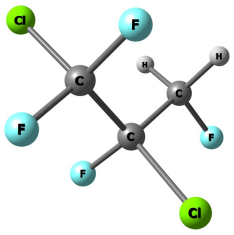
Atom	X	Y	Z
C	-0.578135385586	-1.619675025368	0.523093550333
C	-0.585539862314	-0.308647677366	-0.267020332357
C	0.486348881817	0.735416465003	0.160506602884
H	-1.440646313484	-2.208887861504	0.197226603390
F	0.569407338833	-2.319920660006	0.272805553012
H	-0.659290167684	-1.401227560664	1.591446914402
Cl	-2.205395790663	0.442251154113	0.013388022809
F	-0.433785613368	-0.549845090723	-1.582224561920
Cl	2.140354816184	0.194440795138	-0.257638127469
F	0.264382217666	1.896855159181	-0.448929770224
F	0.411544878598	0.921666302195	1.481749545139

Atom	X	Y	Z
C	-1.783850298662	-0.648252932556	-0.557916427214
C	-0.522176131951	0.219133798571	-0.452125622589
C	0.687233986156	-0.564964691789	0.135336463408
H	-1.551747149418	-1.519666852609	-1.178618145873
F	-2.194441481851	-1.057410055019	0.676853407379
H	-2.563474718752	-0.046886609121	-1.035807363161
Cl	-0.847163363534	1.667266676650	0.543628807655
F	-0.199732429198	0.592798548431	-1.711722016916
Cl	2.218275712234	0.345803282449	-0.011356262182
F	0.470805211090	-0.870550459693	1.408891259886
F	0.808448663887	-1.707848705316	-0.557341100393

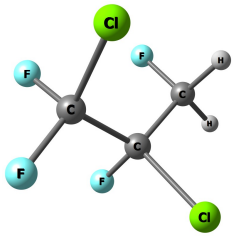
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
45.8609	0.0991
118.1463	0.489
173.2861	0.135
187.4427	0.0414
238.2124	0.403
252.1335	0.494
318.6482	0.303
331.0678	0.0931
353.9354	0.233
406.3112	0.234
427.9399	0.0180
507.8944	0.153
589.9274	6.02
695.6415	4.98
817.5836	40.3
957.8644	9.40
970.5623	4.53
1115.7328	17.6
1132.0547	6.54
1199.8765	32.8
1227.3855	3.89
1240.6034	13.5
1320.8998	1.21
1423.6624	0.718
1491.1373	0.723
3062.5437	1.52
3123.2372	1.35

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
53.3593	0.0602
104.6787	0.330
158.4561	0.0636
203.4795	0.230
211.9412	0.244
294.7855	0.775
313.2501	0.143
329.7404	0.0626
388.2227	0.226
423.3211	0.0297
448.2554	0.285
527.7657	7.25
561.0099	4.10
657.1099	2.05
773.9513	14.1
975.7236	26.1
1082.9489	14.4
1110.1276	7.48
1140.8664	21.4
1171.1881	2.54
1200.3103	31.3
1236.3640	8.60
1289.2327	1.05
1418.9146	2.30
1499.7089	0.972
3054.5187	2.35
3113.1554	1.61



$\Delta E = 0.46$ kcal mol^{-1}
Population = 0.092



$\Delta E = 0.58$ kcal mol^{-1}
Population = 0.075

Optimized Coordinates (Angstroms)

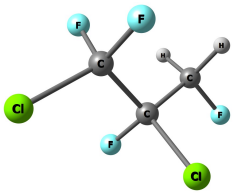
Atom	X	Y	Z
C	-0.970715861404	-1.270026615790	0.613514819526
C	-0.493567287779	-0.084826328527	-0.228715395929
C	0.924020559474	0.411429540060	0.166885334681
H	-0.911892158108	-1.013566056343	1.675086054720
F	-2.256761757191	-1.572102256452	0.272346903899
H	-0.329081894275	-2.130683269443	0.399253059917
Cl	-1.626618927535	1.298726796403	-0.023428147796
F	-0.463679263879	-0.423194838859	-1.534481294910
Cl	2.148791835636	-0.880690543941	-0.114023492050
F	1.266374401382	1.469735689792	-0.555044160157
F	0.944493353679	0.740069883099	1.459765318100

Atom	X	Y	Z
C	-1.339236625775	-0.754150473902	0.941499271691
C	-0.716345784147	0.115143520000	-0.149562386102
C	0.786353264978	-0.162436923563	-0.459571536061
H	-2.406052728364	-0.511990274855	0.985595869613
F	-1.179865532337	-2.074616660970	0.617993838805
H	-0.868829961761	-0.545906352699	1.905143043390
Cl	-0.934677912598	1.832395211376	0.323665196346
F	-1.362099211719	-0.103858470899	-1.319778580112
Cl	1.819608738380	-0.051524008169	1.003518861901
F	0.896267587638	-1.386740657400	-0.970507673167
F	1.223680165707	0.707472091083	-1.365707906304

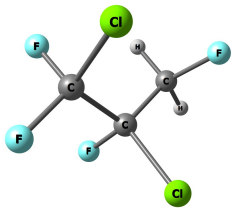
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
60.6241	0.128
90.8860	0.482
155.9856	0.280
182.0252	0.209
240.4281	0.0778
257.8664	0.102
314.3290	0.165
331.6682	0.106
374.2562	0.171
394.7005	0.365
420.9758	0.107
507.2630	0.143
622.7454	7.31
667.0473	3.20
802.9147	43.9
938.5469	3.43
1040.7534	15.5
1093.0412	6.11
1140.1220	10.6
1198.2622	29.7
1227.8683	5.21
1256.3384	13.0
1296.2085	4.26
1426.0422	0.494
1499.2346	0.387
3058.1332	2.01
3118.5307	1.40

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
51.1692	0.0661
119.1730	0.349
170.0689	0.0327
185.8150	0.124
230.2211	0.568
301.1671	0.0107
312.6409	0.405
329.6254	0.358
376.2512	0.130
405.3994	0.357
426.6146	0.567
458.1087	0.710
579.7620	5.26
692.0348	2.97
892.5889	29.9
948.5426	2.45
973.9227	36.9
1104.1933	5.95
1132.4309	12.8
1185.9349	8.78
1219.1264	25.8
1237.5914	10.7
1311.1247	5.16
1422.4661	1.48
1491.2389	1.21
3062.9025	1.54
3128.7344	1.44



$\Delta E = 0.66$ kcal mol^{-1}
Population = 0.065



$\Delta E = 1.10$ kcal mol^{-1}
Population = 0.031

Optimized Coordinates (Angstroms)

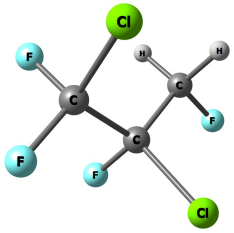
Atom	X	Y	Z
C	-1.613540930634	-0.969796078227	0.280945097528
C	-0.528082428559	-0.005366317243	-0.214656700491
C	0.873655246104	-0.483462636273	0.256245863538
H	-1.555953499979	-1.060372912574	1.369539003492
F	-2.839115421035	-0.500581775456	-0.087618188626
H	-1.441578587172	-1.944556428557	-0.186829170606
Cl	-0.847733149631	1.646687228648	0.394879172146
F	-0.527085685856	0.013480591081	-1.564620692108
Cl	2.201972080871	0.473435935589	-0.444157953426
F	0.942391862734	-0.443582626369	1.588063441812
F	1.020827513157	-1.762411980619	-0.125531873257

Atom	X	Y	Z
C	-1.184385161986	-0.974817497627	-1.009485689810
C	-0.685707381578	0.281064156740	-0.286342652065
C	0.861911624038	0.427721090251	-0.214450310545
H	-0.631512165115	-1.074085831649	-1.950068675799
F	-1.018797585772	-2.097086773477	-0.255189216114
H	-2.247303036393	-0.818910084846	-1.220133310333
Cl	-1.397818269636	0.408616611916	1.345292727189
F	-1.100797025461	1.337979937133	-1.035665916558
Cl	1.659972582406	-0.886622798888	0.689540871747
F	1.321406213743	0.421575863313	-1.474701610070
F	1.176882205755	1.596649327135	0.334431782359

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
62.7394	0.0597
93.7567	0.580
150.3350	0.368
187.6249	0.149
218.6395	0.0690
298.7851	0.158
310.8488	0.211
322.1743	0.274
357.4492	0.0322
419.9861	0.347
430.8196	0.200
488.6883	1.15
643.0282	3.20
657.8377	6.32
832.8416	33.2
924.9014	9.34
1060.3882	24.6
1110.0822	9.21
1140.8296	5.83
1175.8025	14.1
1195.1370	26.1
1238.3827	4.65
1298.1985	6.27
1424.6389	0.742
1501.1543	0.319
3056.1439	1.93
3116.4447	1.58

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
56.7434	0.102
110.5767	0.346
167.8595	0.0228
175.0982	0.0723
236.1338	0.874
298.2333	0.302
310.7986	0.242
318.6218	0.121
371.7860	0.314
427.4089	0.0617
441.3153	0.635
516.1871	1.59
577.5972	3.93
649.3863	4.83
811.9948	13.2
961.1327	30.1
1073.4164	13.5
1115.9489	10.4
1135.0232	28.3
1163.7528	3.15
1197.0472	14.2
1238.2480	14.8
1295.6304	3.39
1422.3023	0.941
1500.3713	0.847
3049.5468	2.24
3107.7084	1.75



$\Delta E = 1.44$ kcal mol^{-1}
Population = 0.018

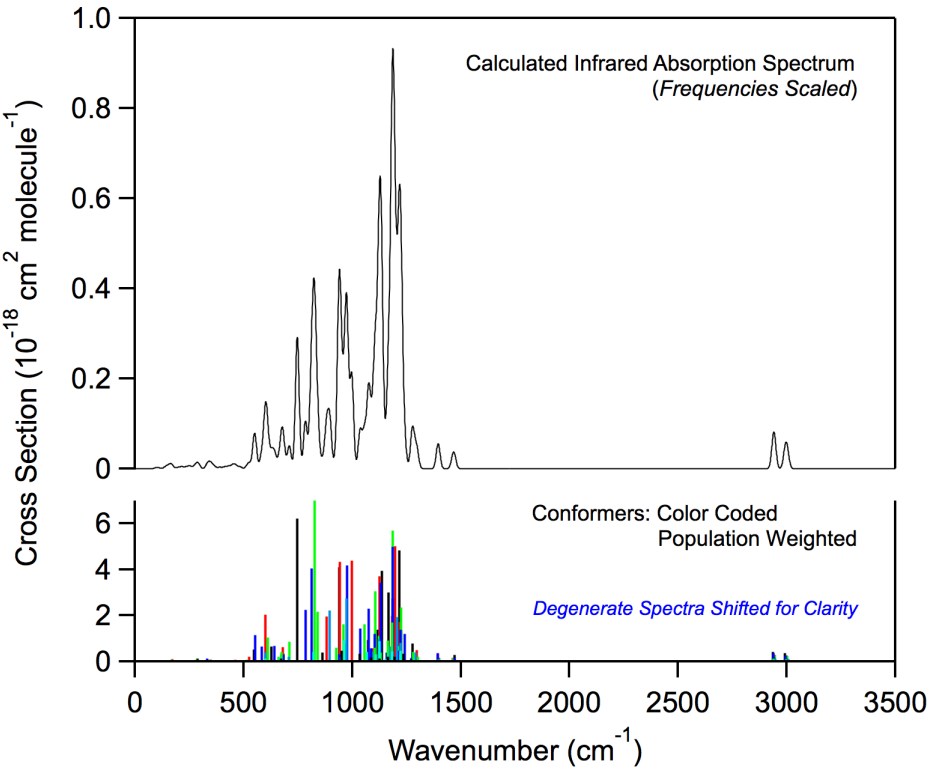
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.189714622629	-0.978069278305	0.810712296746
C	-0.554505929471	-0.087590477916	-0.258370466108
C	0.991973877476	-0.233834399825	-0.337797055335
H	-0.851892774443	-0.679453038138	1.805755330763
F	-2.546650209880	-0.864592805963	0.722464790761
H	-0.896076996895	-2.014473763113	0.609136802462
Cl	-1.001830876871	1.627652613078	-0.010731899436
F	-1.010278004356	-0.476103197619	-1.475228944965
Cl	1.813214744615	0.191539230547	1.198162006610
F	1.265499475183	-1.514197764449	-0.622391263593
F	1.472857317268	0.522050881703	-1.315613597905

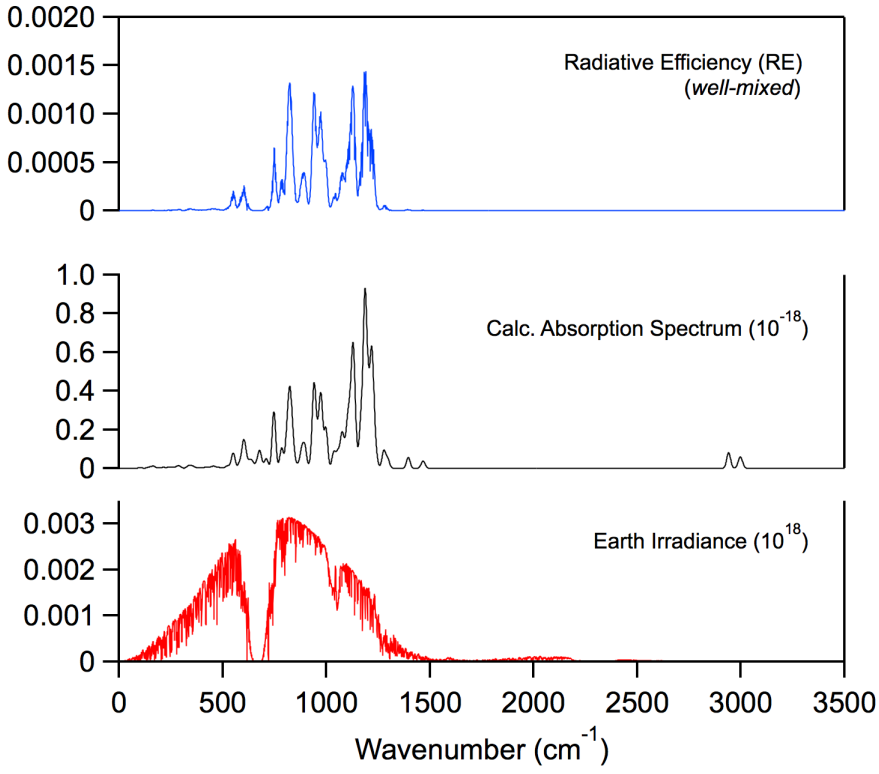
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
64.6346	0.105
94.4260	0.473
154.9191	0.262
170.8575	0.154
229.1001	0.0953
300.5082	0.410
307.6420	0.0542
331.4625	0.133
379.8808	0.0508
396.3472	0.598
431.3813	0.637
460.4142	0.325
634.8097	2.48
656.1254	7.20
857.3327	22.3
950.0459	27.1
1037.9880	19.7
1093.5053	10.9
1134.9699	7.38
1175.5200	11.3
1208.7108	12.4
1250.5942	19.8
1290.8653	5.50
1426.0446	0.514
1500.4444	0.398
3053.5459	2.06
3123.2211	1.41

Infrared Spectrum

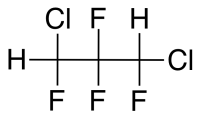


Radiative Efficiency



HCFC-234ca

Molecular Formula: $CHClFCF_2CHClF$
Name: 1,3-Dichloro-1,2,2,3-tetrafluoropropane
CAS number: 70341-81-0
Molecular Weight: 184.95



Global Atmospheric Lifetime (years): 2.74
  Tropospheric Atmospheric Lifetime (years): 2.90
  Stratospheric Atmospheric Lifetime (years): 51.0
Ozone Depletion Potential (ODP): 0.025

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.234	0.205
Global Warming Potential (GWP_H):		
GWP_{20}	781	684
GWP_{100}	212	185
Global Temperature Potentials (GTP_H)		
GTP_{20}		281
GTP_{50}		34
GTP_{100}		26

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 2.02 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 1.29 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 2.81$ years
$\tau^{OH}_{Trop} = 2.90$ years
$\tau^{OH}_{Strat} = 88.0$ years

Fractional Atmospheric Loss: 0.978

O(^{1}D) Reactivity

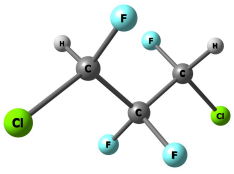
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 1.4 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)} = 265$ years
Fractional Atmospheric Loss: 0.010

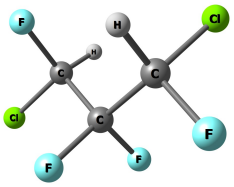
UV Photolysis

UV Spectrum: *No Recommendation*
$\tau_{hv} = 225$ years
Fractional Atmospheric Loss: 0.012

Molecular Structure and Infrared Spectrum (7 conformers)



E = 0
Population = 0.494



$\Delta E = 0.83$ kcal mol^{-1}
Population = 0.121

Optimized Coordinates (Angstroms)

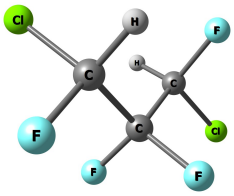
Atom	X	Y	Z
C	-1.260332013087	0.598337679596	-0.136779671696
C	-0.000235219822	-0.279887091462	0.000506197815
C	1.259347669564	0.599555410147	0.134679776076
Cl	-2.730881678259	-0.408485124191	-0.154563433170
F	-1.295813668641	1.452285789835	0.916224258283
H	-1.230743421947	1.161087948998	-1.070039713475
F	0.092810089504	-1.059138134137	-1.090337640452
F	-0.092826518596	-1.055325118080	1.094102438892
H	1.229424983618	1.165596753017	1.065936654730
Cl	2.730485730729	-0.406338376755	0.156044224431
F	1.294337046938	1.449781263033	-0.921348091433

Atom	X	Y	Z
C	1.388557029816	0.210477405831	-0.501893204062
C	-0.017976627474	0.509759624833	0.061480527599
C	-1.007639547790	-0.652012525296	-0.131655071768
F	2.162096016934	1.289186724220	-0.284397936169
Cl	2.112102303393	-1.221224156958	0.304262007854
H	1.334518181212	-0.009169015677	-1.568442167830
F	-0.459766042155	1.601156856098	-0.597856951961
F	0.067691229491	0.803590153598	1.369380982572
H	-0.739799882042	-1.499937647826	0.498377933103
Cl	-2.657819438609	-0.148156656543	0.319704995505
F	-0.974333222775	-1.017673762281	-1.437517114844

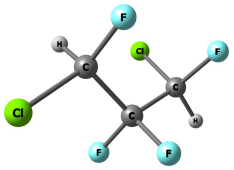
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
59.0258	0.168
62.3643	0.118
119.3128	0.100
211.0518	0.721
228.6541	0.00247
234.1676	0.138
256.1485	0.0548
368.9049	0.00349
369.8671	0.274
441.8090	0.170
494.4096	0.994
589.7399	2.01
701.9637	35.0
777.1228	3.95
815.8152	5.46
878.1219	1.52
1079.6239	6.54
1114.6364	26.2
1115.1615	12.1
1228.9105	21.7
1260.2938	7.44
1285.7217	0.0915
1310.1324	1.82
1362.8182	0.975
1375.9733	0.893
3128.3934	0.0983
3129.6584	1.30

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
51.3922	0.137
71.7874	0.152
126.2341	0.0812
188.2127	0.438
233.3233	0.227
243.1313	0.0569
299.4282	0.248
359.6348	0.229
368.7146	0.280
417.6025	0.873
470.7962	0.602
575.2940	2.45
740.9605	15.3
782.0829	7.26
805.7368	18.3
865.3321	9.23
1074.8892	7.28
1112.9111	18.1
1144.7572	21.3
1217.2385	13.8
1258.1513	14.1
1282.5078	1.20
1304.6966	2.12
1364.3972	0.546
1388.4347	2.03
3128.7216	0.594
3134.0709	0.877



$\Delta E = 0.83$ kcal mol^{-1}
Population = 0.121



$\Delta E = 1.02$ kcal mol^{-1}
Population = 0.088

Optimized Coordinates (Angstroms)

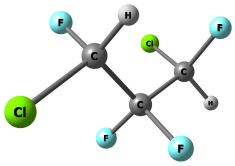
Atom	X	Y	Z
C	1.007296449129	-0.653197376955	-0.126275672242
C	0.019051695253	0.510873326187	0.060168312023
C	-1.387884197371	0.210020624015	-0.501361770468
F	0.973452758811	-1.026405366834	-1.429986903454
Cl	2.658117128050	-0.148720841429	0.322038066397
H	0.738479146933	-1.497120142854	0.508695395529
F	0.462110058144	1.597884415747	-0.605532749360
F	-0.066163681495	0.812406066692	1.366344130393
H	-1.334189137095	-0.015888869852	-1.566619144782
Cl	-2.113099872652	-1.216093425248	0.313152879364
F	-2.160103347707	1.290910590531	-0.290091543399

Atom	X	Y	Z
C	-0.879211183936	0.108804926861	-0.659592547461
C	-0.050898313112	-0.168772096445	0.607855184991
C	1.443302714304	0.216795397861	0.520411705159
Cl	-2.588928047193	-0.338475559448	-0.378561692845
F	-0.790982597851	1.420535896568	-0.960663426519
H	-0.521060705219	-0.493906368785	-1.494540197292
F	-0.115857662236	-1.483914612057	0.894564648454
F	-0.557587845183	0.525743695737	1.646258033717
H	1.934203183910	-0.101587355504	1.443322506590
Cl	2.257121666972	-0.643908651098	-0.828690216281
F	1.571556789545	1.544662726310	0.361030001487

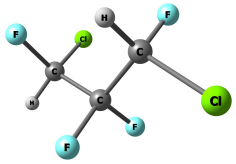
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
51.3922	0.137
71.7873	0.152
126.2340	0.0812
188.2126	0.438
233.3231	0.227
243.1311	0.0569
299.4282	0.248
359.6348	0.229
368.7145	0.280
417.6025	0.873
470.7962	0.602
575.2940	2.45
740.9604	15.3
782.0829	7.26
805.7367	18.3
865.3321	9.23
1074.8891	7.28
1112.9118	18.1
1144.7572	21.3
1217.2385	13.8
1258.1514	14.1
1282.5079	1.20
1304.6966	2.12
1364.3973	0.546
1388.4349	2.03
3128.7212	0.594
3134.0711	0.877

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
38.7238	0.120
80.3262	0.0809
144.5053	0.122
182.6584	0.167
225.0744	0.244
238.0227	0.145
315.9014	0.173
348.0277	0.221
391.7058	0.346
447.4335	0.271
482.1416	1.20
560.0358	11.9
640.8079	3.56
766.6172	3.04
826.1852	20.7
865.5339	7.91
1125.2981	4.39
1133.4984	10.5
1178.2989	27.5
1185.4961	26.8
1211.4816	7.31
1299.2098	1.25
1306.1380	0.793
1362.7042	2.62
1395.7042	2.14
3100.4971	1.19
3128.3510	0.835



ΔE = 1.27 kcal mol^{-1}
Population = 0.057



ΔE = 1.27 kcal mol^{-1}
Population = 0.057

Optimized Coordinates (Angstroms)

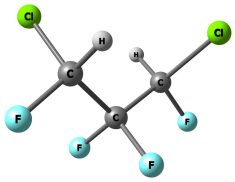
Atom	X	Y	Z
C	0.918185311493	-0.343139001170	0.591218781098
C	0.087407577270	0.551348150427	-0.348270867687
C	-1.413447005325	0.639691839956	0.013495785098
F	0.506275974104	-1.621106854763	0.474057777109
Cl	2.652924759975	-0.228327489713	0.167197179395
H	0.810664592201	-0.006507384719	1.622902141664
F	0.214098130607	0.155028968767	-1.622318541091
F	0.557506653238	1.817462735434	-0.239757555205
H	-1.857353057130	1.458176791908	-0.557460027102
Cl	-2.325563032874	-0.839330087951	-0.380614018679
F	-1.508538903560	0.904840331825	1.339472345401

Atom	X	Y	Z
C	1.411141875039	0.643234697797	0.013699016577
C	-0.087659288442	0.545576470139	-0.354140969593
C	-0.918419382963	-0.347009929697	0.587172089931
F	1.499096315928	0.917047055537	1.338406308930
Cl	2.331933737407	-0.833878950688	-0.367169394482
H	1.853735618989	1.460250202186	-0.560371600853
F	-0.206811692685	0.140817535664	-1.626261824714
F	-0.564169058048	1.810105030581	-0.255543338941
H	-0.817083314165	-0.003522072794	1.617220079197
Cl	-2.651769141883	-0.242991265104	0.154762741943
F	-0.500010669176	-1.623720773621	0.479745892005

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
37.7300	0.109
77.3933	0.0830
141.8220	0.0508
187.2944	0.175
219.1948	0.393
232.4086	0.150
307.0811	0.116
353.4492	0.190
401.7886	0.389
440.3658	0.393
504.3481	1.18
561.7447	9.90
620.4626	4.99
792.3527	3.05
825.6068	24.9
867.5768	2.18
1113.9762	18.8
1136.4346	5.75
1148.3935	32.6
1170.8172	4.21
1236.6764	13.9
1298.6911	4.69
1305.4434	0.732
1366.0980	2.04
1391.8493	1.37
3104.3863	1.14
3125.2642	0.681

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
37.7309	0.109
77.3914	0.0830
141.8187	0.0508
187.2924	0.175
219.1926	0.393
232.4091	0.150
307.0820	0.116
353.4487	0.190
401.7885	0.389
440.3658	0.393
504.3478	1.18
561.7440	9.90
620.4617	4.99
792.3524	3.05
825.6063	24.9
867.5745	2.18
1113.9780	18.8
1136.4350	5.75
1148.3928	32.6
1170.8161	4.21
1236.6738	13.9
1298.6918	4.69
1305.4402	0.732
1366.0977	2.04
1391.8482	1.37
3104.3865	1.14
3125.2650	0.681



$\Delta E = 1.78$ kcal mol^{-1}
Population = 0.024

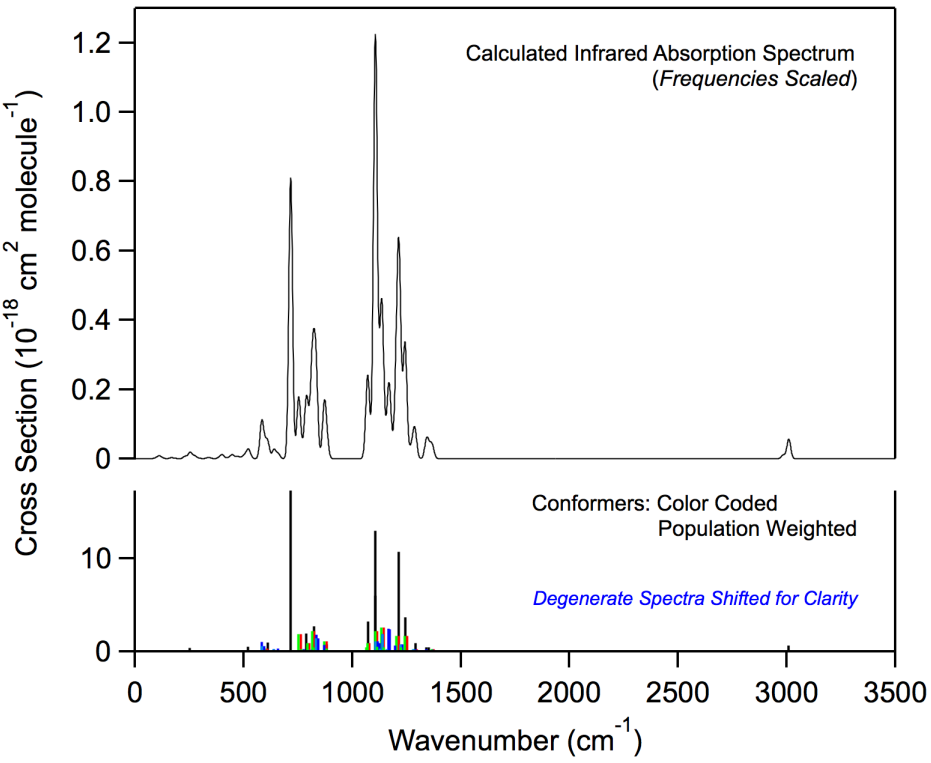
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.157505174735	0.133826189698	0.607552679419
C	0.001819343621	-0.680152884620	0.002189284202
C	1.160427451147	0.130477968394	-0.609011200196
Cl	-1.867250165576	1.240529895456	-0.615663792681
F	-2.094169607677	-0.739034207035	1.023483813990
H	-0.816245843344	0.746861509305	1.441610742496
F	-0.480480385174	-1.476201271227	-0.974177225241
F	0.484817561823	-1.468739659787	0.984248915953
H	0.818630217366	0.737199972738	-1.447453880311
Cl	1.869188539022	1.246573786939	0.606216349853
F	2.097865063529	-0.744521299860	-1.018658687483

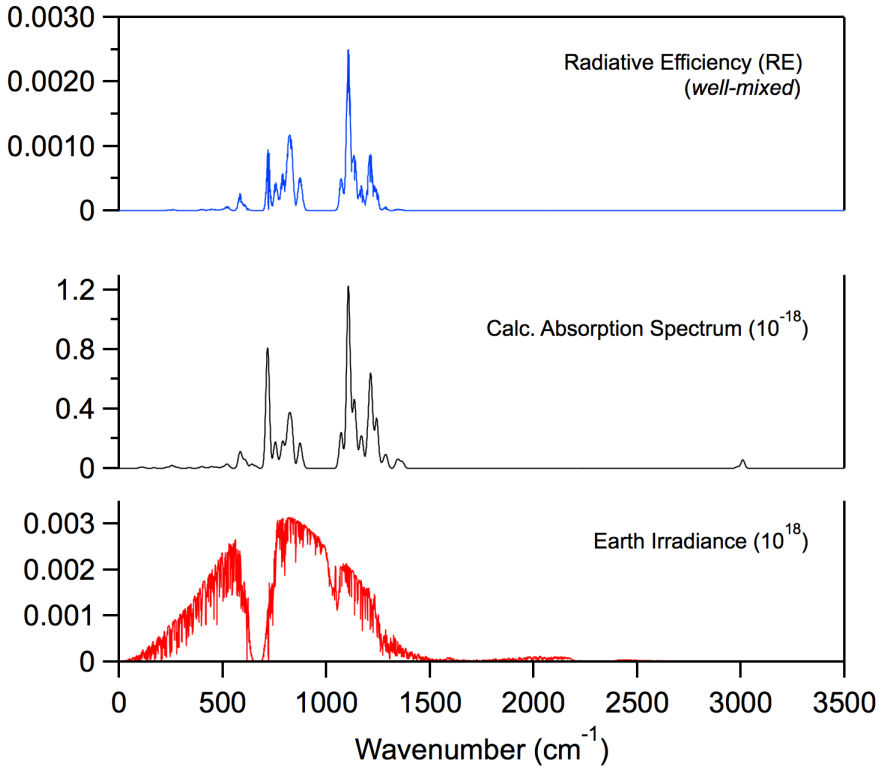
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
49.8816	0.0961
82.7847	0.193
130.1957	0.0366
185.0881	0.530
232.1812	0.0794
279.9799	0.110
290.2583	0.147
355.2759	0.00304
363.2393	0.562
414.2431	1.26
452.8804	0.361
558.4229	2.05
752.9531	9.57
767.6151	4.95
812.9672	18.5
878.1052	12.6
1070.0093	17.8
1122.6997	22.2
1154.5926	17.7
1212.2931	6.43
1239.9565	17.3
1285.8661	3.93
1292.6887	1.16
1369.4990	1.67
1396.8596	2.38
3132.7572	1.45
3132.8215	0.0415

Infrared Spectrum

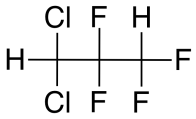


Radiative Efficiency



HCFC-234cb

Molecular Formula: $CHCl_2CF_2CHF_2$
Name: 1,1-Dichloro-2,2,3,3-tetrafluoropropane
CAS number: 4071-01-6
Molecular Weight: 184.95



Global Atmospheric Lifetime (years): 1.65
  Tropospheric Atmospheric Lifetime (years): 1.74
  Stratospheric Atmospheric Lifetime (years): 29.2
Ozone Depletion Potential (ODP): 0.020

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.243	0.199
Global Warming Potential (GWP_H):		
GWP_{20}	488	399
GWP_{100}	132	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) = 3.36×10^{-14}; k_{SAR}(272 K) ≈ 2.15×10^{-14} cm^3 $molecule^{-1}$ s^{-1}

τ^{OH}_{Global} = 1.69 years
τ^{OH}_{Trop} = 1.74 years
τ^{OH}_{Strat} = 55.7 years

Fractional Atmospheric Loss: 0.973

O(^{1}D) Reactivity

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

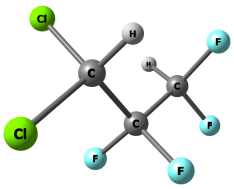
$k_{Est}(T) = 1.4 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)}$ = 265 years
Fractional Atmospheric Loss: 0.006

UV Photolysis

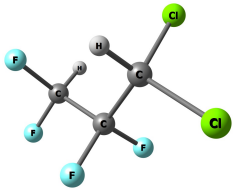
UV Spectrum: *No Recommendation*
τ_{hv} = 80 years
Fractional Atmospheric Loss: 0.021

Papanastasiou et al. (2018)

Molecular Structure and Infrared Spectrum (6 conformers)



E = 0
Population = 0.305



E = 0
Population = 0.305

Optimized Coordinates (Angstroms)

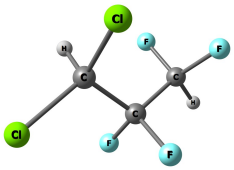
Atom	X	Y	Z
C	-0.840659191099	-0.133023069918	-0.473280339871
C	0.425983117296	0.413116515584	0.211471310502
C	1.673421619794	-0.471918735754	-0.010207720043
Cl	-1.225199621500	-1.769508722723	0.142016869662
Cl	-2.200552713397	0.990149836471	-0.236438177377
H	-0.661965786875	-0.222569733923	-1.541496607394
F	0.237278322044	0.542365623067	1.536711324278
F	0.682804212781	1.630870623876	-0.307810210174
H	1.605126020224	-1.417033037799	0.535582504612
F	1.792772732007	-0.718794633819	-1.335816768241
F	2.751693288724	0.213931334938	0.403446814046

Atom	X	Y	Z
C	-0.842119505256	0.148072775113	-0.471612027775
C	0.419428679154	-0.430607623184	0.195595453315
C	1.670635516608	0.458960008529	0.017590893069
Cl	-2.206577831403	-0.979691801215	-0.289066636430
Cl	-1.224771328115	1.758340463941	0.210416966579
H	-0.657821633445	0.282089129655	-1.534207795100
F	0.675148662401	-1.626159075155	-0.373437857886
F	0.223719658756	-0.615122967006	1.513255547398
H	1.602480395063	1.380383044032	0.602506269989
F	2.744745786879	-0.247244742310	0.407118962237
F	1.797350599358	0.761243787602	-1.295801775396

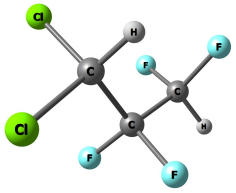
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
52.5926	0.127
71.2220	0.183
135.0650	0.0785
196.4609	0.463
211.8939	0.0638
256.6385	0.101
275.7094	0.210
334.4849	0.0822
370.0414	0.569
431.4575	0.417
553.3163	2.99
584.6678	1.77
746.6574	9.99
752.1862	8.04
789.6070	11.7
866.9932	8.34
1074.2388	15.1
1138.4908	11.2
1167.4937	18.8
1214.5307	14.1
1231.7916	9.39
1262.0948	11.7
1297.1088	2.99
1394.1672	1.31
1414.7913	2.79
3099.5501	2.92
3163.2161	0.385

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
52.5916	0.127
71.2211	0.183
135.0641	0.0785
196.4599	0.463
211.8934	0.0638
256.6381	0.101
275.7089	0.210
334.4847	0.0822
370.0413	0.569
431.4568	0.417
553.3161	2.99
584.6678	1.77
746.6565	9.99
752.1860	8.04
789.6069	11.7
866.9927	8.34
1074.2382	15.1
1138.4903	11.2
1167.4938	18.8
1214.5301	14.1
1231.7920	9.39
1262.0948	11.7
1297.1100	2.99
1394.1668	1.31
1414.7907	2.79
3099.5533	2.92
3163.2161	0.385



$\Delta E = 0.37$ kcal mol^{-1}
Population = 0.164



$\Delta E = 0.37$ kcal mol^{-1}
Population = 0.164

Optimized Coordinates (Angstroms)

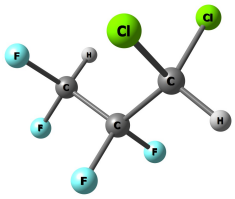
Atom	X	Y	Z
C	-0.706273644150	0.137001035680	-0.511897935791
C	0.336798197700	-0.649168037542	0.305633608120
C	1.808653821181	-0.242151221850	0.061858771509
Cl	-2.314563683367	-0.614947302529	-0.321950406379
Cl	-0.735085130776	1.856223448802	-0.044159337262
H	-0.442811348093	0.087407459949	-1.565033330434
F	0.257888701342	-1.949975734718	-0.067988532770
F	0.087597716907	-0.570564176048	1.621897241694
H	2.463101643144	-1.024046207632	0.466075040173
F	2.010430009846	-0.133697209127	-1.271751643187
F	2.095821716266	0.930838945015	0.644829524328

Atom	X	Y	Z
C	-0.705822809956	-0.132944678211	-0.503885596319
C	0.343324967175	0.635481349532	0.322691583569
C	1.813797110241	0.239816593165	0.053234343913
Cl	-0.724400149117	-1.863699679558	-0.080237952297
Cl	-2.314353844165	0.608458046668	-0.277935350687
H	-0.453577346642	-0.055435196516	-1.558082327233
F	0.108184122088	0.522272524773	1.639019988503
F	0.256471834197	1.945179651885	-0.016527490955
H	2.470021448090	1.013279071969	0.470580278757
F	2.110699888783	-0.946776340789	0.602844646610
F	2.001907779306	0.166310657082	-1.284751123860

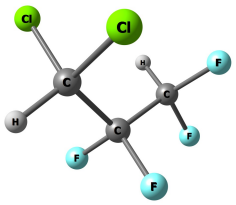
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
38.9096	0.0879
84.5285	0.158
148.0341	0.105
198.4283	0.300
213.1189	0.0262
229.2648	0.236
281.2335	0.280
355.7801	0.285
365.9815	0.0706
493.9436	0.135
545.0640	2.44
574.6774	9.53
649.0613	6.63
752.4548	1.19
814.5248	16.6
849.2957	0.803
1129.3368	17.5
1136.7716	5.70
1167.9765	31.2
1205.4304	2.74
1230.4246	9.90
1237.7478	8.75
1319.9301	3.37
1390.3756	1.58
1411.3972	6.33
3063.9795	4.39
3162.4788	0.318

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
38.9094	0.0879
84.5278	0.158
148.0329	0.105
198.4277	0.300
213.1193	0.0262
229.2649	0.236
281.2335	0.280
355.7804	0.285
365.9816	0.0706
493.9433	0.135
545.0636	2.44
574.6774	9.53
649.0617	6.63
752.4548	1.19
814.5249	16.6
849.2956	0.802
1129.3364	17.5
1136.7701	5.70
1167.9759	31.2
1205.4312	2.74
1230.4252	9.90
1237.7488	8.75
1319.9311	3.37
1390.3757	1.58
1411.3975	6.33
3063.9807	4.39
3162.4781	0.318



$\Delta E = 1.50$ kcal mol^{-1}
Population = 0.024



$\Delta E = 1.50$ kcal mol^{-1}
Population = 0.024

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-0.995847207758	0.144006803796	0.501481345136
C	0.544748989095	0.244173192285	0.551264659775
C	1.322250470656	0.052868458586	-0.767988893784
Cl	-1.663011296395	1.313472962805	-0.679053490942
Cl	-1.567725751519	-1.510354815288	0.190924984819
H	-1.366749284357	0.438325371183	1.481712912663
F	0.990716599366	-0.648725582834	1.454789515214
F	0.838710257398	1.484834550274	1.007295945067
H	1.024155052446	0.788848451846	-1.520874726668
F	2.630934714467	0.202365217850	-0.484801460597
F	1.120824456600	-1.190753610504	-1.241378790684

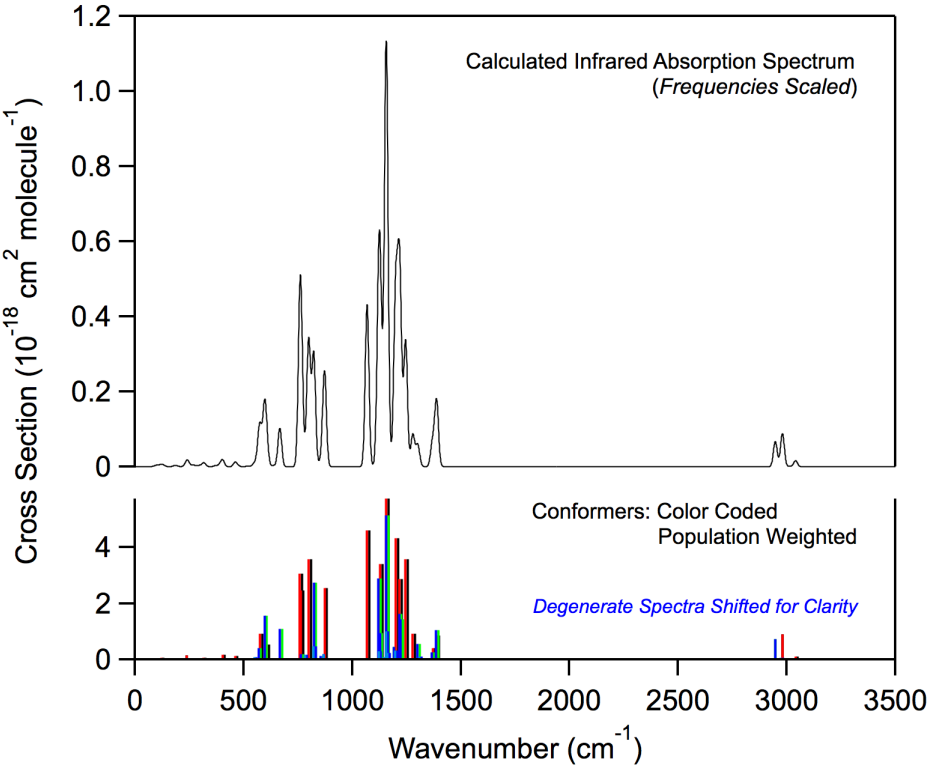
Atom	X	Y	Z
C	-0.997000966873	-0.132507071007	0.497979615385
C	0.539685938131	-0.285528284347	0.531532043691
C	1.319001971911	-0.018951037324	-0.773512083595
Cl	-1.515935649209	1.558237186493	0.317722176878
Cl	-1.705244749267	-1.186302623395	-0.764687134845
H	-1.374283699394	-0.488862419613	1.454909332491
F	0.794684373340	-1.566207976989	0.889935540807
F	1.017055216996	0.520922861645	1.498107626389
H	0.994960965979	-0.685279100835	-1.578725655572
F	1.156540195309	1.263040095486	-1.149504658313
F	2.623003403077	-0.231547630113	-0.509727803317

Infrared Absorption Spectrum (unscaled frequencies)

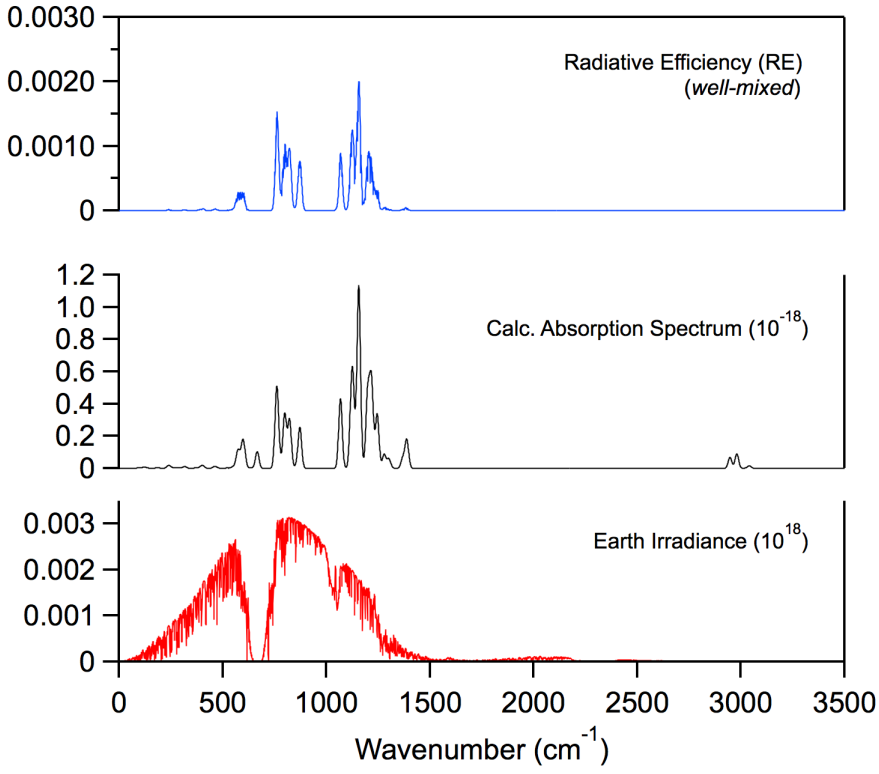
Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
34.2923	0.151
81.4905	0.0649
147.4712	0.0732
181.4312	0.169
226.2954	0.244
246.3801	0.199
285.5225	0.398
344.2781	0.204
371.4660	0.332
445.6881	0.886
524.4124	3.99
616.9623	1.27
634.9596	0.924
771.1619	7.46
813.0457	19.9
862.2627	7.64
1130.8803	12.2
1156.1577	3.90
1165.6931	41.8
1173.6960	9.61
1209.7326	13.4
1229.7009	0.387
1328.4016	4.39
1400.4981	1.51
1425.6430	1.25
3091.3800	3.06
3139.0869	0.451

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
34.2916	0.151
81.4892	0.0649
147.4698	0.0732
181.4307	0.169
226.2955	0.244
246.3798	0.199
285.5228	0.398
344.2784	0.204
371.4661	0.332
445.6880	0.886
524.4122	3.99
616.9621	1.27
634.9595	0.924
771.1619	7.46
813.0461	19.9
862.2626	7.64
1130.8807	12.2
1156.1583	3.90
1165.6934	41.8
1173.6958	9.61
1209.7332	13.4
1229.7024	0.387
1328.4023	4.39
1400.4985	1.51
1425.6432	1.25
3091.3796	3.06
3139.0859	0.451

Infrared Spectrum

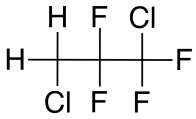


Radiative Efficiency



HCFC-234cc

Molecular Formula:	$CH_2ClCF_2CClF_2$
Name:	1,3-Dichloro-1,1,2,2-tetrafluoropropane
CAS number:	422-00-4
Molecular Weight:	184.95



Global Atmospheric Lifetime (years):	9.46
Tropospheric Atmospheric Lifetime (years):	10.6
Stratospheric Atmospheric Lifetime (years):	85.1
Ozone Depletion Potential (ODP):	0.054

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.281	0.267
Global Warming Potential (GWP_H):		
GWP_{20}	2845	2709
GWP_{100}	876	834
Global Temperature Potentials (GTP_H)		
GTP_{20}		1995
GTP_{50}		301
GTP_{100}		120

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 5.51 \times 10^{-15}$; $k_{SAR}(272\ K) \approx 3.52 \times 10^{-15}$ cm^3 $molecule^{-1}$ s^{-1}

τ^{OH}_{Global} = 10.3 years
τ^{OH}_{Trop} = 10.6 years
τ^{OH}_{Strat} = 284.1 years

Fractional Atmospheric Loss: 0.922

O(^{1}D) Reactivity

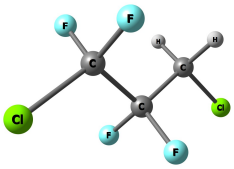
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 1.4 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)}$ = 265 years
Fractional Atmospheric Loss: 0.036

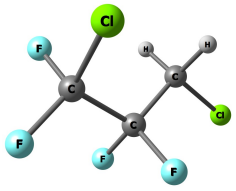
UV Photolysis

UV Spectrum: *No Recommendation*
τ_{hv} = 225 years
Fractional Atmospheric Loss: 0.042

Molecular Structure and Infrared Spectrum (7 conformers)



E = 0
Population = 0.432



$\Delta E = 0.67$ kcal mol^{-1}
Population = 0.140

Optimized Coordinates (Angstroms)

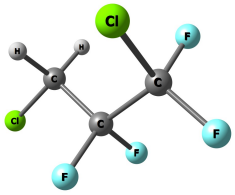
Atom	X	Y	Z
C	-1.601723864354	-0.146500872538	0.000000000000
C	-0.089134178343	-0.358836922496	0.000000000000
C	0.657707228250	1.005865414135	0.000000000000
Cl	-2.464948298406	-1.711853579142	0.000000000000
H	-1.892173759953	0.405312241017	0.892705880404
H	-1.892173759953	0.405312241017	-0.892705880404
F	0.296649920599	-1.041033268654	-1.092936980331
F	0.296649920599	-1.041033268654	1.092936980331
Cl	2.425267085228	0.788524396339	0.000000000000
F	0.295776353202	1.700875809529	-1.083941414647
F	0.295776353202	1.700875809529	1.083941414647

Atom	X	Y	Z
C	-1.169269792113	0.594981099779	0.575973104062
C	-0.282024287885	-0.362246796773	-0.210430103904
C	1.221678226033	-0.270167407311	0.188854192207
Cl	-2.889742937146	0.355863251278	0.147780870770
H	-1.052652065239	0.407229927926	1.642383038370
H	-0.902805544536	1.624675611672	0.344604222236
F	-0.373655103277	-0.140798477837	-1.533142294370
F	-0.641353748428	-1.641828324531	0.028627518346
Cl	1.917330954773	1.336103460277	-0.204178320197
F	1.338402098051	-0.484753748228	1.502842256508
F	1.903643199768	-1.207021596252	-0.458611484027

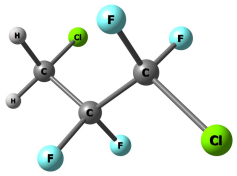
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
58.3725	0.0643
70.1118	0.569
120.6581	0.251
219.3276	0.153
221.5444	0.128
246.5565	0.223
321.8484	0.0965
357.8140	0.0325
367.1430	0.0114
427.0742	0.0132
528.4746	0.00174
542.4316	2.25
650.1755	2.92
725.3831	25.4
786.8072	0.860
908.4294	17.2
910.7836	0.527
1102.6316	28.8
1117.1999	11.8
1188.7585	22.1
1218.0376	13.7
1277.4051	1.00
1287.3515	15.3
1328.2786	1.85
1465.7463	1.12
3111.0057	0.810
3177.8866	0.000

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
62.7652	0.180
68.1795	0.394
131.6416	0.213
189.0833	0.0461
227.7274	0.272
302.5508	0.106
313.3616	0.358
327.4605	0.143
392.5996	0.0734
424.3802	0.203
470.2755	0.634
559.0040	1.28
637.7931	4.00
754.6887	11.2
782.3407	3.89
905.0938	1.61
933.5489	35.4
1069.2040	17.8
1111.8207	10.6
1198.5596	27.2
1239.8054	2.76
1275.3713	22.2
1285.6716	12.7
1331.6029	0.902
1465.1350	1.20
3112.9048	1.04
3180.3839	0.0151



$\Delta E = 0.67$ kcal mol^{-1}
Population = 0.140



$\Delta E = 0.79$ kcal mol^{-1}
Population = 0.113

Optimized Coordinates (Angstroms)

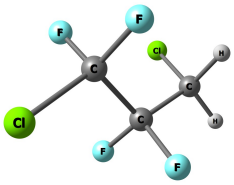
Atom	X	Y	Z
C	-1.169155949385	0.595430767660	-0.575859746745
C	-0.282114836404	-0.362035718584	0.210483016871
C	1.221623805130	-0.270170106727	-0.188714880074
Cl	-2.889691979002	0.356557723197	-0.147783447664
H	-0.902528593128	1.625054135002	-0.344362212484
H	-1.052514489704	0.407778506074	-1.642284533855
F	-0.641651611967	-1.641529223668	-0.028734175873
F	-0.373775155817	-0.140717566175	1.533214912094
Cl	1.917531433883	1.335939307170	0.204526503827
F	1.903395910095	-1.207210842740	0.458683866633
F	1.338377466298	-0.484633981208	-1.502720302729

Atom	X	Y	Z
C	-1.553677600671	-0.704479961731	0.537404291934
C	-0.142694716151	-0.771637403623	-0.053475061201
C	0.746148061877	0.470289503448	0.234669249542
Cl	-2.625081582001	0.467700170228	-0.283398483523
H	-1.992549959709	-1.696164035165	0.426954629356
H	-1.494417547084	-0.440462883870	1.591972429432
F	-0.179297163953	-0.969865932068	-1.379792326560
F	0.457709000758	-1.838278304689	0.526428767426
Cl	2.430095039023	0.191394213975	-0.298300160536
F	0.263854678997	1.539373742739	-0.391209845740
F	0.736518788914	0.705917890756	1.552208509870

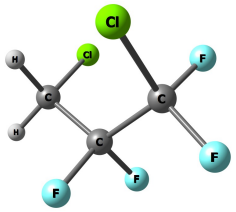
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
62.7651	0.180
68.1798	0.394
131.6417	0.213
189.0834	0.0461
227.7275	0.272
302.5507	0.106
313.3617	0.358
327.4606	0.143
392.5996	0.0734
424.3802	0.203
470.2756	0.634
559.0040	1.28
637.7931	4.00
754.6888	11.2
782.3407	3.89
905.0939	1.61
933.5489	35.4
1069.2040	17.8
1111.8207	10.6
1198.5596	27.2
1239.8056	2.76
1275.3712	22.2
1285.6719	12.7
1331.6030	0.902
1465.1351	1.20
3112.9046	1.04
3180.3838	0.0151

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
36.8753	0.0760
93.1161	0.220
164.0893	0.300
187.4205	0.305
219.6201	0.122
293.2737	0.673
320.2187	0.0450
355.5854	0.0303
375.2715	0.163
423.7506	0.0126
518.0835	1.71
573.4506	4.64
590.1360	5.88
684.4339	0.439
800.1448	11.1
877.5121	3.06
950.2266	29.1
1099.6678	21.9
1152.1282	17.9
1176.7509	4.79
1206.6824	30.2
1243.6707	14.5
1312.3146	0.246
1340.2537	3.46
1463.2169	1.24
3104.5699	0.950
3173.5723	0.00701



$\Delta E = 0.79$ kcal mol^{-1}
Population = 0.113



$\Delta E = 1.55$ kcal mol^{-1}
Population = 0.031

Optimized Coordinates (Angstroms)

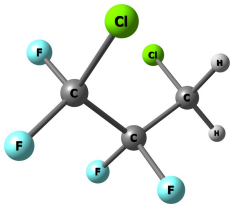
Atom	X	Y	Z
C	-1.553148078048	-0.705515919451	-0.537751686874
C	-0.142289258341	-0.771604160756	0.053544287145
C	0.745914141826	0.470713537247	-0.234886958451
Cl	-2.625455791823	0.466395156613	0.282254746455
H	-1.493750557807	-0.441915818306	-1.592416390767
H	-1.991477075090	-1.697406416716	-0.426998259621
F	0.458890997316	-1.838145393700	-0.525737986150
F	-0.179142117622	-0.969286601713	1.379936132630
Cl	2.429875512729	0.193020712207	0.298664542830
F	0.736511061645	0.705772808717	-1.552529508092
F	0.262830165215	1.539786095859	0.390402080893

Atom	X	Y	Z
C	-1.331866369985	-0.177058410588	0.942591710350
C	-0.153840698633	-0.834456347565	0.228788771783
C	0.904259737248	0.093435822119	-0.437668435268
Cl	-2.455722030807	0.670480945375	-0.160379003690
H	-1.885298529454	-0.975777943100	1.437289430086
H	-0.970760746750	0.535044279674	1.682101085277
F	-0.587969951066	-1.663659521641	-0.741066895035
F	0.502103821512	-1.575673309425	1.152313732626
Cl	1.617854549590	1.233905365582	0.753814241424
F	1.875222700503	-0.670249435181	-0.933519427347
F	0.358797517841	0.785322554749	-1.431825210205

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
36.8753	0.0760
93.1161	0.220
164.0893	0.300
187.4205	0.305
219.6201	0.122
293.2737	0.673
320.2187	0.0450
355.5854	0.0303
375.2715	0.163
423.7506	0.0126
518.0835	1.71
573.4506	4.64
590.1360	5.88
684.4339	0.439
800.1448	11.1
877.5121	3.06
950.2266	29.1
1099.6678	21.9
1152.1283	17.9
1176.7509	4.79
1206.6824	30.2
1243.6707	14.5
1312.3146	0.246
1340.2537	3.46
1463.2169	1.24
3104.5699	0.950
3173.5723	0.00701

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
35.4107	0.0923
99.0498	0.172
167.4902	0.169
187.1375	0.150
232.1501	0.607
308.3499	0.352
316.3606	0.109
335.0037	0.131
393.2551	0.194
422.6656	0.222
455.5120	1.41
588.0736	3.16
613.6815	2.45
682.6142	1.32
805.5425	7.94
892.6499	0.298
939.5611	42.0
1080.8009	6.45
1155.6042	25.4
1184.1224	22.5
1217.0170	30.5
1241.3202	1.82
1314.9270	0.715
1337.5865	8.19
1464.3364	2.66
3105.0572	0.942
3175.5682	0.0183



$\Delta E = 1.55$ kcal mol^{-1}
Population = 0.031

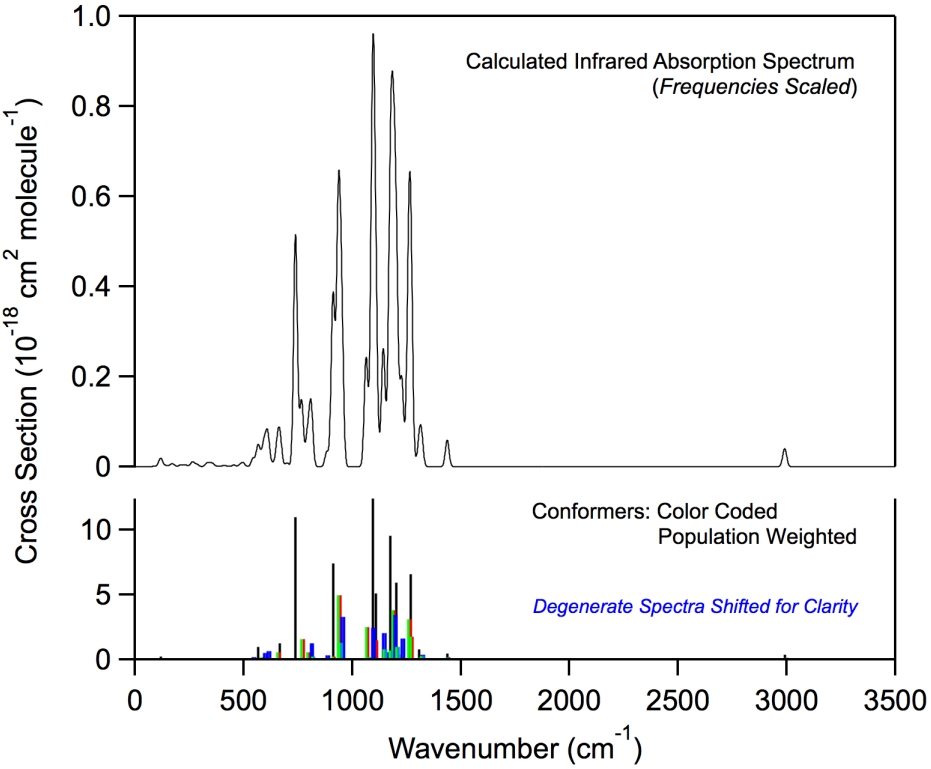
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.331917542685	-0.176960179670	-0.942884690720
C	-0.154179697616	-0.834519690580	-0.228755609649
C	0.904062832159	0.093233220773	0.437669797792
Cl	-2.455721569040	0.671113149964	0.159728164817
H	-0.970505546699	0.534888902887	-1.682488550551
H	-1.885484279359	-0.975637599888	-1.437499823504
F	0.501712747215	-1.576109030839	-1.152018551162
F	-0.588682744442	-1.663399597454	0.741208992861
Cl	1.618150844248	1.233255966994	-0.753944966137
F	0.358627653470	0.785479338417	1.431591268871
F	1.874743302750	-0.670604480604	0.933838967381

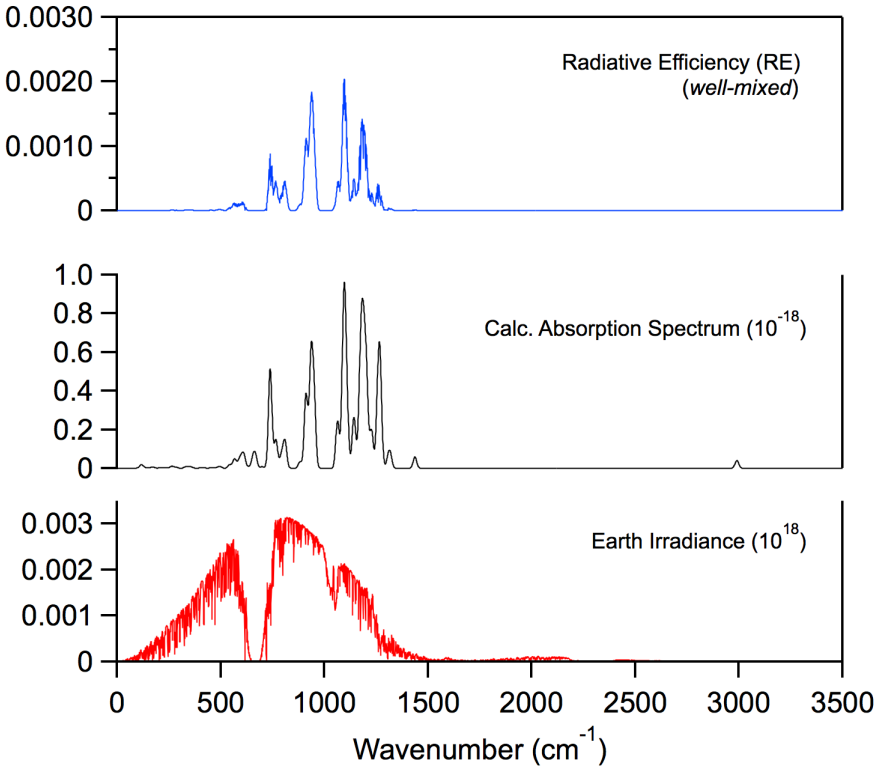
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
35.4107	0.0923
99.0500	0.172
167.4903	0.169
187.1375	0.150
232.1500	0.607
308.3499	0.352
316.3606	0.109
335.0036	0.131
393.2552	0.194
422.6656	0.222
455.5120	1.41
588.0736	3.16
613.6815	2.45
682.6142	1.32
805.5425	7.94
892.6499	0.298
939.5611	42.0
1080.8009	6.45
1155.6043	25.4
1184.1224	22.5
1217.0169	30.5
1241.3201	1.82
1314.9269	0.715
1337.5865	8.19
1464.3364	2.66
3105.0572	0.942
3175.5682	0.0183

Infrared Spectrum

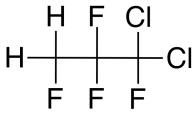


Radiative Efficiency



HCFC-234cd

Molecular Formula:	$CH_2FCF_2CCl_2F$
Name:	1,1-Dichloro-1,2,2,3-tetrafluoropropane
CAS number:	70192-63-1
Molecular Weight:	184.95



Global Atmospheric Lifetime (years):	6.64
Tropospheric Atmospheric Lifetime (years):	7.71
Stratospheric Atmospheric Lifetime (years):	47.6
Ozone Depletion Potential (ODP):	0.063

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.300	0.281
Global Warming Potential (GWP_H):		
GWP_{20}	2304	2159
GWP_{100}	656	615
Global Temperature Potentials (GTP_H)		
GTP_{20}		1367
GTP_{50}		155
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*

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

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

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

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

Fractional Atmospheric Loss: 0.892

O(^{1}D) Reactivity

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

$k_{Est}(T) = 1.4 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 265$ years

Fractional Atmospheric Loss: 0.025

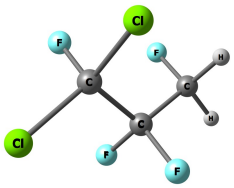
UV Photolysis

UV Spectrum: *No Recommendation*

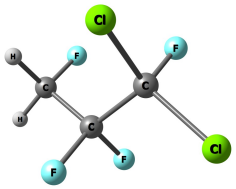
$\tau_{hv} = 80$ years

Fractional Atmospheric Loss: 0.083

Molecular Structure and Infrared Spectrum (9 conformers)



E = 0
Population = 0.189



E = 0
Population = 0.189

Optimized Coordinates (Angstroms)

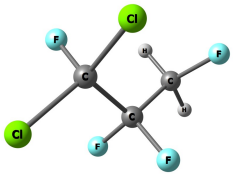
Atom	X	Y	Z
C	1.990495815096	0.267501535477	0.408172044825
C	0.682704608178	-0.527615541507	0.400236209887
C	-0.525289719617	0.163751717180	-0.302454192927
H	2.724611708032	-0.345012807853	0.944042986313
F	2.415880388286	0.490517532699	-0.870504496533
H	1.851234848903	1.217581653030	0.930185732990
F	0.350373181746	-0.781620677338	1.681870225107
F	0.885225492158	-1.700153208377	-0.234312529967
Cl	-1.950902026621	-0.910898373435	-0.255839868964
Cl	-0.905680828451	1.719714853978	0.501579235344
F	-0.204148467709	0.402705316146	-1.574352346075

Atom	X	Y	Z
C	1.988324334107	-0.295614209582	0.403016140586
C	0.687040509347	0.510109528378	0.410637406955
C	-0.525597836085	-0.156178841885	-0.308098036270
H	1.840670305932	-1.255496052130	0.904383168861
F	2.413565249597	-0.494636774383	-0.879661490805
H	2.726681807532	0.299281001007	0.952730677721
F	0.899903057375	1.694291377724	-0.198389159451
F	0.355096795944	0.739279696010	1.697044025144
Cl	-0.919629164783	-1.725895277648	0.461916405810
Cl	-1.942518289736	0.928771326387	-0.240035313165
F	-0.204742769229	-0.370386773879	-1.584468825386

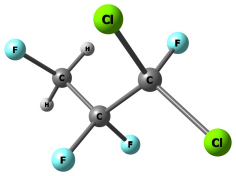
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
37.9367	0.108
107.7828	0.366
183.0819	0.323
194.2907	0.118
204.6460	0.164
272.7642	0.203
308.0910	0.260
328.3835	0.570
375.7272	0.0415
387.4683	0.144
456.8081	1.19
512.2895	0.828
590.7715	12.4
640.1225	1.32
837.6777	26.0
901.9416	18.6
986.3254	8.73
1123.5032	1.47
1159.1254	21.8
1190.4028	30.1
1222.7882	1.71
1233.5098	3.86
1308.5957	6.94
1428.1502	0.862
1497.1308	1.16
3052.8688	2.43
3119.4155	1.92

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
37.9370	0.108
107.7816	0.366
183.0813	0.323
194.2904	0.118
204.6465	0.164
272.7641	0.203
308.0917	0.260
328.3847	0.570
375.7277	0.0415
387.4682	0.144
456.8080	1.19
512.2901	0.828
590.7715	12.4
640.1223	1.32
837.6782	26.0
901.9427	18.6
986.3263	8.73
1123.5046	1.47
1159.1264	21.8
1190.4039	30.1
1222.7888	1.71
1233.5115	3.86
1308.5965	6.94
1428.1516	0.862
1497.1308	1.16
3052.8676	2.43
3119.4167	1.92



$\Delta E = 0.09$ kcal mol^{-1}
Population = 0.164



$\Delta E = 0.09$ kcal mol^{-1}
Population = 0.164

Optimized Coordinates (Angstroms)

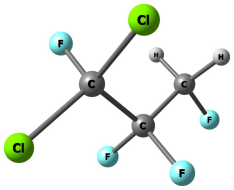
Atom	X	Y	Z
C	1.991219878021	-0.388715155795	-0.388579808933
C	0.603411845532	-0.743121625146	0.156856586348
C	-0.560117124124	0.169405062290	-0.332804512199
H	1.935158124424	-0.257375341339	-1.473124636645
F	2.478149484523	0.741710330085	0.200131314363
H	2.642345301910	-1.237660633175	-0.152628594663
F	0.617257722913	-0.757310126894	1.497909350973
F	0.330597905072	-1.992748313109	-0.290404120661
Cl	-2.125935003620	-0.490820398758	0.215597377757
Cl	-0.361102069206	1.843166448059	0.241592889979
F	-0.537078065445	0.165233753780	-1.675385846319

Atom	X	Y	Z
C	1.988961355625	0.409502667677	-0.380960275085
C	0.597249819599	0.747347182787	0.165039644967
C	-0.557123673429	-0.172776591029	-0.332022198049
H	2.631827399491	1.262943789536	-0.138665133098
F	2.485754485519	-0.720137660767	0.200976003446
H	1.935421976241	0.284730417901	-1.466407633771
F	0.313299726506	1.997271452491	-0.274392667121
F	0.609370399908	0.752890637569	1.506172755064
Cl	-0.343161577110	-1.848335326770	0.231658723896
Cl	-2.129688852171	0.469194489205	0.218741811781
F	-0.532542060180	-0.159592058602	-1.674518032031

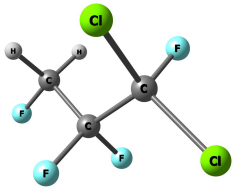
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
42.0588	0.146
111.4922	0.516
168.5272	0.155
196.0481	0.152
215.5712	0.265
262.8166	0.331
303.0362	0.475
315.3544	0.250
383.0322	0.0387
392.5864	0.0496
457.1690	0.622
527.1656	1.97
605.1490	8.09
625.3863	5.93
850.7815	25.4
897.5105	15.1
989.7077	9.56
1127.5688	14.8
1137.1680	16.5
1165.8377	13.8
1220.7738	4.30
1251.7852	11.2
1318.1101	6.17
1428.0457	0.558
1497.9380	0.730
3052.5346	2.44
3113.6794	1.87

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
42.0601	0.146
111.4879	0.516
168.5237	0.155
196.0467	0.152
215.5708	0.265
262.8160	0.331
303.0336	0.475
315.3552	0.250
383.0326	0.0387
392.5867	0.0496
457.1693	0.622
527.1657	1.97
605.1491	8.09
625.3866	5.93
850.7811	25.4
897.5115	15.1
989.7067	9.56
1127.5686	14.8
1137.1710	16.5
1165.8348	13.8
1220.7728	4.30
1251.7860	11.2
1318.1101	6.17
1428.0462	0.558
1497.9375	0.730
3052.5352	2.44
3113.6795	1.87



$\Delta E = 0.38$ kcal mol^{-1}
Population = 0.100



$\Delta E = 0.38$ kcal mol^{-1}
Population = 0.100

Optimized Coordinates (Angstroms)

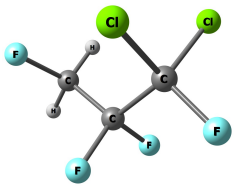
Atom	X	Y	Z
C	1.817902128946	0.656965744824	-0.369558457543
C	0.737955374949	-0.305829054936	0.132846580629
C	-0.699995031759	0.085063665177	-0.320449738087
H	1.685390227270	1.640243774837	0.088762323135
F	3.031165571809	0.139045875233	-0.012022207190
H	1.753313484297	0.738351366481	-1.458668602458
F	0.767846419171	-0.381855846239	1.474729424061
F	0.987833324586	-1.535572370947	-0.363861604099
Cl	-1.870710328211	-1.152201743177	0.194319958951
Cl	-1.156303197897	1.684883937331	0.342845068773
F	-0.704382973160	0.161297651415	-1.659672746174

Atom	X	Y	Z
C	1.819134990829	-0.651259364477	-0.381025166081
C	0.739032542813	0.303189267438	0.136734989581
C	-0.699254246975	-0.082710302480	-0.319757895228
H	1.752862521471	-0.717240579298	-1.471075895983
F	3.032452844626	-0.137214857780	-0.018121377610
H	1.688359904686	-1.641081624580	0.063500100091
F	0.986864838273	1.540118821626	-0.342859715616
F	0.771018626053	0.360184922156	1.479512601661
Cl	-1.152871600489	-1.692258912051	0.321479988291
Cl	-1.870380720606	1.145911127638	0.214413839044
F	-0.705735700680	-0.139921498192	-1.659919468150

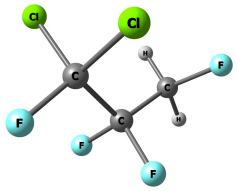
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
58.4350	0.445
80.8956	0.373
144.3024	0.355
190.8960	0.0589
232.4882	0.0652
265.4058	0.163
300.6691	0.155
324.5531	0.442
354.1496	0.0850
386.9120	0.0830
438.4917	0.298
515.5917	0.911
574.6981	2.42
761.1091	15.2
826.4262	28.0
887.2580	21.9
983.9128	6.56
1116.0704	17.5
1128.6635	10.5
1190.9430	5.45
1197.3605	10.7
1261.7350	11.2
1309.1717	6.96
1433.1679	0.470
1501.9670	0.192
3065.2238	1.97
3125.9632	1.69

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
58.4357	0.445
80.8954	0.373
144.3024	0.355
190.8964	0.0589
232.4885	0.0652
265.4059	0.163
300.6694	0.155
324.5533	0.442
354.1497	0.0850
386.9121	0.0830
438.4919	0.298
515.5919	0.911
574.6982	2.42
761.1091	15.2
826.4264	28.0
887.2584	21.9
983.9125	6.56
1116.0718	17.5
1128.6639	10.5
1190.9446	5.45
1197.3605	10.7
1261.7350	11.2
1309.1715	6.96
1433.1677	0.470
1501.9664	0.192
3065.2240	1.97
3125.9636	1.69



$\Delta E = 0.95$ kcal mol^{-1}
Population = 0.038



$\Delta E = 0.95$ kcal mol^{-1}
Population = 0.038

Optimized Coordinates (Angstroms)

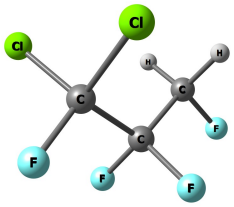
Atom	X	Y	Z
C	1.702074717423	0.168594633611	-0.901897218415
C	0.815567274459	0.518038535670	0.292412910192
C	-0.676281524485	0.058622928765	0.265904029146
H	2.644897056836	0.706854997115	-0.751839239348
F	1.942033730623	-1.174537758915	-0.953696671549
H	1.232277383221	0.503924781252	-1.830472374528
F	0.797599164507	1.868087479630	0.393095292706
F	1.354451547055	0.020714102158	1.422771760827
Cl	-1.517608168091	0.765580705302	-1.150997266984
Cl	-0.816482906006	-1.715640607799	0.252248958359
F	-1.255021275542	0.526354203211	1.375649819595

Atom	X	Y	Z
C	1.688357271397	-0.202174360168	-0.917756791565
C	0.797466113649	-0.548415695406	0.274223415285
C	-0.676084605079	-0.032646410480	0.270984311939
H	1.199866997753	-0.495749211150	-1.850815498195
F	1.978577156173	1.131862024690	-0.937462311221
H	2.611155283044	-0.779191019444	-0.788717890032
F	1.362502925724	-0.100778634493	1.412552671024
F	0.729136013156	-1.898963427012	0.340881534603
Cl	-0.749162414714	1.745406605108	0.303278589247
Cl	-1.553233457768	-0.670995834881	-1.156723387033
F	-1.264490283334	-0.506469036763	1.373036355948

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
43.0723	0.168
111.0204	0.404
176.0523	0.0997
186.4307	0.137
222.6732	0.290
269.9168	0.604
309.7581	0.240
331.5709	0.357
365.9175	0.0640
388.3800	0.168
455.0808	1.60
483.1021	0.415
601.0885	2.33
662.3009	7.17
855.6095	38.2
915.6229	15.8
957.3987	2.09
1134.8064	16.1
1142.1516	17.7
1165.7669	16.0
1217.5519	8.14
1251.4717	5.41
1312.0207	7.52
1432.5318	0.345
1497.9208	1.07
3052.6258	2.40
3116.4727	1.95

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
43.0725	0.168
111.0215	0.404
176.0530	0.0997
186.4307	0.137
222.6728	0.290
269.9168	0.604
309.7579	0.240
331.5703	0.357
365.9174	0.0640
388.3797	0.168
455.0803	1.60
483.1016	0.415
601.0891	2.33
662.2998	7.17
855.6092	38.2
915.6223	15.8
957.3978	2.09
1134.8057	16.1
1142.1517	17.7
1165.7678	16.0
1217.5514	8.14
1251.4700	5.41
1312.0198	7.52
1432.5307	0.345
1497.9202	1.07
3052.6264	2.40
3116.4734	1.95



$\Delta E = 1.32$ kcal mol^{-1}
Population = 0.020

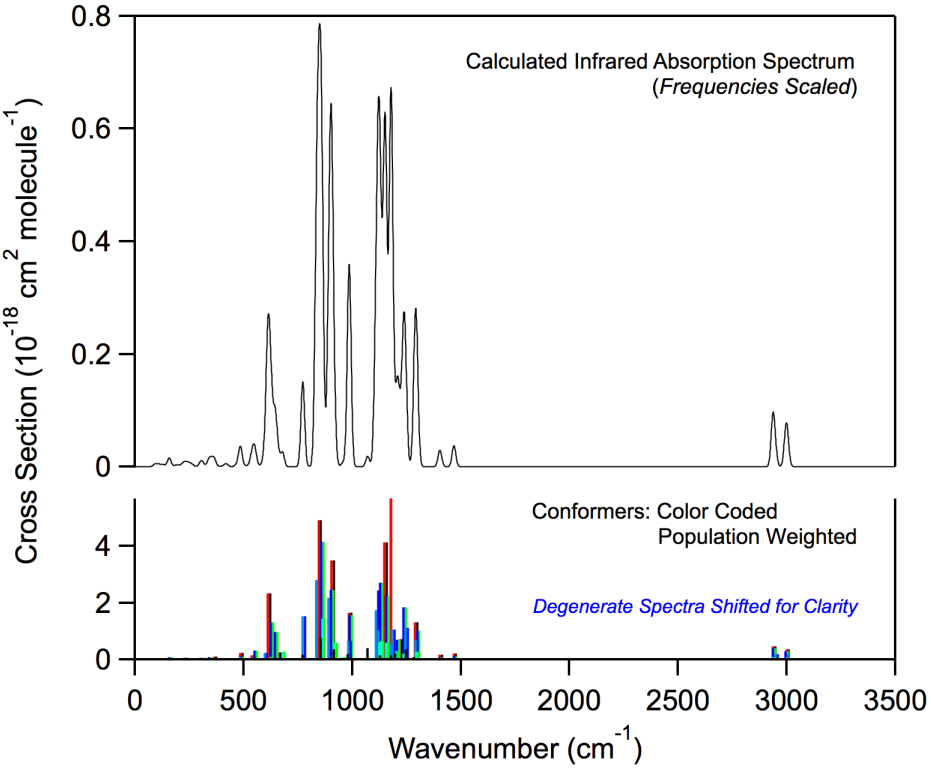
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.520350305566	0.020129489917	-1.009490657432
C	0.780930264932	-0.008604332970	0.326665232659
C	-0.777788749657	-0.000446981449	0.249204318683
H	1.264041193516	0.930434623966	-1.558328868771
F	2.860011715880	0.008113973554	-0.732515415791
H	1.256770764959	-0.860983397145	-1.600877954935
F	1.138003100196	1.061486731867	1.067004817577
F	1.129180092207	-1.115489081347	1.015306394333
Cl	-1.364634143347	1.490375535711	-0.548495324692
Cl	-1.376544330522	-1.446938007664	-0.618215137500
F	-1.246371213729	-0.028162554441	1.496919595868

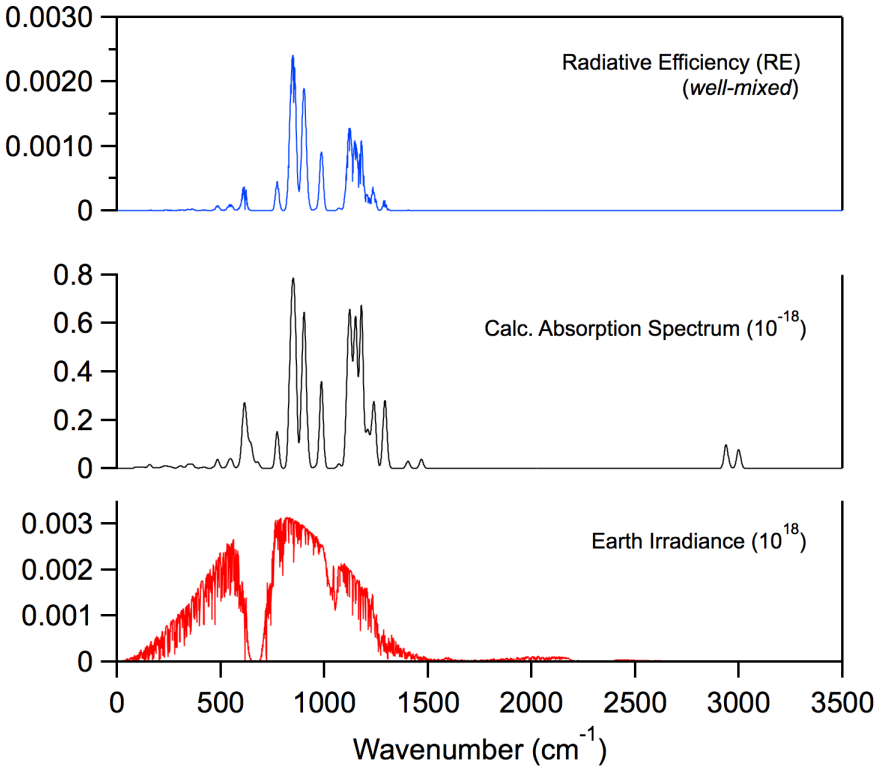
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
57.0754	0.543
79.3474	0.201
154.9334	0.306
176.8714	0.0336
232.6123	0.0628
280.2445	0.211
302.1156	0.142
313.7319	0.490
372.6795	0.0258
382.3726	0.0968
434.5196	0.641
495.3354	0.865
554.7202	1.96
760.3555	8.64
847.1347	37.4
911.2417	17.4
979.9084	9.47
1077.0882	19.5
1137.0904	7.58
1189.7407	6.86
1212.3352	10.4
1262.2341	17.7
1303.1274	4.46
1436.5068	0.460
1500.0978	0.325
3066.8516	2.01
3125.8709	1.62

Infrared Spectrum

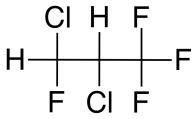


Radiative Efficiency



HCFC-234da

Molecular Formula:	$CHClFCHClCF_3$
Name:	2,3-Dichloro-1,1,1,3-tetrafluoropropane
CAS number:	146916-90-7
Molecular Weight:	184.95



Global Atmospheric Lifetime (years):	2.67
Tropospheric Atmospheric Lifetime (years):	2.82
Stratospheric Atmospheric Lifetime (years):	50.3
Ozone Depletion Potential (ODP):	0.024

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.232	0.203
Global Warming Potential (GWP_H):		
GWP_{20}	754	658
GWP_{100}	204	178
Global Temperature Potentials (GTP_H)		
GTP_{20}		268
GTP_{50}		33
GTP_{100}		25

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 2.08 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 1.33 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 2.73$ years

$\tau^{OH}_{Trop} = 2.82$ years

$\tau^{OH}_{Strat} = 85.9$ years

Fractional Atmospheric Loss: 0.978

O(^{1}D) Reactivity

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

$k_{Est}(T) = 1.4 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 265$ years

Fractional Atmospheric Loss: 0.010

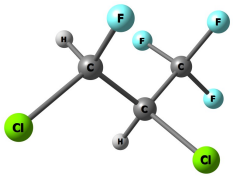
UV Photolysis

UV Spectrum: *No Recommendation*

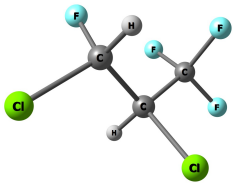
$\tau_{hv} = 225$ years

Fractional Atmospheric Loss: 0.012

Molecular Structure and Infrared Spectrum (6 conformers)



E = 0
Population = 0.371



$\Delta E = 0.27$ kcal mol^{-1}
Population = 0.234

Optimized Coordinates (Angstroms)

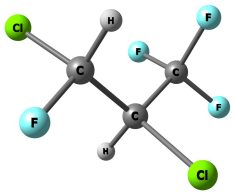
Atom	X	Y	Z
C	0.969938051052	-0.779082854667	-0.018025571471
C	-0.086089045953	0.241765290368	-0.452011665273
C	-1.505016786299	-0.288400203771	-0.183734026440
Cl	2.599064417641	-0.318199660362	-0.620853682720
F	1.001122693750	-0.892902628659	1.324013998624
H	0.746705606706	-1.752625219716	-0.460048324886
H	-0.000720782291	0.403458341407	-1.526896703470
Cl	0.133187609374	1.815998568385	0.359390635868
F	-2.422460379735	0.543941301768	-0.670695350423
F	-1.646749019005	-1.471555709331	-0.810466030733
F	-1.743810365240	-0.476621225423	1.109579720924

Atom	X	Y	Z
C	-1.013371700241	-0.550102883478	-0.379068582845
C	0.068615236069	0.224343988086	0.388723442273
C	1.481941742984	-0.304016343707	0.068543908923
F	-0.831458000865	-1.877694200690	-0.191782556257
Cl	-2.651621743739	-0.109878747339	0.210417174550
H	-0.986160336961	-0.322267412512	-1.445387148800
H	-0.091555038656	0.129708397817	1.463101355361
Cl	-0.027978529993	1.959070605108	-0.036740970136
F	2.417058634336	0.500183631507	0.570203210164
F	1.651131237217	-1.513011787600	0.609285928877
F	1.672980499848	-0.402503247193	-1.251124762112

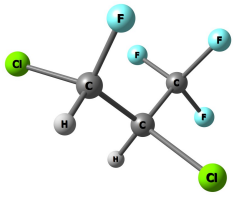
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
50.0971	0.0777
75.1490	0.0610
151.2862	0.355
180.9302	0.0833
202.4284	0.161
256.9987	0.0333
304.3275	0.0511
357.1067	0.0745
399.4564	0.281
529.6866	0.410
549.5109	1.10
642.7452	5.13
671.0187	10.2
794.4282	11.0
812.6866	2.90
892.2137	2.02
976.7547	5.05
1134.9954	6.15
1163.1685	31.5
1214.4531	26.2
1264.3928	1.24
1275.8838	15.2
1290.0894	25.4
1350.7757	19.4
1379.3648	3.71
3103.0861	0.632
3127.0736	0.589

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
51.4310	0.0648
63.3114	0.0297
153.3300	0.102
197.0463	0.0939
219.5502	0.488
272.0255	0.302
310.7128	0.105
373.2729	0.0376
420.2627	1.08
453.5530	1.24
543.9935	0.908
561.1596	0.0659
668.8941	11.7
788.9981	11.4
832.4209	4.32
888.5532	4.46
1069.3624	3.36
1118.4966	6.91
1159.5482	25.8
1201.3306	13.8
1239.6282	24.1
1259.7713	35.6
1290.7460	5.07
1346.1744	14.5
1384.1363	4.23
3118.1253	0.656
3131.6812	0.479



$\Delta E = 0.49$ kcal mol^{-1}
Population = 0.162



$\Delta E = 0.59$ kcal mol^{-1}
Population = 0.136

Optimized Coordinates (Angstroms)

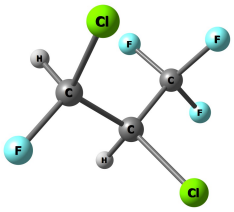
Atom	X	Y	Z
C	1.128827177598	0.539553796985	0.334634037525
C	-0.191206517319	0.380204581031	-0.432348388257
C	-1.017692591762	-0.850271046001	-0.012820269342
Cl	2.263238422957	-0.812242859318	-0.023200636127
F	1.721736270178	1.690214352521	-0.044717300023
H	0.967791146558	0.542645884108	1.413319251937
H	0.003578658443	0.323390108010	-1.503620870705
Cl	-1.171537995842	1.858762287206	-0.136198846281
F	-2.246951108279	-0.792463555361	-0.520166588619
F	-0.450808431689	-1.974002028519	-0.457486230314
F	-1.113074030846	-0.928646520661	1.319351840207

Atom	X	Y	Z
C	-1.061428003017	0.862086310828	0.052433443958
C	0.272550239295	0.328653895241	0.588545867891
C	0.804051504429	-0.943487245284	-0.100460209254
F	-1.067637117209	0.884197888092	-1.294782731141
Cl	-2.445533165109	-0.136136422709	0.641398903070
H	-1.238787535854	1.867923685385	0.435151460478
H	0.174069742730	0.117676315285	1.652624407526
Cl	1.504771003697	1.629988247381	0.419210873501
F	1.908776650375	-1.359779468101	0.525503386825
F	-0.100890465656	-1.923531407339	-0.028749772285
F	1.100179146318	-0.739277798778	-1.379692630568

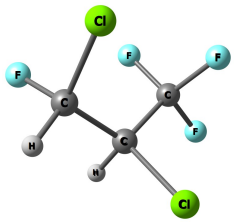
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
37.8291	0.0420
72.6199	0.0389
155.7889	0.0681
204.1582	0.206
225.8008	0.676
262.0685	0.169
333.2944	0.0910
365.4386	0.0344
420.3156	0.649
432.7948	1.99
546.5536	0.718
561.6505	0.258
697.2303	4.67
755.3488	24.0
820.5146	0.333
885.2408	2.96
1061.1746	1.14
1121.3568	24.7
1165.0850	11.8
1209.5666	9.71
1234.0897	26.5
1261.2627	27.9
1298.8984	6.44
1330.9466	10.8
1395.9660	5.50
3119.6922	0.589
3133.7246	0.370

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
37.2546	0.0591
88.5314	0.0740
158.6885	0.0645
188.2298	0.268
204.1321	0.164
260.8819	0.197
303.2313	0.0512
357.0638	0.0732
396.2573	0.240
522.5574	2.55
532.4497	0.804
588.5022	3.46
747.6624	10.4
760.8016	16.1
811.4130	0.704
869.1735	2.96
977.3147	1.46
1151.3594	9.18
1165.9229	29.9
1213.4360	23.2
1236.6717	10.9
1268.5677	20.9
1302.6841	12.3
1347.1190	15.0
1403.8672	3.04
3115.8758	0.905
3138.8516	0.313



$\Delta E = 0.97$ kcal mol^{-1}
Population = 0.072



$\Delta E = 1.59$ kcal mol^{-1}
Population = 0.025

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.127716967214	-0.288189203361	0.759010764752
C	0.163023086480	0.498392556500	0.508487697166
C	1.362106933030	-0.377424268010	0.117978822456
F	-2.044394631834	0.553297183115	1.286964459226
Cl	-1.811605603024	-1.054556769835	-0.708280168578
H	-0.929964835652	-1.098454824575	1.464027610867
H	0.421024608047	0.964688494942	1.462715817850
Cl	-0.057768155548	1.822764132814	-0.666049202496
F	2.490913413492	0.327662322218	0.197045826252
F	1.452018821008	-1.398986736521	0.989703422832
F	1.269185331215	-0.882859887287	-1.105093050327

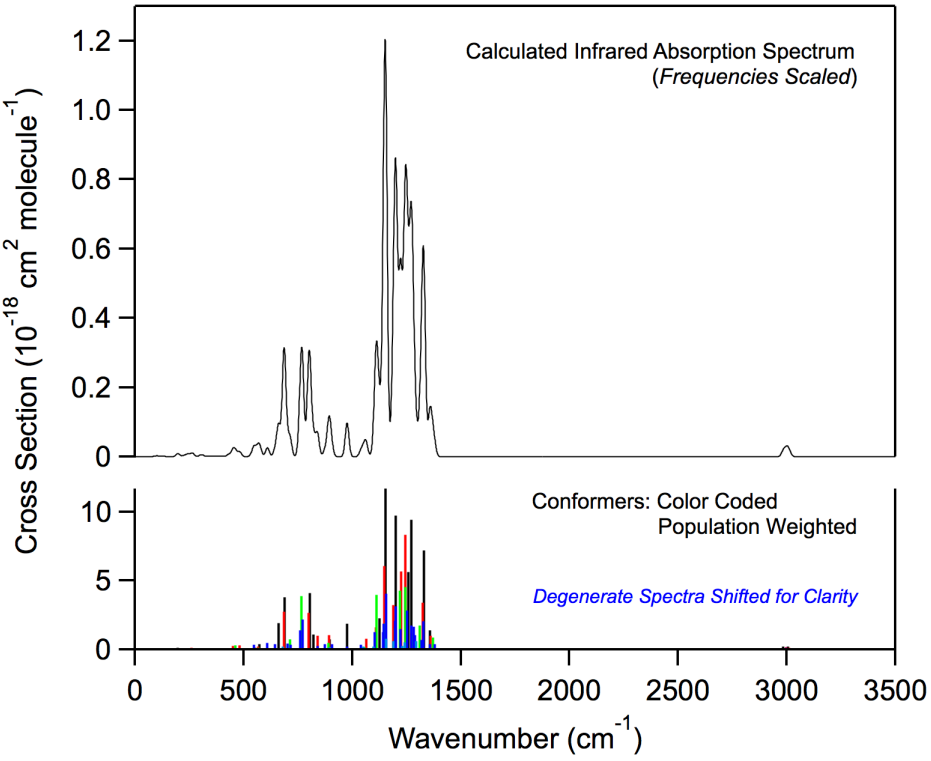
Atom	X	Y	Z
C	1.224160964184	-0.026396120280	-0.762713517003
C	-0.266447306906	0.335021758745	-0.683147182921
C	-1.146596803177	-0.569932526591	0.197814471258
Cl	2.042128406675	-0.136209219131	0.829048066909
F	1.345734963599	-1.210375606198	-1.408536952885
H	1.752927742912	0.747749688489	-1.321549010893
H	-0.653778838403	0.242821079468	-1.700550627039
Cl	-0.464346425926	2.044753686628	-0.200163696966
F	-2.434609414747	-0.319302650772	-0.059768121304
F	-0.908887797756	-1.852330804193	-0.095554369743
F	-0.942687490455	-0.389432286165	1.497570940588

Infrared Absorption Spectrum (unscaled frequencies)

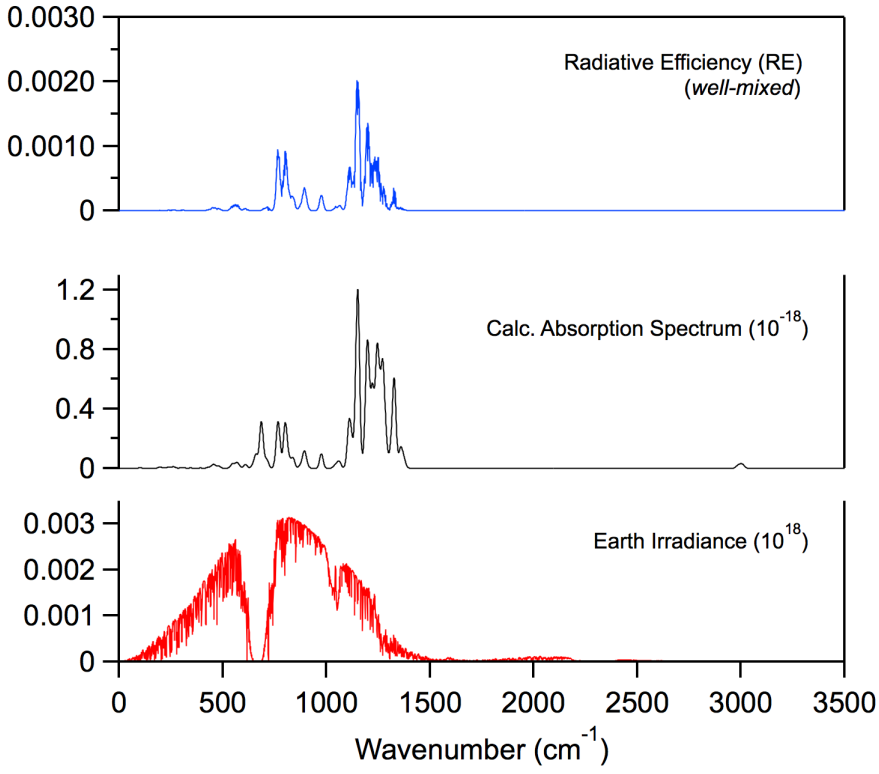
Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
48.7011	0.0522
82.0806	0.0503
150.8538	0.216
175.9037	0.113
192.0060	0.205
271.3947	0.119
323.0262	0.106
356.7861	0.0313
421.2868	0.401
516.5016	1.44
555.0351	0.688
625.6902	5.47
687.3253	6.25
701.7928	4.81
832.1921	3.75
902.7451	5.66
1045.1849	5.12
1112.8058	17.9
1155.0462	26.0
1211.8880	29.1
1249.8146	1.06
1291.1816	24.3
1307.7970	14.4
1340.0990	9.67
1380.5652	5.67
3095.0562	0.191
3105.3547	1.20

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
40.8917	0.0295
89.0982	0.0382
153.6721	0.0807
183.1507	0.0773
200.9858	0.184
272.0290	0.306
316.8740	0.0658
366.7413	0.0649
431.7107	0.178
511.6188	2.09
533.6266	2.06
589.8527	3.40
662.0053	7.85
758.2354	1.31
832.9760	4.22
892.2319	6.63
1056.4050	9.29
1106.0614	8.26
1166.2756	31.0
1202.0855	23.8
1246.3127	9.59
1259.0378	21.1
1312.3081	23.8
1362.9624	2.39
1389.5006	5.40
3099.7657	0.838
3108.6131	0.705

Infrared Spectrum

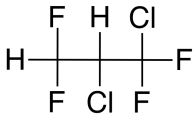


Radiative Efficiency



HCFC-234db

Molecular Formula:	$CHF_2CHClCClF_2$
Name:	1,2-Dichloro-1,1,3,3-tetrafluoropropane
CAS number:	1945188-10-2
Molecular Weight:	184.95



Global Atmospheric Lifetime (years):	5.69
Tropospheric Atmospheric Lifetime (years):	6.18
Stratospheric Atmospheric Lifetime (years):	71.5
Ozone Depletion Potential (ODP):	0.039

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.292	0.271
Global Warming Potential (GWP_H):		
GWP_{20}	1957	1819
GWP_{100}	546	508
Global Temperature Potentials (GTP_H)		
GTP_{20}		1067
GTP_{50}		115
GTP_{100}		71

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 9.50 \times 10^{-15}$; $k_{SAR}(272\ K) \approx 6.06 \times 10^{-15}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 5.96$ years

$\tau^{OH}_{Trop} = 6.18$ years

$\tau^{OH}_{Strat} = 173.9$ years

Fractional Atmospheric Loss: 0.953

$O(^1D)$ Reactivity

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

$k_{Est}(T) = 1.4 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 265$ years

Fractional Atmospheric Loss: 0.022

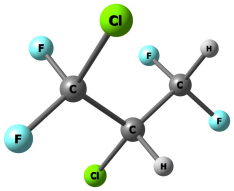
UV Photolysis

UV Spectrum: *No Recommendation*

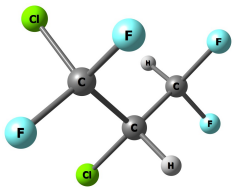
$\tau_{hv} = 225$ years

Fractional Atmospheric Loss: 0.025

Molecular Structure and Infrared Spectrum (9 conformers)



E = 0
Population = 0.310



$\Delta E = 0.44$ kcal mol^{-1}
Population = 0.147

Optimized Coordinates (Angstroms)

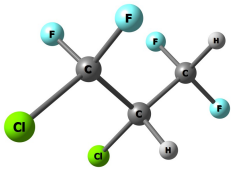
Atom	X	Y	Z
C	1.056699700504	-1.142778622164	-0.097759257326
C	0.373170896817	0.161615972649	-0.531524416047
C	-1.019297458803	0.367907345291	0.081668497470
F	2.222426448833	-1.260129485322	-0.768630855396
F	1.320666132844	-1.126808881885	1.222583072340
H	0.429615413973	-2.012169733922	-0.325347508971
H	0.262674468321	0.150540950168	-1.616152909333
Cl	1.408646780957	1.563217075311	-0.111294913024
Cl	-2.128834302889	-0.966641268585	-0.455439983539
F	-0.984973854096	0.373395757206	1.409372452445
F	-1.546526226461	1.516963891253	-0.334880178620

Atom	X	Y	Z
C	1.425327404427	-0.589091718510	0.385413840165
C	0.468267980065	0.241433032906	-0.482062250660
C	-0.999479163063	-0.220653861120	-0.437665135406
F	1.300436489098	-1.894510315804	0.057249478606
F	2.689722038517	-0.208193129238	0.110102926150
H	1.233625150179	-0.462866175604	1.455391489687
H	0.786237253728	0.152456757724	-1.523948670313
Cl	0.605944474598	1.961189627965	-0.018475453951
Cl	-1.654670795084	-0.325481005031	1.236299537008
F	-1.763769838553	0.618742129247	-1.135646401198
F	-1.094248993911	-1.427186342535	-1.003152360089

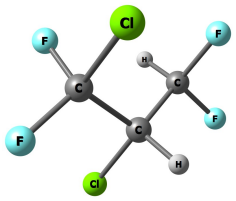
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
48.7026	0.144
85.2667	0.0859
155.1744	0.270
190.5373	0.125
201.6136	0.0940
279.4553	0.488
295.3918	0.00832
337.7013	0.0559
396.5545	0.267
414.4325	0.472
544.5274	2.12
624.9555	1.46
662.7098	8.86
791.8897	23.4
807.8004	3.95
945.5709	13.6
995.9288	8.90
1117.0206	16.6
1178.7949	11.1
1196.2600	23.8
1249.3472	17.5
1264.2138	7.96
1323.4872	7.29
1393.5134	8.35
1412.2636	3.85
3071.0723	3.15
3127.5714	0.576

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
49.3336	0.0618
80.9516	0.0875
151.3640	0.130
183.2632	0.0678
211.5924	0.213
297.0856	0.0248
331.6277	0.351
369.1271	0.108
401.9947	0.858
433.7351	1.39
475.3744	2.21
564.8055	2.20
641.9706	1.85
682.9273	10.6
862.5025	10.8
1038.4887	26.0
1083.1523	6.26
1125.9788	7.58
1138.7983	28.7
1181.2165	27.6
1209.2034	18.3
1241.3805	3.07
1305.5427	7.32
1396.7868	3.05
1414.7763	6.72
3087.7965	2.30
3103.8573	0.927



$\Delta E = 0.48$ kcal mol^{-1}
Population = 0.137



$\Delta E = 0.53$ kcal mol^{-1}
Population = 0.126

Optimized Coordinates (Angstroms)

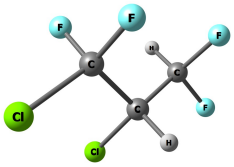
Atom	X	Y	Z
C	1.591315146722	-0.679462146838	-0.346853106871
C	0.345868069164	0.211437745217	-0.488140195807
C	-0.913853041024	-0.514118646224	0.015170697570
F	2.648005703867	-0.044593098800	-0.894373470091
F	1.859833972763	-0.923015207998	0.950466141118
H	1.443725322863	-1.634049612396	-0.865274292004
H	0.207412420454	0.432931030121	-1.546831719781
Cl	0.584101489085	1.757535284759	0.367320508424
Cl	-2.416682472958	0.370969692833	-0.411863831574
F	-0.962924885721	-1.722179337668	-0.578941962458
F	-0.884461725215	-0.704165703006	1.329168231475

Atom	X	Y	Z
C	1.152299672867	-1.008661426586	0.347373901224
C	0.483681653679	0.143740209296	-0.423059439112
C	-0.939289257783	0.474048311147	0.065071708192
F	0.424181864297	-2.138529121913	0.215779926914
F	2.366513181327	-1.236631719274	-0.192367914693
H	1.265097729578	-0.772426146476	1.410482809217
H	0.455813104382	-0.095043680433	-1.485899165883
Cl	1.518113495093	1.599361653228	-0.217287747867
Cl	-2.122876980377	-0.767780772687	-0.480102839647
F	-0.969151592174	0.535621761378	1.401988252763
F	-1.343973870888	1.647980932319	-0.415738491108

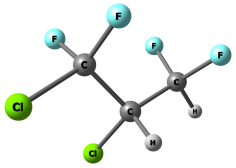
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
53.7103	0.0776
78.7389	0.136
150.4814	0.211
187.6403	0.111
208.4969	0.310
250.1685	0.0965
316.7778	0.104
330.3953	0.0701
421.2112	0.0609
430.7837	0.173
537.8388	3.89
605.7773	1.82
676.8632	7.88
792.0065	10.6
823.7534	8.01
969.9583	13.8
984.8841	14.2
1135.1758	22.0
1150.8784	16.0
1178.2774	19.0
1244.3166	21.4
1266.8929	6.39
1313.0915	6.71
1390.4476	9.69
1412.7483	4.12
3065.9051	3.31
3124.5435	0.631

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
39.2984	0.0667
73.6847	0.0767
162.6904	0.0461
188.8202	0.192
230.0204	0.417
256.7492	0.406
324.2479	0.104
367.7480	0.808
387.2199	0.282
423.7203	0.177
504.5606	2.78
564.3797	2.01
616.8525	0.535
790.2496	28.4
835.6748	2.72
955.5178	17.7
1072.1742	2.80
1128.0418	22.8
1137.6708	23.0
1195.1733	21.8
1222.0001	11.8
1239.2940	6.40
1308.1439	5.48
1397.6481	2.54
1415.2647	7.57
3083.1659	3.05
3137.3311	0.391



$\Delta E = 0.71$ kcal mol^{-1}
Population = 0.093



$\Delta E = 0.92$ kcal mol^{-1}
Population = 0.066

Optimized Coordinates (Angstroms)

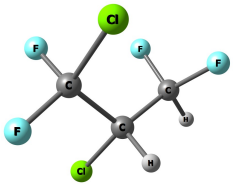
Atom	X	Y	Z
C	1.693124480283	-0.363109701791	0.187985937948
C	0.385583181636	0.239903002438	-0.363701479909
C	-0.855896974360	-0.510727806912	0.152932137515
F	1.797504186890	-1.650251906629	-0.209853393571
F	2.735639002164	0.314749449227	-0.331408418260
H	1.736898412248	-0.315453173660	1.281271976566
H	0.401881049773	0.185546411926	-1.452672589111
Cl	0.326763857988	1.961795055370	0.113146016403
Cl	-2.387487437631	0.195280170469	-0.463938179613
F	-0.805434779352	-1.783906859262	-0.249612083254
F	-0.882582979640	-0.500312641175	1.490196075284

Atom	X	Y	Z
C	1.788859652432	-0.056231999551	-0.361471811034
C	0.318586508200	0.351343562655	-0.577930817597
C	-0.681444972102	-0.537506740453	0.189388498422
F	2.058409795909	-0.214798646288	0.948974698027
F	2.021953609400	-1.229771884854	-0.991429092150
H	2.457291508732	0.707871259732	-0.774488531091
H	0.100319791897	0.272380112779	-1.642654768853
Cl	0.124401201095	2.066268891361	-0.107252327246
Cl	-2.373461507098	-0.223302088037	-0.351497173236
F	-0.403944689110	-1.822111429656	-0.057574731091
F	-0.613755899355	-0.338815037688	1.501007055848

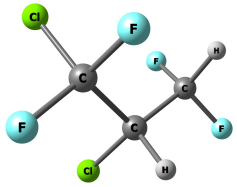
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
40.8236	0.0675
70.7798	0.0874
160.2690	0.140
190.4008	0.0652
213.7599	0.360
277.5463	0.203
319.7575	0.223
370.7956	0.213
410.0807	0.800
425.1691	0.356
473.3004	4.48
568.2228	1.68
614.5590	1.27
793.5911	13.7
861.6942	8.93
953.3918	20.2
1081.0891	19.1
1120.5941	3.94
1149.5934	11.0
1163.9668	39.3
1222.3640	22.1
1239.8963	4.78
1305.4112	3.78
1396.1658	4.18
1412.4965	7.96
3079.2411	3.34
3129.3854	0.451

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
45.3846	0.0605
88.9458	0.114
155.1400	0.0394
193.0641	0.139
206.5932	0.197
250.4345	0.0331
308.7644	0.0352
375.3005	0.0468
413.1578	0.203
423.4818	0.333
523.6267	7.42
572.0514	3.20
633.5036	6.82
807.1367	2.12
879.5455	7.33
943.0402	20.6
987.0688	8.08
1120.3251	10.0
1161.4351	25.1
1183.5440	29.3
1230.2968	11.0
1252.8735	15.8
1329.1525	10.4
1393.8775	5.52
1419.1826	4.33
3066.4645	4.08
3132.2229	0.346



$\Delta E = 1.03$ kcal mol^{-1}
Population = 0.055



$\Delta E = 1.03$ kcal mol^{-1}
Population = 0.054

Optimized Coordinates (Angstroms)

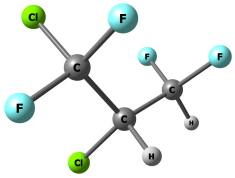
Atom	X	Y	Z
C	0.890151256638	-1.379921959210	-0.247764919091
C	0.514197504774	0.065740409473	-0.620207575144
C	-0.655774951918	0.695850914223	0.157440733577
F	0.952341094499	-1.535353862796	1.088175210949
F	-0.036729469481	-2.235168153970	-0.734931641529
H	1.863542719283	-1.632408757542	-0.683234006561
H	0.268732406530	0.097614749212	-1.681687728776
Cl	1.971879851478	1.094265347489	-0.378259121150
Cl	-2.181940517509	-0.224579025603	-0.109237163806
F	-0.413045383981	0.749879595688	1.462981098460
F	-0.856284510313	1.941823743037	-0.282769886927

Atom	X	Y	Z
C	1.333146273689	-0.869145398642	-0.375372775688
C	0.436710390388	0.366421694606	-0.529034415502
C	-1.066808141191	0.045901498406	-0.501935407697
F	2.589802422894	-0.532426908073	-0.740274507512
F	1.365451721101	-1.302608059288	0.897407021020
H	0.980509644030	-1.682047310415	-1.022018262736
H	0.622335557110	0.775733174200	-1.525446700012
Cl	0.865167370348	1.632493829942	0.648574351120
Cl	-1.660329943493	-0.624081621002	1.044985444616
F	-1.768062255939	1.142191790803	-0.789624510942
F	-1.302315038937	-0.859307690538	-1.472205236667

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
31.9324	0.0732
93.5132	0.136
160.5452	0.0333
205.7815	0.138
208.5206	0.304
255.8273	0.303
295.8371	0.0509
366.5525	0.158
393.6696	0.260
423.3454	0.207
531.6080	3.94
566.3919	1.89
698.7195	7.57
803.3402	1.41
813.3984	22.7
935.3826	13.9
995.4222	4.43
1127.2233	27.9
1157.2067	4.80
1190.2029	25.1
1225.8596	8.25
1252.3458	17.2
1339.6336	11.4
1398.9553	2.48
1422.8217	3.56
3067.9906	4.17
3131.5749	0.290

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
50.1518	0.111
81.3021	0.118
155.5154	0.162
171.9999	0.240
195.6822	0.113
270.5707	0.211
316.5326	0.0649
332.4843	0.188
423.6876	0.0222
444.0201	0.174
554.7620	2.26
634.7620	1.04
661.0663	10.9
680.5169	7.33
838.1143	5.06
991.4416	3.18
1041.5653	22.4
1124.4664	31.2
1164.4824	24.0
1185.2469	16.4
1203.1187	12.3
1266.5532	2.71
1312.5380	7.67
1396.5822	8.65
1413.4489	3.19
3059.7220	3.10
3096.5234	0.785



$\Delta E = 1.91$ kcal mol^{-1}
Population = 0.012

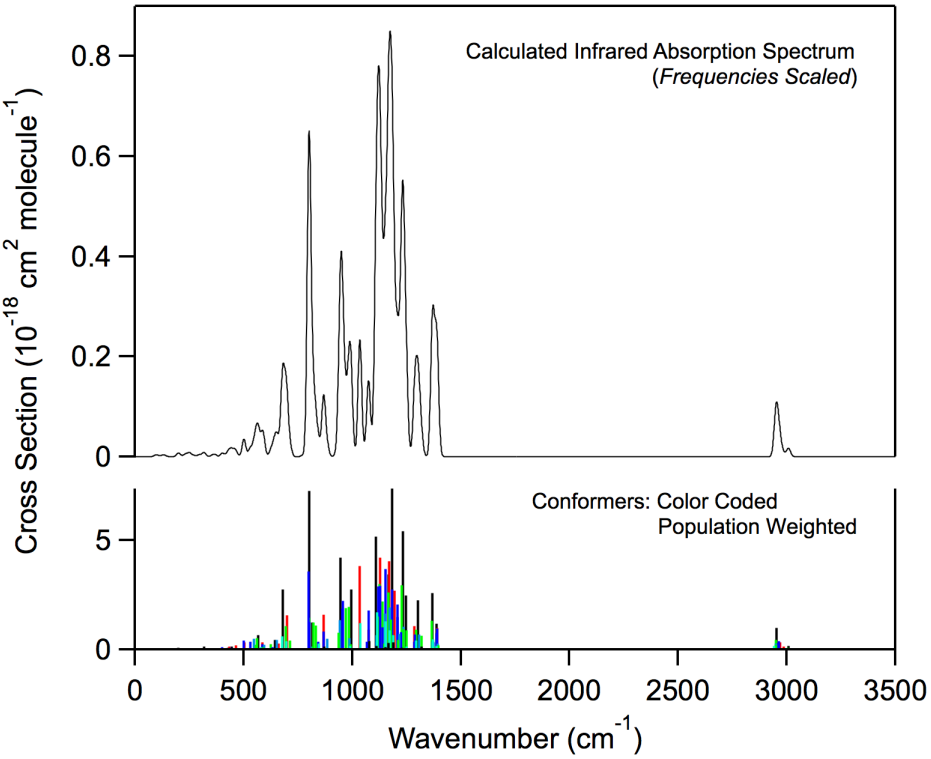
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.678390388968	-0.337332944578	-0.106678536068
C	0.448552685835	0.429108593088	-0.619497552839
C	-0.924217569252	-0.242426944433	-0.410206557592
F	1.613226100682	-0.564366466537	1.217408193451
F	1.753897559992	-1.529416043225	-0.741668885802
H	2.586208680755	0.238848666500	-0.321747989332
H	0.555187624801	0.522067553124	-1.703221902422
Cl	0.467305581720	2.086343379846	0.050026249707
Cl	-1.414144853573	-0.439018606529	1.298649759035
F	-1.857011291920	0.487812530231	-1.031236503194
F	-0.899400908008	-1.449152717487	-0.988589274943

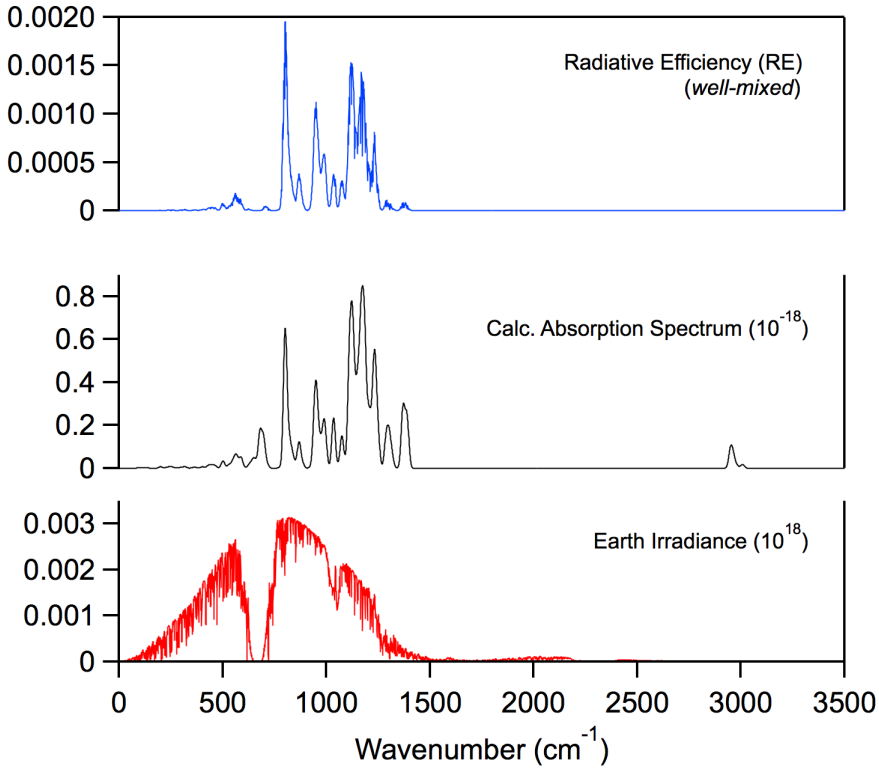
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
31.6994	0.0802
100.5371	0.120
166.3980	0.149
175.7632	0.0317
200.1901	0.107
277.9573	0.257
303.7195	0.0508
372.8241	0.147
422.1063	0.430
426.8859	0.336
541.0720	4.58
558.3785	3.38
643.0419	4.57
760.8006	4.74
866.1641	12.1
920.5444	3.81
1085.8955	30.3
1120.7697	12.9
1164.7665	8.81
1179.2686	25.4
1201.1407	26.2
1243.3226	5.76
1339.4690	10.2
1396.6713	4.22
1426.1369	1.80
3060.1935	4.70
3097.8060	0.386

Infrared Spectrum

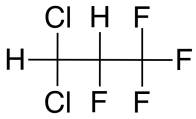


Radiative Efficiency



HCFC-234ea

Molecular Formula:	$CHCl_2CHFCF_3$
Name:	3,3-Dichloro-1,1,1,2-tetrafluoropropane
CAS number:	53063-54-0
Molecular Weight:	184.95



Global Atmospheric Lifetime (years):	1.06
Tropospheric Atmospheric Lifetime (years):	1.11
Stratospheric Atmospheric Lifetime (years):	23.1
Ozone Depletion Potential (ODP):	0.014

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.211	0.158
Global Warming Potential (GWP_H):		
GWP_{20}	271	204
GWP_{100}	74	55
Global Temperature Potentials (GTP_H)		
GTP_{20}		67
GTP_{50}		10
GTP_{100}		8

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 5.29 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 3.38 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 1.08$ years

$\tau^{OH}_{Trop} = 1.11$ years

$\tau^{OH}_{Strat} = 37.0$ years

Fractional Atmospheric Loss: 0.983

$O(^1D)$ Reactivity

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

$k_{Est}(T) = 1.4 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 265$ years

Fractional Atmospheric Loss: 0.004

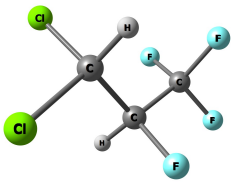
UV Photolysis

UV Spectrum: *No Recommendation*

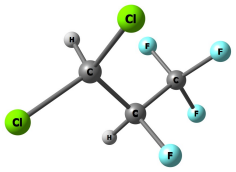
$\tau_{hv} = 80$ years

Fractional Atmospheric Loss: 0.013

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.530



$\Delta E = 0.14$ kcal mol^{-1}
Population = 0.421

Optimized Coordinates (Angstroms)

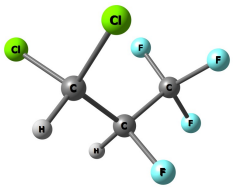
Atom	X	Y	Z
C	0.959762928774	-0.018594144711	0.375496981016
C	-0.221033637215	0.564599906764	-0.412570316729
C	-1.586941078072	-0.035256595309	-0.017296809971
Cl	1.210313389099	-1.742970318719	-0.017764077229
Cl	2.432950838559	0.934680617019	0.027181607509
H	0.779688926002	0.050971811461	1.445557360379
H	-0.070930124076	0.425659480961	-1.487696820324
F	-0.300274149808	1.899571907786	-0.123192897420
F	-2.561184531814	0.724849901207	-0.516144538207
F	-1.740443369320	-1.270890942929	-0.491991705710
F	-1.724519192128	-0.072284623528	1.313760216685

Atom	X	Y	Z
C	0.937978051655	0.060668391034	0.521300781362
C	-0.228436548810	-0.733051058858	-0.072645313697
C	-1.607439868880	-0.098028538168	0.180594663892
Cl	2.418061995395	-0.954485834904	0.486035453312
Cl	1.210539965752	1.605253964479	-0.328958566530
H	0.737995175046	0.293205798943	1.564405242138
H	-0.245741648716	-1.713857104786	0.417325881394
F	-0.078604167561	-0.900001182803	-1.413897467642
F	-2.562105862804	-0.967989747469	-0.157261513823
F	-1.736729921821	0.177785755676	1.488668828063
F	-1.801210169257	1.018373556855	-0.510441988468

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
33.6243	0.0328
75.0893	0.0273
144.8225	0.0958
217.9052	0.503
234.8366	0.268
237.0064	0.345
318.4520	0.205
349.5826	0.139
413.3327	1.55
449.8505	0.886
548.7292	0.392
571.5838	0.924
682.9013	11.3
773.4032	5.50
789.9457	14.8
869.1671	2.64
1076.8733	0.611
1123.2528	10.8
1174.2332	21.9
1227.3581	7.66
1237.6682	29.3
1250.7433	12.9
1278.1195	24.2
1369.7162	0.682
1383.1149	8.81
3086.6487	0.837
3156.2388	0.204

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
36.2319	0.0303
81.0689	0.0872
141.3857	0.341
197.2685	0.134
209.3397	0.103
254.7637	0.0749
266.5658	0.315
336.5243	0.0414
404.3732	0.271
520.2604	1.14
569.6359	0.616
651.3804	6.68
687.0472	16.0
735.5529	1.10
779.4730	7.32
878.7172	0.178
993.6344	2.75
1167.2245	23.2
1180.7266	12.4
1208.6130	33.6
1235.3731	10.4
1275.6831	6.34
1311.4367	23.0
1359.2342	2.56
1398.9926	6.45
3061.1050	1.04
3154.8376	0.255



$\Delta E = 1.41$ kcal mol^{-1}
Population = 0.049

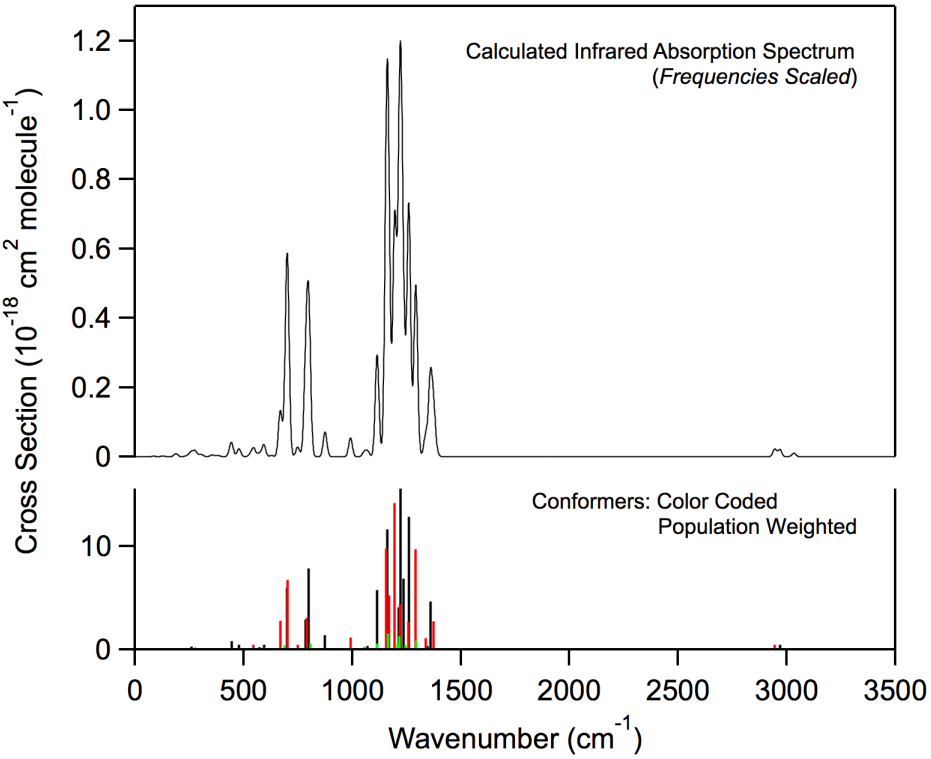
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.104239279909	0.128575450918	-0.587170193926
C	-0.396263720151	0.087337147206	-0.902930408775
C	-1.379552393794	-0.227948599274	0.240113468731
Cl	1.520316419256	1.229933359184	0.755191535479
Cl	1.755744418485	-1.518509775636	-0.326999821263
H	1.605679016827	0.524728653563	-1.467965352980
H	-0.548858731206	-0.672672837460	-1.677799059897
F	-0.750164647392	1.313524296045	-1.399166101637
F	-2.595225717469	-0.408400903793	-0.291624787969
F	-1.037393271046	-1.344391016370	0.883831423742
F	-1.461317653418	0.766240225618	1.118380298493

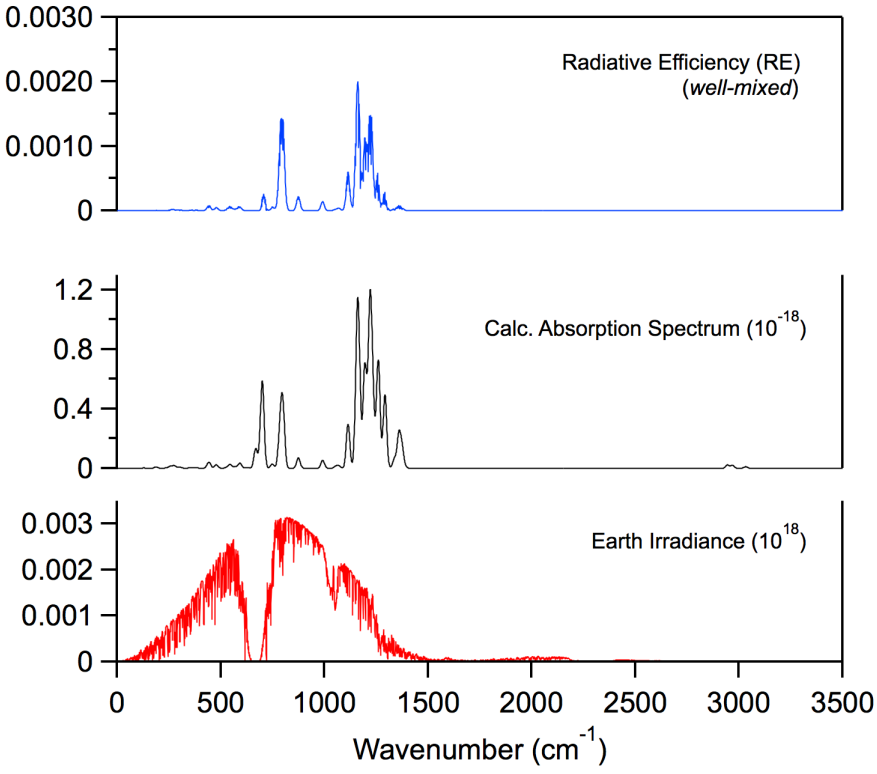
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
27.1374	0.0184
92.8463	0.0483
148.4697	0.0308
182.5615	0.191
231.6227	0.380
244.0185	0.239
291.9961	0.177
342.0572	0.0626
444.5513	0.459
504.5392	2.83
529.0998	1.65
609.0459	1.68
671.6889	8.89
738.2958	2.70
797.9581	12.3
866.7457	1.45
1060.7829	6.12
1121.6550	11.6
1176.8697	31.8
1221.5322	10.8
1232.2090	26.4
1260.5208	9.85
1314.3660	18.5
1354.1357	1.42
1415.5615	3.65
3065.7888	0.954
3138.3814	0.345

Infrared Spectrum

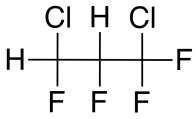


Radiative Efficiency



HCFC-234eb

Molecular Formula:	$CHClFCHFCClF_2$
Name:	1,3-Dichloro-1,1,2,3-tetrafluoropropane
CAS number:	139754-77-1
Molecular Weight:	184.95



Global Atmospheric Lifetime (years):	2.88
Tropospheric Atmospheric Lifetime (years):	3.04
Stratospheric Atmospheric Lifetime (years):	52.4
Ozone Depletion Potential (ODP):	0.026

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.273	0.241
Global Warming Potential (GWP_H):		
GWP_{20}	957	842
GWP_{100}	259	228
Global Temperature Potentials (GTP_H)		
GTP_{20}		353
GTP_{50}		42
GTP_{100}		32

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 1.93 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 1.23 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 2.95$ years

$\tau^{OH}_{Trop} = 3.04$ years

$\tau^{OH}_{Strat} = 92.0$ years

Fractional Atmospheric Loss: 0.976

O(^{1}D) Reactivity

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

$k_{Est}(T) = 1.4 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 265$ years

Fractional Atmospheric Loss: 0.011

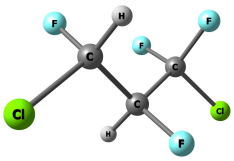
UV Photolysis

UV Spectrum: *No Recommendation*

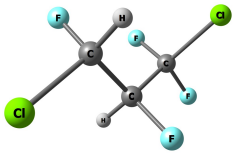
$\tau_{hv} = 225$ years

Fractional Atmospheric Loss: 0.013

Molecular Structure and Infrared Spectrum (12 conformers)



E = 0
Population = 0.288



$\Delta E = 0.18$ kcal mol^{-1}
Population = 0.211

Optimized Coordinates (Angstroms)

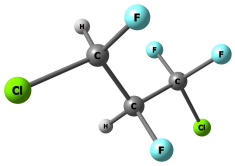
Atom	X	Y	Z
C	1.366477003534	0.359283622793	-0.303830633040
C	0.149677073685	-0.385962254614	0.263925990202
C	-1.167268678299	0.326307791666	-0.108095248582
F	1.401254287698	1.615660035525	0.191401317508
Cl	2.867817437451	-0.507695589772	0.159519255063
H	1.341145230408	0.387555439737	-1.394310396396
H	0.218185093375	-0.444265277380	1.354446694836
F	0.130517258393	-1.635036473505	-0.279731237927
F	-1.212124785341	0.564343143278	-1.425089967850
Cl	-2.581147396749	-0.683806671788	0.340097406970
F	-1.254116524153	1.492098234061	0.533203819218

Atom	X	Y	Z
C	1.183082112231	-0.370721330821	0.347749608002
C	0.192980437964	0.406395371014	-0.524094803084
C	-1.265334409260	-0.081881002303	-0.409439481611
F	1.143537641637	-1.679346145392	0.016091053303
Cl	2.840273427354	0.266169031792	0.071936158781
H	0.973499994181	-0.246426681407	1.411067358617
H	0.473950067600	0.302572661067	-1.579432964166
F	0.220690834225	1.718850055377	-0.162416843571
F	-1.370986491139	-1.335614981573	-0.848726980870
Cl	-1.879727676542	0.000851817854	1.280043940929
F	-2.034512938252	0.696942204391	-1.172642046331

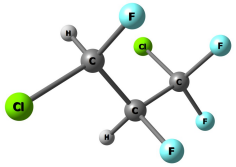
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
39.5302	0.0706
70.1942	0.0526
131.4282	0.140
217.0854	0.231
228.3204	0.595
235.1885	0.0489
323.8302	0.0230
370.3812	0.376
403.6812	1.52
427.6071	0.878
459.2625	2.85
526.2176	0.667
633.1868	3.73
712.0657	31.6
851.4616	1.78
972.9298	25.5
1089.5987	7.15
1130.9064	5.56
1147.3803	7.65
1188.2235	41.7
1233.3712	17.2
1253.5098	2.14
1329.3708	2.57
1363.4248	2.78
1392.5954	1.26
3087.9962	0.603
3119.6252	1.19

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
35.7207	0.0640
78.0683	0.0475
143.7400	0.202
182.7416	0.124
225.7330	0.181
271.2404	0.522
324.3227	0.270
368.0741	0.268
405.0970	0.517
434.3650	1.60
457.8434	1.43
543.2721	1.62
637.2305	9.59
670.6220	12.2
791.6239	15.5
1047.1705	27.4
1101.3205	3.48
1134.1937	5.90
1155.9907	13.4
1199.1327	22.5
1210.8286	31.0
1258.1664	4.52
1328.7500	2.20
1360.9258	5.51
1397.7125	0.590
3059.7347	0.979
3122.5330	1.04



$\Delta E = 0.53$ kcal mol^{-1}
Population = 0.118



$\Delta E = 0.84$ kcal mol^{-1}
Population = 0.070

Optimized Coordinates (Angstroms)

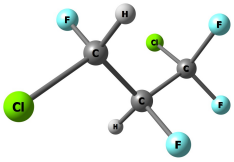
Atom	X	Y	Z
C	1.351382519850	0.465432128290	0.266252168235
C	0.139229307668	-0.466572441080	0.162729414981
C	-1.179150576304	0.330868142959	0.139208242386
Cl	2.848915109129	-0.516853777871	0.433222944256
F	1.444522541103	1.234899685334	-0.837520788071
H	1.288063112848	1.095889489831	1.155024619387
H	0.120234505020	-1.124492004149	1.036840568733
F	0.217749177952	-1.199813144960	-0.979358583229
F	-1.258848205776	1.114613746115	-0.931230983212
Cl	-2.589581368184	-0.780050427765	0.145285119226
F	-1.234191123306	1.102445603295	1.237196277307

Atom	X	Y	Z
C	1.134810808714	-0.540878907213	0.189870784425
C	0.167593653175	0.434435304248	-0.482839643561
C	-1.291021760257	0.298904245784	-0.002916453151
Cl	2.780196643249	-0.311408730052	-0.502907394375
F	1.175888420396	-0.308155132045	1.517988082665
H	0.859945012652	-1.579315578173	0.001622216790
H	0.179284238976	0.273715228070	-1.565127683911
F	0.547484953236	1.714312380906	-0.196607465090
F	-2.038840142326	1.207771571172	-0.629223990161
Cl	-1.935867001487	-1.341464073719	-0.406678133805
F	-1.402140826328	0.496533691021	1.305925680172

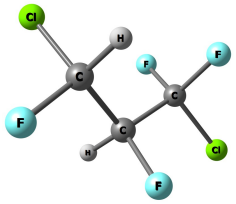
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
39.7626	0.0839
76.6700	0.0821
127.5093	0.324
212.2869	0.340
231.1715	0.0934
235.3973	0.105
271.4519	0.00482
345.7742	0.150
391.1829	0.387
423.1475	0.273
465.1138	0.655
618.2543	4.28
695.8153	33.1
766.6820	6.16
863.9564	1.63
903.4642	4.55
987.6726	22.4
1121.2310	18.6
1166.5463	14.0
1185.9692	18.0
1252.8808	18.1
1278.3581	9.05
1350.8455	4.72
1367.0664	0.884
1395.0694	1.52
3085.8352	0.696
3111.6836	1.27

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
39.5666	0.120
83.7975	0.0689
137.9197	0.249
192.8317	0.310
233.3879	0.107
270.7192	0.0304
290.9109	0.117
340.2564	0.636
379.9873	0.460
418.0669	0.0762
419.9969	0.829
599.6146	6.27
745.0586	9.52
778.7925	19.1
848.0212	6.48
921.7671	14.9
967.4724	25.2
1102.9400	5.44
1171.6017	8.01
1190.4568	25.8
1253.9701	23.8
1279.6924	9.40
1358.1779	3.17
1364.8789	1.39
1391.7274	2.44
3086.9140	0.616
3122.6895	1.19



$\Delta E = 0.88$ kcal mol^{-1}
Population = 0.065



$\Delta E = 0.93$ kcal mol^{-1}
Population = 0.060

Optimized Coordinates (Angstroms)

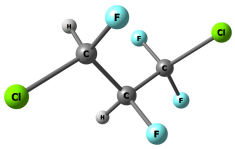
Atom	X	Y	Z
C	1.182416942211	-0.331690390536	0.429092618315
C	0.203755515393	0.505509964705	-0.403453079583
C	-1.266001558444	0.360006841571	0.050826477575
F	0.924814773057	-1.647188803859	0.274600137102
Cl	2.860491167809	0.009774973248	-0.111813202005
H	1.130650034185	-0.062236373278	1.485286563401
H	0.280666658593	0.246568154142	-1.463285262995
F	0.525558073241	1.822085576582	-0.217564961849
F	-1.985010434946	1.340208978933	-0.495904249261
Cl	-1.977342306949	-1.208526645963	-0.448369232133
F	-1.352879864151	0.473614724454	1.382590191432

Atom	X	Y	Z
C	1.462553550152	-0.473292775280	-0.300932185598
C	0.076785034688	-0.638361809648	0.343386314015
C	-0.973425443795	0.363144842989	-0.174847750355
Cl	2.238322293679	1.074594736031	0.166965251016
F	2.232762369314	-1.496620154865	0.126954126803
H	1.400755986446	-0.491219696909	-1.390019137846
H	0.152905621288	-0.547152718723	1.431031793554
F	-0.340940730022	-1.897164183116	0.008712045267
F	-0.938771513064	0.419350749494	-1.512837774616
Cl	-2.621592229646	-0.135093878524	0.333757593575
F	-0.737427939040	1.584714888550	0.302514724186

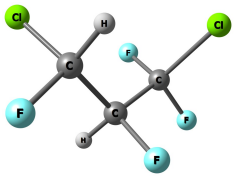
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
33.1039	0.0715
74.9436	0.0367
140.8884	0.0962
196.1536	0.195
230.2383	0.536
279.1717	0.479
314.8664	0.324
355.8930	1.11
391.6258	0.414
425.9054	0.401
479.7592	1.66
518.8527	0.557
593.9642	5.04
772.6050	28.2
851.9367	2.22
957.5513	30.7
1093.1480	4.51
1127.3054	6.50
1142.7722	19.1
1174.8505	24.7
1231.9961	24.4
1256.9808	3.79
1328.6942	2.16
1362.5945	3.56
1396.9359	0.790
3092.9978	0.408
3118.8063	1.16

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
32.7141	0.0408
81.9981	0.0699
138.0258	0.122
195.0311	0.237
229.7103	0.526
297.3351	0.453
315.8411	0.0956
371.3472	0.350
402.7980	1.63
421.4880	0.302
438.3666	2.52
504.1237	1.04
633.1049	1.56
790.9434	30.9
814.5695	7.94
957.9116	22.5
1088.3823	11.6
1118.9757	0.588
1139.0619	29.8
1182.6204	22.0
1232.5808	15.5
1256.8902	5.90
1323.3866	1.36
1365.4527	0.926
1399.6181	2.81
3089.8706	0.362
3121.2850	1.17



ΔE = 1.10 kcal mol^{-1}
Population = 0.045



ΔE = 1.12 kcal mol^{-1}
Population = 0.044

Optimized Coordinates (Angstroms)

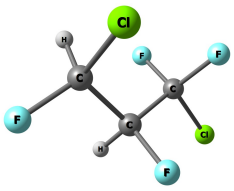
Atom	X	Y	Z
C	1.194082025603	0.291017934620	0.519756455518
C	0.204739584588	-0.682884245026	-0.121923011903
C	-1.263208888967	-0.422918467837	0.273428998220
Cl	2.873879223890	-0.283646057814	0.217248359789
F	1.053181530809	1.526140350426	-0.000576905945
H	1.064699155027	0.325106144687	1.602884176666
H	0.429063678737	-1.694122105171	0.239226558002
F	0.311968113858	-0.644046959879	-1.475469714674
F	-1.336809949743	-0.355228467920	1.613627463406
Cl	-1.946915137861	1.068634986428	-0.428313152657
F	-2.005744335940	-1.458145112514	-0.128943226422

Atom	X	Y	Z
C	1.317298531279	0.400159259271	0.397215341598
C	0.130802821203	0.700956602375	-0.524280412478
C	-1.098840855686	-0.218676977832	-0.404838164577
Cl	2.069193283268	-1.182485071168	0.014912407020
F	2.229436088063	1.378897582038	0.203113037234
H	1.024698471230	0.377178297557	1.447751848901
H	0.462147932098	0.662996676922	-1.569240352560
F	-0.288648673706	1.967711482992	-0.225103454356
F	-0.824302303319	-1.449162182115	-0.833339856021
Cl	-1.715013512976	-0.311568669097	1.284523203255
F	-2.067739781455	0.282901999057	-1.173953598016

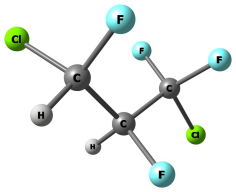
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
36.3290	0.102
79.0882	0.105
143.4000	0.380
189.2805	0.138
221.4544	0.103
241.0838	0.137
292.3678	0.158
346.6494	0.270
400.7372	0.230
423.9960	0.0461
482.0563	0.268
626.3706	9.26
665.9042	16.6
763.6727	3.51
797.0397	13.6
919.5315	0.0322
1065.4069	26.8
1121.3880	19.6
1176.5332	27.8
1192.9691	18.8
1205.0969	10.1
1271.7360	2.40
1355.7511	4.78
1368.0220	0.0833
1398.3209	2.88
3057.5211	1.05
3113.8700	1.06

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
33.2865	0.0348
91.8651	0.0711
142.0525	0.101
184.1839	0.194
232.8814	0.536
302.5981	0.211
331.2936	0.204
353.8276	0.368
401.3790	0.524
423.3950	0.448
453.0276	3.66
522.1999	0.147
650.1279	2.06
681.6631	15.7
807.5267	16.2
1049.7077	26.3
1084.7576	7.04
1128.8601	12.8
1137.3245	19.9
1196.5130	14.2
1210.1631	27.6
1259.0243	3.54
1324.3530	2.64
1361.5217	3.33
1402.6443	2.19
3061.8823	0.695
3123.5443	1.000



$\Delta E = 1.28$ kcal mol^{-1}
Population = 0.033



$\Delta E = 1.39$ kcal mol^{-1}
Population = 0.028

Optimized Coordinates (Angstroms)

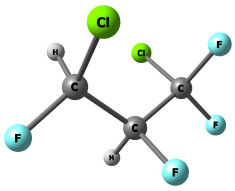
Atom	X	Y	Z
C	1.435135511014	-0.277560529458	0.615187768242
C	0.057908128372	-0.754099455518	0.131940149203
C	-1.033591592983	0.322409995860	0.247316018924
F	2.211375226457	-1.373886332150	0.794563507304
Cl	2.234340457512	0.813008642093	-0.557210948969
H	1.350796874549	0.266923540948	1.557267054285
H	-0.229288241547	-1.583673033681	0.789266391038
F	0.121253778417	-1.193275294250	-1.151665995306
F	-0.803218743211	1.357794548991	-0.553477276524
Cl	-2.641285367401	-0.366588579424	-0.159853540609
F	-1.064136031178	0.764966496588	1.515236872412

Atom	X	Y	Z
C	1.491270905072	-0.619111890122	0.256631818096
C	0.018167577004	-0.520631738831	0.682170993277
C	-0.890297782649	0.264467736579	-0.284593729060
F	1.607622573099	-0.905565573029	-1.055953069768
Cl	2.385269439532	0.895809254462	0.628424478452
H	1.964293430754	-1.411189965663	0.842173380776
H	-0.038234701864	-0.062436143482	1.672814820605
F	-0.463547033579	-1.802416098285	0.737522139991
F	-0.970272386591	-0.344476820245	-1.463894420709
Cl	-2.553200245441	0.376472951013	0.406901294492
F	-0.424165775336	1.499721287603	-0.468413706153

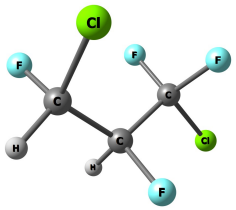
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
34.1076	0.0355
78.7830	0.0871
139.0212	0.414
191.1164	0.108
231.4521	0.177
235.5179	0.173
305.5966	0.164
349.0892	0.133
406.5234	0.602
423.0821	0.345
460.3520	1.11
627.6065	1.37
641.6093	15.7
775.8801	5.61
831.7686	21.2
920.6866	5.01
1019.6747	26.1
1119.3897	17.7
1162.1629	27.8
1181.8813	8.00
1265.6257	18.5
1282.8368	2.89
1325.5193	1.46
1377.1412	3.25
1400.8695	0.940
3060.2715	0.936
3112.4657	1.11

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
32.3630	0.0524
86.8807	0.0693
150.0265	0.0482
184.1635	0.250
230.0153	0.347
261.7902	0.0794
302.0098	0.0557
360.0009	0.168
402.4000	0.350
415.6212	0.216
463.7597	2.39
557.9847	11.4
633.6475	2.78
804.5405	20.9
849.1547	3.86
936.8296	23.5
983.9058	7.17
1117.8207	11.7
1163.3608	20.3
1197.3857	27.6
1237.8182	8.60
1275.0524	12.1
1342.3586	4.98
1364.0332	1.58
1410.9821	1.24
3095.0004	1.41
3101.2791	0.558



$\Delta E = 1.64$ kcal mol^{-1}
Population = 0.018



$\Delta E = 1.99$ kcal mol^{-1}
Population = 0.010

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.236497921218	-0.238873784745	-0.675194378056
C	0.110376477127	0.770719460291	-0.433265300307
C	-1.174469509846	0.218874906042	0.207438618375
F	2.154999027305	0.365435681649	-1.468795341735
Cl	2.032441716339	-0.749210455636	0.845455046950
H	0.870323552233	-1.141755032743	-1.164889032472
H	-0.167564407663	1.178811688285	-1.412562078541
F	0.554211126717	1.784451478239	0.364145638232
F	-2.054755687775	1.214762865345	0.321043813110
Cl	-1.901220774180	-1.061249603669	-0.842734272910
F	-0.961698441475	-0.285981203058	1.417211287354

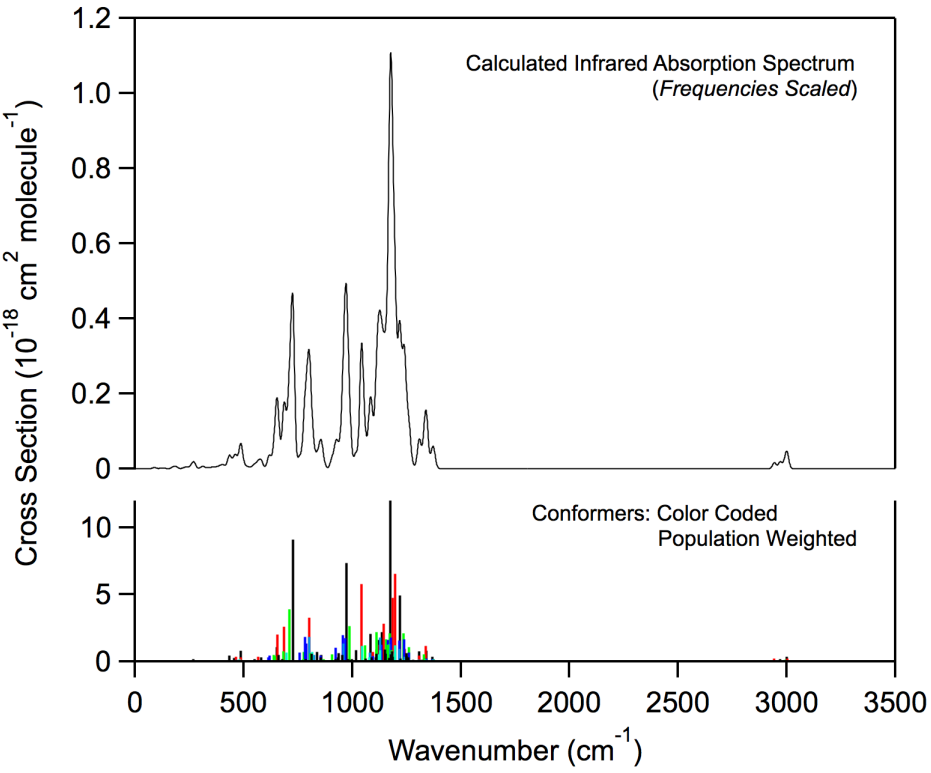
Atom	X	Y	Z
C	1.481914494835	0.145383248080	0.763093499722
C	-0.001076173075	-0.249944434762	0.853635303383
C	-0.914195037336	0.258100928174	-0.278630255616
Cl	2.287157087512	-0.396011043890	-0.743277512143
F	1.595693734877	1.486190500548	0.889058565442
H	2.016163039666	-0.347794410038	1.579021403106
H	-0.376812456643	0.175070000712	1.792007198549
F	-0.081856577254	-1.609173577278	0.898477472851
F	-0.653284317369	-0.346295843141	-1.432474310246
Cl	-2.638490874645	-0.068931855685	0.146910510805
F	-0.757169920568	1.573732487281	-0.433720875853

Infrared Absorption Spectrum (unscaled frequencies)

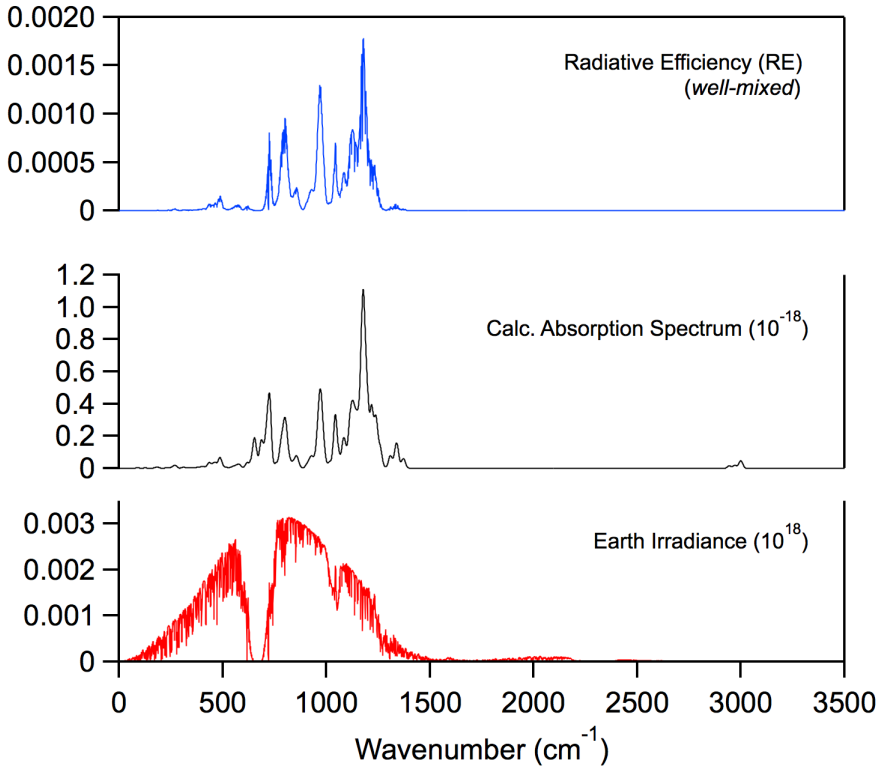
Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
31.8235	0.0644
88.4855	0.0709
141.6971	0.272
192.2893	0.236
223.6153	0.116
278.1884	0.100
312.5277	0.420
337.6600	0.347
379.3241	0.540
419.3506	0.838
433.8458	0.550
620.5782	2.86
660.7320	10.8
768.7487	4.28
847.9837	18.0
951.9326	26.1
999.0279	10.5
1097.1599	18.4
1161.6780	5.59
1189.1701	28.9
1266.4898	21.7
1284.7573	2.68
1327.5848	1.22
1374.0926	3.53
1400.6365	1.81
3060.8766	0.817
3122.8974	1.10

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
23.4917	0.0398
93.5360	0.0447
150.8251	0.111
186.9297	0.0808
209.0183	0.158
241.2686	0.230
323.9508	0.0658
372.2800	0.132
412.5979	0.138
429.3179	0.353
492.3902	5.36
559.9510	10.7
630.5442	3.20
683.6073	6.86
869.7477	2.74
932.2539	29.6
1066.4108	20.5
1127.0998	5.83
1156.2169	10.8
1198.9442	36.4
1250.6948	7.33
1299.0368	13.4
1329.6413	2.92
1368.7122	2.90
1404.4703	0.573
3060.0570	1.11
3092.2224	1.71

Infrared Spectrum

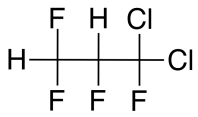


Radiative Efficiency



HCFC-234ec

Molecular Formula: $CHF_2CHFCCl_2F$
Name: 1,1-Dichloro-1,2,3,3-tetrafluoropropane
CAS number: –
Molecular Weight: 184.95



Global Atmospheric Lifetime (years): 5.32
  Tropospheric Atmospheric Lifetime (years): 6.04
  Stratospheric Atmospheric Lifetime (years): 45.1
Ozone Depletion Potential (ODP): 0.052

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.298	0.276
Global Warming Potential (GWP_H):		
GWP_{20}	1888	1748
GWP_{100}	524	485
Global Temperature Potentials (GTP_H)		
GTP_{20}		991
GTP_{50}		106
GTP_{100}		68

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 9.72 \times 10^{-15}$; $k_{SAR}(272\ K) \approx 6.20 \times 10^{-15}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 5.83$ years
$\tau^{OH}_{Trop} = 6.04$ years
$\tau^{OH}_{Strat} = 170.4$ years

Fractional Atmospheric Loss: 0.913

O(^{1}D) Reactivity

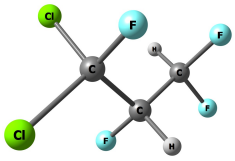
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 1.4 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)} = 265$ years
Fractional Atmospheric Loss: 0.020

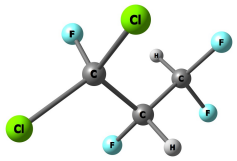
UV Photolysis

UV Spectrum: *No Recommendation*
$\tau_{hv} = 80$ years
Fractional Atmospheric Loss: 0.067

Molecular Structure and Infrared Spectrum (8 conformers)



E = 0
Population = 0.436



$\Delta E = 0.63$ kcal mol^{-1}
Population = 0.150

Optimized Coordinates (Angstroms)

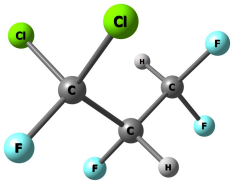
Atom	X	Y	Z
C	-1.819223397051	-0.158606236209	-0.129297408507
C	-0.541097735856	0.665046322148	0.086997792399
C	0.738039712817	-0.172336163756	0.273278919810
F	-2.004840929528	-0.997619837200	0.911429178345
F	-2.853417298915	0.709610763703	-0.169445589587
H	-1.794939220293	-0.728891239089	-1.063488609857
H	-0.668297452672	1.269573171220	0.993142508637
F	-0.389947876242	1.476717179232	-0.996656942322
Cl	1.019459846147	-1.258857638308	-1.127487823840
Cl	2.141672429485	0.925952564530	0.469496173637
F	0.624095922108	-0.915286886270	1.377605801285

Atom	X	Y	Z
C	-1.819559832189	0.002570974257	0.257489984919
C	-0.531759866999	-0.569094371566	-0.361609262877
C	0.759832439717	0.042254792346	0.218948183908
F	-1.949642911886	1.315289378135	-0.020416109791
F	-2.857948431943	-0.653425168280	-0.302701523336
H	-1.842759605258	-0.147943951969	1.342204410539
H	-0.546116139569	-0.432283750045	-1.446609472048
F	-0.540815121458	-1.903456589457	-0.057790961951
Cl	2.169605561747	-0.965070819765	-0.234523854510
Cl	1.001860461102	1.711597169684	-0.373664859054
F	0.677011446735	0.068727336659	1.560209464199

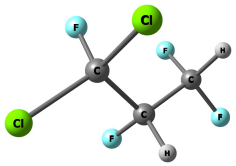
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
36.1402	0.0795
88.3801	0.102
143.5394	0.170
189.6076	0.108
207.0245	0.127
271.0456	0.299
303.5490	0.165
357.7083	0.101
369.7620	0.175
451.0456	5.73
467.0899	1.33
545.5107	1.32
589.7588	1.96
668.1356	10.4
812.2895	32.3
1065.3136	9.41
1116.3105	2.69
1141.8049	5.30
1145.0503	17.9
1162.1411	28.6
1183.8178	22.5
1300.9686	0.256
1344.9213	2.24
1399.7373	2.40
1424.9601	5.58
3062.1707	0.382
3087.3124	4.00

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
32.6584	0.0922
81.2957	0.0905
148.6687	0.0626
205.0601	0.239
221.3631	0.225
265.2544	0.594
308.1947	0.243
323.8653	0.263
376.7072	0.0754
450.3311	2.60
480.3822	2.89
484.1227	2.02
583.6410	1.10
778.6439	17.3
851.8530	30.9
961.2766	10.9
1103.8850	7.85
1118.8893	3.08
1150.9389	19.1
1158.2348	26.5
1187.4297	15.2
1295.5077	0.460
1352.4432	1.20
1400.8062	2.20
1423.6037	6.26
3077.0134	2.44
3097.7570	1.88



$\Delta E = 0.79$ kcal mol^{-1}
Population = 0.115



$\Delta E = 0.91$ kcal mol^{-1}
Population = 0.094

Optimized Coordinates (Angstroms)

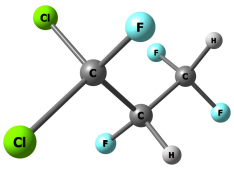
Atom	X	Y	Z
C	-1.655400566237	0.113947104265	0.421795964693
C	-0.630599407622	-0.372424593987	-0.610836974921
C	0.856649314936	-0.115613814542	-0.297411468718
F	-1.606226916473	1.455880901902	0.546515481567
F	-2.877032586129	-0.223626092192	-0.046858250364
H	-1.507408952397	-0.352133655155	1.401576177013
H	-0.848164549598	0.094063133927	-1.578928907482
F	-0.785737855278	-1.727666959817	-0.711198027790
Cl	1.251327075524	1.624476981267	-0.379597158890
Cl	1.311983500431	-0.786886042989	1.304883450824
F	1.579651942844	-0.751691962680	-1.228017285931

Atom	X	Y	Z
C	-1.760544586276	0.392280881810	-0.177935881388
C	-0.515704034259	-0.452947127554	-0.494916049168
C	0.773186635680	0.066667868353	0.167773254536
F	-2.783467939065	-0.107302927400	-0.908985183802
F	-2.074289583020	0.274514629616	1.126869639518
H	-1.628043346782	1.450117242236	-0.426783087747
H	-0.364959398876	-0.468742899136	-1.578630182635
F	-0.748334668837	-1.717669856527	-0.038945720854
Cl	2.121337011699	-1.067378630776	-0.147693591341
Cl	1.175158639873	1.688843909266	-0.506380607258
F	0.616415269863	0.180547910111	1.487331410140

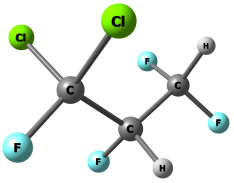
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
32.9018	0.0873
89.8458	0.0863
151.6631	0.0991
180.7442	0.146
221.6792	0.225
277.4249	0.361
309.2201	0.396
335.7288	0.264
379.0186	0.0785
453.3168	4.12
475.3732	1.37
519.3579	0.504
581.6605	2.01
674.9150	12.3
857.6459	32.6
1055.4757	12.3
1095.9417	5.88
1134.0782	7.46
1140.1222	21.0
1156.9569	19.5
1178.2145	19.9
1298.7016	0.223
1345.3109	3.14
1399.5764	1.78
1428.6258	3.69
3064.9510	0.164
3085.1327	3.88

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
40.2698	0.138
87.5101	0.0773
141.7189	0.234
207.3223	0.312
223.8819	0.0789
260.1786	0.119
304.0007	0.160
306.9514	0.210
347.8909	0.347
394.4914	1.01
462.6898	0.521
544.8300	3.72
753.9634	17.3
812.8339	14.0
832.0484	20.0
904.9765	15.2
986.4595	7.99
1134.0490	1.73
1141.7050	20.4
1186.6775	10.0
1219.5326	29.5
1319.2318	1.15
1369.1387	1.74
1411.5485	4.75
1418.2433	3.45
3080.1282	2.15
3087.9764	2.59



ΔE = 1.06 kcal mol^{-1}
Population = 0.073



ΔE = 1.36 kcal mol^{-1}
Population = 0.044

Optimized Coordinates (Angstroms)

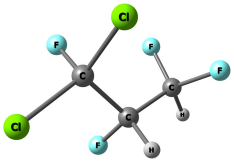
Atom	X	Y	Z
C	-1.791847521050	0.023808528547	0.471618938045
C	-0.512840946007	0.729758323799	-0.007275581198
C	0.782242613711	-0.013023248241	0.368205510350
F	-2.804316657251	0.919907670740	0.398187758769
F	-2.091352436712	-1.012725364838	-0.332460787542
H	-1.700292850026	-0.327664381372	1.505529203774
H	-0.469137187677	1.703186333001	0.496270688421
F	-0.571295013158	0.909872326410	-1.351796449411
Cl	0.922067026013	-1.601342153173	-0.427381541962
Cl	2.197648676231	1.002083133066	-0.055588121403
F	0.773080295926	-0.194221167939	1.702827382158

Atom	X	Y	Z
C	-1.588357273770	0.519372467234	0.357870979196
C	-0.597114830749	0.120325512594	-0.743211571014
C	0.883236152904	0.008832333603	-0.334311842737
F	-2.765914276369	0.802940780463	-0.248400157575
F	-1.789893069928	-0.510082455972	1.202163168872
H	-1.258728977679	1.396676585465	0.923786160790
H	-0.639214544795	0.882985998816	-1.530378264709
F	-0.979368538109	-1.082854607464	-1.258451024113
Cl	1.458065837866	1.609083621556	0.262928688756
Cl	1.175672950034	-1.253720450313	0.887284010094
F	1.587510570594	-0.299548785983	-1.430673147560

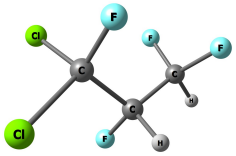
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
38.6168	0.125
82.4154	0.146
142.9328	0.283
187.7917	0.187
232.9031	0.134
252.4152	0.116
267.9236	0.284
308.0455	0.257
378.0151	0.0191
410.6983	0.373
535.5086	1.70
552.0907	2.32
672.3106	13.9
763.4452	20.8
825.2215	12.8
919.1377	5.59
1084.9477	19.5
1135.0350	26.5
1138.1236	7.78
1169.3628	3.64
1206.6778	20.8
1314.8175	1.20
1372.1305	2.97
1416.2351	4.36
1420.6205	3.39
3057.4416	0.681
3071.4392	4.43

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
40.3026	0.152
88.3809	0.120
150.2137	0.210
180.1453	0.169
241.7734	0.182
254.1719	0.0784
297.7171	0.354
306.2688	0.333
370.0458	0.130
396.8508	0.864
480.4910	0.933
570.3948	1.39
674.5658	14.0
773.5102	8.36
847.9422	31.4
924.3284	3.83
1066.2050	12.9
1115.1407	21.0
1144.4852	8.22
1176.1478	16.8
1200.6816	18.3
1316.5387	1.22
1368.8744	1.28
1415.3680	3.88
1419.4487	3.03
3058.8959	0.712
3082.6868	3.95



$\Delta E = 1.38$ kcal mol^{-1}
Population = 0.043



$\Delta E = 1.54$ kcal mol^{-1}
Population = 0.032

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.870724609647	-0.242417493385	-0.364798260067
C	-0.409002932857	-0.626025267332	-0.663898456010
C	0.661602885891	0.012868874980	0.241763612192
F	-2.109561322355	-0.172868902618	0.959362683296
F	-2.162120074721	0.954205676997	-0.918288131115
H	-2.522414216987	-1.009594522918	-0.802691862403
H	-0.190492994873	-0.365636063117	-1.703570848598
F	-0.320800295725	-1.983893658405	-0.496663650630
Cl	2.284305844572	-0.566485958688	-0.279994641353
Cl	0.598415987919	1.797445812788	0.135913385525
F	0.481846728784	-0.358263498301	1.509604169162

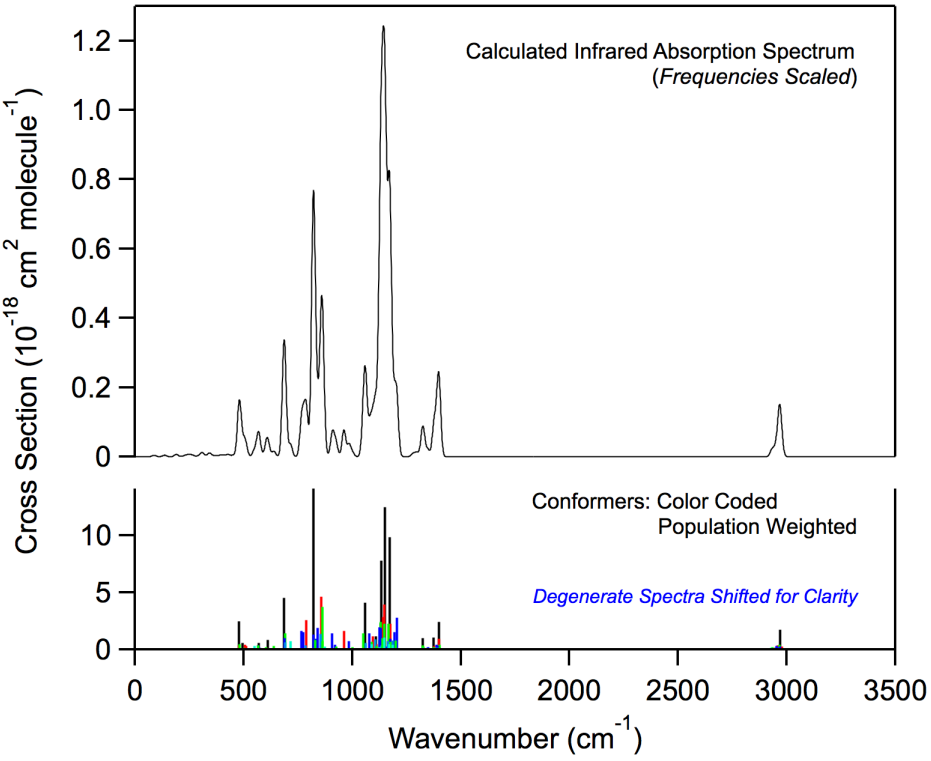
Atom	X	Y	Z
C	-1.877075130960	0.510819182008	-0.056250850168
C	-0.407966061401	0.885295527956	-0.317086388795
C	0.645909436593	-0.061024922405	0.296537645845
F	-2.137242822928	-0.781561106239	-0.328245646843
F	-2.169933106317	0.744701751514	1.242163245280
H	-2.515916818631	1.139158180347	-0.691057090719
H	-0.248668771364	1.873159107872	0.130265959655
F	-0.218009723145	0.961963462405	-1.665095129772
Cl	0.734835517226	-1.626614126856	-0.551073904926
Cl	2.257311768115	0.741846171217	0.223210558442
F	0.340003712813	-0.270188227820	1.582622602001

Infrared Absorption Spectrum (unscaled frequencies)

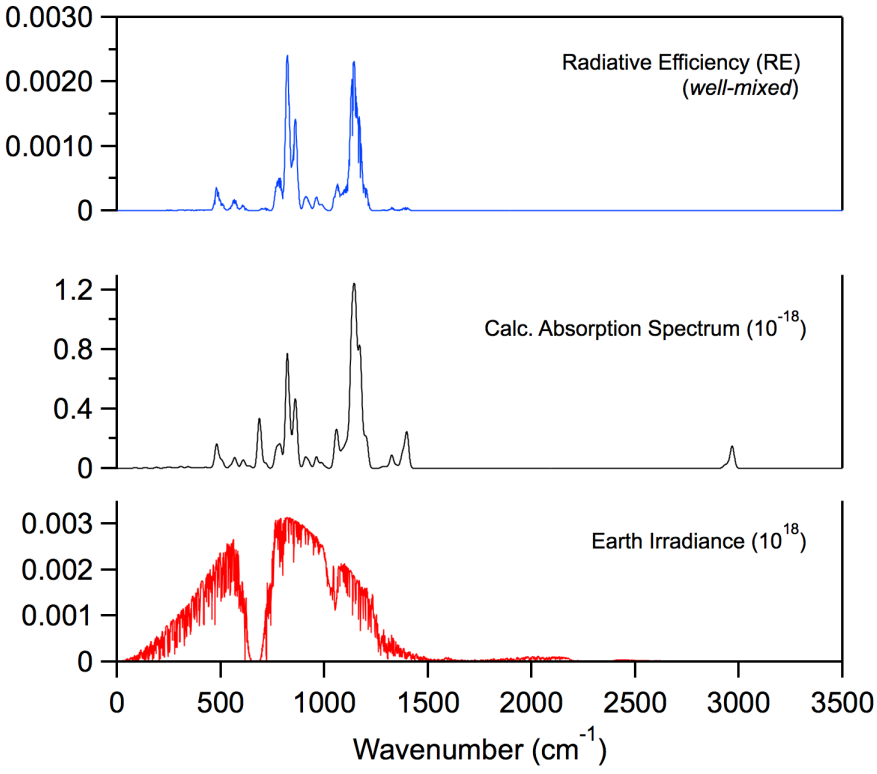
Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
35.6816	0.105
95.0065	0.142
146.6556	0.0352
209.2741	0.170
221.3884	0.289
244.4274	0.210
289.4226	0.0950
335.4401	0.111
379.0264	0.0691
421.5199	1.53
469.4087	0.632
543.6248	8.65
620.2771	7.60
822.7917	19.9
856.2760	17.3
924.5247	5.77
1002.9149	5.46
1119.1422	7.41
1149.9810	23.5
1188.9115	15.9
1214.5805	18.2
1329.3016	0.157
1349.2460	6.37
1404.0640	3.58
1426.3015	4.51
3049.8107	5.43
3090.7412	0.793

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
31.4850	0.0938
96.7673	0.121
155.5707	0.0801
193.8818	0.0836
201.0041	0.202
244.6814	0.180
281.4329	0.160
360.1097	0.0605
376.7830	0.0810
432.4950	1.30
524.6753	9.17
544.1452	1.07
604.3381	2.46
700.8829	23.3
868.5293	8.83
923.7012	2.98
1097.3240	14.3
1133.9605	7.37
1159.0764	32.3
1180.7094	15.1
1199.2594	12.5
1335.7544	1.12
1347.6176	4.34
1405.6536	4.82
1429.3908	3.31
3044.7363	5.55
3065.3423	1.22

Infrared Spectrum

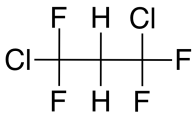


Radiative Efficiency



HCFC-234fa

Molecular Formula:	$CClF_2CH_2CClF_2$
Name:	1,3-Dichloro-1,1,3,3-tetrafluoropropane
CAS number:	76140-39-1
Molecular Weight:	184.95



Global Atmospheric Lifetime (years):	31.0
Tropospheric Atmospheric Lifetime (years):	43.4
Stratospheric Atmospheric Lifetime (years):	108.4
Ozone Depletion Potential (ODP):	0.132

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.354	0.347
Global Warming Potential (GWP_H):		
GWP_{20}	6352	6220
GWP_{100}	3474	3402
Global Temperature Potentials (GTP_H)		
GTP_{20}		5999
GTP_{50}		3323
GTP_{100}		1166

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 1.35 \times 10^{-15}$; $k_{SAR}(272\ K) \approx 0.863 \times 10^{-15}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 41.6$ years

$\tau^{OH}_{Trop} = 43.4$ years

$\tau^{OH}_{Strat} = 1007.2$ years

Fractional Atmospheric Loss: 0.745

$O(^1D)$ Reactivity

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

$k_{Est}(T) = 1.4 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 265$ years

Fractional Atmospheric Loss: 0.117

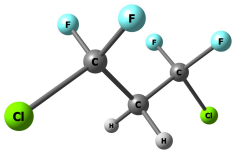
UV Photolysis

UV Spectrum: *No Recommendation*

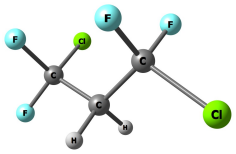
$\tau_{hv} = 225$ years

Fractional Atmospheric Loss: 0.138

Molecular Structure and Infrared Spectrum (5 conformers)



E = 0
Population = 0.685



$\Delta E = 0.97$ kcal mol^{-1}
Population = 0.133

Optimized Coordinates (Angstroms)

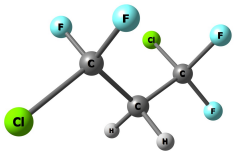
Atom	X	Y	Z
C	-0.189455569798	-1.276639622803	0.000000000000
C	0.650558969087	0.000136453534	0.000000000000
C	-0.189523543354	1.276868139285	0.000000000000
Cl	0.905269573808	-2.719781670917	0.000000000000
F	-0.971224195357	-1.352728901576	1.079917040952
F	-0.971224195357	-1.352728901576	-1.079917040952
H	1.285581477995	0.000153964852	-0.886030605012
H	1.285581477995	0.000153964852	0.886030605012
Cl	0.905123096598	2.720069191653	0.000000000000
F	-0.971296045907	1.352914691389	-1.079917168508
F	-0.971296045907	1.352914691389	1.079917168508

Atom	X	Y	Z
C	-1.350976498149	0.492018317720	0.053789889524
C	0.084409155846	0.664187919307	0.555300172127
C	1.153332291985	-0.121806045566	-0.196505965808
Cl	-2.028183498573	-1.146844561740	0.373849255364
F	-2.123880262879	1.381129564204	0.694530079006
F	-1.447566731213	0.735911068995	-1.255744768205
H	0.121687905142	0.396654788148	1.611287570693
H	0.319773552506	1.726911357616	0.457260692620
Cl	2.780922863008	0.271907197468	0.499879478821
F	0.977206771532	-1.440397525809	-0.098481420584
F	1.175292450795	0.195607919656	-1.493109983557

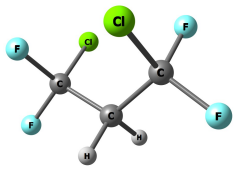
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
25.2470	0.000
113.9951	0.395
130.2694	0.198
229.8919	0.103
242.1421	0.00289
279.7772	0.0
352.6082	0.186
406.4689	0.193
407.8389	0.0
418.0013	0.411
428.1083	0.0
571.2228	3.71
576.4450	5.36
699.7679	29.7
844.0307	2.48
926.0899	4.61
936.1703	32.1
980.1742	22.4
1076.8712	0.0
1217.6810	4.81
1241.8108	51.3
1258.9224	48.0
1320.2720	0.0
1366.6199	14.9
1447.2664	0.867
3110.0901	0.0787
3168.0723	0.0162

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
22.4613	0.00259
110.1171	0.220
146.9867	0.237
212.7943	0.0690
264.7995	0.0603
294.4071	0.0551
352.9142	0.198
396.8575	0.164
411.9667	0.286
415.4082	0.129
431.2648	0.197
579.4188	4.76
591.1773	5.87
670.9965	13.3
822.2165	11.9
897.5382	12.3
944.1276	18.8
1001.7708	16.7
1152.2301	33.0
1173.5658	19.8
1230.5018	27.1
1256.3651	39.2
1310.4529	0.791
1378.7945	13.2
1450.6939	0.888
3091.8859	0.0412
3157.1926	0.0141



$\Delta E = 0.97$ kcal mol^{-1}
Population = 0.133



$\Delta E = 1.97$ kcal mol^{-1}
Population = 0.024

Optimized Coordinates (Angstroms)

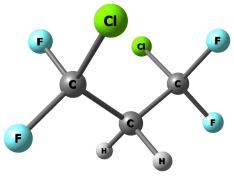
Atom	X	Y	Z
C	-1.351103100054	-0.491849983482	0.053494104849
C	0.084187710664	-0.664301462157	0.555177677654
C	1.153400572994	0.121221696103	-0.196709169967
Cl	-2.027887554700	1.147273360215	0.373110034413
F	-1.447638609960	-0.736020840329	-1.255992852730
F	-2.124311881924	-1.380598986806	0.694369142328
H	0.319265615242	-1.727112853812	0.457404650169
H	0.121442045596	-0.396536111601	1.611107152223
Cl	2.780816057675	-0.272786781846	0.499918849853
F	1.175392696367	-0.196495974669	-1.493238260986
F	0.977635448100	1.439884938383	-0.099004327807

Atom	X	Y	Z
C	-1.266444151906	0.351274286498	0.284323346323
C	0.000253211742	-0.000492883576	1.060669985960
C	1.266610978796	-0.351520313599	0.283435029646
Cl	-1.941361506242	-1.037291255597	-0.645353729723
F	-2.196844737208	0.729501980373	1.174919816906
F	-1.078444803065	1.366732519317	-0.560154678411
H	-0.226226404801	-0.857547472642	1.699695002180
H	0.227012344155	0.855952823673	1.700411788077
Cl	1.941122112234	1.037930053653	-0.645214281735
F	2.197400730940	-0.730595788941	1.173264072641
F	1.078242225355	-1.366173949158	-0.561927351862

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
22.4614	0.00259
110.1163	0.220
146.9864	0.237
212.7941	0.0690
264.7995	0.0603
294.4073	0.0551
352.9139	0.198
396.8574	0.164
411.9667	0.286
415.4083	0.129
431.2648	0.197
579.4189	4.76
591.1774	5.87
670.9969	13.3
822.2165	11.9
897.5384	12.3
944.1273	18.8
1001.7713	16.7
1152.2300	33.0
1173.5658	19.8
1230.5019	27.1
1256.3649	39.2
1310.4532	0.791
1378.7949	13.2
1450.6939	0.888
3091.8857	0.0412
3157.1921	0.0141

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
15.4531	0.0000
115.4966	0.163
145.7401	0.110
228.6335	0.119
259.6912	0.150
313.6155	0.0338
354.0663	0.197
383.1023	0.309
407.2782	0.174
423.6663	0.236
433.0492	0.502
582.3054	3.12
647.0914	0.00
683.3699	19.6
685.0993	9.32
920.9088	6.85
951.3228	3.46
1073.2389	32.2
1127.7200	43.8
1188.5840	31.2
1219.1257	15.1
1235.0318	31.9
1298.1234	1.56
1388.9540	10.8
1453.7628	0.769
3081.6504	0.000
3137.8324	0.0314



$\Delta E = 1.97$ kcal mol^{-1}
Population = 0.024

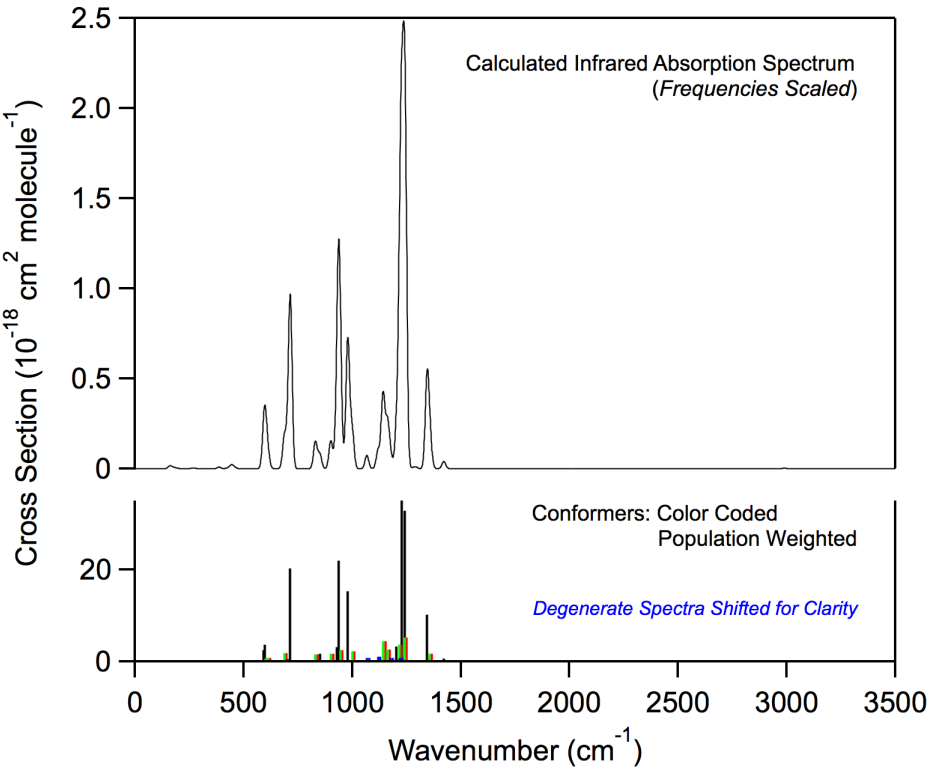
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.266533791210	-0.351552446680	0.283796601145
C	-0.000061619616	-0.000092299326	1.060649460573
C	1.266460365563	0.351464320904	0.283921501664
Cl	-1.941335353429	1.037451241708	-0.645309710644
F	-1.078235893415	-1.366544356000	-0.561175391015
F	-2.197126098191	-0.730334029434	1.173957327373
H	0.226612194387	-0.856862430538	1.699986996094
H	-0.226776447793	0.856598385934	1.700078898563
Cl	1.941321059616	-1.037423725533	-0.645314704557
F	1.078216780874	1.366561632572	-0.560935977851
F	2.196995803214	0.730134706393	1.174188998655

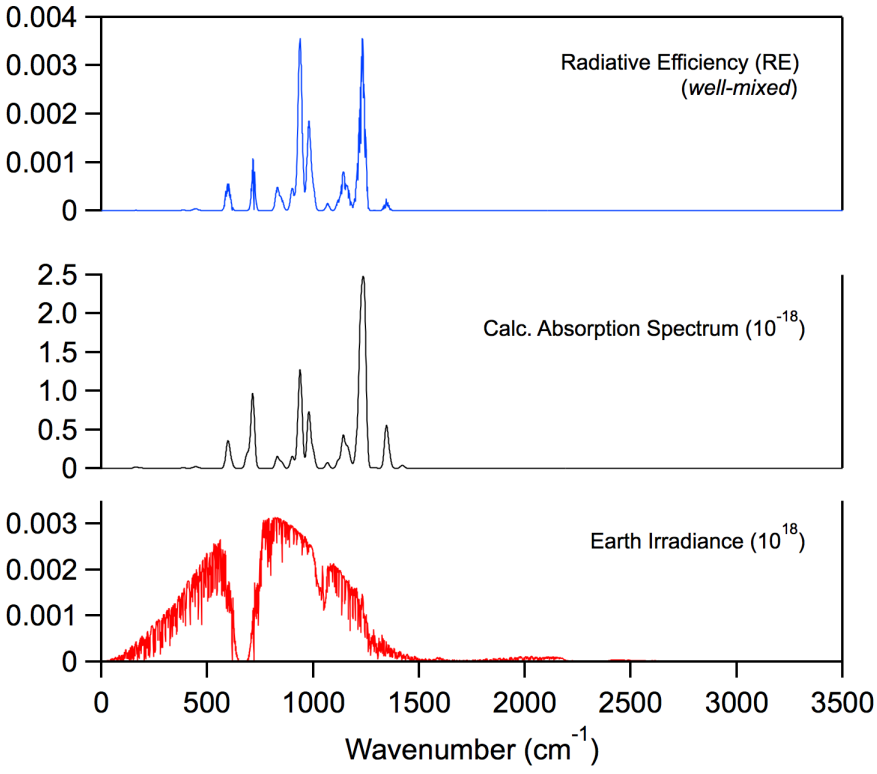
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
15.4530	0.0000
115.4971	0.163
145.7401	0.110
228.6339	0.119
259.6907	0.150
313.6155	0.0338
354.0663	0.197
383.1023	0.309
407.2783	0.174
423.6664	0.236
433.0491	0.502
582.3054	3.12
647.0916	0.00
683.3703	19.6
685.0986	9.32
920.9087	6.85
951.3233	3.46
1073.2385	32.2
1127.7203	43.8
1188.5836	31.2
1219.1256	15.1
1235.0318	31.9
1298.1235	1.56
1388.9540	10.8
1453.7626	0.769
3081.6503	0.000
3137.8324	0.0314

Infrared Spectrum

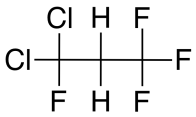


Radiative Efficiency



HCFC-234fb

Molecular Formula:	$CCl_2FCH_2CF_3$
Name:	1,1-Dichloro-1,3,3,3-tetrafluoropropane
CAS number:	64712-27-2
Molecular Weight:	184.95



Global Atmospheric Lifetime (years):	26.2	~45 #
Tropospheric Atmospheric Lifetime (years):	47.6	98 #
Stratospheric Atmospheric Lifetime (years):	58.1	~85 #
Ozone Depletion Potential (ODP):	0.215	

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.271	0.264
Global Warming Potential (GWP_H):		
GWP_{20}	4605	4499
GWP_{100}	2283	2230
Global Temperature Potentials (GTP_H)		
GTP_{20}		4245
GTP_{50}		2043
GTP_{100}		627

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

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

OH Reactivity

$k_{Rec}(T) = 1.8 \times 10^{-12} \exp(-2300/T)$; $k_{Rec}(272\ K) = 3.8 \times 10^{-16}$ cm^3 $molecule^{-1}$ s^{-1}

$k_{SAR}(298\ K) = 1.23 \times 10^{-15}$; $k_{SAR}(272\ K) \approx 0.787 \times 10^{-15}$ cm^3 $molecule^{-1}$ s^{-1}

τ^{OH}_{Global} = 45.6 years
τ^{OH}_{Trop} = 47.6 years
τ^{OH}_{Strat} = 1094.4 years

Fractional Atmospheric Loss: 0.574

O(^{1}D) Reactivity

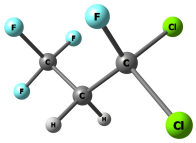
$k_{Rec}(T)$, *No recommendation*

$k_{Est}(T) = 1.4 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)}$ = 265 years
Fractional Atmospheric Loss: 0.099

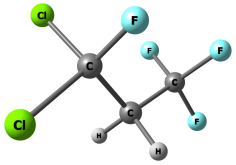
UV Photolysis

UV Spectrum: *No Recommendation*
τ_{hv} = 80 years
Fractional Atmospheric Loss: 0.327

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.443



E = 0
Population = 0.443

Optimized Coordinates (Angstroms)

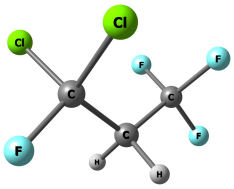
Atom	X	Y	Z
C	-0.876804995694	-0.102569193668	-0.186876350300
C	0.332715872055	-0.728303594226	0.505980599414
C	1.701412379711	-0.194221006138	0.085789408303
Cl	-1.110440767113	1.622417429176	0.248859048381
F	-0.758261076444	-0.182877639091	-1.517257969398
Cl	-2.353461131682	-1.027616668305	0.291319073152
H	0.325901847592	-1.796212929504	0.274679917909
H	0.232060681357	-0.608134365841	1.584937176308
F	2.643944967443	-0.904044305824	0.725818522830
F	1.911572464115	-0.328690253953	-1.226796589837
F	1.880210758660	1.090486527375	0.401835163237

Atom	X	Y	Z
C	-0.876411203159	-0.104744101039	0.192262469461
C	0.333018545107	-0.731610113128	-0.499730818089
C	1.701510522996	-0.193401478547	-0.084163416752
Cl	-2.352313008258	-1.034354349073	-0.279369348401
F	-0.755588706559	-0.178865205358	1.522798499874
Cl	-1.113588145895	1.617877617888	-0.250854291107
H	0.230426178405	-0.616463122391	-1.579052561228
H	0.328333511416	-1.798477333382	-0.263618023814
F	2.644175834768	-0.904547713401	-0.722526113743
F	1.877682586847	1.090164257430	-0.406265044055
F	1.914010884332	-0.321626458998	1.228670647855

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
23.3684	0.00497
119.2550	0.219
148.6612	0.210
223.3462	0.00857
234.1879	0.121
300.2167	0.0815
318.8549	0.0138
370.7419	0.0555
400.4420	0.302
451.8482	0.491
530.6903	0.745
540.0601	0.221
634.4141	10.4
675.8244	14.8
803.0055	16.9
862.9183	4.47
931.0232	5.87
1002.8410	5.56
1154.8493	10.1
1182.0876	35.4
1219.9585	35.2
1277.4874	38.8
1323.5467	9.24
1385.7383	16.8
1451.9712	1.05
3091.7448	0.0378
3155.0611	0.00678

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
23.3686	0.00497
119.2551	0.219
148.6611	0.210
223.3461	0.00857
234.1878	0.121
300.2167	0.0815
318.8548	0.0138
370.7418	0.0555
400.4421	0.302
451.8480	0.491
530.6904	0.745
540.0601	0.221
634.4140	10.4
675.8243	14.8
803.0053	16.9
862.9181	4.47
931.0232	5.87
1002.8404	5.56
1154.8489	10.1
1182.0880	35.4
1219.9580	35.2
1277.4873	38.8
1323.5467	9.24
1385.7382	16.8
1451.9712	1.05
3091.7445	0.0378
3155.0609	0.00678



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

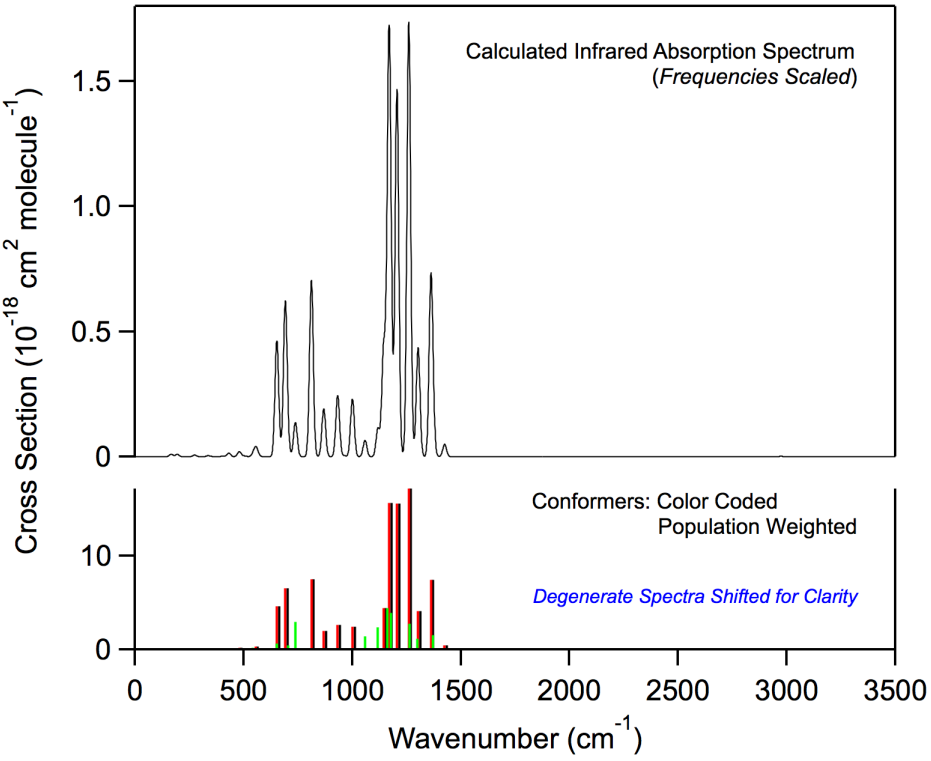
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-0.985006103045	-0.001828810180	0.420306591026
C	0.433255107574	0.026129615525	0.989830535133
C	1.623871389478	0.018086316927	0.037212197115
Cl	-1.325522997183	-1.493158754104	-0.517829381706
F	-1.826836692493	0.012156841361	1.470415053207
Cl	-1.357387122680	1.438996774066	-0.582424656726
H	0.532315761013	-0.844589736280	1.642917930504
H	0.513065435856	0.926703863242	1.603902781104
F	2.744133901413	0.046564480697	0.777856825650
F	1.671920127826	-1.078069637123	-0.723343726795
F	1.648472192243	1.080491045869	-0.770874148512

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
22.9624	0.00071
119.1168	0.138
148.8538	0.154
233.8259	0.108
234.9811	0.0979
295.9163	0.129
339.0801	0.0413
370.3044	0.0204
401.3688	0.337
477.5055	0.573
518.1806	1.61
539.7189	0.508
634.9724	5.74
689.4893	3.94
725.0225	25.9
867.9630	1.23
961.8440	0.874
1064.2026	12.3
1126.9654	21.2
1172.9653	39.3
1190.1543	34.9
1281.0448	24.4
1319.9725	10.2
1396.7159	13.8
1454.5176	1.18
3079.9880	0.00814
3135.9487	0.0333

Infrared Spectrum



Radiative Efficiency