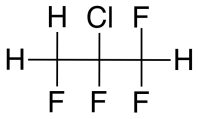
HCFC-244ba

Molecular Formula:	$CH_2FCClFCHF_2$
Name:	2-Chloro-1,1,2,3-tetrafluoropropane
CAS number:	149329-28-2
Molecular Weight:	150.5



Global Atmospheric Lifetime (years):	5.17
Tropospheric Atmospheric Lifetime (years):	5.49
Stratospheric Atmospheric Lifetime (years):	90.5
Ozone Depletion Potential (ODP):	0.017

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.187	0.173
Global Warming Potential (GWP_H):		
GWP_{20}	1416	1308
GWP_{100}	392	362
Global Temperature Potentials (GTP_H)		
GTP_{20}		731
GTP_{50}		78
GTP_{100}		51

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 1.07 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 0.682 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 5.30$ years

$\tau^{OH}_{Trop} = 5.49$ years

$\tau^{OH}_{Strat} = 156.3$ years

Fractional Atmospheric Loss: 0.976

O(^{1}D) Reactivity

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

$k_{Est}(T) = 0.9 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 410$ years

Fractional Atmospheric Loss: 0.013

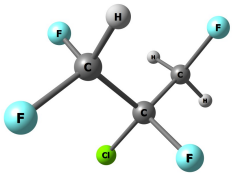
UV Photolysis

UV Spectrum: *No Recommendation*

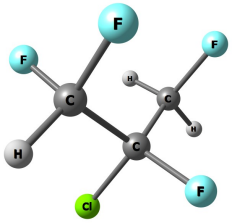
$\tau_{hv} = 450$ years

Fractional Atmospheric Loss: 0.011

Molecular Structure and Infrared Spectrum (5 conformers)



E = 0
Population = 0.533



$\Delta E = 0.75$ kcal mol^{-1}
Population = 0.149

Optimized Coordinates (Angstroms)

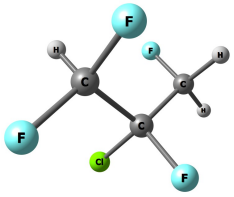
Atom	X	Y	Z
C	1.512088614782	-0.368321911402	-0.551888841341
C	0.200970981355	-0.279848201613	0.219350507251
C	-0.456480356426	1.107289483642	0.111458257202
F	2.335354381575	0.644216567286	-0.112038432620
H	1.982257899022	-1.335677130873	-0.352000887604
H	1.324926975235	-0.249937161639	-1.621849388236
F	0.429999055468	-0.504379441451	1.536634082694
Cl	-0.906647684726	-1.545800290217	-0.412590062597
H	0.202143900009	1.859804384087	0.559507035714
F	-0.658209482152	1.405582028307	-1.190294374729
F	-1.638045284142	1.110839673872	0.750160104265

Atom	X	Y	Z
C	0.242154345940	-1.230757049451	-0.812833579880
C	-0.264302582460	-0.261596490924	0.251994492607
C	0.458705383000	1.099765204068	0.291695390192
F	1.557163213712	-1.523961589227	-0.565934036111
H	-0.353943987180	-2.147532125039	-0.763909346446
H	0.141985730904	-0.771282056487	-1.799938829300
F	-0.147752607024	-0.813702169406	1.480331945257
Cl	-2.011446466940	0.052624642612	-0.086734020647
H	-0.032692806363	1.784490468949	0.992125520613
F	1.735304972059	0.909105332497	0.674283661541
F	0.455593804353	1.638427832407	-0.946623197827

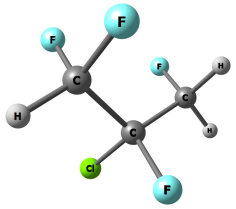
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
73.0105	0.251
116.7207	0.600
174.3958	0.164
191.3932	0.185
235.8416	0.947
327.9604	0.165
332.9297	0.321
398.0595	0.0997
488.6298	0.200
544.2323	4.22
646.8554	6.42
701.4257	9.45
945.2029	4.84
1013.6487	12.8
1090.9681	6.56
1145.0120	11.9
1167.8114	23.5
1196.7024	7.44
1212.0820	12.3
1293.1207	2.47
1388.1959	2.46
1401.1155	3.85
1417.9421	1.45
1489.7073	0.874
3066.8270	1.34
3075.4497	3.19
3131.4597	1.44

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
61.7111	0.0976
127.7295	0.596
180.6545	0.0651
193.0152	0.199
265.6469	1.68
313.1461	0.136
325.8654	0.122
411.3825	0.548
460.9948	3.13
496.5986	2.84
598.2203	1.35
832.7927	2.33
900.8078	24.2
984.8270	6.40
1103.4270	3.75
1145.7682	16.2
1150.6725	19.4
1204.1725	17.2
1236.5403	5.88
1304.7075	1.95
1386.3679	1.79
1392.1297	2.29
1435.6414	3.18
1490.2511	0.782
3059.6891	1.92
3072.2441	3.72
3121.3444	1.62



$\Delta E = 0.95$ kcal mol^{-1}
Population = 0.108



$\Delta E = 1.01$ kcal mol^{-1}
Population = 0.097

Optimized Coordinates (Angstroms)

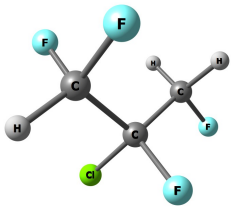
Atom	X	Y	Z
C	1.016420610799	1.219518525622	0.474575068412
C	0.165807148334	-0.043353032138	0.369500461134
C	-1.055421380343	0.140980814187	-0.550174954300
F	1.418284877516	1.603349908921	-0.778717525350
H	0.401952524806	2.009404979184	0.919147138407
H	1.887950251801	1.019621756286	1.104550416179
F	-0.268358664144	-0.354222326343	1.613190794122
Cl	1.148517323243	-1.407684788488	-0.273743727519
H	-0.752720334758	0.341446467749	-1.582014306100
F	-1.833158670443	-0.952641710716	-0.499702177319
F	-1.769002686810	1.193114405736	-0.077537187665

Atom	X	Y	Z
C	-0.227192332651	-1.094315639200	1.043810410771
C	-0.249006124074	0.273568968833	0.362040776622
C	1.008061878958	0.595060307549	-0.467811160871
F	-0.238740919010	-2.096445286990	0.117647625982
H	0.687024173500	-1.157321868344	1.644290847137
H	-1.104993599840	-1.170109580371	1.693600953578
F	-0.316269679879	1.210063347180	1.345179397917
Cl	-1.687198203243	0.436940248661	-0.700009769665
H	0.973403402025	1.624141818814	-0.843388767526
F	2.082454712290	0.455848489972	0.346883934947
F	1.136882691923	-0.264635806104	-1.490606248892

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
69.7054	0.199
98.9711	0.444
163.5771	0.0584
219.6636	0.876
252.3612	0.317
304.0921	0.390
338.8916	0.455
405.9949	0.347
482.4933	1.57
541.3986	2.19
618.0551	5.58
784.0293	12.2
861.2621	6.21
1080.0010	13.6
1116.4229	16.5
1121.6256	10.3
1162.0639	15.3
1176.1638	2.35
1222.5785	17.0
1273.1905	1.88
1391.9731	0.961
1407.6650	3.19
1420.8492	1.58
1499.4711	1.04
3055.7023	2.32
3095.4198	2.84
3116.8680	1.77

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
60.0026	0.158
114.8397	0.340
173.9994	0.0465
198.2295	0.219
264.9292	1.60
317.1601	0.103
379.5652	0.698
395.4202	0.543
450.2907	4.67
533.8000	0.932
602.9058	1.40
730.9553	10.4
913.4558	2.97
1076.4784	14.7
1116.4949	10.2
1130.3552	5.79
1162.0160	28.4
1178.7817	15.7
1233.8963	4.14
1285.0665	0.420
1381.8820	2.55
1387.2711	2.16
1436.4813	2.16
1499.2471	0.995
3048.6534	2.64
3071.6790	3.90
3106.4424	1.97



$\Delta E = 1.11$ kcal mol^{-1}
Population = 0.082

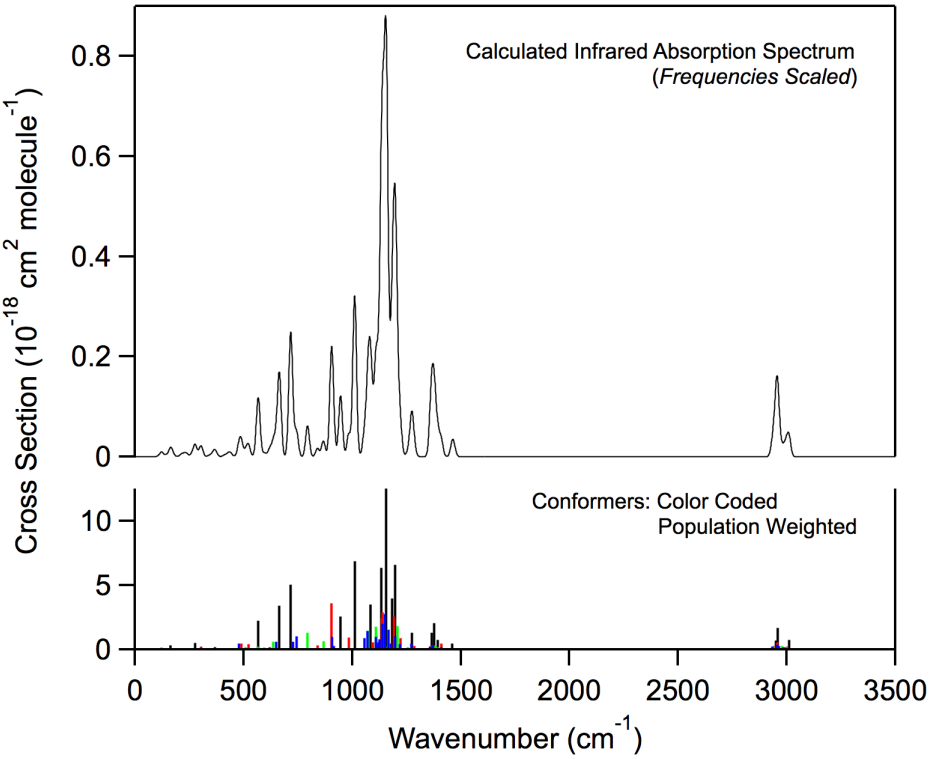
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-0.607677124916	-1.098840514073	-0.720695868483
C	-0.132962800448	-0.047904551751	0.278141013204
C	1.368652450223	0.257481191332	0.141243526119
F	-1.948654777842	-1.306654336610	-0.574407995017
H	-0.385713028884	-0.762315114129	-1.737288850833
H	-0.068710436230	-2.029341532046	-0.510852649160
F	-0.334484073559	-0.490852475532	1.543671387181
Cl	-1.043941478480	1.489337554253	0.064829043223
H	1.692284403419	0.998851724020	0.879430493341
F	2.049767710999	-0.897054202770	0.334899693660
F	1.636402155719	0.699574257306	-1.104135793235

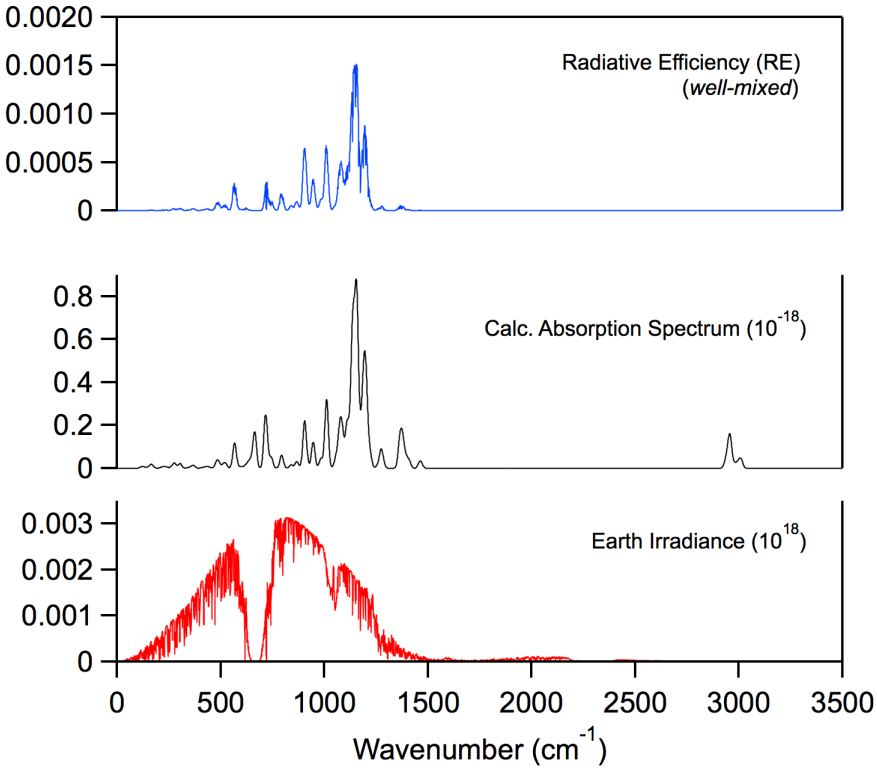
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
77.0751	0.445
94.5764	0.285
165.8063	0.433
184.6501	0.174
263.2973	0.631
314.4096	0.217
328.7647	0.0557
403.7684	0.394
462.1173	1.25
573.6928	1.95
632.4682	7.34
713.1426	7.62
903.7529	12.3
1060.6549	10.7
1125.5307	4.63
1133.6447	9.62
1149.9807	24.4
1189.5742	6.01
1209.9081	12.6
1289.5136	5.90
1383.9716	1.55
1396.2117	3.95
1428.8085	0.409
1501.6995	0.482
3052.8099	1.99
3082.5723	3.47
3113.9696	1.66

Infrared Spectrum

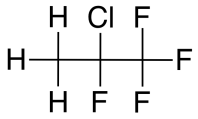


Radiative Efficiency



HCFC-244bb

Molecular Formula:	$CH_3CClFCF_3$
Name:	2-Chloro-1,1,1,2-tetrafluoropropane
CAS number:	421-73-8
Molecular Weight:	150.5



Global Atmospheric Lifetime (years):	16.6
Tropospheric Atmospheric Lifetime (years):	18.7
Stratospheric Atmospheric Lifetime (years):	147.6
Ozone Depletion Potential (ODP):	0.027

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.246	0.238
Global Warming Potential (GWP_H):		
GWP_{20}	4265	4130
GWP_{100}	1644	1592
Global Temperature Potentials (GTP_H)		
GTP_{20}		3590
GTP_{50}		1073
GTP_{100}		279

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

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

OH Reactivity

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

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

$\tau^{OH}_{Global} = 18.0$ years

$\tau^{OH}_{Trop} = 18.7$ years

$\tau^{OH}_{Strat} = 471.3$ years

Fractional Atmospheric Loss: 0.923

O(^{1}D) Reactivity

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

$k_{Est}(T) = 0.9 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 410$ years

Fractional Atmospheric Loss: 0.040

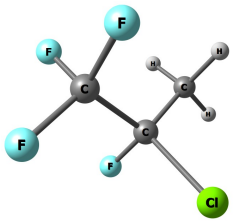
UV Photolysis

UV Spectrum: *No Recommendation*

$\tau_{hv} = 450$ years

Fractional Atmospheric Loss: 0.037

Molecular Structure and Infrared Spectrum (1 conformer)



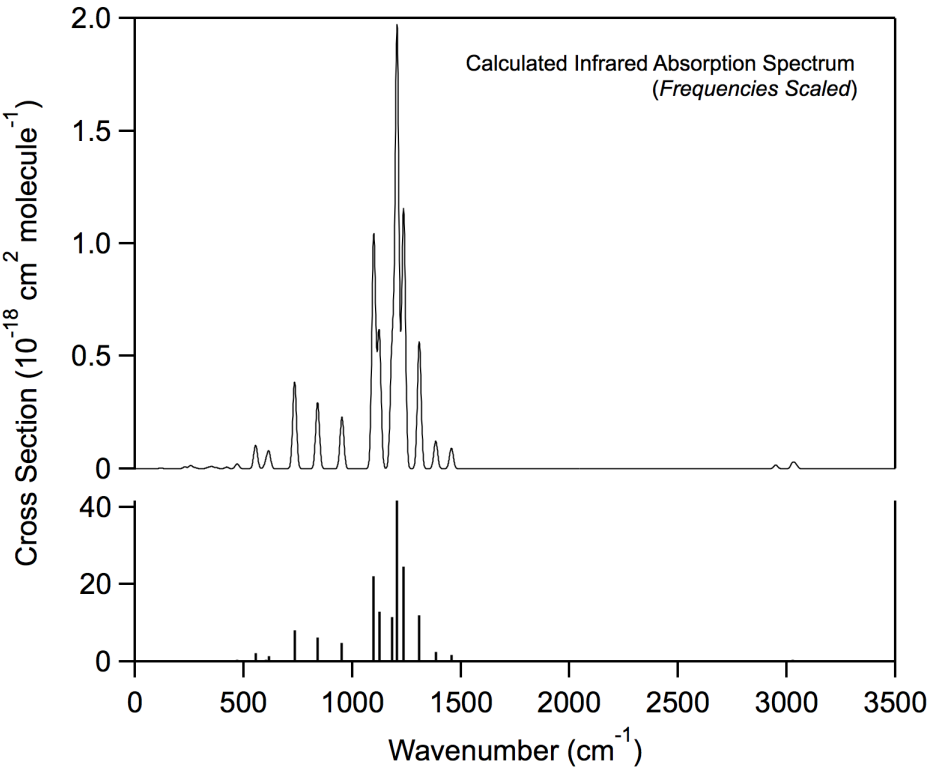
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-0.939391555506	-0.217846900915	0.053125607159
C	0.447751754295	0.447485782896	-0.114213965277
C	0.661106206730	1.610325255101	0.832608714351
F	-1.111933402696	-1.213253045082	-0.807280759992
F	-1.094659052856	-0.683136747247	1.293343569594
F	-1.888409723295	0.700024416655	-0.171255560926
F	0.513303806552	0.869176530334	-1.401694174849
Cl	1.712352517034	-0.817927840062	0.129628261328
H	1.644104434217	2.045989138004	0.648633908745
H	-0.110548405968	2.362132060960	0.648927956426
H	0.601054421493	1.273814349355	1.868108443441

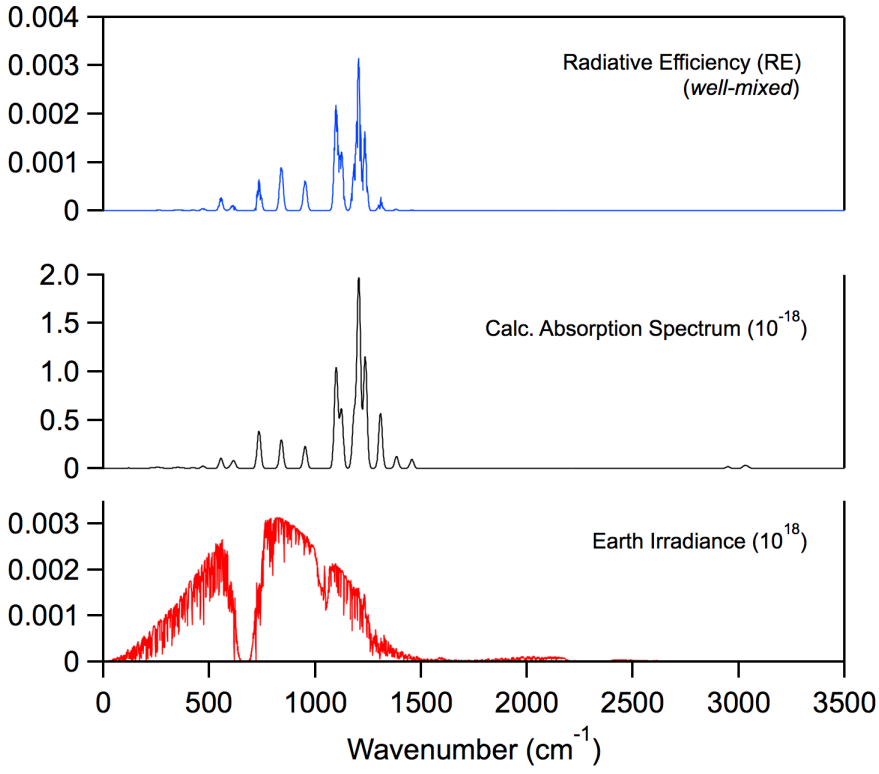
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
68.8854	0.0688
185.9089	0.174
214.5494	0.307
236.3596	0.0900
297.6968	0.112
316.7205	0.199
338.8522	0.112
390.5805	0.148
440.9630	0.467
530.9358	2.24
581.4021	0.519
595.4720	1.52
720.9838	8.19
833.1125	6.25
951.8159	4.89
1106.8606	22.1
1133.3716	12.9
1196.6715	11.5
1220.2833	41.6
1252.2927	24.5
1328.7367	12.0
1408.8581	2.62
1478.1555	0.188
1486.0336	1.82
3066.2777	0.356
3148.8916	0.544
3164.3790	0.356

Infrared Spectrum

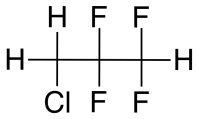


Radiative Efficiency



HCFC-244ca

Molecular Formula:	$CH_2ClCF_2CHF_2$
Name:	3-Chloro-1,1,2,2-tetrafluoropropane
CAS number:	679-85-6
Molecular Weight:	150.5



Global Atmospheric Lifetime (years):	6.39
Tropospheric Atmospheric Lifetime (years):	6.82
Stratospheric Atmospheric Lifetime (years):	100.9
Ozone Depletion Potential (ODP):	0.018

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.184	0.173
Global Warming Potential (GWP_H):		
GWP_{20}	1686	1577
GWP_{100}	477	447
Global Temperature Potentials (GTP_H)		
GTP_{20}		980
GTP_{50}		109
GTP_{100}		63

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 8.60 \times 10^{-15}$; $k_{SAR}(272\ K) \approx 5.49 \times 10^{-15}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 6.59$ years

$\tau^{OH}_{Trop} = 6.82$ years

$\tau^{OH}_{Strat} = 190.3$ years

Fractional Atmospheric Loss: 0.970

O(^{1}D) Reactivity

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

$k_{Est}(T) = 0.9 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 410$ years

Fractional Atmospheric Loss: 0.016

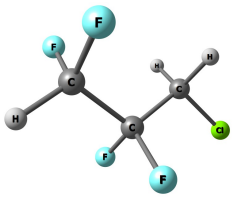
UV Photolysis

UV Spectrum: *No Recommendation*

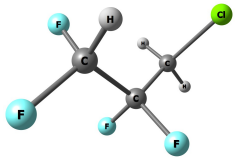
$\tau_{hv} = 450$ years

Fractional Atmospheric Loss: 0.014

Molecular Structure and Infrared Spectrum (7 conformers)



E = 0
Population = 0.504



$\Delta E = 0.76$ kcal mol^{-1}
Population = 0.141

Optimized Coordinates (Angstroms)

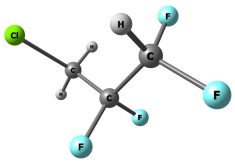
Atom	X	Y	Z
C	1.663784190207	0.086025884780	-0.027030158126
C	0.162715634343	0.419083424336	-0.106935912828
C	-0.718285310338	-0.783233970578	0.196921812983
F	1.952929173910	-0.359717172602	1.214809102990
F	1.947735581721	-0.893514379541	-0.912653337109
H	2.268160622948	0.972638199791	-0.250963313219
F	-0.073712106802	0.890563994183	-1.351943357007
F	-0.068525735140	1.422789190499	0.769043701058
H	-0.513060874751	-1.572341121349	-0.525178823065
H	-0.508823296446	-1.138165178281	1.205081149859
Cl	-2.454216879651	-0.362315871238	0.095550134464

Atom	X	Y	Z
C	0.968030754528	-0.701756055861	0.336594280725
C	0.233188099065	0.577564866350	-0.101596250265
C	-1.092265746659	0.348590890303	-0.817523545178
F	1.091178664314	-1.514246917181	-0.739174611717
F	2.196353771755	-0.363838696957	0.768512081133
H	0.429110594025	-1.226596288366	1.131367292704
F	1.033891592160	1.251152223677	-0.964286236487
F	0.058747887424	1.347891357942	0.994340868913
H	-1.504434338518	1.316376298343	-1.102303738584
H	-0.929363536023	-0.270633541439	-1.697727298671
Cl	-2.289360742072	-0.478772136809	0.233769157427

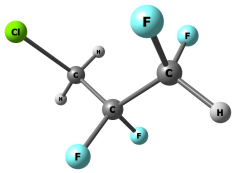
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
73.4987	0.339
76.6877	0.441
144.5323	0.287
211.0751	0.193
226.5345	0.456
344.5073	0.0875
358.5128	0.0618
503.0273	0.00706
525.6777	2.72
570.1539	5.72
643.1688	6.65
780.7875	0.926
836.7244	0.452
906.4555	0.815
1102.9024	10.4
1135.4037	19.6
1146.5380	24.8
1200.1270	0.439
1232.5863	10.8
1275.5390	15.9
1337.1937	2.51
1384.1411	1.70
1409.7006	5.96
1467.0954	1.42
3072.7921	4.40
3109.8885	0.835
3175.3021	0.00448

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
56.2127	0.263
94.2619	0.428
160.3573	0.189
220.7945	0.800
255.0018	0.159
327.9485	0.327
363.6636	0.404
438.0061	0.447
540.2031	2.75
579.9560	1.45
661.6702	2.41
773.8547	4.98
854.3692	9.26
894.2658	0.655
1087.7293	11.0
1137.3248	8.65
1159.1748	17.5
1180.1777	31.0
1232.4366	14.4
1282.9000	6.22
1322.1093	1.71
1397.2722	0.844
1427.3466	1.06
1462.1534	2.41
3090.3837	3.27
3107.7838	1.00
3179.6249	0.00757



$\Delta E = 0.76$ kcal mol^{-1}
Population = 0.141



$\Delta E = 1.07$ kcal mol^{-1}
Population = 0.083

Optimized Coordinates (Angstroms)

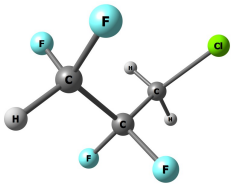
Atom	X	Y	Z
C	0.965899743219	-0.705775519739	-0.323894945124
C	0.229758985738	0.579393453147	0.094558269164
C	-1.094286646073	0.360099400809	0.816100394460
F	2.193068361926	-0.373079323826	-0.763086537704
F	1.091871204689	-1.500496276427	0.764744491478
H	0.426607835301	-1.244265595793	-1.109228494351
F	0.052529301842	1.331550560054	-1.013484983901
F	1.030711319153	1.268105282111	0.944988703203
H	-0.929143364863	-0.244497363080	1.706002178212
H	-1.507503836827	1.331766807606	1.085739581707
Cl	-2.291675904104	-0.486024424861	-0.219812657143

Atom	X	Y	Z
C	1.189542520399	-0.674381445603	-0.218693573002
C	0.431685595561	0.663479485939	-0.155547013571
C	-0.789695798384	0.718652676405	0.756209997958
F	1.430070524338	-1.091243178317	1.045935469698
F	0.458186488505	-1.606869466086	-0.851547651606
H	2.143457264695	-0.535845566144	-0.742438788521
F	0.124122006497	1.028479746847	-1.415960824300
F	1.320895091814	1.572531774762	0.335959897205
H	-0.522235435655	0.329357186909	1.737245689585
H	-1.099549961117	1.760406419068	0.838607879996
Cl	-2.178232296652	-0.225015633779	0.135474916558

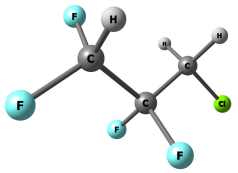
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
56.2130	0.263
94.2615	0.428
160.3569	0.189
220.7944	0.800
255.0026	0.159
327.9484	0.327
363.6635	0.404
438.0061	0.447
540.2029	2.75
579.9561	1.45
661.6701	2.41
773.8548	4.98
854.3694	9.26
894.2657	0.655
1087.7294	11.0
1137.3243	8.65
1159.1742	17.5
1180.1773	31.0
1232.4364	14.4
1282.8999	6.22
1322.1091	1.71
1397.2719	0.844
1427.3465	1.06
1462.1533	2.41
3090.3847	3.27
3107.7838	1.00
3179.6247	0.00757

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
46.3421	0.124
104.5899	0.284
166.7688	0.243
211.2348	0.152
254.2306	1.67
340.1491	0.0759
362.8697	0.0124
471.8970	4.69
512.7240	1.52
550.2007	1.20
643.8463	0.115
782.1793	6.68
832.2832	1.47
916.9709	2.34
1112.7377	14.3
1127.3970	8.44
1150.6431	23.2
1175.1572	19.8
1249.4644	16.4
1290.8823	4.38
1323.2098	1.31
1388.9490	1.72
1425.4423	1.28
1465.2096	2.75
3061.6896	5.20
3104.3663	1.12
3173.3063	0.0140



$\Delta E = 1.07$ kcal mol^{-1}
Population = 0.083



$\Delta E = 1.79$ kcal mol^{-1}
Population = 0.025

Optimized Coordinates (Angstroms)

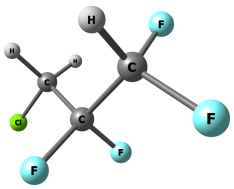
Atom	X	Y	Z
C	1.181708525493	-0.684423174053	0.218168452108
C	0.437086674895	0.660802179332	0.154041361432
C	-0.787739999900	0.725367640830	-0.752461937202
F	0.443838674074	-1.607454877923	0.857293090750
F	1.412365601300	-1.107740754570	-1.046155012893
H	2.139304061916	-0.553835515452	0.737217899889
F	1.333199041426	1.559263487969	-0.344355616412
F	0.138850569860	1.032919195956	1.414615299479
H	-1.087457217770	1.769922946888	-0.836863796141
H	-0.528599276364	0.330258872684	-1.733406556946
Cl	-2.182916654930	-0.202265001660	-0.122513184064

Atom	X	Y	Z
C	1.551054147716	-0.226887820291	0.451666303746
C	0.147815512912	0.253746493858	0.024945601800
C	-0.943767933931	-0.723237035054	0.441942237883
F	1.735383943224	-1.495547331534	0.015914453198
F	2.474833159802	0.565342552276	-0.114981623453
H	1.665183736515	-0.198173115670	1.542286817855
F	0.142894547115	0.422075236917	-1.312438861548
F	-0.044884092314	1.462633159331	0.603073214129
H	-0.785403848394	-1.677478058471	-0.057742388292
H	-0.925449838862	-0.863528246811	1.523580913594
Cl	-2.565751333784	-0.113655834551	-0.004281668911

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
46.3429	0.124
104.5904	0.284
166.7690	0.243
211.2354	0.152
254.2316	1.67
340.1491	0.0759
362.8699	0.0124
471.8974	4.69
512.7235	1.52
550.2005	1.20
643.8463	0.115
782.1795	6.68
832.2832	1.47
916.9711	2.34
1112.7378	14.3
1127.3966	8.44
1150.6428	23.2
1175.1573	19.8
1249.4652	16.4
1290.8823	4.38
1323.2100	1.31
1388.9492	1.72
1425.4424	1.28
1465.2097	2.75
3061.6892	5.20
3104.3661	1.12
3173.3059	0.0140

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
64.1644	0.187
77.1551	0.481
138.7314	0.128
223.1896	0.355
257.2172	0.260
314.4059	0.133
356.4072	0.101
428.4024	0.230
540.5013	1.37
577.8885	2.57
727.1110	9.87
778.2020	4.76
854.3991	4.96
904.3576	1.23
1080.4536	14.2
1115.7269	4.24
1147.9821	25.8
1188.1297	6.25
1251.7113	14.1
1290.9070	16.8
1330.6084	1.74
1392.1362	1.63
1422.9448	3.77
1463.9170	1.02
3057.6609	5.01
3098.6303	1.60
3169.0162	0.0802



$\Delta E = 1.79$ kcal mol^{-1}
Population = 0.025

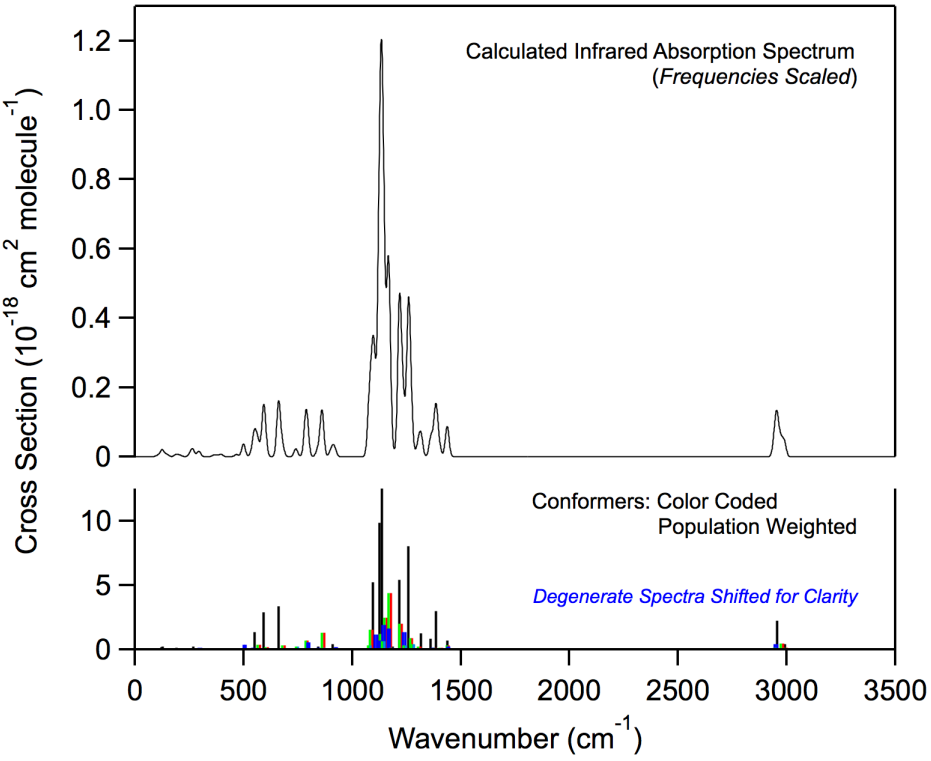
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.549517475030	-0.225996581892	-0.452515729347
C	0.146420284274	0.251982503460	-0.022362834245
C	-0.944901213516	-0.724346644403	-0.441571677809
F	2.473358903964	0.564910598217	0.115876358424
F	1.735372797895	-1.496076807595	-0.021577030520
H	1.662303003053	-0.193249129525	-1.543162442572
F	-0.047928416785	1.462800326782	-0.595878657203
F	0.142988889346	0.415467875906	1.315627134859
H	-0.927783188773	-0.860710665685	-1.523732161904
H	-0.785184470913	-1.680263377192	0.054466108278
Cl	-2.566820063575	-0.117661098072	0.008813932038

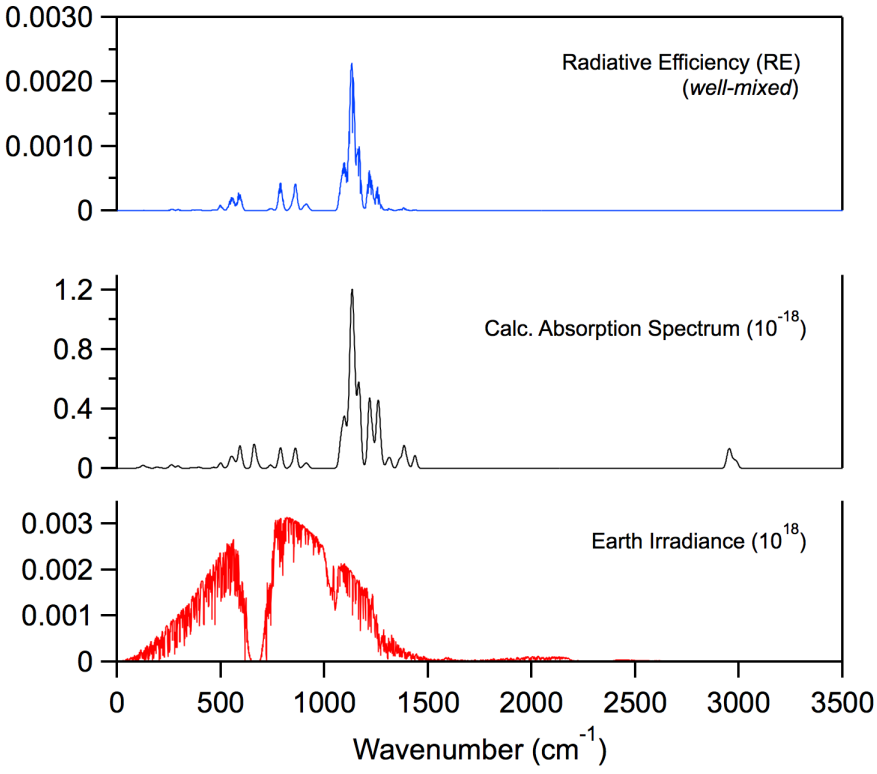
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
64.1647	0.187
77.1553	0.481
138.7313	0.128
223.1896	0.355
257.2175	0.260
314.4061	0.133
356.4072	0.101
428.4027	0.230
540.5012	1.37
577.8884	2.57
727.1110	9.87
778.2019	4.76
854.3993	4.96
904.3575	1.23
1080.4538	14.2
1115.7267	4.24
1147.9820	25.8
1188.1294	6.25
1251.7112	14.1
1290.9067	16.8
1330.6082	1.74
1392.1361	1.63
1422.9447	3.77
1463.9169	1.02
3057.6609	5.01
3098.6302	1.60
3169.0164	0.0802

Infrared Spectrum

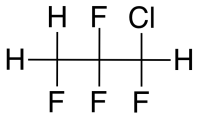


Radiative Efficiency



HCFC-244cb

Molecular Formula:	CH_2FCF_2CHFCl
Name:	1-Chloro-1,2,2,3-tetrafluoropropane
CAS number:	67406-66-0
Molecular Weight:	150.5



Global Atmospheric Lifetime (years):	4.02
Tropospheric Atmospheric Lifetime (years):	4.24
Stratospheric Atmospheric Lifetime (years):	78.6
Ozone Depletion Potential (ODP):	0.015

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.196	0.178
Global Warming Potential (GWP_H):		
GWP_{20}	1169	1061
GWP_{100}	319	289
Global Temperature Potentials (GTP_H)		
GTP_{20}		520
GTP_{50}		57
GTP_{100}		41

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 1.38 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 0.883 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 4.10$ years

$\tau^{OH}_{Trop} = 4.24$ years

$\tau^{OH}_{Strat} = 123.9$ years

Fractional Atmospheric Loss: 0.981

$O(^1D)$ Reactivity

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

$k_{Est}(T) = 0.9 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 410$ years

Fractional Atmospheric Loss: 0.010

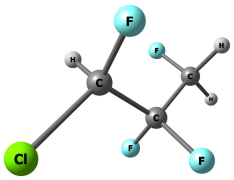
UV Photolysis

UV Spectrum: *No Recommendation*

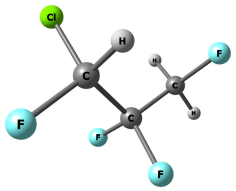
$\tau_{hv} = 450$ years

Fractional Atmospheric Loss: 0.009

Molecular Structure and Infrared Spectrum (5 conformers)



E = 0
Population = 0.628



$\Delta E = 0.88$ kcal mol^{-1}
Population = 0.143

Optimized Coordinates (Angstroms)

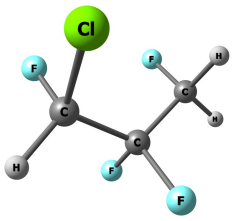
Atom	X	Y	Z
C	0.534929317369	0.592005133855	0.281992217679
C	-0.496280974167	-0.433655475536	-0.214799828922
C	-1.898283686119	0.159032973547	-0.330611708094
Cl	2.173664946888	-0.116370335749	0.325869036104
F	0.515461355428	1.653693382798	-0.560290566295
H	0.286832655803	0.916877698219	1.292943338440
F	-0.510418891503	-1.470355459708	0.651934887404
F	-0.144688169091	-0.897573067213	-1.433737878494
H	-1.904462580634	0.937757518729	-1.097865853454
H	-2.593346652646	-0.643256061038	-0.598795358040
F	-2.253350321328	0.697311692094	0.882375713673

Atom	X	Y	Z
C	0.661199158487	0.208691783427	0.609076305856
C	-0.590841764484	0.394573059426	-0.267026005357
C	-1.437395102919	-0.858143169009	-0.451840839093
Cl	1.796810825898	-0.966012477930	-0.136807756910
F	1.272270434814	1.401241187212	0.743346843072
H	0.383572072105	-0.187476724044	1.586347674771
F	-0.241747184578	0.862206049825	-1.484229499025
F	-1.334859396572	1.349272015805	0.348241894723
H	-2.370125489780	-0.570416497427	-0.948286495201
H	-0.898695234100	-1.590740985650	-1.057974038863
F	-1.713131318869	-1.389330241634	0.785289916028

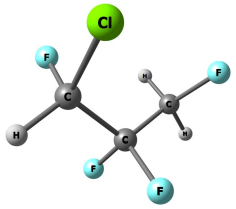
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
59.4435	0.162
99.6941	0.576
171.3147	0.254
208.7334	0.585
233.6672	0.228
315.6160	0.744
370.5658	0.0470
421.8368	0.0938
481.9005	1.52
586.3322	5.90
606.4411	7.02
792.3261	4.42
849.7065	6.23
960.4127	5.89
1110.2863	16.3
1116.8351	18.0
1155.6517	9.69
1222.5759	5.86
1233.5845	16.0
1286.9216	4.69
1313.2847	2.52
1380.7281	0.929
1423.6320	0.455
1495.4352	0.819
3059.4393	2.45
3123.4147	1.86
3126.2146	0.930

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
54.7743	0.172
99.8471	0.491
177.1566	0.211
204.3679	0.656
254.6607	0.507
319.5055	0.362
371.7671	0.220
407.9104	0.748
450.5641	0.440
572.8067	1.91
647.9238	6.74
786.0560	8.20
848.8081	11.4
943.6197	5.15
1107.9747	12.8
1138.8081	22.0
1155.0698	12.7
1227.6301	8.00
1231.4943	10.6
1271.7679	6.58
1309.2434	1.60
1390.0243	2.82
1428.5389	0.298
1496.8805	1.29
3059.7309	2.34
3124.7636	2.08
3126.6575	0.781



$\Delta E = 1.29$ kcal mol^{-1}
Population = 0.072



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

Optimized Coordinates (Angstroms)

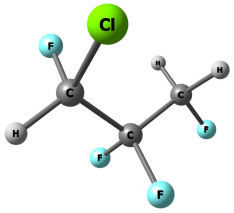
Atom	X	Y	Z
C	0.692729117153	-0.019873337142	0.720048549109
C	-0.610088835047	-0.551541806050	0.093437514639
C	-1.190588347119	0.222325868157	-1.085418560397
Cl	2.032003819546	-0.018413906878	-0.476669064245
F	0.497784805582	1.226653267770	1.186853703501
H	0.995998904313	-0.683284104042	1.533657898205
F	-1.517763723516	-0.585964739426	1.100159217715
F	-0.388840082555	-1.825036569872	-0.312408628029
H	-0.467406389920	0.245987838941	-1.905636152116
H	-2.097420868387	-0.302645473333	-1.406773326388
F	-1.502298400050	1.496303961874	-0.698654151994

Atom	X	Y	Z
C	0.585480794775	0.850545815655	0.077422651905
C	-0.799081447685	0.208731492288	0.278465554135
C	-1.223650299765	-0.848268998595	-0.737315645189
Cl	1.923905607602	-0.292618887397	0.378898267964
F	0.653641950822	1.311748210499	-1.194280558334
H	0.702872342228	1.681203960424	0.776917808112
F	-1.693571119572	1.231772826957	0.170345401912
F	-0.873338704462	-0.278581468449	1.532070398403
H	-2.287495300162	-1.051301312694	-0.571297745116
H	-1.075486119157	-0.455150189424	-1.747631983626
F	-0.501615704623	-1.995817449263	-0.569211150166

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
42.5354	0.131
118.3031	0.485
181.7212	0.189
192.4186	0.195
271.1919	1.61
318.1387	0.270
368.1347	0.165
429.1930	0.372
461.5894	3.41
504.7789	2.79
631.2419	1.21
776.5039	5.46
847.9494	13.9
974.5384	3.79
1121.2057	2.98
1150.3089	12.8
1171.9738	36.1
1176.7313	16.8
1242.6015	2.02
1294.3070	2.45
1311.9009	2.00
1375.0298	2.70
1442.0943	1.00
1497.3213	1.12
3050.5847	2.70
3099.8838	1.48
3112.7030	2.40

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
46.1148	0.154
108.3616	0.413
177.7717	0.351
195.0763	0.0697
265.0264	1.80
310.5306	0.173
371.9361	0.0715
426.4499	0.662
467.2112	3.95
530.5208	1.58
612.9931	1.38
792.8384	7.18
847.9650	10.7
980.7544	3.30
1119.1818	10.4
1131.9531	18.3
1133.6084	23.6
1207.3464	8.38
1251.0514	7.10
1293.8123	5.72
1313.0940	3.26
1374.2405	2.23
1440.1482	0.330
1497.7839	0.810
3050.8485	2.83
3103.2873	1.35
3111.1588	2.40



$\Delta E = 1.39$ kcal mol^{-1}
Population = 0.060

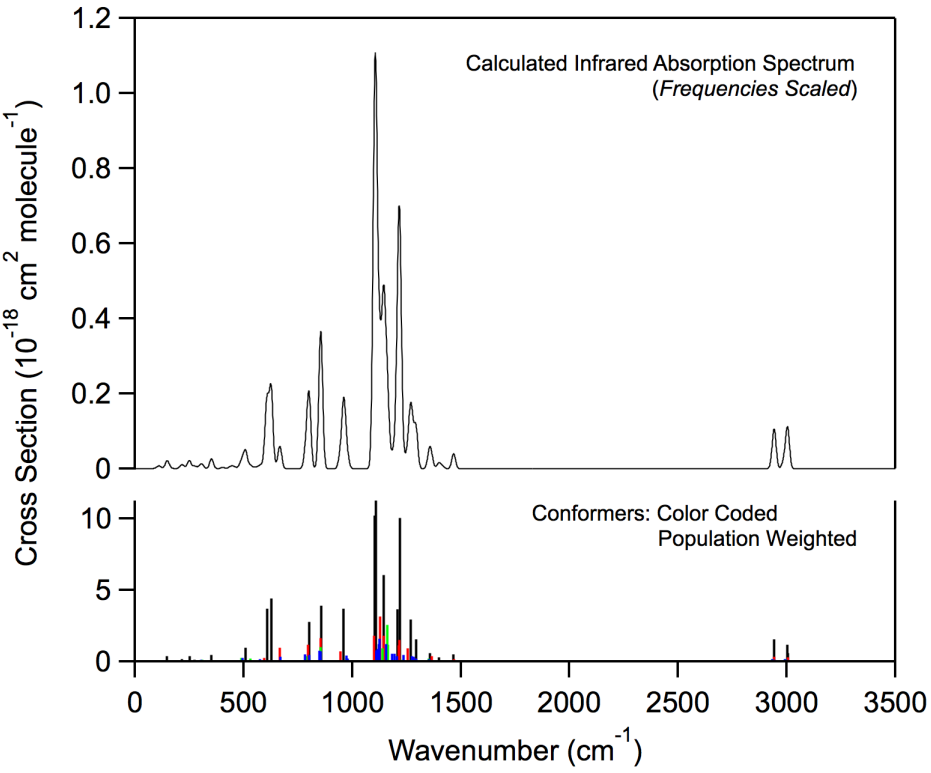
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	0.937436022059	-0.597372889442	-0.207159180597
C	-0.534592062614	-0.168978210138	-0.337892618601
C	-1.121101502157	0.503944368807	0.898191167867
Cl	2.022849366165	0.816899084884	-0.012352526618
F	1.058654940293	-1.412268569345	0.865095243147
H	1.248636990493	-1.122207197114	-1.112806043781
F	-1.231124242526	-1.304691137706	-0.599190059956
F	-0.652095919663	0.635320234366	-1.416262917959
H	-0.989952677553	-0.154982301745	1.761990694105
H	-0.613467038028	1.456130979406	1.076610939427
F	-2.452984876468	0.722130638026	0.674879302966

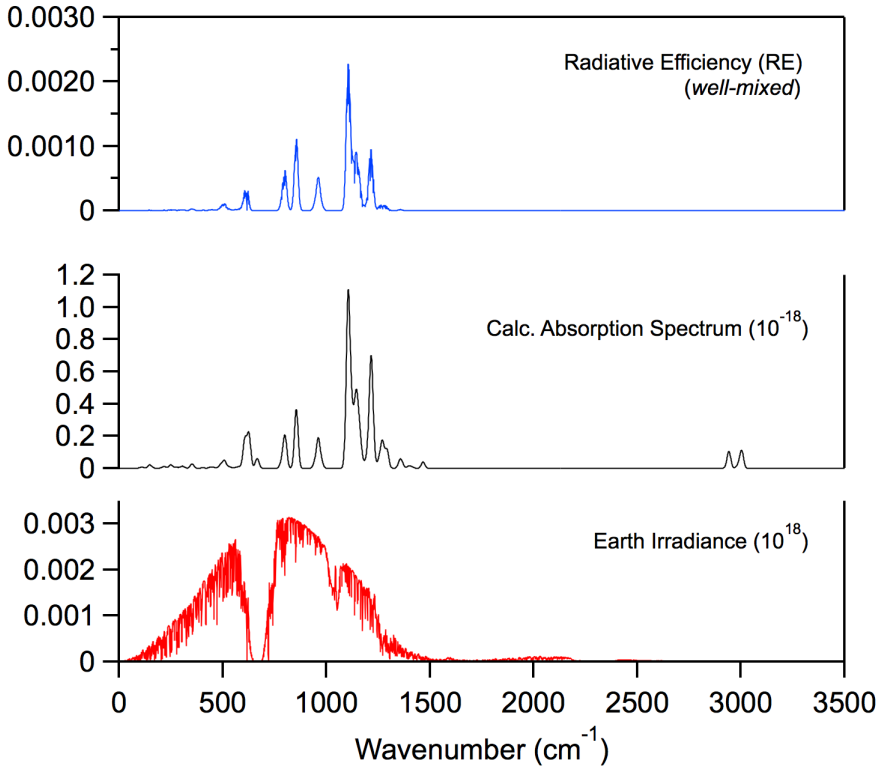
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
65.6539	0.657
83.3512	0.218
160.6533	0.457
190.8716	0.158
272.3332	0.575
314.0361	0.331
338.9589	0.0690
411.9156	0.143
482.1615	0.405
553.3174	3.17
652.6737	5.54
773.1999	8.10
841.8325	12.8
974.2310	7.38
1121.5250	13.5
1127.3742	15.0
1167.0116	19.9
1196.2053	8.92
1221.1584	6.05
1300.0391	2.61
1302.5516	5.62
1379.2072	2.76
1441.3844	0.878
1502.1059	0.329
3061.0737	2.05
3109.0407	1.31
3118.7697	1.87

Infrared Spectrum

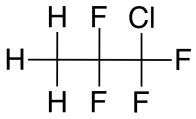


Radiative Efficiency



HCFC-244cc

Molecular Formula:	$CH_3CF_2CF_2Cl$
Name:	1-Chloro-1,1,2,2-tetrafluoropropane
CAS number:	421-75-0
Molecular Weight:	150.5



Global Atmospheric Lifetime (years):	31.2
Tropospheric Atmospheric Lifetime (years):	38.1
Stratospheric Atmospheric Lifetime (years):	173.3
Ozone Depletion Potential (ODP):	0.039

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.283	0.277
Global Warming Potential (GWP_H):		
GWP_{20}	6259	6130
GWP_{100}	3439	3369
Global Temperature Potentials (GTP_H)		
GTP_{20}		5918
GTP_{50}		3300
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*

$k_{SAR}(298\ K) = 1.54 \times 10^{-15}$; $k_{SAR}(272\ K) \approx 0.982 \times 10^{-15}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 36.6$ years

$\tau^{OH}_{Trop} = 38.1$ years

$\tau^{OH}_{Strat} = 896.6$ years

Fractional Atmospheric Loss: 0.855

$O(^1D)$ Reactivity

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

$k_{Est}(T) = 0.9 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 410$ years

Fractional Atmospheric Loss: 0.076

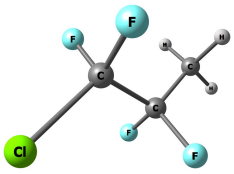
UV Photolysis

UV Spectrum: *No Recommendation*

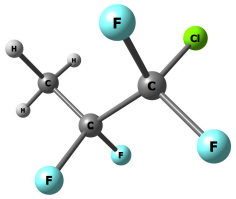
$\tau_{hv} = 450$ years

Fractional Atmospheric Loss: 0.069

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.609



$\Delta E = 0.67$ kcal mol^{-1}
Population = 0.195

Optimized Coordinates (Angstroms)

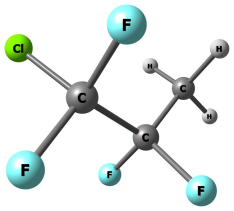
Atom	X	Y	Z
C	0.419857071895	-0.485569789847	-0.000622920446
C	-0.917641001838	0.300714298823	-0.002382292563
C	-2.131295764779	-0.605704867754	-0.012135400849
F	0.464890895022	-1.272744990485	1.079171421090
F	0.474152006351	-1.261840712206	-1.087860007096
Cl	1.835137602576	0.604562788481	0.010910471670
F	-0.917233741942	1.101865603644	-1.091952221594
F	-0.926584494028	1.090851988273	1.095164516746
H	-3.025802898331	0.020259173801	-0.012804881373
H	-2.123281268617	-1.230673686648	-0.906196090463
H	-2.130896406310	-1.239649806082	0.875619404878

Atom	X	Y	Z
C	0.456020331641	0.449372315125	-0.108664098844
C	-0.945355946965	-0.190573242428	0.097135779736
C	-1.312795942413	-1.271365107943	-0.892678046622
F	0.541825850068	0.930064562916	-1.352372320493
F	0.617674909670	1.454448734174	0.746347422132
Cl	1.775377918736	-0.743537154880	0.144750144040
F	-1.822601039709	0.843027307347	0.004824807516
F	-0.997900848335	-0.653042825862	1.366038370520
H	-2.339191003000	-1.582975124136	-0.687772919140
H	-1.248995269450	-0.882016896046	-1.909871059949
H	-0.646238960243	-2.127874568265	-0.787195078895

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
64.3541	0.180
180.4145	0.320
200.3817	0.0183
222.2982	0.144
293.5747	0.470
328.1096	0.0452
357.4546	0.00402
375.9649	0.00141
424.4720	0.0116
532.1355	0.00912
534.9527	4.16
606.1264	4.82
690.5716	2.56
876.2054	13.2
980.5539	4.08
1010.9378	29.1
1143.8561	24.4
1191.4391	20.9
1229.5725	28.4
1238.7507	12.2
1310.7585	2.04
1409.2982	3.04
1477.9455	0.140
1488.9698	0.431
3070.7151	0.253
3156.1687	0.571
3162.6549	0.524

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
66.3312	0.127
184.6126	0.0836
199.6720	0.0488
222.5266	0.408
310.8184	0.288
322.2470	0.174
337.5810	0.127
398.9621	0.172
422.7053	0.224
469.9251	0.729
570.6862	1.11
603.0303	3.44
696.7925	2.73
915.5716	21.1
960.7481	14.0
977.8778	13.7
1148.3879	22.7
1205.8802	28.9
1216.8969	26.8
1250.5960	7.21
1312.0465	9.06
1414.4599	5.35
1478.9402	0.259
1487.5580	0.328
3071.4730	0.155
3154.4451	0.666
3165.1180	0.482



$\Delta E = 0.67$ kcal mol^{-1}
Population = 0.195

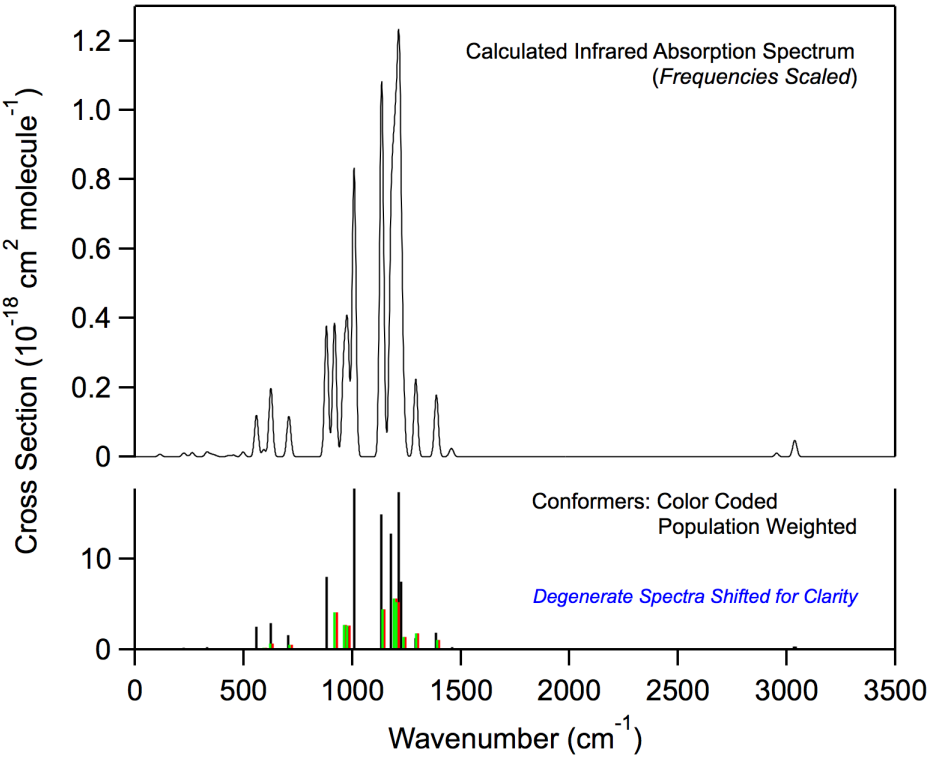
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	0.456920956486	0.447864222862	0.109373250737
C	-0.944339189502	-0.191465765009	-0.099103915175
C	-1.306361070871	-1.285327096406	0.878272602228
F	0.613794129195	1.463995064045	-0.733375051462
F	0.546917375681	0.912789850354	1.358766087691
Cl	1.776965854201	-0.739779527664	-0.164377784345
F	-1.001196793190	-0.637799181555	-1.373586784239
F	-1.822682538379	0.839583851749	0.009800010696
H	-2.333107723134	-1.595808821617	0.673416949443
H	-0.639006465637	-2.139441284865	0.759274949445
H	-1.239126534851	-0.908884311895	1.900091684980

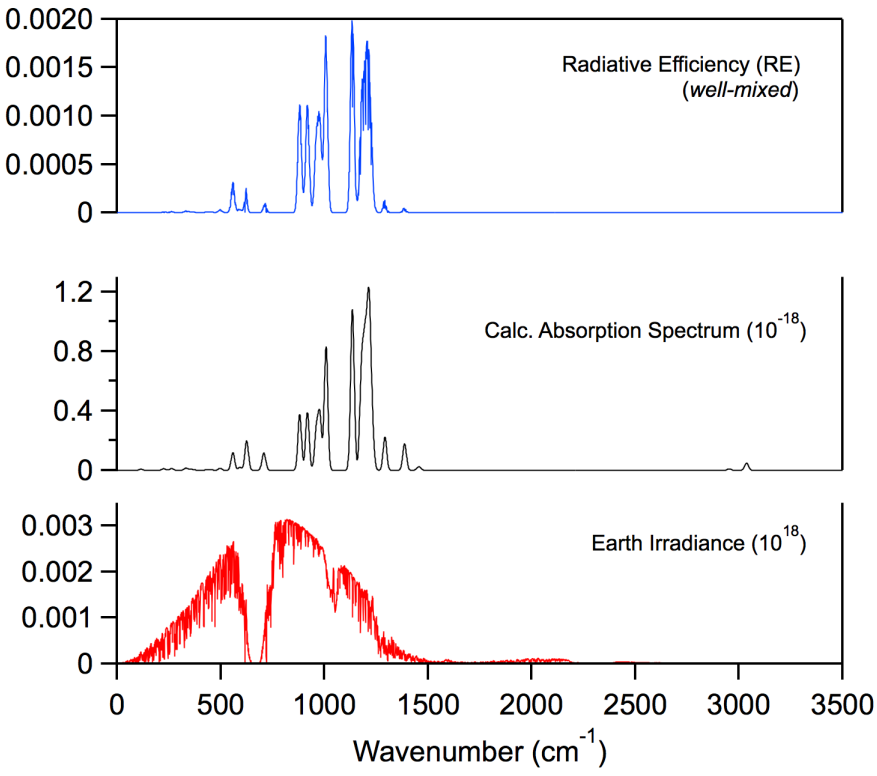
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
66.3326	0.127
184.6135	0.0836
199.6701	0.0488
222.5273	0.408
310.8189	0.288
322.2473	0.174
337.5810	0.127
398.9619	0.172
422.7053	0.224
469.9252	0.729
570.6861	1.11
603.0302	3.44
696.7926	2.73
915.5712	21.1
960.7483	14.0
977.8775	13.7
1148.3880	22.7
1205.8802	28.9
1216.8969	26.8
1250.5951	7.21
1312.0479	9.06
1414.4593	5.35
1478.9402	0.259
1487.5579	0.328
3071.4736	0.155
3154.4461	0.666
3165.1177	0.482

Infrared Spectrum

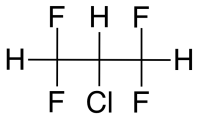


Radiative Efficiency



HCFC-244da

Molecular Formula:	$CHF_2CHClCHF_2$
Name:	2-Chloro-1,1,3,3-tetrafluoropropane
CAS number:	19041-02-2
Molecular Weight:	150.5



Global Atmospheric Lifetime (years):	3.88
Tropospheric Atmospheric Lifetime (years):	4.09
Stratospheric Atmospheric Lifetime (years):	77.0
Ozone Depletion Potential (ODP):	0.015

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.201	0.182
Global Warming Potential (GWP_H):		
GWP_{20}	1163	1053
GWP_{100}	317	287
Global Temperature Potentials (GTP_H)		
GTP_{20}		507
GTP_{50}		56
GTP_{100}		40

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 1.43 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 0.916 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 3.95$ years

$\tau^{OH}_{Trop} = 4.09$ years

$\tau^{OH}_{Strat} = 120.0$ years

Fractional Atmospheric Loss: 0.982

O(^{1}D) Reactivity

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

$k_{Est}(T) = 0.9 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 410$ years

Fractional Atmospheric Loss: 0.009

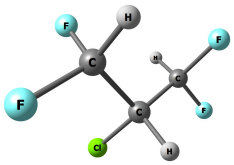
UV Photolysis

UV Spectrum: *No Recommendation*

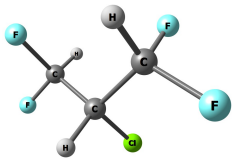
$\tau_{hv} = 450$ years

Fractional Atmospheric Loss: 0.009

Molecular Structure and Infrared Spectrum (8 conformers)



E = 0
Population = 0.287



E = 0
Population = 0.287

Optimized Coordinates (Angstroms)

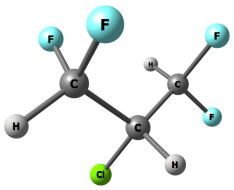
Atom	X	Y	Z
C	1.339698970939	-0.317058708542	0.246123700185
C	0.044818356222	0.131129914169	-0.432326814963
C	-1.087183675942	-0.861486340872	-0.173236970236
F	1.610109791136	-1.585120320639	-0.170262638215
F	2.359547791559	0.472647525290	-0.139220072631
H	1.264465586992	-0.308903452956	1.338090899059
H	0.219643804710	0.200279477797	-1.507925700022
Cl	-0.397276504176	1.766321135537	0.151439342314
H	-0.827529952791	-1.850435200562	-0.569335770642
F	-1.307845636822	-0.973241482330	1.158272968597
F	-2.223553531827	-0.438059546892	-0.760708943447

Atom	X	Y	Z
C	1.086751725460	-0.861443437920	-0.171388062829
C	-0.045541275393	0.130195072208	-0.432940359059
C	-1.340189541011	-0.316484763318	0.246946791209
F	2.222912201717	-0.439316530099	-0.760198985178
F	1.307679136836	-0.969567147133	1.160377727189
H	0.827271365229	-1.851516597688	-0.564782306862
H	-0.220577519081	0.196410290214	-1.508689633805
Cl	0.396257447228	1.767057769594	0.146348798045
H	-1.264761803645	-0.305375626724	1.338874531507
F	-2.360301104334	0.471933705199	-0.140334206481
F	-1.610365633005	-1.585726734335	-0.165981293737

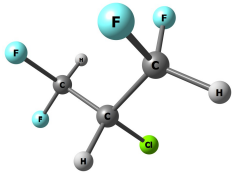
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
73.2145	0.289
77.1149	0.220
160.1574	0.216
191.6258	0.0922
223.3777	0.780
331.1624	0.233
382.4520	0.0922
488.6330	3.25
540.4210	1.69
578.8639	0.331
675.2653	7.51
826.6060	3.40
977.8375	3.14
1077.5394	3.87
1105.8855	21.2
1131.0222	20.4
1167.1871	26.4
1180.7879	7.01
1245.1148	1.43
1287.3599	3.62
1388.2878	2.58
1393.9224	5.94
1405.2231	3.34
1423.4002	8.63
3063.4694	3.42
3085.7754	2.60
3112.2877	1.37

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
73.2147	0.289
77.1150	0.220
160.1571	0.216
191.6260	0.0922
223.3778	0.780
331.1624	0.233
382.4521	0.0922
488.6331	3.25
540.4210	1.69
578.8640	0.331
675.2652	7.51
826.6059	3.40
977.8371	3.14
1077.5395	3.87
1105.8851	21.2
1131.0221	20.4
1167.1868	26.4
1180.7877	7.01
1245.1148	1.43
1287.3599	3.62
1388.2876	2.58
1393.9220	5.94
1405.2228	3.34
1423.4001	8.63
3063.4703	3.42
3085.7755	2.60
3112.2874	1.37



$\Delta E = 0.49$ kcal mol^{-1}
Population = 0.125



$\Delta E = 0.49$ kcal mol^{-1}
Population = 0.125

Optimized Coordinates (Angstroms)

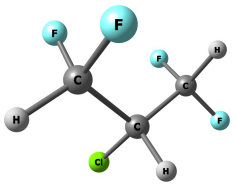
Atom	X	Y	Z
C	0.694224126684	-0.933410645892	0.387747817035
C	0.149315457761	0.189649977795	-0.500868199450
C	-1.335180551953	0.481038641603	-0.259517861496
F	-0.020688100009	-2.057159350541	0.147011470079
F	1.980544020253	-1.179072322648	0.061746664757
H	0.632545965698	-0.686423377311	1.452061499979
H	0.296048730575	-0.082567122877	-1.547255055816
Cl	1.089374216029	1.690623682795	-0.193569654793
H	-1.644008026076	1.417035154429	-0.737883942317
F	-2.077013470360	-0.534009364459	-0.755111415395
F	-1.576777368602	0.570685727105	1.070276677418

Atom	X	Y	Z
C	1.352006215758	0.431466805363	-0.262382152140
C	-0.141579619774	0.189253983776	-0.502006630725
C	-0.723811381580	-0.910420962316	0.392168260323
F	1.596986853655	0.519332423600	1.066912676254
F	2.058930392011	-0.610456121108	-0.753201542286
H	1.692109974745	1.354166803099	-0.745344240567
H	-0.297819019221	-0.082917471419	-1.547028398389
Cl	-1.030252714525	1.722618485855	-0.201808604996
H	-0.653423947318	-0.660500909026	1.455256265301
F	-2.017821913532	-1.114032530399	0.067630417962
F	-0.047387840218	-2.058851507426	0.156747949264

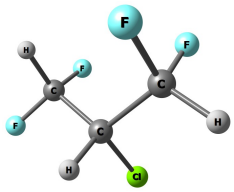
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
55.5039	0.185
87.8382	0.137
166.6104	0.0531
199.5219	0.177
237.5362	0.919
332.2368	0.285
388.6896	0.712
434.6382	3.07
539.7177	1.66
571.1480	0.813
701.0158	3.35
852.8614	10.1
926.6523	0.315
1105.1895	17.7
1113.6909	2.29
1139.0734	9.36
1146.8637	27.6
1171.9416	25.7
1230.0431	1.70
1294.1993	3.11
1379.2306	4.40
1401.2925	4.08
1406.0583	5.36
1434.3338	4.08
3070.7855	4.48
3087.8694	2.92
3120.4356	0.723

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
55.5042	0.185
87.8368	0.137
166.6075	0.0531
199.5207	0.177
237.5367	0.919
332.2369	0.285
388.6890	0.712
434.6391	3.07
539.7179	1.66
571.1482	0.813
701.0151	3.35
852.8609	10.1
926.6527	0.315
1105.1908	17.7
1113.6922	2.29
1139.0727	9.36
1146.8645	27.6
1171.9413	25.7
1230.0428	1.70
1294.1999	3.11
1379.2317	4.40
1401.2926	4.08
1406.0594	5.36
1434.3341	4.08
3070.7843	4.48
3087.8694	2.92
3120.4345	0.723



$\Delta E = 0.85$ kcal mol^{-1}
Population = 0.068



$\Delta E = 0.85$ kcal mol^{-1}
Population = 0.068

Optimized Coordinates (Angstroms)

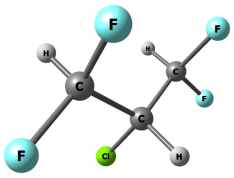
Atom	X	Y	Z
C	0.705867959007	-1.054110751405	-0.119655742347
C	0.045245319633	0.240289136296	-0.599839731723
C	-1.446863479212	0.295554662654	-0.268143325990
F	1.955822541228	-1.134125333365	-0.628694676237
F	0.791628050375	-1.088398502892	1.223393195333
H	0.127033486044	-1.921099931830	-0.462367367040
H	0.150688384623	0.287205873495	-1.685334946830
Cl	0.869551654838	1.679901921308	0.076445758310
H	-1.909137721716	1.224865423411	-0.618651461031
F	-2.045154101485	-0.757396890094	-0.892245766258
F	-1.658331093336	0.169029392422	1.054685063813

Atom	X	Y	Z
C	1.448413013508	0.280367132060	-0.284927897995
C	-0.045524460338	0.229526697863	-0.609012900874
C	-0.713012492544	-1.051035878857	-0.101980659752
F	1.664943008856	0.176882689074	1.039084339618
F	2.036505075343	-0.788179002330	-0.891986383635
H	1.915596244428	1.199726672029	-0.654643534769
H	-0.155527053398	0.257052949403	-1.694720548127
Cl	-0.856684054580	1.687228774853	0.044020693204
H	-0.141800031878	-1.928305338395	-0.431048503722
F	-0.792967519026	-1.059792125970	1.241835146019
F	-1.965772730371	-1.131636569729	-0.603981749966

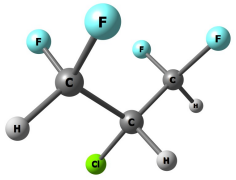
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
54.4596	0.303
94.1520	0.0333
170.9731	0.337
189.8612	0.301
204.8264	0.129
316.0960	0.196
371.7226	0.142
500.6084	3.28
551.7220	1.24
655.5719	4.95
719.9065	5.53
800.2951	2.00
953.3807	1.21
1004.0535	4.15
1101.7505	22.1
1141.2763	9.57
1184.0262	17.0
1185.9004	22.5
1249.2283	3.01
1311.0196	5.40
1380.0963	4.90
1395.8310	5.76
1415.2024	5.53
1425.9364	3.59
3054.4435	3.44
3072.3546	4.80
3110.3248	0.744

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
54.4588	0.303
94.1532	0.0333
170.9745	0.337
189.8615	0.301
204.8289	0.129
316.0964	0.196
371.7225	0.142
500.6083	3.28
551.7222	1.24
655.5725	4.95
719.9080	5.53
800.2964	2.00
953.3814	1.21
1004.0547	4.15
1101.7498	22.1
1141.2753	9.57
1184.0259	17.0
1185.8997	22.5
1249.2282	3.01
1311.0195	5.40
1380.0962	4.90
1395.8320	5.76
1415.2027	5.53
1425.9361	3.59
3054.4428	3.44
3072.3555	4.80
3110.3248	0.744



$\Delta E = 1.52$ kcal mol^{-1}
Population = 0.022



$\Delta E = 1.88$ kcal mol^{-1}
Population = 0.012

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.286254487341	-0.421312783292	0.298034812168
C	-0.000002805798	0.187024007421	-0.271459728863
C	-1.280663781936	-0.431744174041	0.299406937672
F	1.331641795682	-1.737089884371	-0.009135705036
F	2.352496549128	0.174664894964	-0.274250577858
H	1.356563637942	-0.303898718494	1.386935168390
H	-0.000096007507	0.067211697834	-1.356827102203
Cl	-0.006955674297	1.945876396598	0.093151947290
H	-1.350761945654	-0.314898252730	1.388381970215
F	-2.352325497674	0.155543494286	-0.271738042517
F	-1.315682757226	-1.747848678174	-0.007717679258

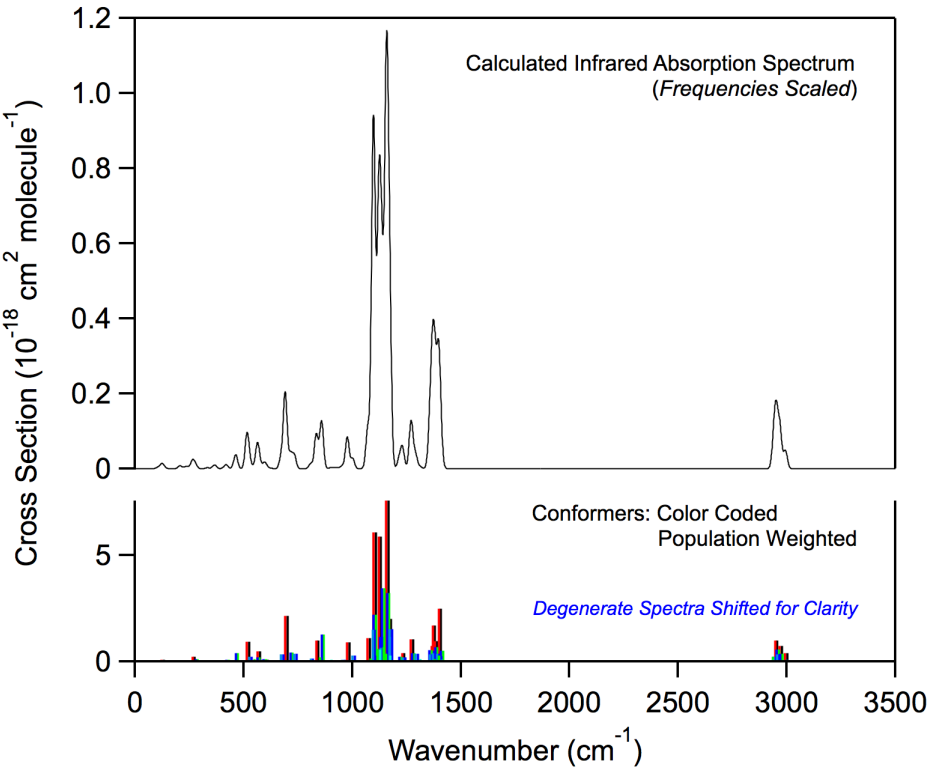
Atom	X	Y	Z
C	-0.293191320421	-1.302313785656	-0.142006973460
C	0.314978639361	0.010763529546	-0.652876524438
C	-0.332516129278	1.296027536208	-0.120074553856
F	-0.277133158125	-1.361439955950	1.202731687250
F	-1.579956048074	-1.376620431181	-0.557810056098
H	0.257760204567	-2.163459848486	-0.539582235705
H	0.229668820005	0.018657862776	-1.741037135549
Cl	2.070003859219	0.034036918882	-0.263454819710
H	0.192033188505	2.180037762127	-0.502906226055
F	-1.621040402267	1.338379275097	-0.534909344882
F	-0.317928653493	1.332900136636	1.225475182504

Infrared Absorption Spectrum (unscaled frequencies)

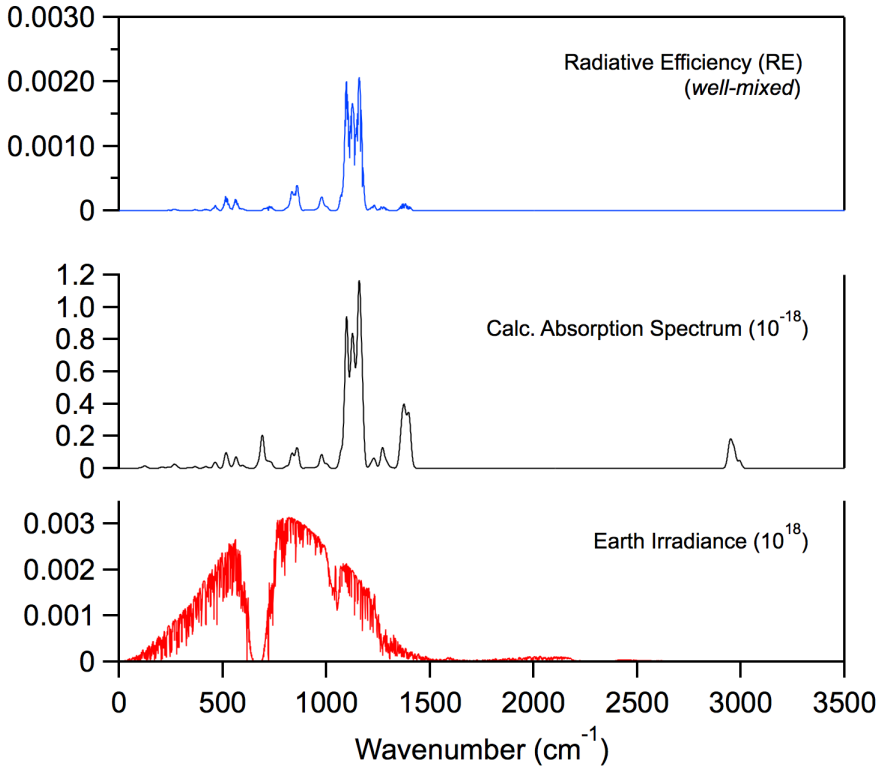
Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
39.1683	0.0357
78.0244	0.105
177.4583	0.123
203.5599	0.155
295.3365	2.53
331.8617	0.197
344.6389	0.153
430.1197	0.390
524.6089	4.67
588.7487	0.908
602.4147	1.47
845.1724	8.95
1063.9238	2.24
1092.3559	6.59
1113.2796	2.19
1126.5839	27.1
1154.3900	30.9
1167.6992	17.2
1228.6500	1.18
1270.8877	0.493
1384.0051	0.282
1402.7133	5.64
1422.6101	0.999
1424.7630	13.4
3047.4510	0.00339
3052.7049	9.76
3115.3326	0.807

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
28.3897	0.000
112.5162	0.387
181.5758	0.000
204.9836	0.418
209.3413	0.0591
337.2118	0.108
389.6761	0.136
422.1323	5.07
549.2417	1.76
579.2313	0.873
791.6015	2.07
855.6096	4.66
900.4024	6.24
1003.4779	0.713
1110.7189	0.209
1137.6414	46.3
1186.3736	23.5
1189.9831	3.28
1232.2153	5.51
1333.6816	9.44
1367.0227	2.91
1405.9342	4.27
1422.5308	0.0889
1440.2449	7.01
3053.3829	6.43
3056.0697	4.18
3110.9448	0.512

Infrared Spectrum

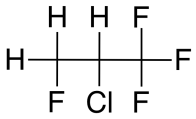


Radiative Efficiency



HCFC-244db

Molecular Formula:	$CH_2FCHClCF_3$
Name:	2-Chloro-1,1,1,3-tetrafluoropropane
CAS number:	117970-90-8
Molecular Weight:	150.5



Global Atmospheric Lifetime (years):	2.44
Tropospheric Atmospheric Lifetime (years):	2.54
Stratospheric Atmospheric Lifetime (years):	57.4
Ozone Depletion Potential (ODP):	0.012

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.189	0.164
Global Warming Potential (GWP_H):		
GWP_{20}	690	596
GWP_{100}	187	162
Global Temperature Potentials (GTP_H)		
GTP_{20}		234
GTP_{50}		29
GTP_{100}		23

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 2.31 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 1.47 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 2.46$ years

$\tau^{OH}_{Trop} = 2.54$ years

$\tau^{OH}_{Strat} = 78.2$ years

Fractional Atmospheric Loss: 0.989

O(^{1}D) Reactivity

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

$k_{Est}(T) = 0.9 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 410$ years

Fractional Atmospheric Loss: 0.006

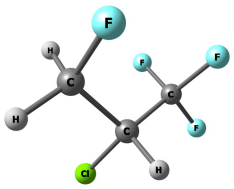
UV Photolysis

UV Spectrum: *No Recommendation*

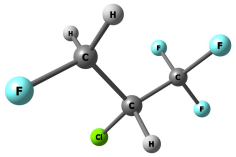
$\tau_{hv} = 450$ years

Fractional Atmospheric Loss: 0.005

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.399



$\Delta E = 0.12$ kcal mol^{-1}
Population = 0.328

Optimized Coordinates (Angstroms)

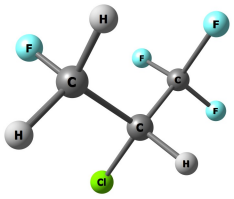
Atom	X	Y	Z
C	-0.343393134864	-0.897857739205	0.003413629443
C	0.234142778016	0.446608818478	-0.454331498139
C	-0.432608138525	1.646521490829	0.220057111991
F	0.322692521505	-1.921621341937	-0.532732632707
F	-0.300930184539	-1.021181900229	1.333894530662
F	-1.620675740332	-0.992069896392	-0.381569549215
H	0.123873376759	0.504980082094	-1.538075594676
Cl	1.991576886635	0.505284990172	-0.085263834115
H	-0.370706372738	1.547532720882	1.308408970393
H	0.078312709119	2.562507094720	-0.091351324964
F	-1.751067701036	1.709220680587	-0.159748808672

Atom	X	Y	Z
C	-1.139771495864	0.168916285435	-0.041220971767
C	0.340107845907	0.043554920038	-0.406743001146
C	1.170694732324	1.142350563562	0.247279272628
F	-1.599236134418	1.352560922872	-0.486045323070
F	-1.874379450028	-0.789415778775	-0.598657988973
F	-1.327533083942	0.130839880569	1.281011588424
H	0.423150861068	0.110515954772	-1.492705306121
Cl	0.950587262618	-1.579866591514	0.059863579470
H	0.732130823596	2.115955805195	-0.001593431882
H	1.183609356095	1.014876870697	1.334103971749
F	2.451259282644	1.089336167149	-0.234474389309

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
45.4137	0.0678
128.6129	0.722
185.2655	0.186
210.0913	0.344
242.6715	0.460
321.2723	0.0576
388.3657	0.0697
447.5104	2.33
532.2881	1.15
571.3681	0.981
645.3447	2.36
800.4838	2.33
855.9524	6.56
1011.6701	4.89
1085.8461	5.16
1102.5114	3.28
1167.9084	30.7
1223.2608	25.3
1235.7004	8.10
1264.8514	20.3
1284.4840	11.4
1384.5313	8.14
1425.6023	2.46
1509.5941	0.691
3055.5072	2.39
3106.8574	1.97
3124.1141	1.03

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
60.9990	0.0373
99.8076	0.731
175.1221	0.765
186.4465	0.149
272.8696	0.0886
341.0569	0.0969
362.1606	0.0392
447.6801	1.78
542.2651	0.920
563.7111	0.155
692.8033	4.82
730.4572	4.29
882.5910	2.87
1011.3009	4.53
1083.4311	6.34
1115.6946	12.8
1150.4248	24.0
1220.3356	24.3
1249.6778	0.978
1277.1123	26.0
1310.8449	3.03
1342.4678	17.2
1430.8725	2.76
1508.0917	0.618
3042.3136	3.04
3098.2338	1.26
3119.5877	1.37



$\Delta E = 0.23$ kcal mol^{-1}
Population = 0.273

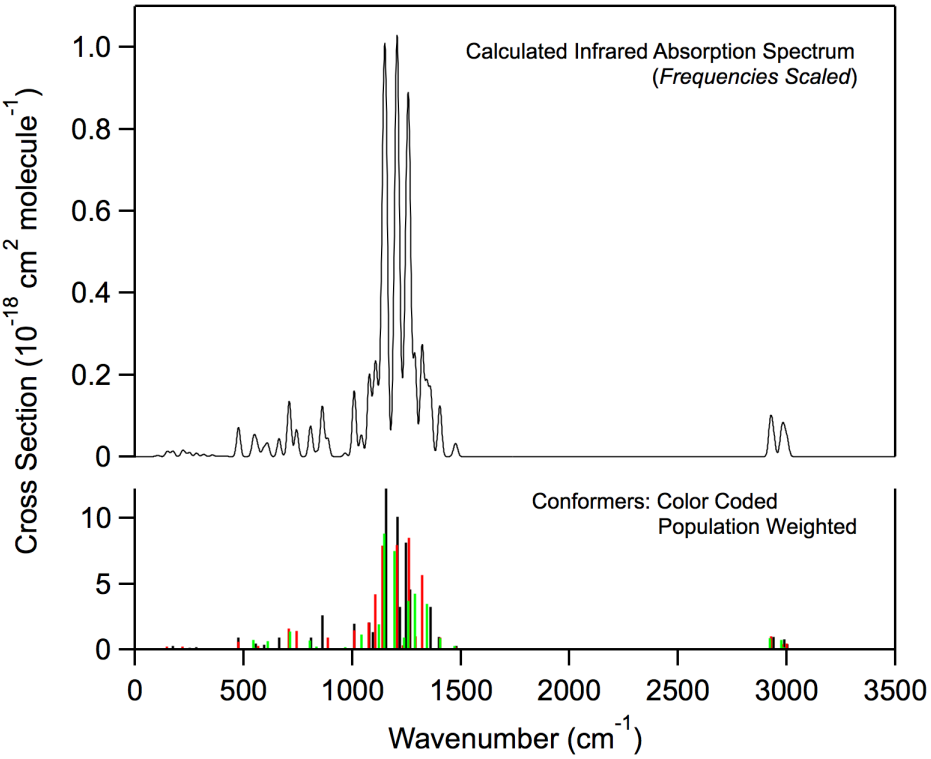
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.025743008199	-0.026954193706	0.009644170606
C	0.349082145093	-0.107914129683	-0.665317332472
C	1.092068959312	1.221370891215	-0.668098148458
F	-1.704078501773	-1.165733783347	-0.147213285094
F	-0.948331593122	0.239828081467	1.308309431580
F	-1.734583771396	0.955046275469	-0.577803338687
H	0.178451190048	-0.418558654927	-1.698409640135
Cl	1.327669402521	-1.395526253776	0.116791213662
H	2.043157830762	1.103235543133	-1.197549989004
H	0.477079787704	1.968154707746	-1.184804966068
F	1.335553559049	1.648553516410	0.609494884071

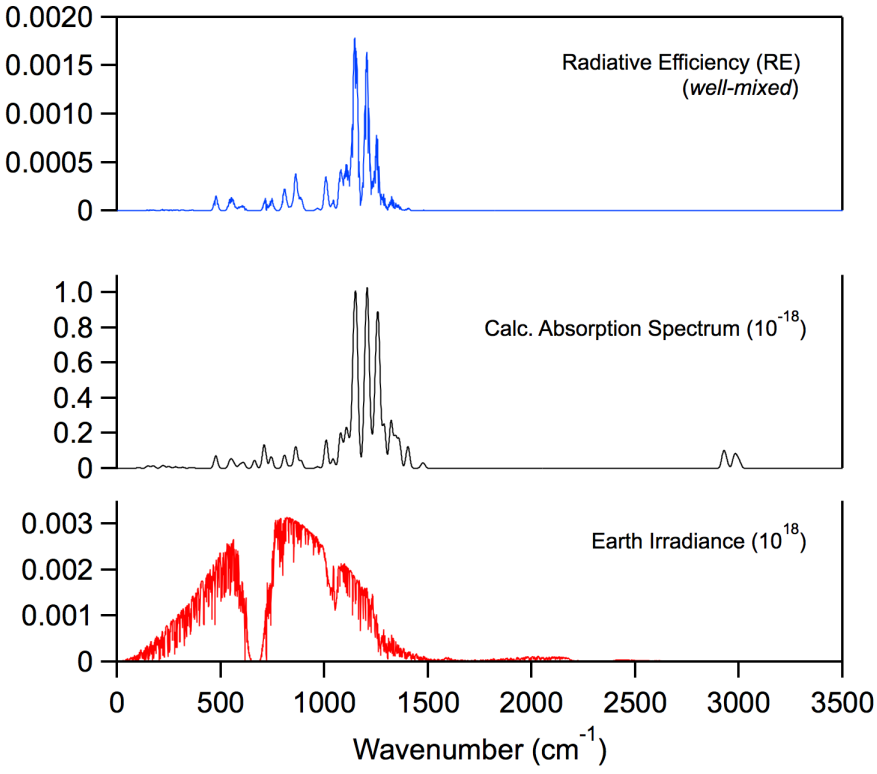
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
56.2019	0.129
109.0684	0.274
175.8489	0.0758
205.1504	0.304
279.8070	0.350
318.6688	0.230
363.1645	0.0211
519.8255	2.71
527.7975	0.579
589.3601	2.40
697.2364	5.04
796.3535	2.57
828.2528	0.907
967.5458	0.682
1046.3904	4.15
1132.9362	7.11
1158.2139	32.4
1209.4598	27.5
1253.4881	3.39
1275.4322	13.5
1306.7445	15.5
1364.6871	12.8
1430.4474	3.15
1499.7192	1.08
3039.1056	3.27
3093.2920	2.74
3104.6531	0.696

Infrared Spectrum

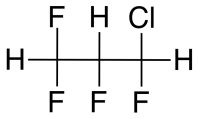


Radiative Efficiency



HCFC-244ea

Molecular Formula:	$CHF_2CHFCHFCl$
Name:	1-Chloro-1,2,3,3-tetrafluoropropane
CAS number:	149447-91-6
Molecular Weight:	150.5



Global Atmospheric Lifetime (years):	2.39
Tropospheric Atmospheric Lifetime (years):	2.50
Stratospheric Atmospheric Lifetime (years):	56.6
Ozone Depletion Potential (ODP):	0.012

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.222	0.191
Global Warming Potential (GWP_H):		
GWP_{20}	793	684
GWP_{100}	215	185
Global Temperature Potentials (GTP_H)		
GTP_{20}		267
GTP_{50}		33
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*

$k_{SAR}(298\ K) = 2.35 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 1.50 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 2.42$ years

$\tau^{OH}_{Trop} = 2.50$ years

$\tau^{OH}_{Strat} = 76.9$ years

Fractional Atmospheric Loss: 0.989

O(^{1}D) Reactivity

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

$k_{Est}(T) = 0.9 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 410$ years

Fractional Atmospheric Loss: 0.006

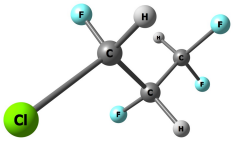
UV Photolysis

UV Spectrum: *No Recommendation*

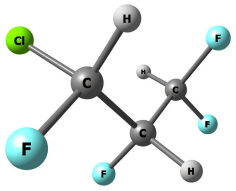
$\tau_{hv} = 450$ years

Fractional Atmospheric Loss: 0.005

Molecular Structure and Infrared Spectrum (12 conformers)



E = 0
Population = 0.255



$\Delta E = 0.31$ kcal mol^{-1}
Population = 0.150

Optimized Coordinates (Angstroms)

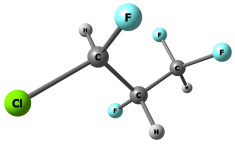
Atom	X	Y	Z
C	1.640941476389	0.167803300794	-0.159153026179
C	0.292470972226	-0.425758405479	0.256562549348
C	-0.836542898855	0.571465746147	0.024601427510
F	1.824851308368	1.334309723825	0.512262933109
F	2.624179122423	-0.684967462605	0.191656546720
H	1.693553237614	0.356061474855	-1.236574129062
H	0.336432895770	-0.690852607254	1.319053534195
F	0.088184084432	-1.550139799491	-0.493772857190
F	-0.846401905634	0.943670268979	-1.280745603210
Cl	-2.422342718531	-0.157725860176	0.443302447627
H	-0.715085574200	1.454725620405	0.653564177132

Atom	X	Y	Z
C	1.426218142567	-0.371922380493	0.127847475210
C	0.348827548016	0.665692381755	-0.180115631934
C	-0.963748330560	0.052438397639	-0.655391842739
F	1.569776313618	-1.176451269689	-0.957594487011
F	2.595287974679	0.266553179431	0.341721583095
H	1.185481076362	-0.983101363193	1.003840595252
H	0.718159982103	1.313170867271	-0.987237917339
F	0.141165738207	1.420916336641	0.939012810112
H	-0.800045142268	-0.620089801973	-1.498801179847
Cl	-1.737962431799	-0.928481910373	0.643053011080
F	-1.807886870926	1.045160562983	-1.015265415880

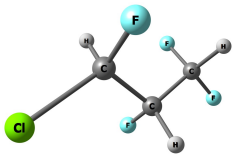
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
62.3188	0.170
78.2236	0.323
139.4479	0.299
216.5595	0.322
231.9601	0.396
298.2369	0.374
392.3936	0.323
445.4008	0.623
470.4374	5.26
577.1881	1.31
758.8060	7.98
787.4085	14.9
917.7189	3.89
1085.3395	7.47
1109.7809	9.15
1130.4712	19.6
1159.9038	21.8
1174.7718	14.2
1261.7267	0.727
1311.6703	0.886
1356.9383	1.90
1384.0107	3.62
1400.5641	0.354
1428.9424	6.47
3066.2573	0.278
3085.8618	4.84
3116.4709	1.41

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
55.7105	0.153
84.4957	0.303
145.9114	0.259
200.7536	0.335
244.7973	0.354
312.8891	0.480
407.2179	0.683
443.4394	1.86
493.5891	2.26
572.8804	2.50
662.2645	9.83
772.5725	5.32
979.6098	3.93
1094.2829	16.3
1117.8621	18.2
1138.8559	10.8
1156.4734	16.0
1176.5838	16.6
1279.0865	1.42
1288.3112	2.25
1358.7006	4.85
1381.6430	1.24
1400.0858	0.680
1435.9781	4.21
3039.5795	1.12
3085.9427	3.86
3117.3224	1.21



$\Delta E = 0.40$ kcal mol^{-1}
Population = 0.129



$\Delta E = 0.42$ kcal mol^{-1}
Population = 0.126

Optimized Coordinates (Angstroms)

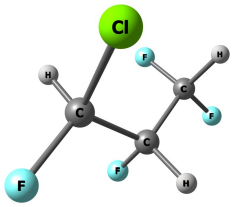
Atom	X	Y	Z
C	1.710802975075	0.193704239708	-0.263878830550
C	0.227635449804	0.460456309326	-0.548413977241
C	-0.695927599035	-0.320759173195	0.386602127518
F	1.942797413350	0.250291310680	1.070522796351
F	2.055043310326	-1.033499026467	-0.705817982045
H	2.334399132051	0.948974097371	-0.758294894585
H	0.010504123024	0.196212375543	-1.589004643735
F	0.016702582904	1.801654640289	-0.356195395512
H	-0.533696007043	-0.050887624766	1.430666643170
Cl	-2.413422362898	0.059599688112	0.015884955689
F	-0.479200017558	-1.643714836602	0.212097200941

Atom	X	Y	Z
C	1.599041088164	-0.384429148033	-0.188510159788
C	0.266602303043	0.345625608898	-0.375097732992
C	-0.878554946589	-0.450068787777	0.247142959547
F	2.590307220844	0.374858219655	-0.699841058575
F	1.834056489261	-0.558118303889	1.135296190618
H	1.599923271666	-1.362593299487	-0.682244593410
H	0.081463214896	0.482944755550	-1.446772202228
F	0.346045282516	1.562657246564	0.240027995802
H	-0.759046124357	-0.549704351374	1.326992102357
Cl	-2.446586319307	0.371118701697	-0.032109958372
F	-0.901325480138	-1.681307641804	-0.327994542958

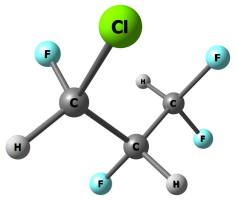
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
47.2745	0.166
87.7701	0.117
151.1400	0.0691
219.4718	0.291
227.2022	0.588
343.8866	0.0764
373.9436	3.92
425.1858	0.912
511.9627	0.655
565.4933	3.99
641.0376	10.1
830.3580	6.35
932.7134	3.20
1106.0553	4.71
1123.6083	7.11
1136.4382	5.53
1159.7336	38.2
1175.1179	15.4
1249.9361	1.07
1326.5498	3.17
1337.9176	1.13
1374.4542	5.93
1408.2777	3.24
1432.1642	2.32
3055.3045	5.54
3073.9375	1.59
3125.7121	1.21

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
62.3288	0.217
74.7227	0.233
139.2465	0.312
226.2397	0.569
243.4908	0.201
279.2249	0.818
373.1868	0.204
462.5031	2.09
496.4164	0.657
541.5218	2.80
763.3283	25.0
814.1869	2.06
898.0803	3.10
1097.2934	13.1
1119.0100	12.6
1124.6458	8.27
1149.9168	11.6
1190.2572	22.7
1241.4912	1.63
1328.3528	2.09
1354.1881	1.60
1391.5471	2.58
1412.4463	4.19
1421.4005	4.00
3061.9477	0.629
3073.8372	5.38
3121.2078	1.26



$\Delta E = 0.66$ kcal mol^{-1}
Population = 0.083



$\Delta E = 0.88$ kcal mol^{-1}
Population = 0.058

Optimized Coordinates (Angstroms)

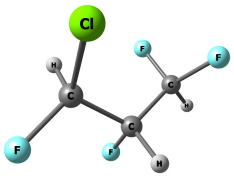
Atom	X	Y	Z
C	1.287446431137	-0.635612322356	-0.107203883569
C	0.308708263890	0.497321842408	-0.416007109778
C	-1.009514493889	0.385850404619	0.345257728676
F	2.463116033365	-0.362882641266	-0.711796211378
F	1.498609867140	-0.687219254347	1.231711459611
H	0.924242442432	-1.610470787868	-0.447910384936
H	0.108692070679	0.528919169121	-1.493153029857
F	0.891879507627	1.676981088380	-0.027516932841
F	-1.778523991003	1.453080035304	0.049845957312
Cl	-1.878555561263	-1.120418425629	-0.140535318093
H	-0.852535570115	0.329808891634	1.423448724853

Atom	X	Y	Z
C	1.267379578544	-0.392034798310	0.398314088927
C	0.455732459536	0.478014731929	-0.565474280162
C	-0.994465218142	0.707031970361	-0.140022064757
F	0.744694763016	-1.635637217999	0.451044358092
F	2.528987829284	-0.479056749839	-0.078311951060
H	1.295582445994	0.036279983185	1.405648588393
H	0.492253930985	0.044396161703	-1.569627856816
F	1.059490997195	1.716623013979	-0.580235540811
H	-1.405009139265	1.563306289371	-0.679292784893
Cl	-2.038088006871	-0.700301559091	-0.530409040170
F	-1.049609640276	0.956648174712	1.192573483257

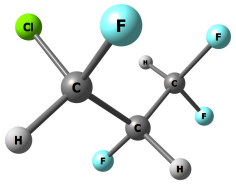
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
58.1554	0.259
87.0800	0.249
143.0451	0.181
225.9180	0.988
255.1447	0.191
303.2962	0.242
386.8846	0.729
418.4678	0.487
472.9729	2.65
554.3254	1.36
766.1900	9.71
810.5101	15.8
908.9401	5.01
1084.6544	10.6
1100.2886	7.78
1136.8710	13.3
1162.8800	20.5
1180.6569	22.1
1241.3097	0.0516
1308.6468	1.56
1368.9733	0.286
1393.1889	1.67
1411.3858	3.80
1426.3446	3.83
3066.0644	0.717
3083.8214	4.45
3122.5727	1.18

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
42.9657	0.160
86.7066	0.0885
155.0277	0.0507
208.2164	0.498
263.9263	1.27
307.6136	0.146
386.6710	1.10
429.6815	2.94
475.4375	1.38
579.0634	1.14
675.0638	2.91
813.2337	17.4
936.5583	2.60
1098.0646	7.99
1113.4438	16.1
1142.5326	11.6
1152.3479	23.7
1159.4998	16.6
1260.6868	2.74
1302.1555	1.11
1351.0991	0.953
1374.3484	3.24
1403.8701	1.96
1445.1965	2.87
3077.6505	0.790
3090.3377	4.24
3103.8372	1.50



$\Delta E = 0.94$ kcal mol^{-1}
Population = 0.052



$\Delta E = 1.03$ kcal mol^{-1}
Population = 0.045

Optimized Coordinates (Angstroms)

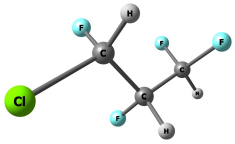
Atom	X	Y	Z
C	1.531381462616	-0.272914085293	-0.253326195762
C	0.338128250916	0.638289122790	-0.557898557011
C	-0.860928070440	0.467561773754	0.374203828375
F	1.704431150987	-0.379756279757	1.087335333575
F	1.336171036804	-1.508021194858	-0.757462853133
H	2.441846740214	0.156984968060	-0.689115205260
H	0.024299952535	0.497188522848	-1.597515468739
F	0.783645251191	1.931700268424	-0.389746904024
F	-1.773031752407	1.418009810898	0.071665878272
Cl	-1.607076540135	-1.152932458814	0.165155742776
H	-0.572596482280	0.557148551950	1.421929400930

Atom	X	Y	Z
C	1.270152093341	-0.097002316765	0.485412543834
C	0.407107751479	0.384698561775	-0.681395071039
C	-1.030303439937	-0.136994944719	-0.703722103903
F	1.293048449595	-1.448027975528	0.492141464498
F	2.529972140639	0.352885095503	0.286603446284
H	0.910452469319	0.269365201200	1.452131835128
H	0.888284432188	0.062711356950	-1.614564088300
F	0.361915660019	1.753437930271	-0.641351425913
F	-1.034554093363	-1.463161555589	-0.950776075322
Cl	-1.891884514870	0.191039242147	0.847116869607
H	-1.602065948410	0.387211404755	-1.472863394873

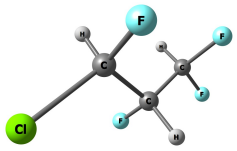
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
44.9571	0.175
94.7719	0.120
146.9805	0.0518
226.4359	0.595
263.9124	1.31
315.1942	0.195
377.3590	1.92
424.5656	0.916
483.7854	1.28
567.9580	1.25
697.3000	6.61
803.3718	15.2
931.5359	1.92
1090.4962	7.70
1121.1023	1.74
1130.3804	31.8
1153.7912	14.4
1175.2538	15.2
1250.8280	3.65
1319.9303	0.529
1335.9951	1.97
1390.0350	4.12
1409.4667	2.55
1432.1145	2.03
3056.2803	5.74
3077.6532	1.15
3127.6147	1.20

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
42.9705	0.160
94.0858	0.0864
156.2489	0.131
189.6177	0.132
261.4235	1.02
339.8689	0.240
399.4673	2.52
421.1173	2.31
511.6068	1.54
580.4923	2.77
632.7359	5.61
719.9272	5.59
1010.0709	5.28
1120.8498	2.68
1133.3413	4.42
1144.9415	22.6
1153.4567	3.51
1159.8409	44.1
1278.0293	3.51
1322.2148	0.653
1329.0082	3.41
1366.9921	2.78
1405.4173	2.24
1444.8870	2.43
3043.7187	1.31
3088.6560	4.14
3098.9407	1.87



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



$\Delta E = 1.43$ kcal mol^{-1}
Population = 0.023

Optimized Coordinates (Angstroms)

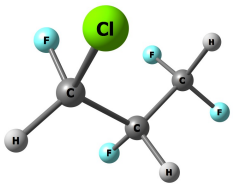
Atom	X	Y	Z
C	1.717681813181	-0.242608729614	0.326940009214
C	0.233014304287	-0.605243563764	0.437145649774
C	-0.682499356245	0.550079518250	0.038275341802
F	2.030555092925	0.164782609122	-0.917448735328
F	1.966408844706	0.777915836444	1.189615873464
H	2.352167366444	-1.098090411101	0.589474307963
H	0.029785152024	-0.870313276908	1.480843109219
F	0.000855747613	-1.685999910413	-0.366888595786
F	-0.573187359645	0.802327837574	-1.281416674661
Cl	-2.397089776753	0.135322812135	0.415095913798
H	-0.445476828537	1.448667278275	0.611629800542

Atom	X	Y	Z
C	1.651215327568	-0.033736826013	0.291153424427
C	0.272813611901	0.427450134366	-0.197258645067
C	-0.875806692627	-0.400786908099	0.382847455844
F	1.869672428273	-1.315814037989	-0.070048323581
F	2.586745025256	0.741908243153	-0.297249476465
H	1.752128095324	0.059744500514	1.380806591943
H	0.246026936363	0.376598315679	-1.291627378784
F	0.126509268445	1.724951123364	0.216818501250
H	-0.879339521133	-0.391620966513	1.476226648961
Cl	-2.451842466534	0.299418126498	-0.126331527919
F	-0.787288012836	-1.671966704959	-0.063371270610

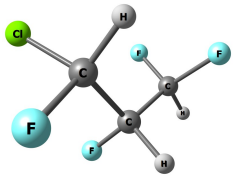
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
40.7133	0.213
89.4841	0.127
162.9110	0.361
204.0863	0.310
231.0090	0.124
267.7662	0.0304
381.5685	0.808
430.6299	0.410
541.5534	6.68
608.1081	8.15
759.1503	6.62
852.7664	1.87
856.4501	7.43
999.8620	0.504
1117.4281	17.4
1124.7631	11.8
1180.0995	8.41
1194.7810	28.6
1267.6825	1.69
1338.0494	1.71
1358.9278	6.30
1387.4228	2.61
1406.9771	1.28
1429.3916	5.31
3055.6099	4.68
3067.6593	2.98
3106.9941	1.34

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
30.4662	0.0316
78.5523	0.0722
152.0673	0.164
222.4354	0.211
280.0833	1.16
336.7464	2.06
345.9038	1.00
431.0012	0.304
503.5497	5.48
543.7811	1.49
598.4696	0.264
778.5747	17.9
1087.8717	1.26
1097.7373	1.11
1127.9183	1.95
1135.5549	4.69
1149.1081	23.1
1165.4559	42.4
1246.4078	3.63
1321.4866	0.496
1325.1351	3.31
1382.8937	1.71
1408.4234	2.06
1431.6431	6.66
3041.0408	4.64
3071.1128	1.03
3090.6806	4.00



$\Delta E = 1.51$ kcal mol^{-1}
Population = 0.020



$\Delta E = 1.89$ kcal mol^{-1}
Population = 0.011

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.134099936371	-0.680404535446	0.196547109057
C	0.349083947093	0.250885196382	-0.732145333336
C	-1.050570053331	0.608063107072	-0.236323006139
F	2.269817244315	-1.052115549684	-0.441908813020
F	1.479681753638	-0.024011651524	1.321623241344
H	0.563995005735	-1.578632532307	0.459376241255
H	0.264789464082	-0.226077683731	-1.714449265894
F	1.048024976351	1.425961470965	-0.856071212941
H	-1.496324340419	1.374878521971	-0.873552100902
Cl	-2.126266524163	-0.841076217458	-0.345160189813
F	-1.018215409672	1.046384873760	1.037391330389

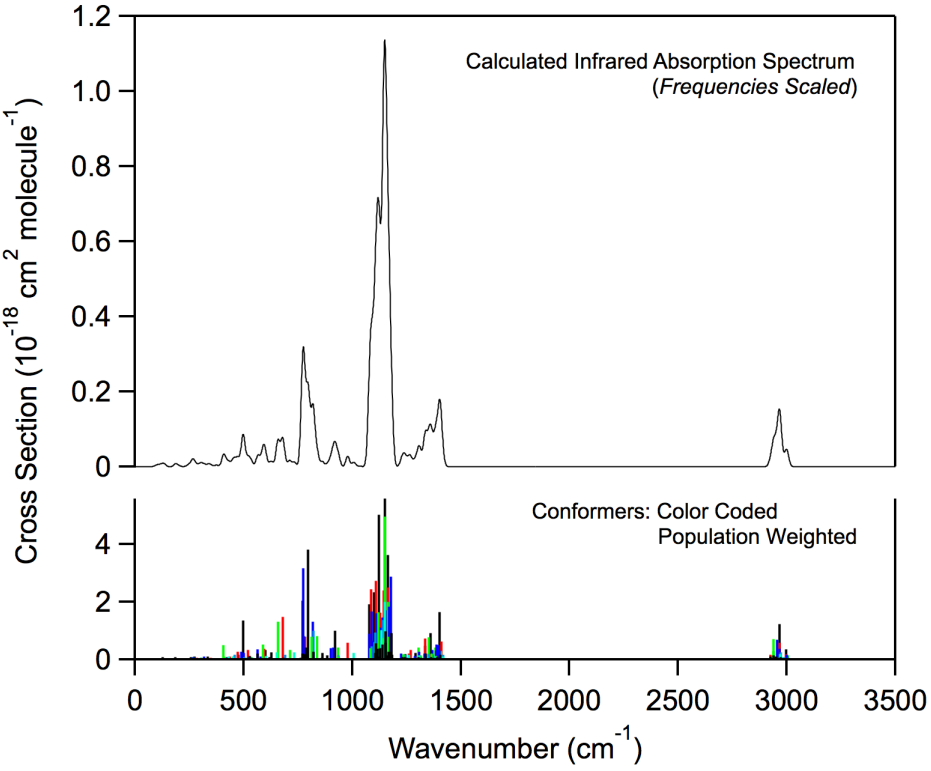
Atom	X	Y	Z
C	1.636256314562	0.182024476445	0.019707584581
C	0.302660981740	0.921151672217	0.133340496069
C	-0.852373994987	0.243543276751	-0.606742757747
F	1.551284702212	-1.075970312477	0.491718986536
F	1.971116943236	0.123323764674	-1.296610038127
H	2.425014124305	0.711496474998	0.568107777305
H	0.431894488133	1.903845660489	-0.339866730717
F	0.013410994880	1.102169680093	1.455997806571
H	-0.514111454278	-0.138202468850	-1.572180433933
Cl	-1.531616803866	-1.141260055076	0.302597435937
F	-1.835607295937	1.158147830736	-0.804335126476

Infrared Absorption Spectrum (unscaled frequencies)

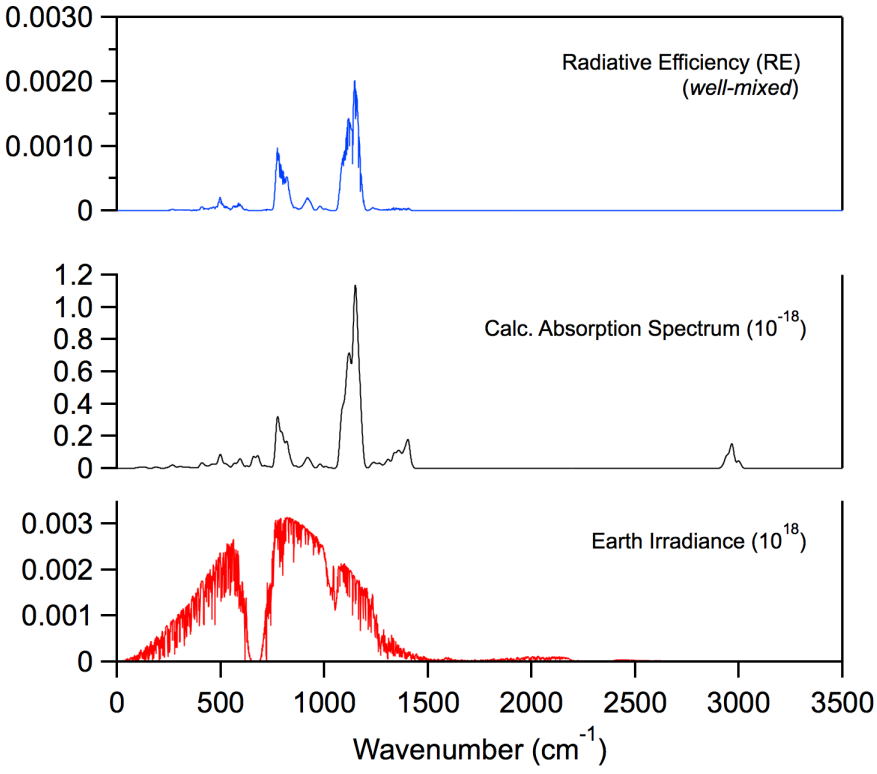
Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
46.1550	0.272
88.7166	0.138
163.8677	0.364
204.8434	0.427
250.8532	0.0943
305.5687	0.293
341.6507	0.475
404.4015	0.573
508.1648	3.48
666.5081	3.09
767.7506	9.58
812.6597	13.9
881.1077	7.80
989.4453	0.253
1116.7395	4.13
1136.4957	19.6
1163.5356	29.0
1186.1790	13.2
1257.9561	3.92
1319.3299	0.313
1367.0280	1.37
1400.3527	3.08
1415.2104	4.52
1432.1789	2.50
3067.9139	2.14
3074.8888	3.56
3104.5510	1.57

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
40.7314	0.221
90.5659	0.0816
159.2752	0.444
204.2745	0.297
222.4158	0.149
303.0420	0.278
390.4242	1.41
423.2051	0.562
559.0499	2.47
599.4941	7.01
751.2944	6.13
775.3845	7.24
893.9792	1.29
1037.0131	4.05
1113.9302	21.6
1123.3904	16.3
1170.1257	13.2
1197.1760	15.3
1283.5739	2.50
1319.6836	0.541
1352.4661	4.69
1396.7365	4.06
1412.2644	1.38
1430.4896	1.87
3039.0238	2.02
3059.7886	6.17
3106.9149	1.20

Infrared Spectrum

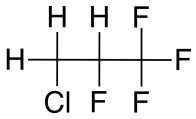


Radiative Efficiency



HCFC-244eb

Molecular Formula: $CH_2ClCHFCF_3$
Name: 3-Chloro-1,1,1,2-tetrafluoropropane
CAS number: 151771-09-4
Molecular Weight: 150.5



Global Atmospheric Lifetime (years): 2.04
  Tropospheric Atmospheric Lifetime (years): 2.12
  Stratospheric Atmospheric Lifetime (years): 50.8
Ozone Depletion Potential (ODP): 0.011

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.178	0.151
Global Warming Potential (GWP_H):		
GWP_{20}	544	460
GWP_{100}	147	124
Global Temperature Potentials (GTP_H)		
GTP_{20}		171
GTP_{50}		22
GTP_{100}		17

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 2.76 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 1.76 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 2.06$ years
$\tau^{OH}_{Trop} = 2.12$ years
$\tau^{OH}_{Strat} = 66.5$ years

Fractional Atmospheric Loss: 0.991

O(^{1}D) Reactivity

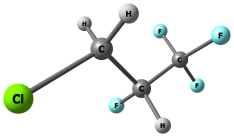
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 0.9 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)} = 410$ years
Fractional Atmospheric Loss: 0.005

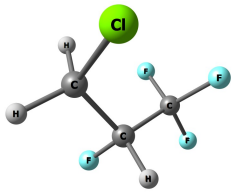
UV Photolysis

UV Spectrum: *No Recommendation*
$\tau_{hv} = 450$ years
Fractional Atmospheric Loss: 0.004

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.773



$\Delta E = 0.97$ kcal mol^{-1}
Population = 0.150

Optimized Coordinates (Angstroms)

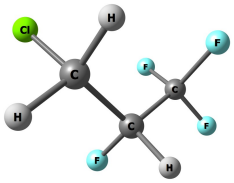
Atom	X	Y	Z
C	-1.376353147901	-0.142692059248	0.054897191791
C	0.059493884802	0.309987917635	0.348354878219
C	1.068879916315	-0.611472993865	-0.314875759479
F	-1.582495335180	-1.362870477499	0.574074855761
F	-2.257219750693	0.696657391763	0.595609863662
F	-1.609610639587	-0.205146680749	-1.259892696289
H	0.191721322049	0.319911213383	1.435783363425
F	0.190422877915	1.585231496028	-0.131015984402
H	0.896776443184	-1.643861802790	-0.011590193050
H	1.000926672137	-0.526275181811	-1.399217086656
Cl	2.744695756960	-0.171700822848	0.161070567020

Atom	X	Y	Z
C	-1.015112392924	-0.407169968068	-0.025962743445
C	-0.144142728362	0.753489322036	0.470119892194
C	1.167848503840	0.924308316785	-0.290788412926
F	-2.201600447506	-0.381895964759	0.584658170814
F	-1.225164074808	-0.317239985669	-1.344877761419
F	-0.438439148155	-1.583832430984	0.227354764142
H	0.033688601216	0.618163294756	1.541797644032
F	-0.878998735646	1.900315253761	0.271581463307
H	1.011582078155	0.823557084150	-1.364332414944
H	1.563092181550	1.914820712871	-0.067732557203
Cl	2.406625162640	-0.277779634879	0.206113955449

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
66.3348	0.0501
77.9040	0.633
149.0535	0.747
217.7251	0.251
256.7515	0.00682
316.7269	0.108
399.0128	0.450
474.4780	1.21
556.2748	0.527
568.9505	0.678
685.1538	9.53
776.5007	4.31
855.6984	0.975
892.6357	2.05
1047.4841	2.77
1142.5738	11.3
1171.0107	26.7
1207.7569	11.8
1231.6447	22.0
1290.0602	14.4
1295.0047	18.1
1381.1171	4.62
1398.2775	6.99
1467.4590	0.687
3071.3199	1.68
3102.1219	1.05
3168.3796	0.109

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
40.1028	0.114
102.4506	0.321
184.1604	0.586
229.8146	0.847
242.8749	0.0897
329.8429	0.100
431.6734	2.12
442.7842	0.257
535.9503	1.22
581.8719	0.118
666.4594	3.43
784.6418	6.53
803.3919	0.125
956.6748	5.36
1075.9500	1.88
1106.0256	12.4
1152.1175	12.3
1212.4910	23.6
1234.2318	34.3
1267.5443	14.0
1302.7708	11.2
1365.8675	0.148
1416.4027	3.74
1481.8169	1.70
3079.1557	1.25
3102.8057	1.27
3168.3409	0.114



$\Delta E = 1.37$ kcal mol^{-1}
Population = 0.076

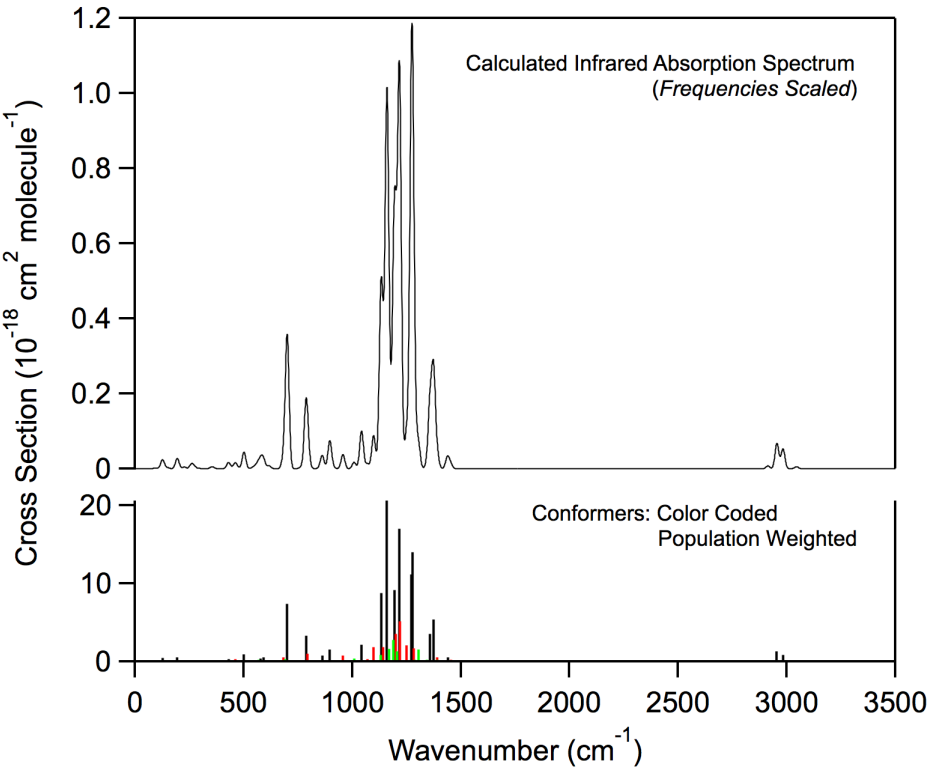
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.123469494511	-0.248600750862	-0.001752103499
C	-0.141862818354	0.824983439135	0.487325538310
C	1.190898895839	0.303296719078	1.000714591663
F	-2.322818294122	0.302111714190	-0.218498000889
F	-0.731852946711	-0.836169295351	-1.126458687162
F	-1.264166399719	-1.188649749799	0.947006011592
H	-0.641839199666	1.331308123321	1.325237935881
F	0.037499027887	1.722529956099	-0.527855146802
H	1.761146798353	1.135421101860	1.413688066666
H	1.021992166033	-0.444911443523	1.775144700952
Cl	2.214664264970	-0.442000814149	-0.274799906711

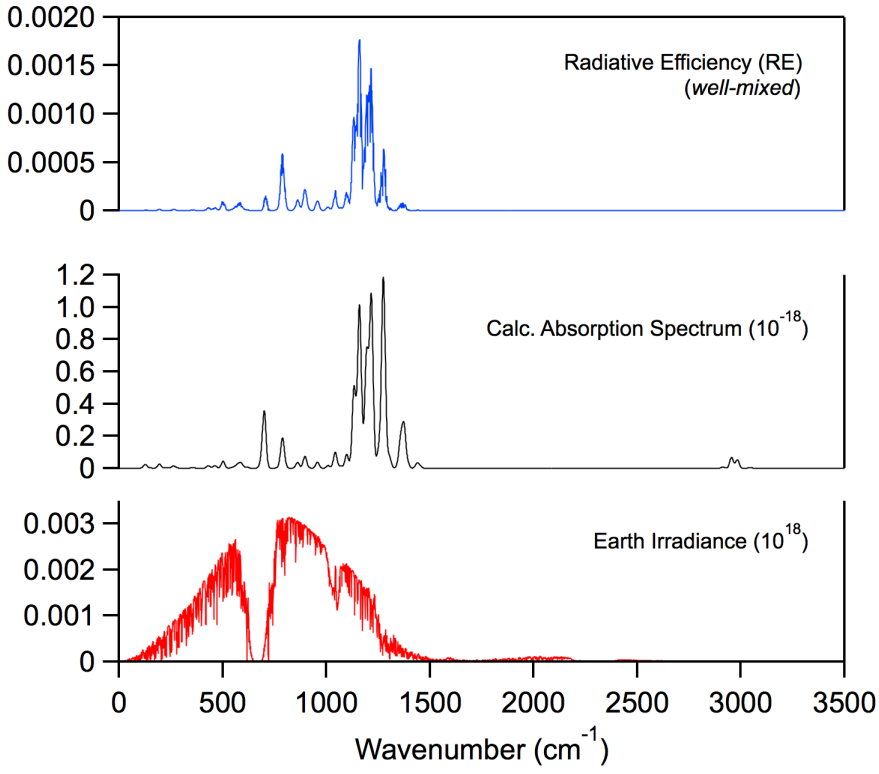
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
43.5759	0.168
102.9087	0.0741
170.8338	0.150
218.5754	0.522
255.3300	0.148
322.9713	0.287
410.9428	0.178
519.1434	1.19
546.9877	2.74
596.7748	2.11
674.9327	4.56
751.1585	1.07
840.2860	0.369
910.7550	0.707
1011.0776	4.74
1141.7729	10.9
1182.4755	21.4
1202.3107	36.8
1219.5924	17.1
1306.2885	2.94
1323.7638	20.3
1366.0842	2.59
1414.4870	3.07
1462.0738	2.08
3028.1179	2.07
3098.6630	1.60
3160.7436	0.142

Infrared Spectrum

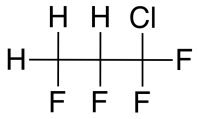


Radiative Efficiency



HCFC-244ec

Molecular Formula:	$CH_2FCHFCF_2Cl$
Name:	1-Chloro-1,1,2,3-tetrafluoropropane
CAS number:	149448-09-9
Molecular Weight:	150.5



Global Atmospheric Lifetime (years):	2.88
Tropospheric Atmospheric Lifetime (years):	3.01
Stratospheric Atmospheric Lifetime (years):	64.0
Ozone Depletion Potential (ODP):	0.013

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.257	0.226
Global Warming Potential (GWP_H):		
GWP_{20}	1106	974
GWP_{100}	300	264
Global Temperature Potentials (GTP_H)		
GTP_{20}		408
GTP_{50}		49
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*

$k_{SAR}(298\ K) = 1.95 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 1.24 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 2.92$ years

$\tau^{OH}_{Trop} = 3.01$ years

$\tau^{OH}_{Strat} = 91.1$ years

Fractional Atmospheric Loss: 0.987

$O(^1D)$ Reactivity

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

$k_{Est}(T) = 0.9 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 410$ years

Fractional Atmospheric Loss: 0.007

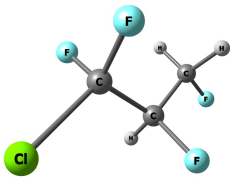
UV Photolysis

UV Spectrum: *No Recommendation*

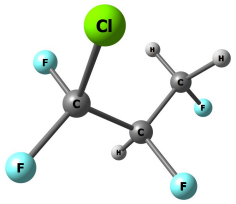
$\tau_{hv} = 450$ years

Fractional Atmospheric Loss: 0.006

Molecular Structure and Infrared Spectrum (9 conformers)



E = 0
Population = 0.222



$\Delta E = 0.06$ kcal mol^{-1}
Population = 0.200

Optimized Coordinates (Angstroms)

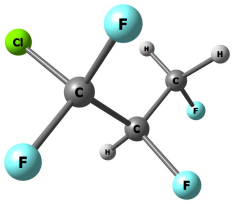
Atom	X	Y	Z
C	0.658907386285	-0.403171552928	0.039711795102
C	-0.642971154720	0.334638644087	-0.294467795551
C	-1.858405539732	-0.509987672222	0.067272129576
F	0.665495465313	-0.793625488250	1.320258233229
F	0.749347606199	-1.500084102103	-0.727306762192
Cl	2.099199823117	0.623372162199	-0.251400763707
H	-0.647290886118	0.554721441473	-1.367485915849
F	-0.676289588772	1.509125460806	0.406102016728
H	-1.753609655154	-1.518429941213	-0.347149319512
H	-1.954867450018	-0.567430769708	1.156283130723
F	-2.977294006400	0.085929817861	-0.457275748547

Atom	X	Y	Z
C	0.775938489200	0.393307772888	-0.240674648864
C	-0.701995019250	0.513814227127	0.147251144438
C	-1.598583860254	-0.504539483868	-0.536839884711
F	0.900810814815	0.564791923728	-1.564624513270
F	1.485761799362	1.341367111349	0.371156963432
Cl	1.474249169562	-1.205815589246	0.200341341758
H	-1.013334455463	1.525510234852	-0.145967640227
F	-0.801253223711	0.400234408719	1.506561276129
H	-1.366572877340	-0.552066941036	-1.606184624423
H	-1.457567845487	-1.491201289250	-0.084818891617
F	-2.904882991435	-0.113305375263	-0.369467522645

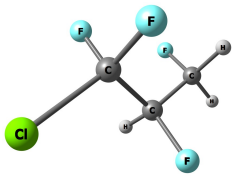
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
63.0490	0.0798
91.0140	0.774
150.4222	0.647
221.2204	0.328
280.4734	0.403
313.0053	0.280
348.9048	0.108
416.5026	0.150
433.8920	1.65
522.9213	2.18
629.5592	1.42
809.0951	22.3
903.1154	1.45
972.2078	31.3
1115.4573	7.37
1118.8022	6.64
1155.1909	27.0
1163.6944	9.67
1245.9831	13.8
1282.0291	1.72
1319.8680	3.43
1393.6792	0.401
1435.0960	1.77
1503.2646	0.452
3048.4702	2.56
3072.8403	0.918
3107.2146	3.34

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
68.3394	0.168
87.6481	0.640
159.1284	0.503
202.0494	0.349
282.9528	0.418
326.1597	0.109
347.1846	0.389
415.3046	0.0729
489.8473	1.45
499.7012	1.46
650.6923	1.97
682.6576	17.0
914.0448	2.30
1049.4925	26.3
1100.6253	23.0
1121.4738	3.35
1157.2824	16.2
1192.5246	19.9
1217.2428	7.94
1283.3557	1.61
1320.7326	5.95
1391.1975	2.51
1437.7201	0.998
1500.7450	0.513
3042.6732	1.31
3051.5636	2.73
3109.9793	2.57



$\Delta E = 0.35$ kcal mol^{-1}
Population = 0.124



$\Delta E = 0.41$ kcal mol^{-1}
Population = 0.111

Optimized Coordinates (Angstroms)

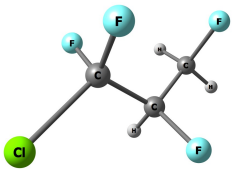
Atom	X	Y	Z
C	0.774044255432	0.322955119153	0.047418901466
C	-0.687165209028	0.248087618832	-0.414312379279
C	-1.520109527799	-0.747160169699	0.378100438618
F	1.390869643271	1.343729468819	-0.543528525322
F	0.845195719802	0.502837266703	1.371002625333
Cl	1.657388366333	-1.196486589695	-0.372729493423
H	-0.704697789621	-0.001149204999	-1.480377952371
F	-1.213022860700	1.506116918596	-0.243813687551
H	-1.050750433761	-1.735781239508	0.377001420478
H	-1.628339871100	-0.392154242280	1.408381342453
F	-2.759652292829	-0.829788945920	-0.206096690402

Atom	X	Y	Z
C	0.454173676403	-0.331725054067	0.176467168315
C	-0.558904672158	0.653500947674	-0.422270953160
C	-1.984042948706	0.401951531684	0.076082879594
F	0.406580525160	-0.298812457931	1.513331445466
F	0.166127271716	-1.572346611915	-0.223068739196
Cl	2.130757833682	0.067463716273	-0.339616541007
H	-0.515553600411	0.568704821753	-1.513023825615
F	-0.205483386128	1.919761796049	-0.036804887544
H	-1.999674762258	0.340115552270	1.168997515823
H	-2.608928166835	1.241380264303	-0.248094024553
F	-2.463442770465	-0.766072506092	-0.459580038123

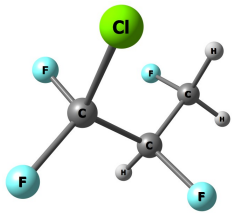
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
66.7500	0.288
84.9150	0.522
170.8418	0.747
205.7077	0.352
299.5389	0.132
318.6769	0.503
334.1919	0.251
409.9576	0.339
424.5111	0.651
519.6386	2.13
613.1628	2.16
840.1679	16.7
912.1272	5.08
954.8123	34.3
1093.2637	16.7
1121.2126	4.62
1138.4585	2.90
1190.8944	22.9
1249.6201	16.4
1283.8727	4.38
1323.7551	2.92
1388.9106	1.94
1438.7645	1.07
1502.4821	0.602
3052.0385	2.32
3077.9138	0.895
3110.5471	3.13

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
36.5289	0.122
116.0605	0.563
179.9023	0.361
209.9685	0.510
245.5664	0.0305
329.9259	0.0942
399.5010	2.14
406.7841	0.177
442.6540	5.33
503.0068	0.553
625.2374	1.85
724.2874	5.82
957.0667	32.6
1013.3569	5.13
1109.3265	2.37
1120.0756	12.5
1135.1143	7.90
1189.4170	35.5
1242.7519	9.70
1260.3705	5.62
1331.3709	0.552
1391.7301	0.335
1429.0886	1.54
1513.5645	0.564
3046.9387	3.42
3075.9700	1.36
3105.3394	3.46



$\Delta E = 0.42$ kcal mol^{-1}
Population = 0.109



$\Delta E = 0.60$ kcal mol^{-1}
Population = 0.081

Optimized Coordinates (Angstroms)

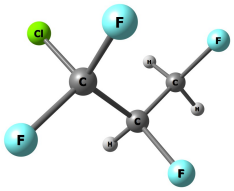
Atom	X	Y	Z
C	0.496442882695	-0.383342151108	0.008958853368
C	-0.539015756291	0.591074315060	-0.574417268681
C	-1.935920588309	-0.007132428798	-0.665392905972
F	0.225526418447	-0.691957128949	1.272309578712
F	0.489719578598	-1.511123145169	-0.718014634746
Cl	2.152673140384	0.325901138818	-0.058764006106
H	-0.208080976112	0.859612137193	-1.585005878695
F	-0.558610260278	1.709219950705	0.213569151766
H	-2.614221837511	0.763424365179	-1.050534462860
H	-1.926613807543	-0.859211122588	-1.354350951061
F	-2.376392794080	-0.416397930343	0.566008524276

Atom	X	Y	Z
C	0.601638601373	-0.141350880309	-0.420856270747
C	-0.667351174338	0.720936417875	-0.375250868864
C	-1.794116557190	0.164306236160	0.490903753135
F	0.295789180996	-1.372487671402	-0.835752143201
F	1.473245575022	0.388901421216	-1.283330102488
Cl	1.404941220714	-0.252801924948	1.187801632579
H	-1.012127756641	0.806661154864	-1.414224600946
F	-0.326005312178	1.960830843070	0.094085010987
H	-1.428203500700	-0.113179574909	1.484660905243
H	-2.555023419958	0.946347806442	0.593102618205
F	-2.340450857099	-0.934964828059	-0.122311933903

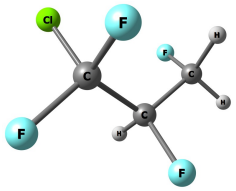
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
48.3732	0.214
115.9001	0.334
171.7781	0.171
220.7005	0.386
256.4982	0.129
309.8629	0.532
345.6273	0.178
416.5149	0.150
468.3912	0.301
553.2723	9.81
644.5089	4.96
839.2632	3.38
879.8269	8.08
976.1290	25.4
1010.6194	4.73
1127.4174	13.5
1167.4695	2.69
1172.2973	32.9
1257.6197	13.0
1295.8006	8.07
1361.8170	1.71
1384.2085	0.377
1429.2796	2.34
1493.9493	1.02
3036.7482	2.33
3057.8525	3.32
3091.0272	3.10

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
43.4962	0.130
119.9385	0.570
189.6777	0.125
201.4360	0.359
242.8089	0.884
332.3509	0.210
393.5084	0.714
414.5815	0.149
470.3511	2.08
531.4190	2.10
602.3267	9.12
662.6239	2.37
919.0752	15.4
1103.5006	14.2
1107.0666	5.08
1112.9544	8.45
1150.7527	20.2
1200.7976	30.3
1219.0659	12.4
1253.7374	0.949
1330.9002	0.322
1391.2435	3.52
1432.6065	0.632
1514.0831	0.957
3043.8848	0.591
3046.4084	4.63
3102.5845	3.22



$\Delta E = 0.74$ kcal mol^{-1}
Population = 0.064



$\Delta E = 0.85$ kcal mol^{-1}
Population = 0.052

Optimized Coordinates (Angstroms)

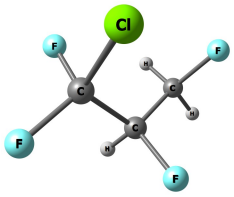
Atom	X	Y	Z
C	0.608628588258	0.370666325305	0.155958473437
C	-0.650006622299	0.345572008351	-0.726411984429
C	-1.538697950182	-0.877100872289	-0.574660284081
F	1.285082708293	1.499568400839	-0.072963992167
F	0.311254816797	0.322746406282	1.449331346226
Cl	1.691199489511	-1.022425843741	-0.249049840902
H	-0.318109607192	0.422806694118	-1.768911128991
F	-1.364553075914	1.472136426396	-0.394607120202
H	-2.434186702918	-0.718971145703	-1.187454635175
H	-1.014884580015	-1.772579566605	-0.924247990286
F	-1.915691064340	-1.044445832952	0.732468156570

Atom	X	Y	Z
C	0.659188084003	0.380901241617	0.088537202023
C	-0.744978824814	0.525823911203	-0.511567272223
C	-1.833692406695	-0.280735983100	0.196990222725
F	1.503309468053	1.208334828911	-0.531495569169
F	0.645720431649	0.702769666931	1.387317354529
Cl	1.272061042159	-1.299740428362	-0.084478615910
H	-0.701529141082	0.256525682709	-1.571884542933
F	-1.068956773800	1.857831584075	-0.385219857670
H	-1.694353436978	-0.252477520132	1.282509944121
H	-2.794307407394	0.180848834527	-0.056433746891
F	-1.822850035101	-1.581919818379	-0.234653118601

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
45.8067	0.251
118.7008	0.217
185.9788	0.294
213.2969	0.383
279.4240	0.0653
316.1659	0.502
354.2726	0.250
405.5245	0.246
419.6210	0.870
545.0076	4.56
692.6214	3.39
833.8085	8.17
909.7080	15.0
937.7543	22.3
1011.5754	7.93
1119.0539	5.36
1156.0492	9.21
1182.7839	28.1
1257.2647	14.9
1296.9516	8.61
1364.6154	0.328
1384.4496	2.87
1432.2681	2.09
1496.1272	1.33
3040.4219	2.24
3058.9745	2.92
3097.8709	3.14

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
47.6228	0.155
112.4457	0.621
173.1865	0.362
240.9408	0.0612
248.0665	1.06
315.1177	0.286
351.6345	0.936
417.5729	0.207
470.2916	1.56
510.6415	2.25
593.9083	1.55
775.0120	5.98
941.6559	32.4
1015.9392	8.67
1093.1517	1.15
1116.5189	26.3
1124.2959	1.96
1190.3691	23.0
1244.2020	16.1
1263.0961	4.24
1327.5581	0.350
1393.6003	2.13
1432.7618	0.295
1514.0778	0.692
3047.2613	3.19
3078.1168	1.30
3104.9351	3.25



$\Delta E = 1.05$ kcal mol^{-1}
Population = 0.038

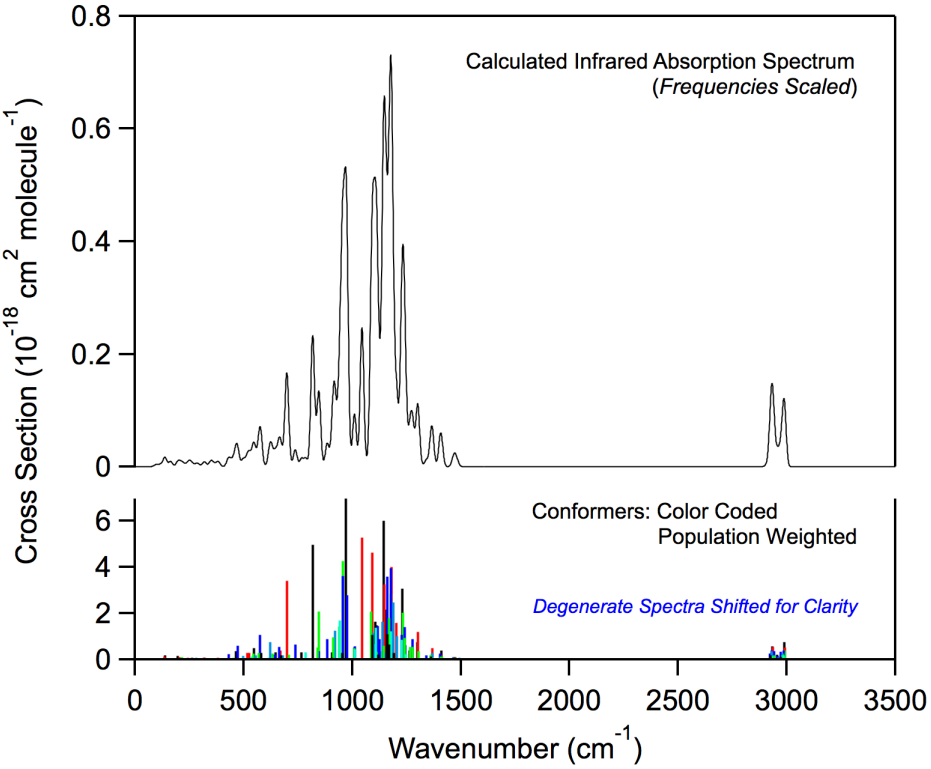
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	0.742448607763	0.277046902415	-0.249556851981
C	-0.633144629478	0.909108783442	0.021299872566
C	-1.814414061785	0.204900215039	-0.624545952074
F	0.877200951833	0.092884577309	-1.573040241558
F	1.700138112802	1.124841120604	0.145787043205
Cl	0.998283239123	-1.280151815624	0.588317677198
H	-0.570125747814	1.921633865596	-0.403900624607
F	-0.809011503092	1.005160609374	1.373624908713
H	-2.720737370628	0.776189189784	-0.390933314293
H	-1.673272174436	0.181288680913	-1.711030733389
F	-1.961785424289	-1.071795128851	-0.151712783780

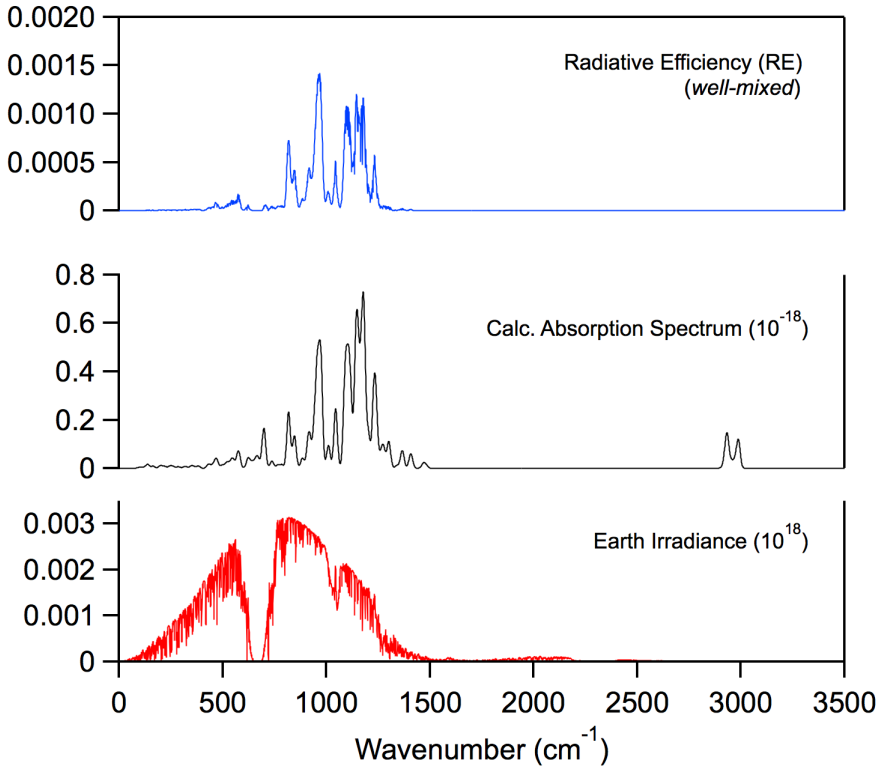
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
46.4658	0.349
113.0026	0.335
180.9948	0.0768
197.8840	0.213
265.2706	0.542
322.7042	0.233
348.0429	0.221
422.2036	0.0246
483.8251	0.272
557.0574	7.55
653.7631	4.95
754.6644	8.02
902.6955	1.93
952.8037	7.85
1099.8198	28.2
1129.8119	5.50
1173.4295	29.2
1181.5262	17.5
1203.8763	7.52
1291.3614	1.60
1367.8909	1.41
1385.4785	3.56
1434.0729	0.756
1495.6345	0.884
3020.4620	1.44
3040.6530	5.09
3089.8485	3.13

Infrared Spectrum

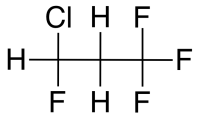


Radiative Efficiency



HCFC-244fa

Molecular Formula:	$CHFClCH_2CF_3$
Name:	3-Chloro-1,1,1,3-tetrafluoropropane
CAS number:	149329-29-3
Molecular Weight:	150.5



Global Atmospheric Lifetime (years):	2.37
Tropospheric Atmospheric Lifetime (years):	2.48
Stratospheric Atmospheric Lifetime (years):	56.3
Ozone Depletion Potential (ODP):	0.012

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.215	0.185
Global Warming Potential (GWP_H):		
GWP_{20}	764	658
GWP_{100}	207	178
Global Temperature Potentials (GTP_H)		
GTP_{20}		256
GTP_{50}		32
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*

$k_{SAR}(298\ K) = 2.37 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 1.51 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 2.40$ years

$\tau^{OH}_{Trop} = 2.48$ years

$\tau^{OH}_{Strat} = 76.4$ years

Fractional Atmospheric Loss: 0.989

O(^{1}D) Reactivity

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

$k_{Est}(T) = 0.9 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 410$ years

Fractional Atmospheric Loss: 0.006

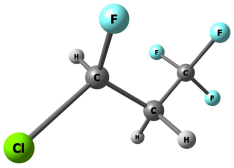
UV Photolysis

UV Spectrum: *No Recommendation*

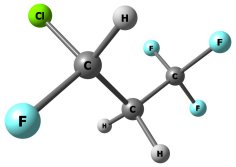
$\tau_{hv} = 450$ years

Fractional Atmospheric Loss: 0.005

Molecular Structure and Infrared Spectrum (2 conformers)



E = 0
Population = 0.800



$\Delta E = 0.90$ kcal mol^{-1}
Population = 0.174

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.016005363727	0.210358591993	0.340252516665
C	-0.055958566828	-0.634573310163	-0.329026591759
C	-1.461666455743	-0.142843523604	-0.014320193308
Cl	2.645588609582	-0.508459420864	0.026982772747
F	0.995740736771	1.472578380738	-0.146525419045
H	0.907493267337	0.245652245063	1.425485936898
H	0.023246965704	-1.665728170366	0.020207765917
H	0.086129084132	-0.620335224074	-1.411920828195
F	-2.371377272302	-0.995841813575	-0.503248891699
F	-1.656437023547	-0.055989402976	1.313467730628
F	-1.708269708831	1.061099647828	-0.537881798848

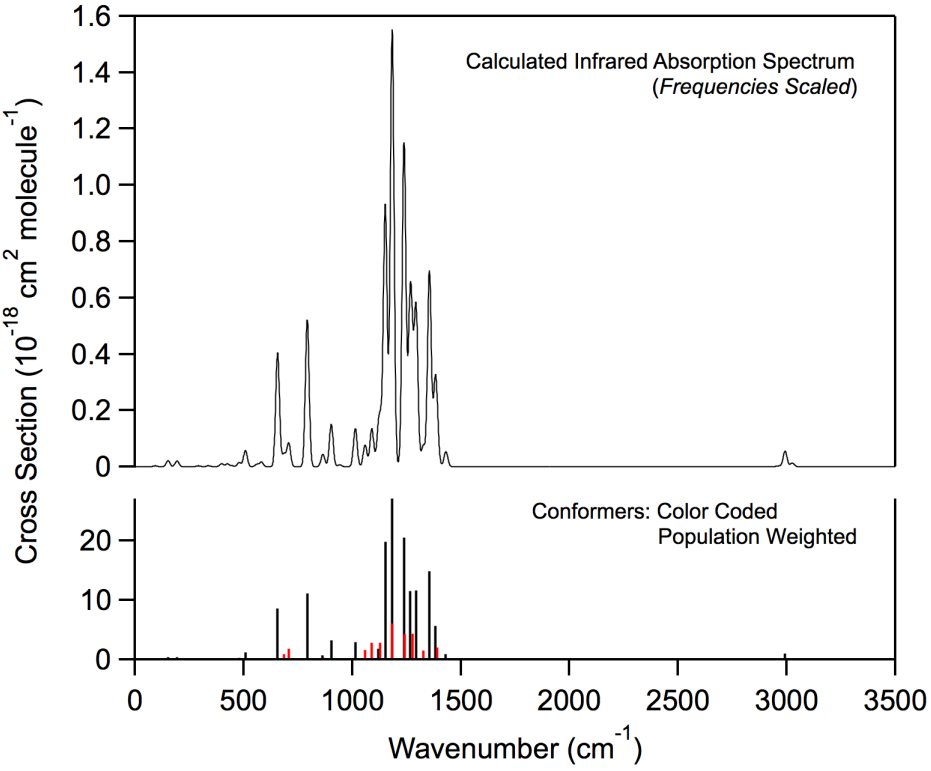
Atom	X	Y	Z
C	1.133548393308	0.561273754365	0.334162078374
C	-0.150007614898	0.860473488955	-0.427357781160
C	-1.350458762388	0.033788436948	0.000832630769
Cl	1.857789541851	-1.021199811738	-0.138686101736
F	2.031811014102	1.539953691231	0.060109750127
H	0.977015834061	0.508992103035	1.412713657177
H	0.006668317216	0.733783272356	-1.500486822801
H	-0.398713646096	1.908581423359	-0.234774136523
F	-2.464569486533	0.521579031511	-0.562157241802
F	-1.250394117973	-1.250615955817	-0.349103140322
F	-1.515031472649	0.079688565795	1.334989107897

Infrared Absorption Spectrum (unscaled frequencies)

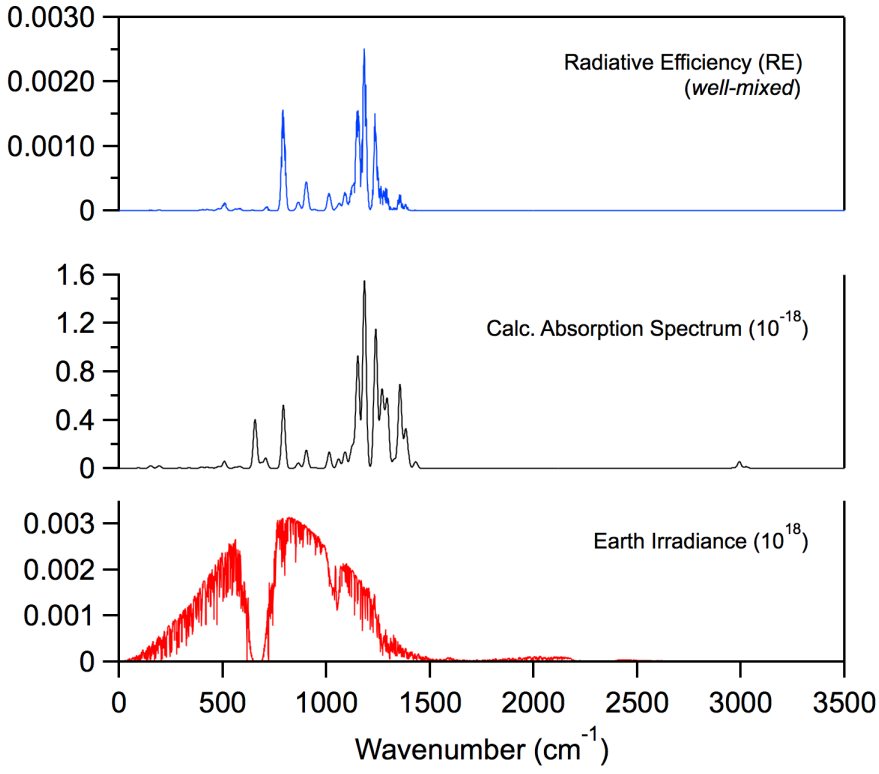
Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
42.7401	0.0781
103.8552	0.504
146.8959	0.450
247.8686	0.0419
300.1629	0.0916
364.5469	0.224
393.3680	0.266
481.3130	1.54
536.9467	0.155
559.1590	0.320
638.1402	10.8
782.7003	13.9
857.7643	0.876
899.7889	4.02
1016.9812	3.60
1127.8128	2.25
1162.7204	24.7
1196.8653	33.8
1253.8879	25.6
1284.3625	14.4
1313.1825	14.5
1378.0772	18.5
1406.2007	7.11
1457.4027	1.17
3089.7898	0.0591
3111.9465	1.24
3148.4676	0.291

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
38.3921	0.0447
107.0708	0.334
152.9353	0.512
255.3149	0.246
325.0278	0.0797
367.6365	0.301
417.4372	0.395
451.2203	1.81
536.7463	0.347
560.7844	0.524
668.7659	5.37
692.1721	10.3
862.5798	1.49
940.7225	0.867
1064.5293	9.44
1097.4652	16.5
1138.6105	16.3
1196.0200	34.8
1257.0078	24.1
1295.4194	25.0
1330.4177	1.22
1348.4987	8.92
1416.0903	11.5
1463.4682	1.40
3074.2104	0.256
3111.6600	1.10
3137.7820	0.422

Infrared Spectrum

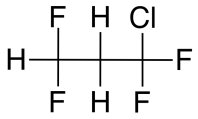


Radiative Efficiency



HCFC-244fb

Molecular Formula:	$CHF_2CH_2CF_2Cl$
Name:	1-Chloro-1,1,3,3-tetrafluoropropane
CAS number:	2730-64-5
Molecular Weight:	150.5



Global Atmospheric Lifetime (years):	7.76
Tropospheric Atmospheric Lifetime (years):	8.35
Stratospheric Atmospheric Lifetime (years):	110.7
Ozone Depletion Potential (ODP):	0.020

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.301	0.285
Global Warming Potential (GWP_H):		
GWP_{20}	3233	3053
GWP_{100}	948	895
Global Temperature Potentials (GTP_H)		
GTP_{20}		2076
GTP_{50}		260
GTP_{100}		127

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 7.02 \times 10^{-15}$; $k_{SAR}(272\ K) \approx 4.48 \times 10^{-15}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 8.05$ years

$\tau^{OH}_{Trop} = 8.35$ years

$\tau^{OH}_{Strat} = 228.3$ years

Fractional Atmospheric Loss: 0.964

O(^{1}D) Reactivity

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

$k_{Est}(T) = 0.9 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 410$ years

Fractional Atmospheric Loss: 0.019

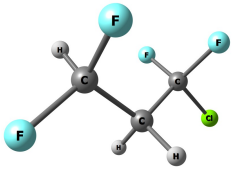
UV Photolysis

UV Spectrum: *No Recommendation*

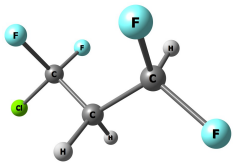
$\tau_{hv} = 450$ years

Fractional Atmospheric Loss: 0.017

Molecular Structure and Infrared Spectrum (9 conformers)



E = 0
Population = 0.236



E = 0
Population = 0.236

Optimized Coordinates (Angstroms)

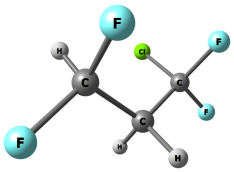
Atom	X	Y	Z
C	1.742156695160	-0.110108490787	0.268224676080
C	0.407636826207	-0.724384548072	-0.143032250226
C	-0.766512932611	0.199519366476	0.131061221674
F	2.715092974786	-1.033117456879	0.068504160052
F	2.022686719895	0.966604425295	-0.502786605240
H	1.765085515386	0.200049922220	1.319261933004
H	0.261226345838	-1.649829737338	0.416907364225
H	0.439013245106	-0.959918119289	-1.208926167481
Cl	-2.336433775908	-0.625847046375	-0.229355859073
F	-0.784234471627	0.570996713238	1.422457781038
F	-0.707741142232	1.310181971511	-0.606970254054

Atom	X	Y	Z
C	1.742827393523	0.112069404013	0.271639805946
C	0.407327237331	0.730354737544	-0.130320997624
C	-0.765515786886	-0.198801566129	0.131334189932
F	2.024353699542	-0.953342182067	-0.514557960663
F	2.714490388848	1.039038529816	0.084455458405
H	1.766661404994	-0.212798827856	1.318203689220
H	0.437881567630	0.980864725219	-1.192818644832
H	0.260018382495	1.647662181351	0.442622416489
Cl	-2.336658818809	0.629532774933	-0.216736148394
F	-0.705691591083	-1.298927875043	-0.622230645262
F	-0.782138877584	-0.588378901780	1.417400836784

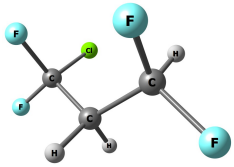
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
42.3488	0.0872
109.0080	0.603
143.0979	0.338
246.9230	0.129
315.0719	0.197
339.9147	0.170
409.4734	0.0369
421.9105	0.257
490.5244	5.81
555.6579	1.25
595.6970	0.822
798.8846	14.0
884.6720	5.55
946.9693	29.4
1023.6215	3.69
1125.8873	14.9
1138.4702	18.8
1188.5462	31.3
1236.8026	19.3
1291.2157	8.85
1333.7140	5.06
1419.4228	5.69
1423.4740	12.7
1456.6782	0.649
3064.9373	5.24
3091.6080	0.0682
3149.2751	0.250

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
42.3477	0.0872
109.0067	0.603
143.0974	0.338
246.9231	0.129
315.0711	0.197
339.9153	0.170
409.4735	0.0369
421.9099	0.257
490.5237	5.81
555.6574	1.25
595.6978	0.822
798.8843	14.0
884.6723	5.55
946.9685	29.4
1023.6217	3.69
1125.8867	14.9
1138.4707	18.8
1188.5460	31.3
1236.8021	19.3
1291.2152	8.85
1333.7133	5.06
1419.4228	5.69
1423.4743	12.7
1456.6780	0.649
3064.9369	5.24
3091.6089	0.0682
3149.2762	0.250



$\Delta E = 0.24$ kcal mol^{-1}
Population = 0.157



$\Delta E = 0.24$ kcal mol^{-1}
Population = 0.157

Optimized Coordinates (Angstroms)

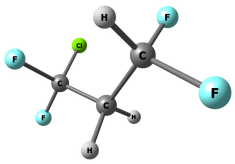
Atom	X	Y	Z
C	1.562123436548	-0.343396555406	-0.032719032299
C	0.475994295775	0.439349044138	-0.756640166840
C	-0.888142407154	0.417875748424	-0.088859913561
F	2.697018665177	-0.269251078609	-0.773275456532
F	1.815043845179	0.214197377473	1.174574020514
H	1.312085521290	-1.399487822579	0.116934510586
H	0.369291984457	0.048250223815	-1.770137989605
H	0.791055176551	1.486352574553	-0.815544928466
Cl	-1.565933856336	-1.264612246126	0.014550180002
F	-0.845448539664	0.916258525442	1.148053390762
F	-1.751132121823	1.154646208875	-0.799152614560

Atom	X	Y	Z
C	1.563644834424	0.342991223526	-0.056927249455
C	0.478345638584	-0.480937402739	-0.734937003506
C	-0.887003282297	-0.418968395754	-0.072183492293
F	1.813994661472	-0.141785339424	1.181924049986
F	2.699848989576	0.224238783021	-0.789625331200
H	1.314007086877	1.406256693856	0.029046991632
H	0.792839643391	-1.529758331483	-0.730734852779
H	0.373760425344	-0.150892426991	-1.770144097262
Cl	-1.563899913793	1.267052992164	-0.070518800794
F	-1.749159001681	-1.196308647001	-0.738912338830
F	-0.846906081897	-0.842756149175	1.192316124501

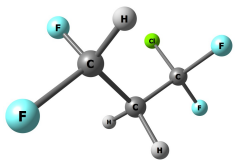
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
41.5921	0.105
110.0033	0.422
152.4549	0.215
287.3313	0.157
305.4021	0.532
339.6452	0.0958
390.1930	0.336
417.3479	0.862
519.3507	2.92
552.6431	2.30
624.4215	1.14
683.9933	12.5
894.6868	4.81
963.9619	12.1
1093.9241	22.8
1111.9234	17.4
1141.5536	22.0
1188.2539	24.9
1222.5645	16.8
1281.1302	11.6
1341.2944	4.23
1418.7621	4.90
1428.9868	10.9
1456.4386	0.463
3067.6969	1.26
3075.5150	3.22
3138.3844	0.342

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
41.5918	0.105
110.0026	0.422
152.4540	0.215
287.3312	0.157
305.4026	0.532
339.6448	0.0958
390.1928	0.336
417.3479	0.862
519.3503	2.92
552.6429	2.30
624.4216	1.14
683.9934	12.5
894.6867	4.81
963.9620	12.1
1093.9246	22.8
1111.9231	17.4
1141.5537	22.0
1188.2542	24.9
1222.5646	16.8
1281.1301	11.6
1341.2947	4.23
1418.7626	4.90
1428.9872	10.9
1456.4390	0.463
3067.6967	1.26
3075.5148	3.22
3138.3845	0.342



$\Delta E = 0.68$ kcal mol^{-1}
Population = 0.075



$\Delta E = 0.68$ kcal mol^{-1}
Population = 0.075

Optimized Coordinates (Angstroms)

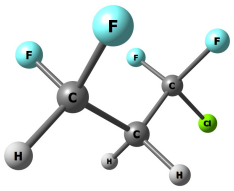
Atom	X	Y	Z
C	1.614437254143	-0.078475961211	0.294996930490
C	0.496028378678	-0.746971171428	-0.493425168785
C	-0.904737954206	-0.476908832275	0.031545502815
F	2.793866605855	-0.610898300279	-0.114350517922
F	1.654777702995	1.250150583903	0.045199529470
H	1.520277788628	-0.227091923114	1.376903963754
H	0.641705463605	-1.829872847988	-0.429764368918
H	0.561574586644	-0.446148055348	-1.540805021812
Cl	-1.443349170591	1.226686280207	-0.201026679464
F	-1.782296171662	-1.270435163922	-0.596359316725
F	-0.973462484089	-0.754771608545	1.345149147097

Atom	X	Y	Z
C	1.616657501171	0.081483130701	0.293540550629
C	0.496452423098	0.754067355073	-0.488827836532
C	-0.903065467271	0.481780744440	0.038316169446
F	1.656052485082	-1.245919914555	0.037174733732
F	2.795192869443	0.615620556932	-0.116147226511
H	1.525228576986	0.224850248424	1.376389624805
H	0.559312832870	0.458328882454	-1.537819277989
H	0.642553719469	1.836612692467	-0.420262089469
Cl	-1.442669685663	-1.220537634739	-0.201192137489
F	-0.968447114307	0.753270481027	1.353422148647
F	-1.781992140879	1.278554457774	-0.583533659268

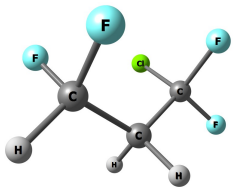
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
37.4772	0.0891
105.8615	0.385
158.6516	0.471
249.6940	0.186
315.8950	0.0911
351.4785	0.432
396.6509	0.111
428.5524	0.376
523.3827	3.21
557.9099	1.21
619.0155	0.499
684.5862	14.0
897.8548	4.31
957.0691	8.38
1086.2908	4.05
1113.1255	37.8
1157.9658	39.8
1184.2449	17.7
1216.3007	15.1
1260.9549	3.08
1338.4105	4.28
1419.9413	3.52
1430.5116	11.5
1458.6071	0.657
3065.6656	4.85
3072.9929	0.214
3139.5132	0.313

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
37.4768	0.0891
105.8618	0.385
158.6520	0.471
249.6942	0.186
315.8955	0.0911
351.4794	0.432
396.6517	0.111
428.5532	0.376
523.3833	3.21
557.9101	1.21
619.0158	0.499
684.5873	14.0
897.8563	4.31
957.0706	8.38
1086.2915	4.05
1113.1265	37.8
1157.9658	39.8
1184.2450	17.7
1216.3020	15.1
1260.9551	3.08
1338.4112	4.28
1419.9410	3.52
1430.5126	11.5
1458.6073	0.657
3065.6659	4.85
3072.9903	0.214
3139.5116	0.313



$\Delta E = 0.98$ kcal mol^{-1}
Population = 0.045



$\Delta E = 1.96$ kcal mol^{-1}
Population = 0.009

Optimized Coordinates (Angstroms)

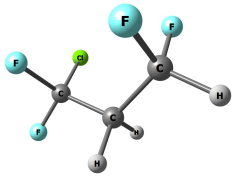
Atom	X	Y	Z
C	1.788830226855	0.001487296369	-0.597066489069
C	0.311922205190	0.002407392344	-0.985339964054
C	-0.649310305207	-0.000765094538	0.196776261145
F	2.094043662610	1.094821517462	0.141420273598
F	2.094195848073	-1.095691549636	0.135633459399
H	2.423920356712	0.003897362778	-1.493000924781
H	0.110020476020	-0.880854037585	-1.595051596293
H	0.109898201707	0.888834082241	-1.590399475363
Cl	-2.366402776269	0.000682687001	-0.404243718055
F	-0.490084708282	-1.082594098095	0.962449296202
F	-0.490247187409	1.077058441658	0.968111877272

Atom	X	Y	Z
C	1.727133690952	0.141947893783	-0.404033277565
C	0.386384862139	0.622533359113	-0.946926705495
C	-0.836668014701	0.417435775074	-0.058968204962
F	2.016489733224	0.755742286935	0.768086983162
F	1.727917245550	-1.193502766118	-0.187042439237
H	2.529809699961	0.371237210117	-1.117653183895
H	0.197791209008	0.143504928042	-1.909976591516
H	0.463148402756	1.702114613462	-1.114106202576
Cl	-1.313952685490	-1.315315846557	0.106652894684
F	-0.648529397388	0.915722224347	1.165608622398
F	-1.877517746011	1.066662321802	-0.606428894997

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
23.9788	0.155
131.9705	0.0528
163.9811	0.162
234.0806	0.00206
292.9242	0.0231
375.4180	0.0962
405.6516	0.251
423.0015	0.000
500.6390	6.57
536.9628	1.89
635.1062	9.34
823.3142	2.37
916.4476	4.89
943.0354	31.8
951.4063	0.0884
1058.6680	0.482
1171.6113	15.0
1199.3055	43.7
1242.0945	25.7
1305.3214	5.78
1368.5089	18.3
1415.3077	3.22
1420.3809	5.00
1451.8747	1.71
3036.3745	7.78
3089.9008	0.262
3142.0684	0.179

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
22.9650	0.139
131.1306	0.0223
167.8081	0.132
253.6306	0.196
290.2908	0.0769
384.9038	0.113
393.9281	0.188
426.5519	0.369
513.0939	4.34
538.6823	1.55
652.0519	6.62
777.5440	7.39
869.7274	8.04
938.7963	1.61
996.8769	6.34
1132.4897	34.2
1158.8712	17.9
1181.9436	23.4
1225.0167	29.5
1284.9996	4.19
1383.7131	15.0
1418.7077	3.23
1425.0580	1.91
1454.4583	1.32
3035.0805	7.83
3069.6172	0.908
3130.5472	0.265



$\Delta E = 1.96$ kcal mol^{-1}
Population = 0.009

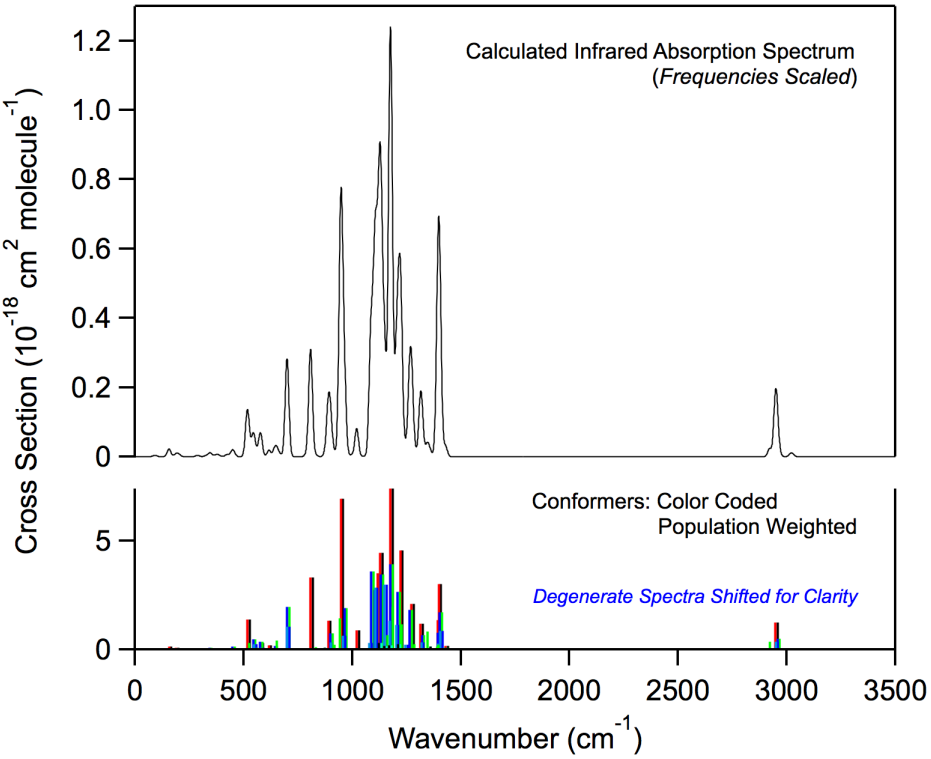
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.727284909474	-0.138741493203	-0.405339096267
C	0.387371382896	-0.624413145015	-0.945763277761
C	-0.835478512473	-0.420108524143	-0.057342696119
F	1.724684218725	1.197308965592	-0.192083902056
F	2.019248768701	-0.748478606332	0.768251102591
H	2.529978237153	-0.367885911201	-1.118985898709
H	0.466875804270	-1.704246703266	-1.110006062376
H	0.196692562581	-0.148569735232	-1.909980765090
Cl	-1.317226849171	1.311821746336	0.103891055297
F	-1.875057420416	-1.073608872277	-0.602126549860
F	-0.644990101739	-0.914504721259	1.168447090351

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
22.9631	0.139
131.1351	0.0223
167.8103	0.132
253.6309	0.196
290.2905	0.0769
384.9038	0.113
393.9283	0.188
426.5519	0.369
513.0939	4.34
538.6822	1.55
652.0519	6.62
777.5434	7.39
869.7289	8.04
938.7946	1.61
996.8770	6.34
1132.4882	34.2
1158.8719	17.9
1181.9424	23.4
1225.0158	29.5
1284.9987	4.19
1383.7121	15.0
1418.7072	3.23
1425.0569	1.91
1454.4582	1.32
3035.0818	7.83
3069.6178	0.908
3130.5482	0.265

Infrared Spectrum



Radiative Efficiency