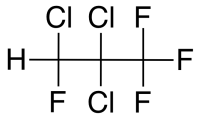
HCFC-224aa

Molecular Formula:	$CHClFCCl_2CF_3$
Name:	2,2,3-Trichloro-1,1,1,3-tetrafluoropropane
CAS number:	139754-75-9
Molecular Weight:	219.39



Global Atmospheric Lifetime (years):	3.15
Tropospheric Atmospheric Lifetime (years):	3.54
Stratospheric Atmospheric Lifetime (years):	28.9
Ozone Depletion Potential (ODP):	0.049

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.278	0.247
Global Warming Potential (GWP_H):		
GWP_{20}	896	796
GWP_{100}	243	216
Global Temperature Potentials (GTP_H)		
GTP_{20}		347
GTP_{50}		40
GTP_{100}		30

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

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

OH Reactivity

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

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

$\tau^{OH}_{Global} = 3.42$ years

$\tau^{OH}_{Trop} = 3.54$ years

$\tau^{OH}_{Strat} = 105.3$ years

Fractional Atmospheric Loss: 0.921

$O(^1D)$ Reactivity

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

$k_{Est}(T) = 1.9 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 195$ years

Fractional Atmospheric Loss: 0.016

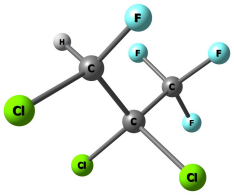
UV Photolysis

UV Spectrum: *No Recommendation*

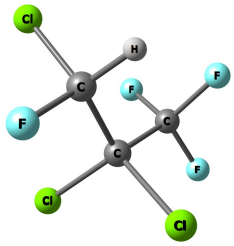
$\tau_{hv} = 50$ years

Fractional Atmospheric Loss: 0.063

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.612



$\Delta E = 0.51$ kcal mol^{-1}
Population = 0.257

Optimized Coordinates (Angstroms)

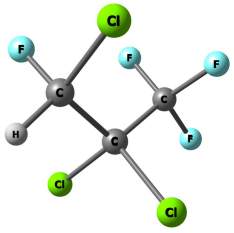
Atom	X	Y	Z
C	0.990452346759	-0.584097859144	-0.655714587549
C	-0.086120245680	0.222364644196	0.117189201576
C	-1.511509840626	-0.312322933648	-0.243914529510
Cl	2.651249672699	-0.027261313446	-0.313864246125
F	0.884134443600	-1.887428229505	-0.323248468139
H	0.824831077589	-0.462173432547	-1.727340710916
Cl	-0.008280606834	1.928167971170	-0.408804519213
Cl	0.133881673254	0.072055083483	1.875568460988
F	-2.453492191897	0.468005479602	0.267095714994
F	-1.647636730563	-0.333215142473	-1.575612872402
F	-1.690853598302	-1.546105267687	0.212019556297

Atom	X	Y	Z
C	1.127666882129	0.365876029770	0.709256521510
C	-0.205361198764	0.352209334056	-0.084648986564
C	-1.032991241273	-0.952580660740	0.130455035008
Cl	2.244222362379	-0.954195051630	0.242311070799
F	1.744018606575	1.543250162338	0.504535592066
H	0.910851224158	0.235163930468	1.770256123726
Cl	0.074351151882	0.593931134620	-1.822371723452
Cl	-1.178475731360	1.709417564332	0.586425765488
F	-2.267826548384	-0.809349041427	-0.331103407028
F	-0.476832369471	-1.989624735628	-0.483524849225
F	-1.091277137870	-1.219030666158	1.441000857672

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
62.2451	0.0560
80.5971	0.0239
141.0505	0.0642
174.0484	0.0271
207.0786	0.101
212.2230	0.216
254.2340	0.0328
287.7923	0.0832
313.7014	0.0887
362.4314	0.0521
392.4245	0.160
441.1616	0.234
546.5034	1.18
557.1954	1.25
639.2743	5.76
702.9701	11.9
801.3297	9.28
877.5021	19.7
931.7805	3.15
1054.1502	3.89
1130.4871	7.80
1210.3432	28.2
1243.2459	37.2
1258.7580	32.3
1283.8819	6.35
1360.5872	2.90
3117.8491	0.465

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
55.9965	0.0401
86.3064	0.0371
144.1520	0.0449
169.3281	0.0774
199.3796	0.213
231.2737	0.0214
245.5824	0.126
277.9487	0.154
334.0366	0.0608
358.1249	0.0313
386.5440	0.158
423.5834	0.392
550.1091	0.972
559.5466	1.16
642.1247	5.56
725.4073	4.90
765.2710	26.2
854.3200	7.01
943.9776	7.95
1045.4939	3.78
1149.7795	11.6
1215.8175	26.1
1247.0386	27.4
1259.9824	31.6
1281.4806	7.68
1364.4344	2.56
3121.4428	0.467



$\Delta E = 0.91$ kcal mol^{-1}
Population = 0.131

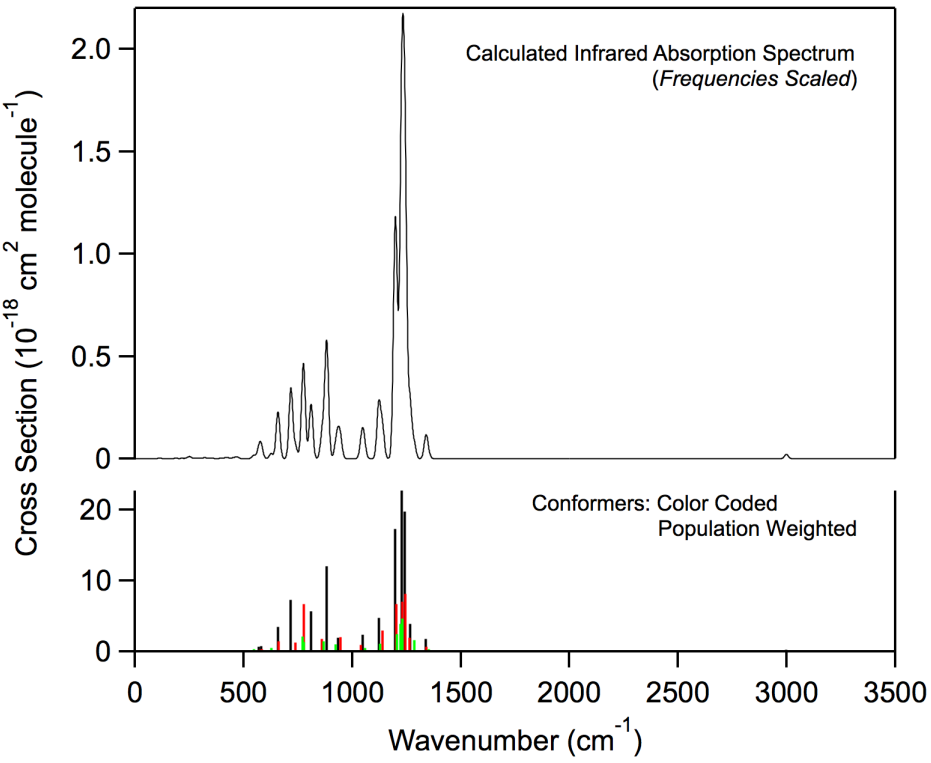
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.096312034115	0.860556088240	-0.272027726171
C	-0.280495588529	0.339078747857	0.226790037284
C	-0.732021926516	-1.034328027370	-0.362594294484
Cl	2.469231875145	-0.214631063073	0.143345592456
F	1.061085084010	1.017248486733	-1.609497290097
H	1.291590818456	1.818724544148	0.211978883268
Cl	-1.486361322501	1.567119822425	-0.287953916839
Cl	-0.252884627149	0.222938508274	2.004801769383
F	-1.970591142812	-1.314925834992	0.029597808830
F	-0.703799367931	-0.993689408187	-1.691914645495
F	0.067767163712	-2.013280864056	0.049012781865

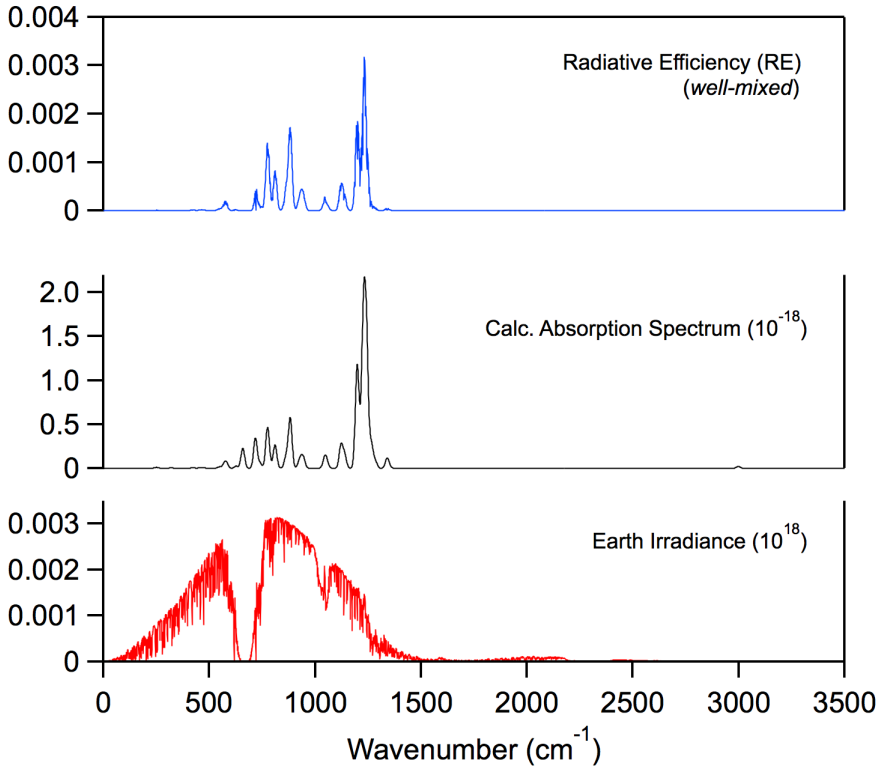
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
43.5111	0.0153
102.2102	0.0434
152.1698	0.0141
165.5102	0.0157
199.6061	0.0792
241.5641	0.119
246.5889	0.0603
278.9044	0.248
324.5367	0.0360
367.4196	0.0735
383.8959	0.0993
438.7514	0.240
521.9111	2.61
559.7578	0.974
606.7927	4.07
759.3445	16.2
764.6644	10.6
861.2855	11.0
921.2319	8.05
1064.4871	3.82
1137.1311	8.71
1218.4784	18.6
1236.8580	30.0
1246.9315	35.4
1303.3694	12.3
1374.5504	2.58
3115.0759	0.564

Infrared Spectrum

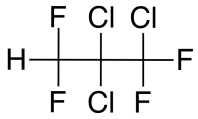


Radiative Efficiency



HCFC-224ab

Molecular Formula:	$CHF_2CCl_2CClF_2$
Name:	1,2,2-Trichloro-1,1,3,3-tetrafluoropropane
CAS number:	422-32-2
Molecular Weight:	219.39



Global Atmospheric Lifetime (years):	11.3
Tropospheric Atmospheric Lifetime (years):	15.1
Stratospheric Atmospheric Lifetime (years):	44.6
Ozone Depletion Potential (ODP):	0.141

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.319	0.306
Global Warming Potential (GWP_H):		
GWP_{20}	3063	2935
GWP_{100}	999	957
Global Temperature Potentials (GTP_H)		
GTP_{20}		2298
GTP_{50}		426
GTP_{100}		141

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 3.89 \times 10^{-15}$; $k_{SAR}(272\ K) \approx 2.48 \times 10^{-15}$ cm^3 $molecule^{-1}$ s^{-1}

τ^{OH}_{Global} = 14.5 years
τ^{OH}_{Trop} = 15.1 years
τ^{OH}_{Strat} = 389.0 years

Fractional Atmospheric Loss: 0.776

O(^{1}D) Reactivity

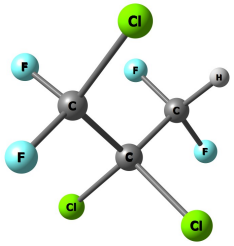
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 1.9 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)}$ = 195 years
Fractional Atmospheric Loss: 0.058

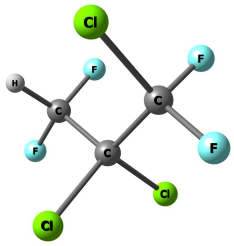
UV Photolysis

UV Spectrum: *No Recommendation*
τ_{hv} = 68 years
Fractional Atmospheric Loss: 0.166

Molecular Structure and Infrared Spectrum (9 conformers)



E = 0
Population = 0.220



E = 0
Population = 0.220

Optimized Coordinates (Angstroms)

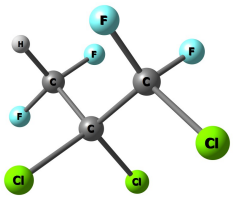
Atom	X	Y	Z
C	-1.012808663227	0.833273047548	-0.884100078771
C	-0.369516347836	-0.241566710014	0.033540696609
C	1.077647416062	0.130627454227	0.491365110030
F	-2.282394486949	0.486897436464	-1.146651315469
F	-1.012955528294	2.020522086958	-0.249503222943
H	-0.455421725752	0.918500197586	-1.821820659887
Cl	-0.320538439052	-1.775988191419	-0.877546581928
Cl	-1.361472429311	-0.420591218134	1.508869322737
Cl	2.147679395052	0.491728646090	-0.913676015456
F	1.046197237538	1.206192389249	1.271492899325
F	1.609442571771	-0.874073138554	1.176728845754

Atom	X	Y	Z
C	-1.012728841946	0.841439628509	0.877378898976
C	-0.371256982819	-0.242095165037	-0.031266484447
C	1.077105233138	0.123119714842	-0.490918249690
F	-1.009645121998	2.023642494759	0.233437629968
F	-2.283310833372	0.500091142388	1.141688985001
H	-0.455840875992	0.932769159292	1.814821376721
Cl	-1.362536675838	-0.430457230874	-1.505886949522
Cl	-0.326516603319	-1.769388792744	0.891935114952
Cl	2.146936969733	0.492815725469	0.912038531593
F	1.607070065653	-0.888187716874	-1.167931848954
F	1.048729666760	1.192565040269	-1.279531004597

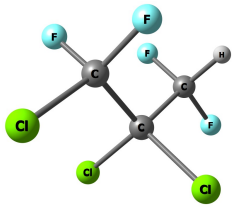
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
60.0386	0.0690
92.6756	0.0854
147.7091	0.0582
172.8895	0.0506
199.4704	0.148
228.5816	0.0234
241.9021	0.0716
304.4558	0.0207
314.1001	0.353
340.7724	0.0625
382.6689	0.221
424.2336	0.157
451.9158	0.268
563.9108	2.09
638.7229	4.65
661.5605	8.27
806.4010	28.5
883.4736	16.2
1011.6388	15.3
1057.8225	0.896
1150.9260	7.12
1179.6963	21.5
1208.8421	24.7
1228.4549	25.2
1379.0601	5.96
1395.2148	1.97
3092.5634	2.01

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
60.0384	0.0690
92.6752	0.0854
147.7088	0.0582
172.8896	0.0506
199.4703	0.148
228.5817	0.0234
241.9020	0.0716
304.4559	0.0207
314.1000	0.353
340.7724	0.0625
382.6688	0.221
424.2337	0.157
451.9158	0.268
563.9108	2.09
638.7228	4.65
661.5606	8.27
806.4010	28.5
883.4734	16.2
1011.6389	15.3
1057.8224	0.896
1150.9259	7.12
1179.6962	21.5
1208.8419	24.7
1228.4548	25.2
1379.0601	5.96
1395.2147	1.97
3092.5636	2.01



$\Delta E = 0.25$ kcal mol^{-1}
Population = 0.143



$\Delta E = 0.25$ kcal mol^{-1}
Population = 0.143

Optimized Coordinates (Angstroms)

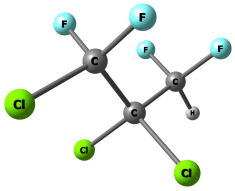
Atom	X	Y	Z
C	-1.567412499502	0.467755128565	0.606812784751
C	-0.332275578806	-0.228896853718	-0.040881041989
C	0.972393493950	0.556512485396	0.314217522953
F	-1.692738164041	1.716666210271	0.122430802258
F	-2.677106574774	-0.219920690628	0.298744019807
H	-1.447347899436	0.506198589618	1.694336101667
Cl	-0.540815363253	-0.285540801468	-1.803656047400
Cl	-0.244608927045	-1.868345409383	0.662794546253
Cl	2.463914224809	-0.252209394804	-0.238264143741
F	0.925240709841	1.771926853814	-0.224478296330
F	1.022076578257	0.695857882336	1.647097751773

Atom	X	Y	Z
C	-1.565765958313	0.464501130781	-0.612502796010
C	-0.331550576552	-0.227704900470	0.041682652712
C	0.973765191765	0.554591769534	-0.317888050297
F	-2.676020572824	-0.220465401034	-0.300442788905
F	-1.691154041233	1.717050583245	-0.137625591201
H	-1.444560417636	0.494749967634	-1.700157959116
Cl	-0.243708149412	-1.872395455050	-0.649628101887
Cl	-0.541983604133	-0.271099499496	1.804609250875
Cl	2.464427344647	-0.250477617073	0.242193402820
F	1.024910087499	0.683965381537	-1.651717132501
F	0.926455696194	1.774009040392	0.211671113511

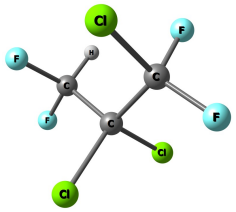
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
59.8693	0.0695
88.2241	0.0943
145.0390	0.0770
174.9108	0.0255
201.0087	0.0398
216.9110	0.311
254.0620	0.0454
281.6118	0.105
318.8435	0.1000
343.7200	0.107
408.3317	0.284
430.7885	0.108
450.1465	0.313
560.9855	3.70
631.5037	2.12
674.0402	9.80
816.1715	20.9
886.0586	17.0
1011.7520	8.05
1068.2416	21.5
1152.9098	7.62
1166.6317	11.5
1184.7106	23.4
1209.4635	33.9
1376.3443	7.81
1396.0738	2.19
3085.6412	2.06

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
59.8689	0.0695
88.2239	0.0944
145.0384	0.0770
174.9114	0.0255
201.0083	0.0398
216.9119	0.311
254.0613	0.0454
281.6113	0.105
318.8450	0.1000
343.7190	0.107
408.3320	0.284
430.7892	0.108
450.1463	0.313
560.9846	3.70
631.5034	2.12
674.0397	9.80
816.1718	20.9
886.0602	17.0
1011.7501	8.05
1068.2413	21.5
1152.9096	7.62
1166.6328	11.5
1184.7100	23.4
1209.4615	33.9
1376.3419	7.81
1396.0718	2.19
3085.6445	2.06



$\Delta E = 0.66$ kcal mol^{-1}
Population = 0.072



$\Delta E = 0.79$ kcal mol^{-1}
Population = 0.058

Optimized Coordinates (Angstroms)

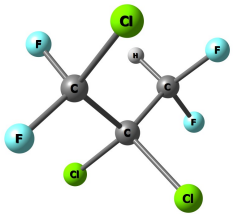
Atom	X	Y	Z
C	-1.790587213596	0.120301011930	-0.001533732074
C	-0.320183719647	-0.405838558237	-0.001636480979
C	0.736101910559	0.749171258602	0.002450545467
F	-2.015060051517	0.872330229323	1.090030470210
F	-2.013075211470	0.878294996120	-1.089372695266
H	-2.472160934768	-0.737153715023	-0.004500524388
Cl	-0.123720125675	-1.391737337536	-1.474771064330
Cl	-0.126367985197	-1.399742923800	1.466453377765
Cl	2.423632943161	0.148769133585	0.002382699155
F	0.557684873968	1.510196244555	-1.075807762736
F	0.555698514181	1.504370660482	1.084468167176

Atom	X	Y	Z
C	-1.010110549199	0.930161402581	-0.825680055122
C	-0.425954659145	-0.176063297229	0.097073581940
C	1.072335199303	-0.495945614351	-0.217315415025
F	-2.323732870267	1.058921587976	-0.583157502547
F	-0.419571910449	2.110793265713	-0.568527473414
H	-0.851875490646	0.660970530565	-1.875573425537
Cl	-1.347136578241	-1.676980164727	-0.264663224449
Cl	-0.620352856497	0.275664377944	1.802336763114
Cl	2.189556038421	0.852279018688	0.142504554894
F	1.463957374769	-1.558605101480	0.475720708155
F	1.168920301951	-0.778802005681	-1.524473512009

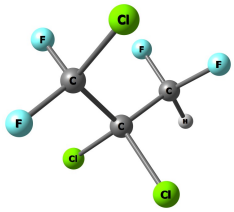
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
47.5552	0.0132
107.1770	0.137
153.9702	0.00335
169.7170	0.00131
209.6066	0.0743
214.3329	0.116
252.7343	0.0175
282.0149	0.00254
315.1162	0.00002
392.8733	0.193
402.4157	0.0768
424.6063	0.0173
448.6860	0.435
541.2732	9.65
591.3619	4.36
643.4152	3.64
873.3631	22.6
918.1279	8.28
943.0533	13.0
1079.7732	15.2
1152.1052	7.88
1164.0784	16.4
1200.9606	29.0
1207.4707	30.3
1391.2674	1.82
1392.0053	8.90
3077.4781	2.49

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
54.7650	0.0737
87.8962	0.0840
153.2891	0.0660
163.0902	0.00975
201.1858	0.202
231.1581	0.0182
247.8155	0.303
273.9276	0.0932
324.1914	0.0172
345.4314	0.186
389.0403	0.236
431.2191	0.0183
452.6810	0.0515
570.9369	2.36
635.0085	1.34
676.8975	9.67
789.9108	32.0
887.9126	10.4
1018.1697	13.6
1052.5563	2.03
1156.5151	23.4
1172.3154	8.85
1183.3307	27.7
1221.9843	19.6
1380.4231	6.31
1395.0643	2.37
3080.7602	2.03



$\Delta E = 0.79$ kcal mol^{-1}
Population = 0.058



$\Delta E = 0.98$ kcal mol^{-1}
Population = 0.042

Optimized Coordinates (Angstroms)

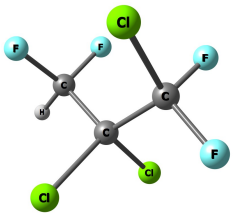
Atom	X	Y	Z
C	-1.009229168355	0.937982110757	0.819250839872
C	-0.427755188558	-0.175157051762	-0.096860594646
C	1.068793001920	-0.499093711107	0.221655128249
F	-0.413789263277	2.115037333321	0.557053186754
F	-2.321951341078	1.070474051383	0.573882223363
H	-0.853748470986	0.673571942330	1.870769069397
Cl	-0.617635248287	0.268565625904	-1.804732242851
Cl	-1.355218402404	-1.670705048604	0.271011645607
Cl	2.191709561973	0.843037027008	-0.143184421914
F	1.162152999648	-0.775624345746	1.530399975681
F	1.457525519405	-1.566757933484	-0.465288809514

Atom	X	Y	Z
C	-0.841990327404	1.425064103070	-0.047305754209
C	-0.520145367406	-0.087257001169	-0.227149673907
C	0.760890500019	-0.602863390078	0.509560059100
F	-0.849022278327	1.734275535803	1.261980546893
F	0.080296545764	2.188381468722	-0.657476985764
H	-1.826824768148	1.628824627547	-0.481150345289
Cl	-0.391212124708	-0.425228896938	-1.971144028462
Cl	-1.912913569969	-0.982604122552	0.470758194916
Cl	2.254967424101	0.228311844049	-0.021946898274
F	0.622389993921	-0.420118592980	1.821055988369
F	0.902587972156	-1.906342575473	0.279424896627

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
54.7659	0.0737
87.8966	0.0840
153.2897	0.0660
163.0895	0.00975
201.1855	0.202
231.1573	0.0182
247.8153	0.303
273.9271	0.0932
324.1909	0.0172
345.4308	0.186
389.0399	0.236
431.2191	0.0183
452.6806	0.0515
570.9367	2.36
635.0089	1.34
676.8973	9.67
789.9103	32.0
887.9124	10.4
1018.1678	13.6
1052.5539	2.03
1156.5159	23.4
1172.3146	8.85
1183.3298	27.7
1221.9847	19.6
1380.4204	6.31
1395.0628	2.37
3080.7623	2.03

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
45.4240	0.0465
107.8906	0.0884
155.4133	0.0251
166.4971	0.0329
202.5023	0.0315
240.1350	0.118
250.8093	0.0815
275.0467	0.270
308.6631	0.0119
380.8088	0.127
389.1682	0.228
428.6494	0.498
432.3557	0.301
560.6934	3.16
588.0476	3.31
696.2301	7.53
816.0246	28.4
882.5697	15.6
972.9609	9.71
1091.0467	6.58
1150.1380	7.58
1169.7254	13.0
1199.5682	27.3
1216.0794	32.2
1392.3491	2.35
1398.3182	4.08
3078.3819	2.62



$\Delta E = 0.98$ kcal mol^{-1}
Population = 0.042

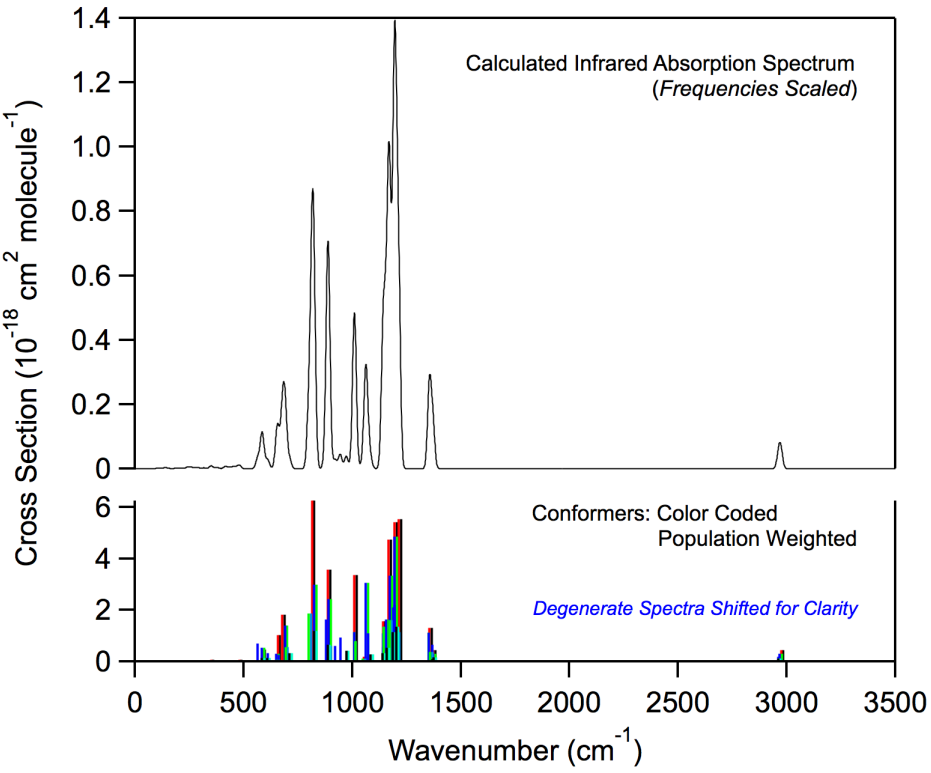
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-0.832014759358	1.431618133354	0.049537532111
C	-0.522388425314	-0.083797206870	0.224715673053
C	0.757767863215	-0.606213164623	-0.508718152676
F	0.093474681099	2.185506014633	0.666545143825
F	-0.831241044057	1.746021302510	-1.258530364955
H	-1.817078740195	1.641140719112	0.480104383078
Cl	-1.918975541859	-0.965792022115	-0.482499086751
Cl	-0.403297543078	-0.429591798523	1.967876300488
Cl	2.255866165163	0.211505624836	0.032257849261
F	0.888628939781	-1.911624081540	-0.283160788733
F	0.626127404603	-0.417272520773	-1.820042488700

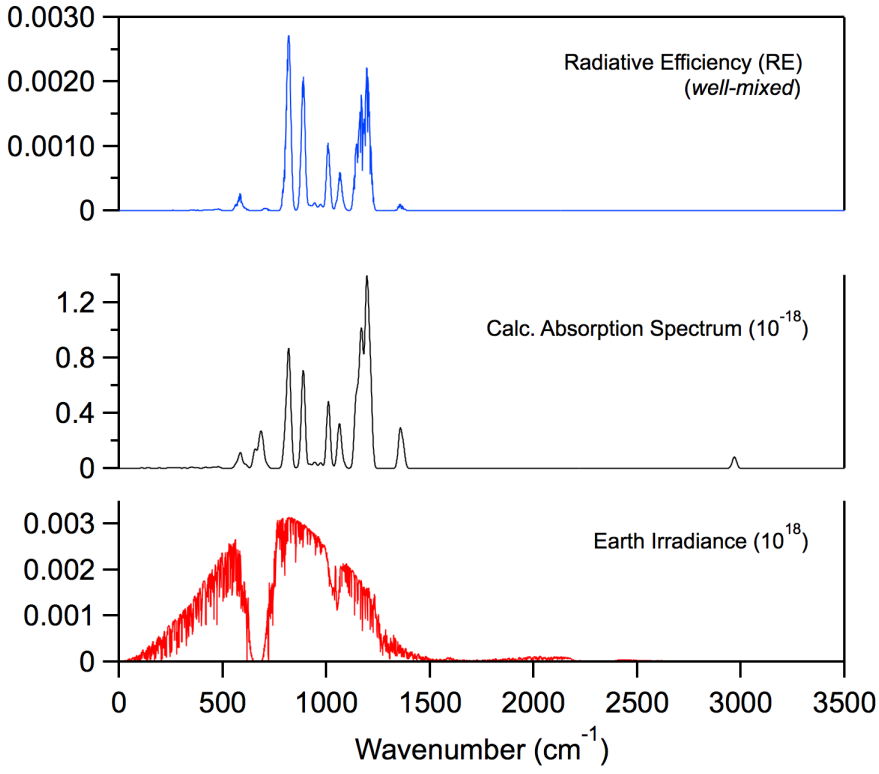
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
45.4245	0.0465
107.8908	0.0884
155.4134	0.0251
166.4971	0.0329
202.5024	0.0315
240.1349	0.118
250.8094	0.0815
275.0468	0.270
308.6631	0.0119
380.8092	0.127
389.1686	0.228
428.6494	0.498
432.3558	0.301
560.6936	3.16
588.0477	3.31
696.2306	7.53
816.0249	28.4
882.5696	15.6
972.9615	9.71
1091.0478	6.58
1150.1384	7.58
1169.7249	13.0
1199.5688	27.3
1216.0797	32.2
1392.3488	2.35
1398.3186	4.08
3078.3811	2.62

Infrared Spectrum

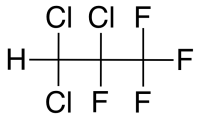


Radiative Efficiency



HCFC-224ba

Molecular Formula:	$CHCl_2CClFCF_3$
Name:	2,3,3-Trichloro-1,1,1,2-tetrafluoropropane
CAS number:	422-47-9
Molecular Weight:	219.39



Global Atmospheric Lifetime (years):	1.39
Tropospheric Atmospheric Lifetime (years):	1.47
Stratospheric Atmospheric Lifetime (years):	24.5
Ozone Depletion Potential (ODP):	0.023

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.271	0.215
Global Warming Potential (GWP_H):		
GWP_{20}	386	307
GWP_{100}	105	83
Global Temperature Potentials (GTP_H)		
GTP_{20}		105
GTP_{50}		14
GTP_{100}		12

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

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

OH Reactivity

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

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

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

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

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

Fractional Atmospheric Loss: 0.973

O(^{1}D) Reactivity

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

$k_{Est}(T) = 1.9 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 195$ years

Fractional Atmospheric Loss: 0.007

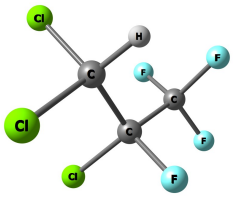
UV Photolysis

UV Spectrum: *No Recommendation*

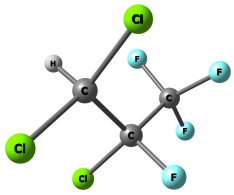
$\tau_{hv} = 68$ years

Fractional Atmospheric Loss: 0.020

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.640



$\Delta E = 0.57$ kcal mol^{-1}
Population = 0.242

Optimized Coordinates (Angstroms)

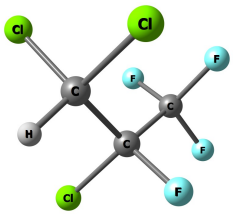
Atom	X	Y	Z
C	0.985864912098	-0.342120107826	0.552520733157
C	-0.230874980687	0.495318610643	0.088156919912
C	-1.587310953054	-0.260382505203	0.250374198217
Cl	1.247781635162	-1.796418022862	-0.437342700939
Cl	2.447602600212	0.675477695692	0.622884755594
H	0.783505079004	-0.675295206044	1.568196880313
Cl	-0.080514633156	1.080793363240	-1.585338996613
F	-0.315749890237	1.554185596984	0.928044949136
F	-2.588910280657	0.601183485734	0.128445459302
F	-1.742371375913	-1.229289408867	-0.639743731895
F	-1.635359112773	-0.794832501491	1.478377533817

Atom	X	Y	Z
C	1.021273615825	-0.144998442545	-0.495980392689
C	-0.224297813932	0.347195424653	0.280976971863
C	-1.532880354799	-0.438969327246	-0.064761558070
Cl	2.463934328771	0.793029659457	-0.026121428785
Cl	1.321009758436	-1.888388813492	-0.227234946173
H	0.861523982393	-0.004638621177	-1.561180757065
Cl	-0.508806914608	2.068136558214	-0.158228828007
F	-0.031610259426	0.245150745449	1.605059918842
F	-2.602094398807	0.215403582785	0.371033308324
F	-1.627384252692	-0.592435691664	-1.388156371977
F	-1.525423691159	-1.635219074436	0.511660083737

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
48.5594	0.0311
77.9855	0.0123
140.1798	0.0920
167.8134	0.0209
191.7918	0.198
231.1372	0.0410
249.8469	0.194
312.7558	0.0599
328.4762	0.152
356.3494	0.160
385.1925	0.0570
477.6228	0.646
549.8213	1.92
586.1025	0.735
609.8496	3.00
712.6808	12.3
782.5349	5.42
812.3037	14.7
941.6503	16.2
1072.8295	7.79
1137.6720	12.2
1217.4039	25.7
1232.3723	0.0398
1263.5550	37.3
1275.1946	13.3
1292.6720	16.5
3148.4462	0.442

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
44.3747	0.0185
63.2277	0.0198
148.7339	0.0501
201.1696	0.277
207.4733	0.0671
219.3026	0.0171
247.7868	0.0744
289.8881	0.124
318.8469	0.166
337.9671	0.0173
387.1981	0.0553
441.0170	0.569
544.5705	1.18
582.3606	0.305
693.8427	12.2
743.7433	9.37
756.9505	15.4
782.9624	3.93
919.3743	10.8
1017.6786	5.88
1189.4375	18.8
1218.3736	3.79
1235.0671	20.0
1249.9166	29.5
1267.6974	21.9
1307.8602	10.8
3168.1109	0.525



$\Delta E = 1.00$ kcal mol^{-1}
Population = 0.118

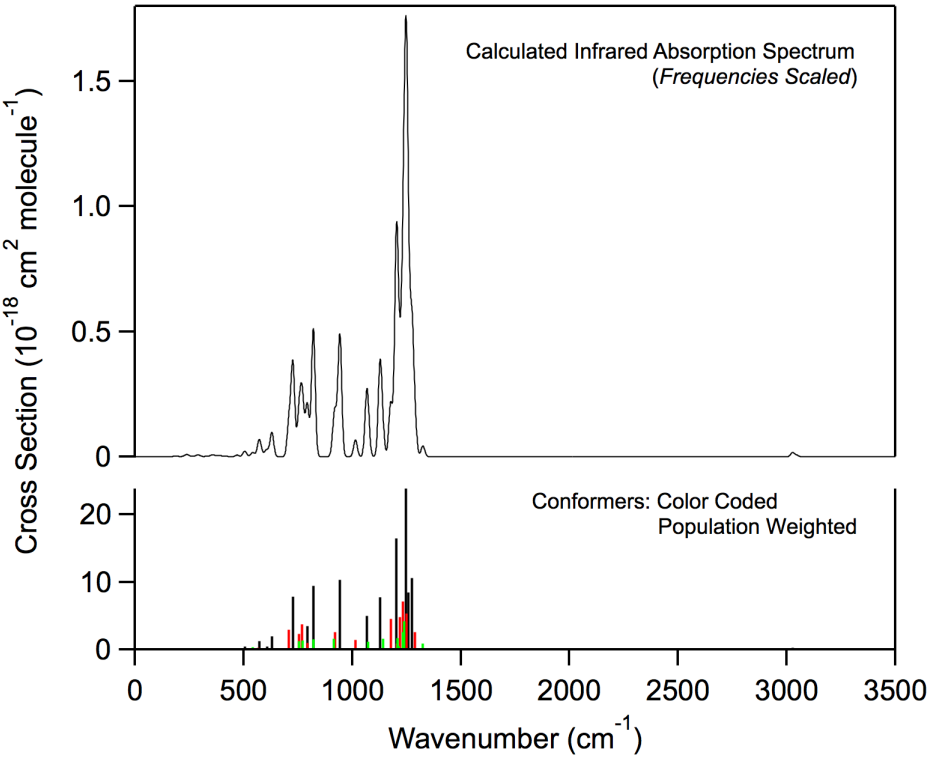
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.136924568252	0.322456879083	0.480038132097
C	-0.397992834146	0.112457306256	0.567975272035
C	-1.100851814941	-0.670735432428	-0.583493320094
Cl	2.021985869524	-1.211506769591	0.730802326034
Cl	1.652226093387	1.128067860796	-1.021741179608
H	1.413233332588	0.973632557217	1.306135352399
Cl	-1.176981392752	1.724361605494	0.709380803758
F	-0.643624942383	-0.577823807833	1.702026115983
F	-2.368321700315	-0.883962642308	-0.240069939332
F	-1.074528429577	0.000288242656	-1.727859935805
F	-0.511037749637	-1.850371799340	-0.763875627466

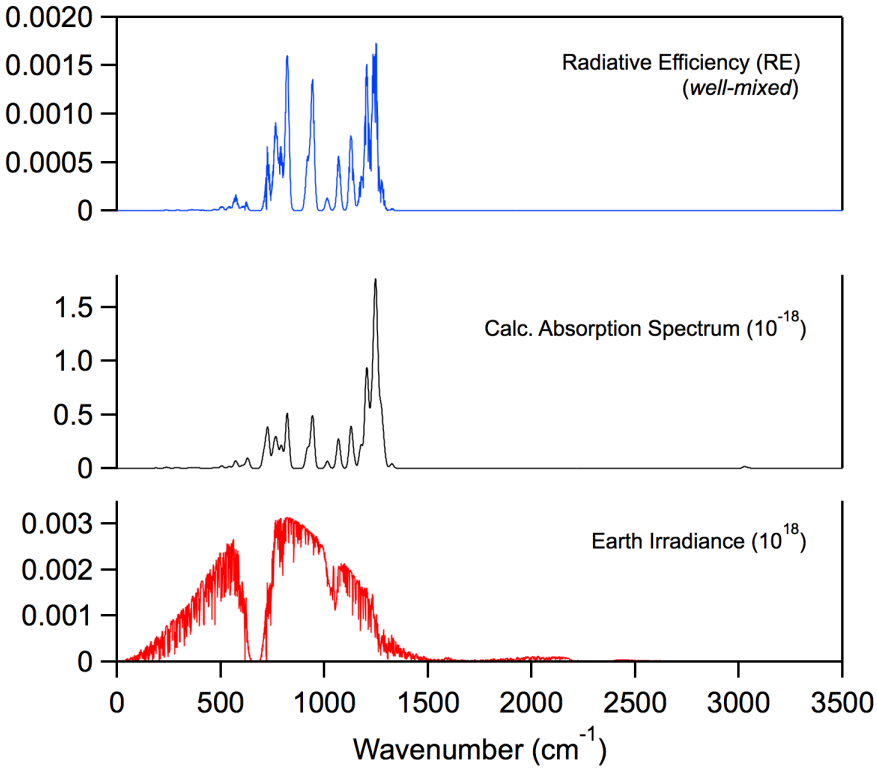
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
33.8552	0.00952
87.3517	0.0252
148.8493	0.00888
168.5917	0.0213
196.4828	0.104
230.3753	0.0723
261.9757	0.264
310.0350	0.0828
315.3363	0.167
349.2302	0.153
389.4195	0.00518
481.1335	0.552
516.6348	3.12
570.6797	1.27
614.4643	1.41
741.7371	10.6
760.3163	11.6
813.1972	12.6
911.7983	13.8
1080.4289	9.75
1151.3612	13.4
1222.5147	14.4
1227.6556	4.30
1247.5388	21.9
1254.0680	35.4
1346.5542	7.77
3147.5639	0.562

Infrared Spectrum

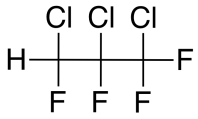


Radiative Efficiency



HCFC-224bb

Molecular Formula:	$CHClFCClFCClF_2$
Name:	1,2,3-Trichloro-1,1,2,3-tetrafluoropropane
CAS number:	422-42-4
Molecular Weight:	219.39



Global Atmospheric Lifetime (years):	4.10
Tropospheric Atmospheric Lifetime (years):	4.45
Stratospheric Atmospheric Lifetime (years):	51.2
Ozone Depletion Potential (ODP):	0.047

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.312	0.283
Global Warming Potential (GWP_H):		
GWP_{20}	1300	1182
GWP_{100}	355	322
Global Temperature Potentials (GTP_H)		
GTP_{20}		585
GTP_{50}		64
GTP_{100}		45

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 1.32 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 0.841 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 4.30$ years

$\tau^{OH}_{Trop} = 4.45$ years

$\tau^{OH}_{Strat} = 129.5$ years

Fractional Atmospheric Loss: 0.952

O(^{1}D) Reactivity

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

$k_{Est}(T) = 1.9 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 195$ years

Fractional Atmospheric Loss: 0.021

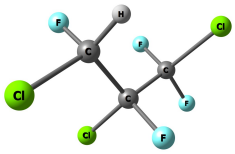
UV Photolysis

UV Spectrum: *No Recommendation*

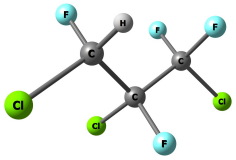
$\tau_{hv} = 150$ years

Fractional Atmospheric Loss: 0.027

Molecular Structure and Infrared Spectrum (12 conformers)



E = 0
Population = 0.325



$\Delta E = 0.04$ kcal mol^{-1}
Population = 0.305

Optimized Coordinates (Angstroms)

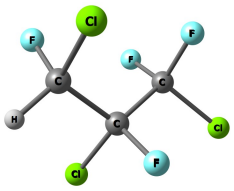
Atom	X	Y	Z
C	-1.008281151888	0.833354197013	-0.286056325621
C	-0.123697082276	-0.278656232360	0.324734984435
C	1.369520151146	-0.182098350237	-0.127830098923
Cl	-2.654629543573	0.788920506179	0.405059813974
H	-0.591651929167	1.810095980537	-0.034576513840
F	-1.059748184620	0.687005810239	-1.622913412051
Cl	-0.722800226198	-1.894805283818	-0.148262950968
F	-0.139863663965	-0.159241583541	1.664824479120
Cl	2.081894335291	1.395241714644	0.377789408831
F	2.068014651861	-1.152896637505	0.448167193683
F	1.471303643390	-0.294228121151	-1.446164578640

Atom	X	Y	Z
C	-1.313987764174	0.754738975620	0.100287436310
C	-0.115829980024	-0.221377987237	0.226357431447
C	1.226899989557	0.546094352249	-0.008669595018
Cl	-2.843176530491	-0.040477017317	0.562646774855
H	-1.168962388527	1.585855955584	0.792351547649
F	-1.391358568088	1.216586230531	-1.161844542543
Cl	-0.253229321374	-1.563020968620	-0.931744978877
F	-0.095110662909	-0.687185573374	1.489748156072
Cl	2.643753669120	-0.452386594678	0.410396274267
F	1.322003749534	0.951704991682	-1.268700185374
F	1.221557807375	1.630835635558	0.783282681212

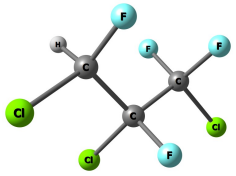
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
46.5477	0.0652
77.7797	0.0363
136.6545	0.124
175.9374	0.0828
196.0981	0.0921
230.6955	0.113
260.8263	0.136
291.6790	0.0867
333.3274	0.0484
362.4783	0.188
390.7837	0.398
421.6525	0.147
451.8294	0.0460
565.7516	1.77
623.7811	8.54
656.7202	2.76
774.5172	35.0
825.6005	22.8
1015.9403	5.72
1088.0085	7.67
1149.6867	12.7
1187.5315	20.7
1233.9018	27.3
1235.7586	13.0
1293.6434	4.05
1363.0101	2.50
3117.2061	0.667

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
52.2807	0.0697
72.3417	0.0437
130.3834	0.0970
180.0395	0.0134
204.9210	0.314
224.3546	0.111
237.3761	0.0681
309.6177	0.0637
325.5408	0.0359
360.3868	0.0622
419.1743	0.309
431.4138	0.254
453.8740	0.137
561.9316	0.659
626.8690	12.5
658.9609	1.97
728.8518	31.3
888.6546	8.73
1022.7600	21.8
1091.7201	10.6
1148.9378	16.8
1159.9783	5.80
1198.4147	32.2
1233.0552	15.7
1294.2665	3.68
1361.2800	3.09
3117.2980	0.509



$\Delta E = 1.11$ kcal mol^{-1}
Population = 0.050



$\Delta E = 1.16$ kcal mol^{-1}
Population = 0.046

Optimized Coordinates (Angstroms)

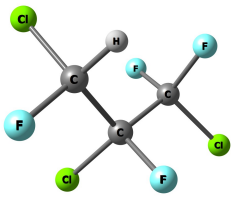
Atom	X	Y	Z
C	1.521630829455	-0.568887962848	-0.039512975736
C	0.021701760669	-0.437141856515	-0.426553739976
C	-0.777150452963	0.628936794884	0.392759920259
Cl	2.502410028192	0.813353016681	-0.619299467896
F	1.636561771484	-0.683764099370	1.296908791082
H	1.925581633388	-1.456400425055	-0.529128179446
Cl	-0.716318618516	-2.051452165145	-0.152085303618
F	-0.057024792550	-0.128520667628	-1.730510363370
Cl	-2.425491962592	0.843767820937	-0.274282383768
F	-0.861798205283	0.264464425269	1.666895918065
F	-0.143160991283	1.799724118789	0.328405784403

Atom	X	Y	Z
C	1.342070438062	0.542915553584	0.432783753319
C	0.123463931162	-0.187594262590	-0.194788411770
C	-1.220487243968	0.501417635823	0.218802317264
Cl	2.874880179031	-0.132101909077	-0.190774706539
F	1.287588305861	1.854495548995	0.117531137618
H	1.339291546639	0.419180384104	1.515952222558
Cl	0.129695499160	-1.878050551484	0.385587494161
F	0.199655986879	-0.148383066168	-1.533639815611
Cl	-2.648310552700	-0.376991302539	-0.396363868831
F	-1.277054496427	0.575537436923	1.552043990247
F	-1.252318593699	1.735980532430	-0.277095112415

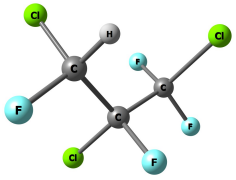
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
38.2889	0.0198
85.3317	0.0817
148.7539	0.0120
171.3164	0.0610
200.0144	0.0837
223.1406	0.128
256.3885	0.0415
307.7053	0.0751
324.7489	0.0237
373.3618	0.0160
412.4963	0.174
423.0746	0.0518
451.7233	0.251
540.4735	10.3
566.6778	4.73
664.6058	1.83
769.1339	28.2
893.4025	17.3
952.9428	15.2
1106.3571	12.2
1154.7092	26.8
1188.4724	3.72
1210.9268	23.7
1222.5346	15.0
1303.4523	6.14
1371.5631	1.99
3113.4623	0.680

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
46.4831	0.0593
62.3132	0.0305
138.0393	0.0523
188.1239	0.0338
209.2081	0.345
235.2039	0.0296
239.7444	0.103
298.7414	0.0445
320.3136	0.106
351.8007	0.0307
407.8732	0.408
430.0294	0.105
448.4099	0.444
500.1567	0.685
641.1429	4.19
699.5358	33.8
789.6689	5.26
905.6421	6.00
947.6742	21.2
1069.3871	18.8
1121.8331	13.9
1190.2807	16.5
1199.0991	15.0
1233.3290	25.3
1288.2501	5.08
1369.3601	1.09
3128.3349	0.570



$\Delta E = 1.19$ kcal mol^{-1}
Population = 0.044



$\Delta E = 1.20$ kcal mol^{-1}
Population = 0.043

Optimized Coordinates (Angstroms)

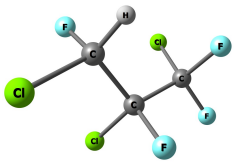
Atom	X	Y	Z
C	1.442789259747	0.068217342011	-0.714891876307
C	0.061674431610	-0.483365017829	-0.268928927981
C	-1.016929316867	0.632047217085	-0.097941267186
Cl	2.177314187766	1.198965646742	0.452521130116
F	2.262188896966	-0.981906886681	-0.906266078104
H	1.312212788187	0.609017623244	-1.653700823872
Cl	0.196405494413	-1.457458290466	1.210480777554
F	-0.340135428077	-1.272522502055	-1.293487715592
Cl	-2.665258956228	-0.053684210393	-0.074697889487
F	-0.819296177098	1.331114947885	1.011292254523
F	-0.913450180420	1.463851130458	-1.147017583664

Atom	X	Y	Z
C	-1.118072235398	-0.598491615789	-0.700434423104
C	-0.104413624476	0.516280584722	-0.346097876846
C	1.200731059887	0.067167907064	0.379063246865
Cl	-1.719793307127	-1.495807641133	0.718351452285
F	-2.149330786483	-0.019098618484	-1.344374412829
H	-0.634689555592	-1.320607031577	-1.360270127280
Cl	-0.877763777475	1.793649498279	0.633886844976
F	0.283000898330	1.047413268596	-1.529532578725
Cl	2.006556908893	-1.260044059611	-0.536594798833
F	2.033457902304	1.101870451655	0.427172706396
F	0.960180517136	-0.347719743720	1.614490967095

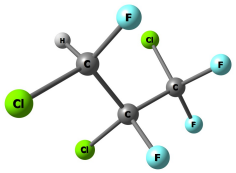
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
50.1180	0.0447
78.7630	0.0439
135.4494	0.0858
180.3166	0.192
189.3770	0.0982
215.5664	0.109
299.8423	0.277
307.4383	0.0994
320.3217	0.0454
353.0924	0.163
414.9292	0.706
428.0649	0.210
445.5726	0.360
514.7799	1.30
639.3923	8.40
654.7227	1.27
815.3749	35.0
841.9009	14.6
1017.2053	18.4
1099.3482	22.4
1125.3324	1.08
1157.9649	24.1
1193.0232	22.2
1239.1021	10.4
1279.6723	6.13
1368.7193	3.17
3116.2984	0.608

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
48.5788	0.0447
86.9023	0.0379
137.9366	0.0753
177.7055	0.199
186.4789	0.0594
249.5024	0.129
262.0019	0.130
305.3122	0.114
334.6440	0.0357
351.6432	0.208
394.3204	0.420
422.0222	0.152
433.4120	0.416
544.8612	0.307
624.5292	9.54
657.6143	1.17
815.3000	42.3
827.8017	14.8
1023.0793	6.24
1070.8881	15.4
1144.1004	11.4
1161.3110	19.4
1230.0868	26.6
1244.3590	10.8
1281.4768	3.77
1368.7819	2.79
3118.6944	0.715



$\Delta E = 1.23$ kcal mol^{-1}
Population = 0.041



$\Delta E = 1.24$ kcal mol^{-1}
Population = 0.040

Optimized Coordinates (Angstroms)

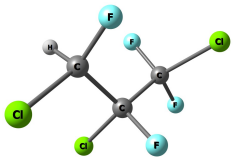
Atom	X	Y	Z
C	-1.088109425092	0.740420915682	0.426204160650
C	-0.160893417987	-0.466771575537	0.143021997199
C	1.343010918855	-0.150918832723	0.443861971337
Cl	-2.796180289149	0.221245494817	0.494111107068
H	-0.843565288590	1.155847781452	1.406086436189
F	-0.936208960846	1.681303046654	-0.522556819601
Cl	-0.349843409365	-1.067630621567	-1.518090082387
F	-0.477484471930	-1.445716641043	1.020957893054
Cl	2.051701247825	1.112604449421	-0.592527354467
F	1.413859237650	0.251556123557	1.722183651484
F	2.049276858630	-1.268594140713	0.320491039472

Atom	X	Y	Z
C	1.093695966295	0.611948266697	0.503322546339
C	0.150908971533	-0.250556149298	-0.368722947091
C	-1.337836614462	0.240652066363	-0.347506979032
Cl	2.801715734301	0.206092755902	0.171194485479
F	0.884720827760	1.914582201175	0.210907029167
H	0.911925086763	0.433462918837	1.562355218787
Cl	0.221673106904	-1.946908855424	0.185550914359
F	0.527725026724	-0.178511388271	-1.660463847601
Cl	-1.965724821711	0.433365690919	1.322143208286
F	-1.416409170851	1.408673248209	-0.977912011638
F	-2.097293113256	-0.633445755109	-0.999152617055

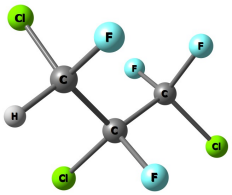
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
48.1681	0.0592
76.9506	0.0399
139.3698	0.0988
170.3331	0.0466
192.1880	0.0819
216.8875	0.216
285.0083	0.140
311.3999	0.177
319.6357	0.117
367.5331	0.172
402.8440	0.427
431.4828	0.144
452.9359	0.233
541.8046	1.20
622.3784	4.61
641.7190	7.49
786.1551	25.0
891.2552	15.6
1017.6387	28.9
1082.4553	5.60
1139.8934	14.0
1163.8953	21.1
1192.4357	11.8
1227.3621	25.5
1293.6153	3.71
1363.4752	2.83
3108.8478	0.582

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
55.5234	0.0571
70.9111	0.0166
137.2472	0.0517
180.7547	0.0834
196.9725	0.0694
233.7204	0.0916
291.6147	0.111
303.4830	0.108
322.0024	0.211
346.7091	0.220
401.2674	0.526
430.2015	0.589
435.7665	0.0743
460.6373	0.999
625.6464	6.11
751.9528	12.2
795.6415	11.8
896.9699	28.4
977.0391	29.6
1045.9888	10.1
1112.7275	10.2
1185.8853	1.77
1223.1988	22.2
1229.2913	33.4
1288.3907	3.96
1369.8503	0.829
3139.1715	0.632



$\Delta E = 1.25$ kcal mol^{-1}
Population = 0.039



$\Delta E = 1.68$ kcal mol^{-1}
Population = 0.019

Optimized Coordinates (Angstroms)

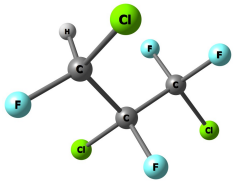
Atom	X	Y	Z
C	1.059237158149	0.628648705146	0.568366671706
C	0.161241478450	-0.314612715222	-0.271424261229
C	-1.350529544403	-0.227570064990	0.138731738113
Cl	2.726616941933	0.646249734451	-0.073351082932
F	0.563231695811	1.883774056434	0.524861818834
H	1.103186624982	0.284098121467	1.601280156102
Cl	0.703860701739	-2.000185962003	0.030876932520
F	0.262808403930	-0.037557494845	-1.578750922133
Cl	-2.136147424043	1.249425175600	-0.487973674553
F	-2.014578583793	-1.274877684217	-0.339273502509
F	-1.430731452756	-0.242407871820	1.473886126080

Atom	X	Y	Z
C	-1.515768026407	0.035732513226	0.664401365006
C	-0.018845594989	-0.365351726385	0.529031967155
C	0.858184598198	0.591638916684	-0.341303649142
Cl	-2.367070088796	0.201727840996	-0.896445162000
H	-2.020024323865	-0.753956887903	1.225178332632
F	-1.591492821492	1.194719448534	1.347467348791
Cl	0.083428967578	-2.032793869697	-0.096529897645
F	0.467180607802	-0.329282009984	1.789164692875
Cl	2.601612559947	0.272639612476	-0.082626069786
F	0.579034861201	0.447599740979	-1.631368528214
F	0.598746260821	1.851227421073	0.012818600328

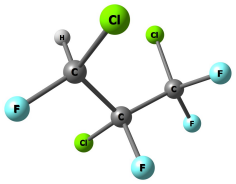
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
45.5396	0.0709
62.8334	0.0264
143.1637	0.0286
182.0162	0.0853
211.8832	0.253
231.3701	0.0380
253.0294	0.196
301.2421	0.161
320.6817	0.176
359.7269	0.210
385.7470	0.291
430.1866	0.0136
442.0941	0.227
500.3875	0.571
634.3009	5.47
751.2720	25.7
792.1255	8.12
836.1962	32.1
972.2948	1.56
1057.3866	13.3
1123.0778	16.8
1186.0849	30.1
1222.5697	18.9
1232.5128	7.21
1287.6904	3.52
1373.5003	0.913
3132.9107	0.512

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
41.8836	0.00566
87.4452	0.0613
146.1393	0.0361
180.1399	0.00956
192.4608	0.0761
214.7386	0.130
300.2255	0.0187
315.1346	0.106
323.3001	0.131
368.2413	0.0423
413.3188	0.148
426.5260	0.122
449.3443	0.662
515.1903	0.762
555.7193	13.8
660.5135	1.10
822.1766	18.7
910.1619	22.4
958.3464	22.2
1100.9968	19.5
1130.3015	10.4
1163.0815	12.3
1202.4552	16.0
1220.3836	22.8
1299.7141	7.55
1374.6570	2.06
3106.1385	0.796



$\Delta E = 1.80$ kcal mol^{-1}
Population = 0.016



$\Delta E = 1.96$ kcal mol^{-1}
Population = 0.012

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.495021069194	-0.294357629907	-0.388550106680
C	-0.078753307160	-0.425349423061	0.241206121316
C	0.926849483447	0.642855870903	-0.294411025932
Cl	-2.350395339618	1.171107736294	0.183927279017
H	-1.417663556981	-0.229519348592	-1.474454410316
F	-2.227045151715	-1.368168872232	-0.035773973268
Cl	0.528265084161	-2.056382503859	-0.199361106373
F	-0.149068045743	-0.314034488444	1.575371246638
Cl	2.561374163380	0.429330369279	0.389546166656
F	0.978743582183	0.556449277996	-1.627374070792
F	0.502492157240	1.863231011624	0.028906879733

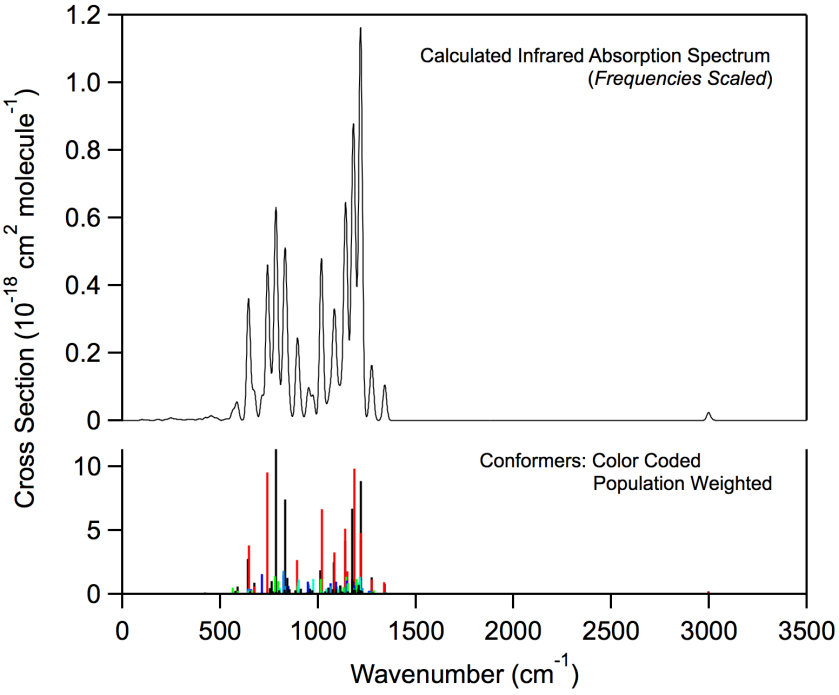
Atom	X	Y	Z
C	-1.283865100620	-0.196754632252	-0.617906336984
C	-0.102989210043	-0.508675510028	0.332071179435
C	1.056448381300	0.540287937764	0.377271970390
Cl	-2.103387038554	1.335015197923	-0.178578705052
H	-0.942441767731	-0.101684703576	-1.647797283381
F	-2.173672798312	-1.202696136695	-0.509197341287
Cl	0.575557262492	-2.092160515757	-0.176038587819
F	-0.563373346287	-0.613569702828	1.593297951403
Cl	1.633206774208	0.981934594826	-1.263422480306
F	0.635808663705	1.637919680706	0.998816575655
F	2.071136179843	0.039680789917	1.074472057945

Infrared Absorption Spectrum (unscaled frequencies)

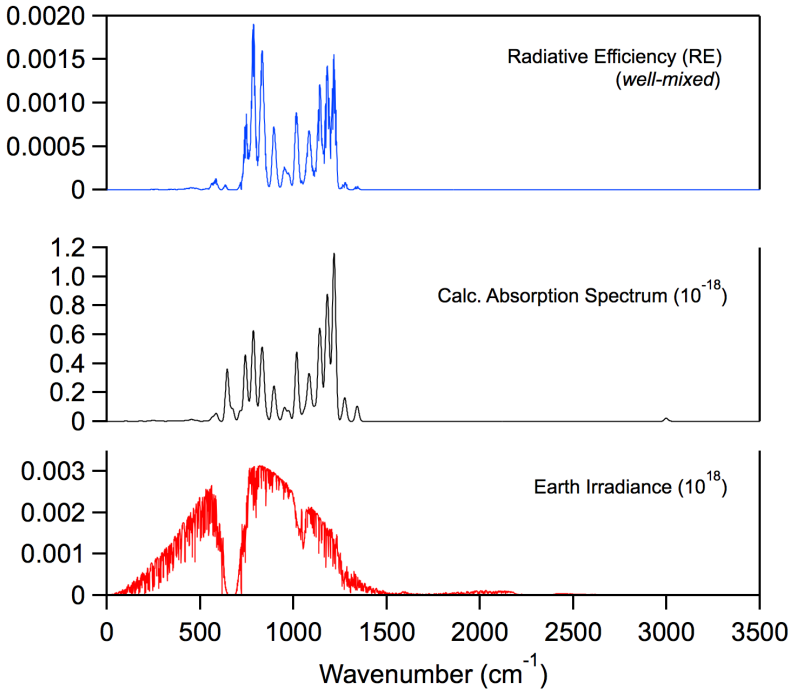
Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
34.6133	0.0310
69.2893	0.0424
143.0120	0.125
185.0967	0.0620
198.4097	0.206
237.0435	0.108
258.5848	0.0758
307.0268	0.163
317.3529	0.177
344.2560	0.0358
414.6412	0.629
422.1949	0.392
431.5694	0.282
492.7723	0.880
648.0096	1.53
741.1307	30.8
785.6364	7.71
848.1467	25.0
940.1433	8.90
1082.1225	23.5
1135.8025	10.2
1195.1042	15.8
1197.0096	22.6
1240.6062	15.0
1283.1616	1.15
1378.7878	1.69
3123.9488	0.553

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
45.7375	0.0282
80.8786	0.0280
140.5673	0.0614
176.1891	0.0930
204.5107	0.130
249.4291	0.0261
269.8495	0.0909
305.1707	0.219
321.4481	0.145
348.4100	0.142
401.9484	0.613
414.3165	0.365
435.7905	0.888
458.4629	0.451
643.1763	2.33
757.5754	18.9
775.4917	14.0
880.0465	23.3
971.8783	24.0
1040.9261	16.2
1133.5601	10.6
1191.0514	8.20
1220.0952	20.8
1237.1859	23.0
1282.5751	3.29
1373.0856	1.26
3139.8107	0.606

Infrared Spectrum

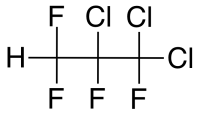


Radiative Efficiency



HCFC-224bc

Molecular Formula:	$CHF_2CClFCCl_2F$
Name:	1,1,2-Trichloro-1,2,3,3-tetrafluoropropane
CAS number:	139754-76-0
Molecular Weight:	219.39



Global Atmospheric Lifetime (years):	11.3
Tropospheric Atmospheric Lifetime (years):	15.1
Stratospheric Atmospheric Lifetime (years):	44.6
Ozone Depletion Potential (ODP):	0.141

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.322	0.308
Global Warming Potential (GWP_H):		
GWP_{20}	3091	2962
GWP_{100}	1008	966
Global Temperature Potentials (GTP_H)		
GTP_{20}		2319
GTP_{50}		430
GTP_{100}		142

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 3.89 \times 10^{-15}$; $k_{SAR}(272\ K) \approx 2.48 \times 10^{-15}$ cm^3 $molecule^{-1}$ s^{-1}

τ^{OH}_{Global} = 14.5 years
τ^{OH}_{Trop} = 15.1 years
τ^{OH}_{Strat} = 389.0 years

Fractional Atmospheric Loss: 0.776

O(^{1}D) Reactivity

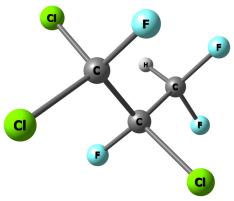
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 1.9 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)}$ = 195 years
Fractional Atmospheric Loss: 0.058

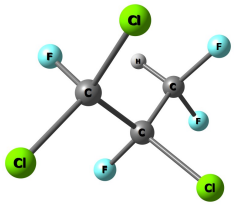
UV Photolysis

UV Spectrum: *No Recommendation*
τ_{hv} = 68 years
Fractional Atmospheric Loss: 0.166

Molecular Structure and Infrared Spectrum (9 conformers)



E = 0
Population = 0.549



ΔE = 1.03 kcal mol^{-1}
Population = 0.096

Optimized Coordinates (Angstroms)

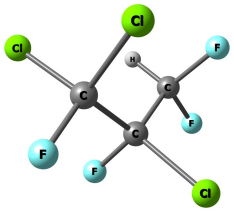
Atom	X	Y	Z
C	-1.543811085301	-0.899671387127	-0.088879720988
C	-0.472063203014	0.192791765196	-0.353449324085
C	0.909931395805	-0.115280700894	0.307385540667
F	-1.716260963684	-1.064622738909	1.233596851446
F	-2.701797576778	-0.498794055039	-0.639222076183
H	-1.239481495451	-1.846687423323	-0.544979362990
Cl	-1.075010934092	1.758034811814	0.260049414250
F	-0.298447755897	0.259187880086	-1.687659789606
Cl	1.465197682287	-1.753414495711	-0.198100758995
Cl	2.129562235228	1.086562264757	-0.188446721766
F	0.789165700897	-0.103296920851	1.631908948250

Atom	X	Y	Z
C	-1.655629436010	-0.499001225174	-0.582994967352
C	-0.483390692195	0.436488439805	-0.174626098941
C	0.918928224000	-0.234462366315	-0.353921458530
F	-1.791252296044	-1.513091272623	0.285780897998
F	-2.784293527999	0.229910090211	-0.578707844960
H	-1.481253609538	-0.893197972722	-1.590020618992
Cl	-0.725479286365	1.052372764336	1.472619829446
F	-0.520565892823	1.464104011730	-1.055047661421
Cl	2.215276095163	0.979674337771	-0.198878015825
Cl	1.196991653839	-1.587448896055	0.764268299599
F	0.942349767973	-0.713956910963	-1.614087361022

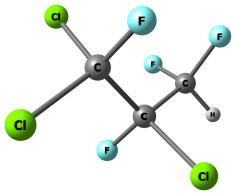
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
49.0911	0.107
80.4525	0.0844
146.1058	0.0879
193.2613	0.0573
202.9697	0.194
213.5994	0.0634
249.3682	0.0800
287.0166	0.100
303.7526	0.246
361.9692	0.0540
379.2419	0.0545
386.8457	0.292
480.6085	0.307
550.1954	2.89
608.7935	1.05
661.3070	14.6
769.5401	25.2
816.3161	27.0
1043.2487	0.735
1102.0605	2.69
1161.3983	6.05
1176.7624	32.0
1191.3937	26.4
1205.8852	8.14
1382.1664	6.69
1397.6583	2.11
3091.5432	2.45

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
48.1829	0.112
82.9403	0.0817
147.7231	0.0786
170.0529	0.00656
197.0207	0.232
220.4410	0.127
251.1687	0.0990
298.4182	0.314
320.1093	0.205
358.4643	0.0731
383.3030	0.0217
394.4695	0.0771
496.1870	0.441
520.2882	1.81
582.2047	2.97
676.6319	11.9
798.1092	21.9
873.5085	28.4
1037.4672	17.2
1090.8093	4.16
1113.0300	2.35
1167.5632	15.7
1175.1610	28.3
1190.4602	13.3
1384.2724	7.08
1399.4532	2.65
3080.1777	2.46



$\Delta E = 1.07$ kcal mol^{-1}
Population = 0.089



$\Delta E = 1.09$ kcal mol^{-1}
Population = 0.087

Optimized Coordinates (Angstroms)

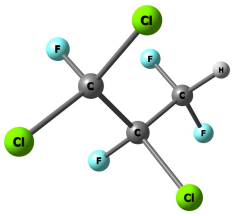
Atom	X	Y	Z
C	-1.238726958286	-0.946927392147	0.621420860875
C	-0.530419560523	-0.078090338422	-0.448805233392
C	1.000391504255	0.163223797505	-0.232840481900
F	-1.281368037441	-0.311493539456	1.803556005802
F	-2.496217069849	-1.166812131859	0.199858402214
H	-0.723171049560	-1.906501627599	0.735835536503
Cl	-1.362416975623	1.493732555035	-0.605000803440
F	-0.640198040927	-0.746202466915	-1.619723688959
Cl	1.369172519591	1.060831527469	1.255186932415
Cl	1.845609400248	-1.428032761318	-0.209361068171
F	1.456535268116	0.849576377707	-1.280962461948

Atom	X	Y	Z
C	-1.821061236215	-0.355499091527	-0.180946505790
C	-0.466474881492	0.367943931506	-0.444821127918
C	0.764022812836	-0.155825466976	0.366717463148
F	-1.816250840467	-1.568955079857	-0.759251546512
F	-2.019377943033	-0.499657957833	1.140277120199
H	-2.629860990228	0.242306207733	-0.615738108925
Cl	-0.733344444132	2.095918126661	-0.026749455938
F	-0.201618000460	0.258870963968	-1.757197021297
Cl	0.998845034511	-1.908812007135	0.098406840004
Cl	2.245405933273	0.711312787529	-0.140643905823
F	0.559813555406	0.054533585931	1.665927248852

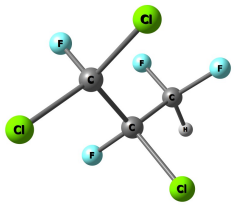
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
46.9658	0.106
85.1147	0.0851
150.8873	0.0928
168.0199	0.0226
195.4531	0.150
230.2443	0.0475
259.0352	0.223
290.0680	0.110
314.7819	0.186
352.0554	0.0227
380.2777	0.187
390.0679	0.250
481.5335	0.931
533.5827	0.288
589.1935	1.50
661.5085	14.9
783.1589	27.4
868.1237	25.8
1038.2331	7.09
1072.7027	6.68
1155.8078	11.0
1170.2267	15.5
1189.1874	27.4
1197.3397	7.61
1388.2526	4.65
1397.1605	2.55
3081.5030	2.48

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
40.0810	0.0449
90.5819	0.145
155.5872	0.0298
193.9236	0.0308
204.4831	0.108
216.1071	0.0972
237.9211	0.0676
288.3017	0.0357
317.2828	0.0823
363.8677	0.0779
385.8540	0.0343
400.7808	0.118
473.8367	0.432
547.9907	5.61
583.1121	11.5
611.7496	0.972
794.6581	44.0
884.2606	5.96
947.4776	2.33
1128.9085	4.42
1153.5738	3.23
1176.5716	37.3
1197.0522	11.2
1210.2017	19.7
1393.9594	4.02
1399.2434	4.45
3073.3634	3.03



$\Delta E = 1.38$ kcal mol^{-1}
Population = 0.053



$\Delta E = 1.59$ kcal mol^{-1}
Population = 0.037

Optimized Coordinates (Angstroms)

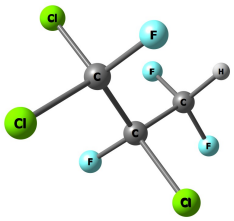
Atom	X	Y	Z
C	-1.689818719316	-0.547947866092	0.274574951735
C	-0.499423366935	0.325179697875	-0.215318591369
C	0.881172629711	-0.410570417690	-0.176842782538
F	-2.821126584472	0.144918254284	0.058717347220
F	-1.740859922960	-1.677604583281	-0.456538821917
H	-1.600929110055	-0.795199623856	1.335702014241
Cl	-0.470339399345	1.809342685532	0.776859598130
F	-0.725726055800	0.643065785501	-1.504811382620
Cl	2.185684577273	0.654811333597	-0.763238554853
Cl	1.248984364718	-1.008704836117	1.470119718674
F	0.805983587180	-1.459414429753	-1.000863496703

Atom	X	Y	Z
C	-1.871841020746	0.012638374942	-0.195235069913
C	-0.427392698234	0.589503297191	-0.242165207319
C	0.735724935779	-0.458796111953	-0.246856355241
F	-2.041778167733	-0.865153845107	-1.200629960660
F	-2.121843221171	-0.607017033362	0.967778644800
H	-2.566899518052	0.850976238822	-0.324980330764
Cl	-0.261019690554	1.753557110189	1.098466595172
F	-0.347600552387	1.249402322583	-1.420946435115
Cl	2.304584683515	0.369854251315	-0.484420462408
Cl	0.774485976956	-1.441845652862	1.236497013193
F	0.538733272626	-1.268294951758	-1.293612431745

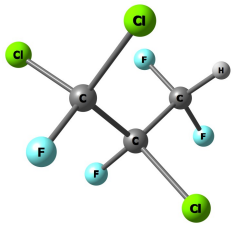
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
45.0470	0.0793
81.2854	0.0533
146.3117	0.0931
174.0761	0.0168
199.0923	0.111
232.6283	0.0254
265.4901	0.145
301.6326	0.182
316.4734	0.157
338.7569	0.318
377.9454	0.103
394.0936	0.229
446.0670	1.42
497.1728	0.600
565.9749	3.42
766.9782	21.7
827.3650	15.6
877.3868	24.0
959.8890	25.1
1080.3959	3.18
1145.2330	6.06
1148.3846	7.04
1175.8278	17.8
1222.1081	31.7
1393.1923	4.60
1399.4837	1.71
3102.7595	2.45

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
35.3083	0.0395
100.8717	0.145
156.8310	0.0198
170.4651	0.00988
200.7894	0.0425
216.2871	0.154
260.6941	0.0766
303.7061	0.0969
317.6936	0.180
360.1239	0.0206
385.6638	0.0419
412.0056	0.162
480.3167	1.82
508.6397	0.570
559.8095	10.6
618.7509	6.19
858.5894	31.6
898.3888	10.2
956.8007	19.4
1107.8496	3.66
1131.2406	7.33
1168.1067	7.21
1186.6509	36.0
1196.9399	14.6
1391.6634	2.23
1400.8560	7.90
3064.1215	3.32



ΔE = 1.63 kcal mol^{-1}
Population = 0.035



ΔE = 1.66 kcal mol^{-1}
Population = 0.033

Optimized Coordinates (Angstroms)

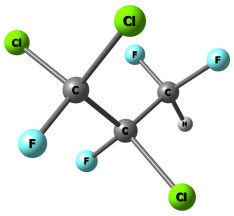
Atom	X	Y	Z
C	-1.657279819390	-0.586078268415	0.384336174309
C	-0.509892483377	0.264136574371	-0.239835446607
C	0.906690173039	-0.096000886613	0.317259565432
F	-2.834547043060	-0.086158601132	-0.027979807769
F	-1.573375852764	-1.852614470127	-0.061716281857
H	-1.605559740405	-0.569311130746	1.477564210553
Cl	-0.860765015645	1.977340391452	0.168939107573
F	-0.512799383798	0.101420468076	-1.570324566874
Cl	1.347312275452	-1.783542863992	-0.073982695554
Cl	2.155847961779	0.987719057487	-0.350454341433
F	0.868046928171	0.035126729641	1.651270082227

Atom	X	Y	Z
C	-1.310838908127	-0.719306195745	0.748456592674
C	-0.580476035047	0.103648891862	-0.345166706207
C	0.977499023871	0.200284133739	-0.211672032021
F	-2.606420971026	-0.797381007630	0.398633031604
F	-0.809524924336	-1.968936458856	0.786133050435
H	-1.216810085535	-0.253412929715	1.732649011332
Cl	-1.260017560870	1.765447504236	-0.303588910530
F	-0.847938434906	-0.444081053934	-1.545103203789
Cl	1.444933784799	0.712218413691	1.440542808936
Cl	1.748481593856	-1.358858351718	-0.611964860343
F	1.422323517321	1.107108054069	-1.082891782091

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
31.7878	0.0869
68.5006	0.0606
155.6852	0.0538
187.4504	0.0794
211.1362	0.186
237.2174	0.0497
241.4953	0.284
282.7440	0.0651
294.9566	0.0255
348.6717	0.354
379.2011	0.0127
399.0978	0.0676
439.2745	0.649
547.8213	1.22
571.9643	2.94
769.6643	25.3
801.0305	41.1
834.3764	2.61
955.2581	3.30
1089.2342	9.16
1142.7790	8.74
1155.1386	22.4
1178.4004	13.4
1239.5727	19.3
1392.2862	3.39
1402.4333	2.81
3087.9460	2.58

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
43.4198	0.0926
78.5979	0.0535
152.2509	0.0346
170.9465	0.0646
212.8586	0.162
224.1304	0.0150
267.2622	0.0769
294.7367	0.0577
311.5280	0.398
348.3952	0.331
361.3659	0.165
396.0193	0.164
447.7180	1.31
491.6328	0.574
578.6497	1.45
770.5669	23.8
812.1150	23.3
870.1863	26.0
966.5484	11.0
1056.3467	7.01
1145.0610	6.73
1165.3450	14.8
1184.3086	19.3
1228.0956	16.5
1397.4415	1.92
1399.8262	3.01
3105.1018	2.27



$\Delta E = 1.97$ kcal mol^{-1}
Population = 0.020

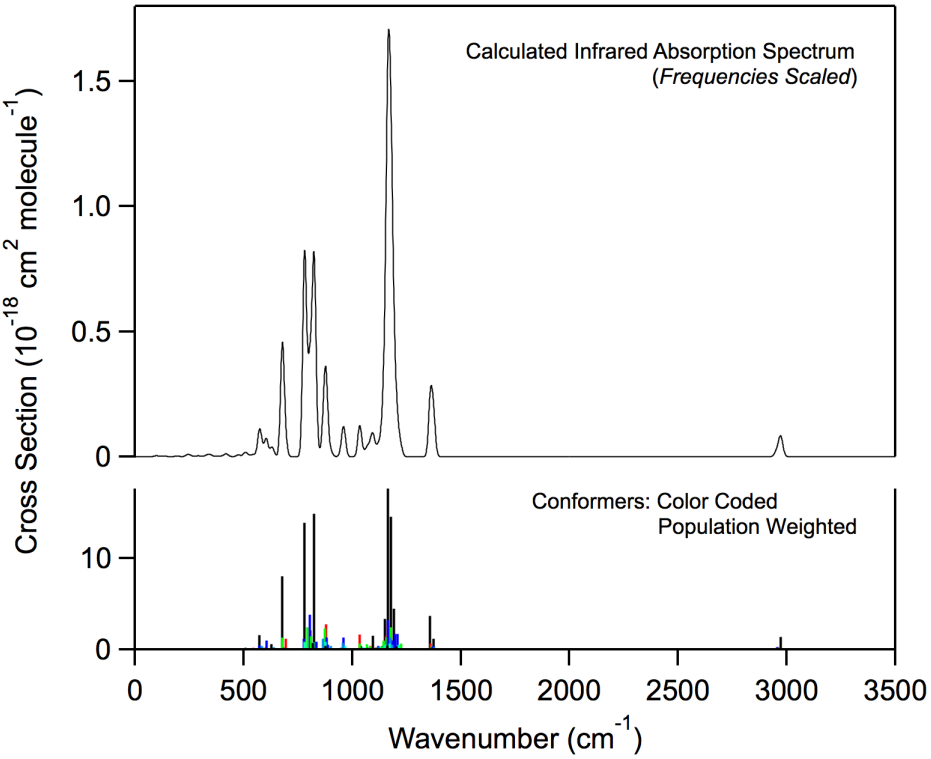
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.264349572278	-1.191929382700	0.288819985756
C	-0.623125415870	-0.031097865667	-0.517390557607
C	0.826970309727	0.438394003628	-0.154813632350
F	-0.473051179728	-2.279409075832	0.244595523547
F	-1.460365637371	-0.854227719155	1.572110988146
H	-2.225969877324	-1.426477361351	-0.183486818385
Cl	-1.734659341090	1.372258718630	-0.405481249781
F	-0.587167046994	-0.443435465927	-1.804709875194
Cl	0.974023385462	0.930530656293	1.549995929784
Cl	2.013426656283	-0.846995590832	-0.529945395468
F	1.113705719183	1.488048082912	-0.932185898448

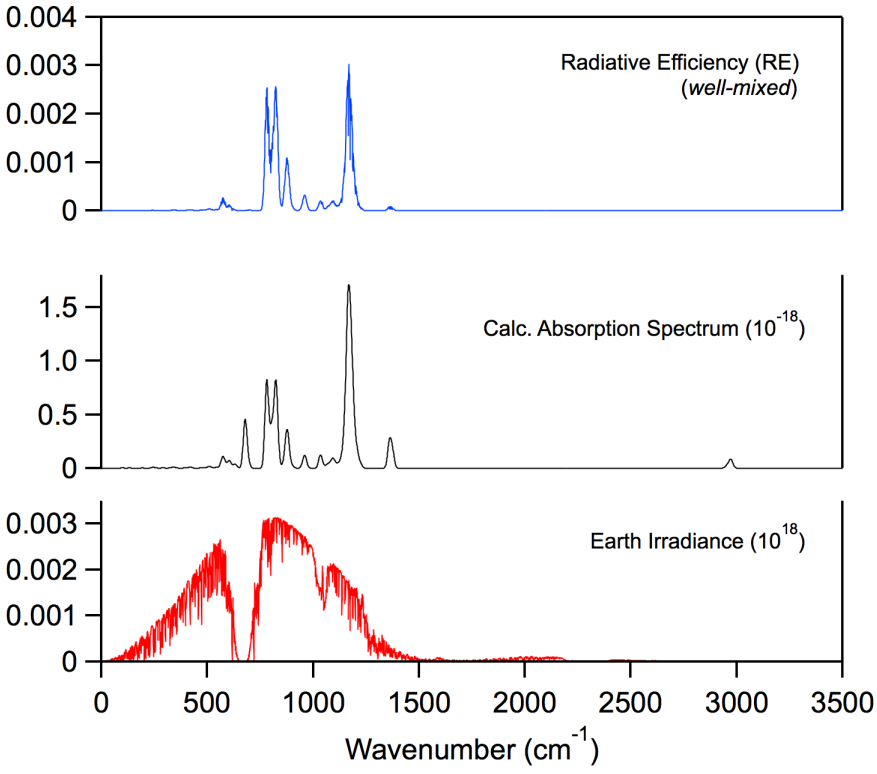
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
32.6120	0.0538
102.0702	0.105
160.1160	0.103
167.8289	0.00332
199.0062	0.0292
226.2920	0.0392
264.7430	0.257
309.9180	0.324
315.2663	0.0778
325.7565	0.239
391.2068	0.0580
408.7203	0.0927
458.3680	2.01
499.9728	0.991
588.6341	1.45
670.2621	11.0
810.8273	36.7
872.4075	20.7
965.3767	5.83
1120.6524	9.96
1132.0545	6.44
1172.8574	12.5
1173.7319	22.9
1215.8302	15.7
1392.3996	1.72
1407.0882	3.89
3064.1195	3.41

Infrared Spectrum

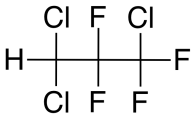


Radiative Efficiency



HCFC-224ca

Molecular Formula: $CHCl_2CF_2CClF_2$
Name: 1,3,3-Trichloro-1,1,2,2-tetrafluoropropane
CAS number: 422-54-8
Molecular Weight: 219.39



Global Atmospheric Lifetime (years): 1.79
  Tropospheric Atmospheric Lifetime (years): 1.92
  Stratospheric Atmospheric Lifetime (years): 27.5
Ozone Depletion Potential (ODP): 0.028

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.316	0.262
Global Warming Potential (GWP_H):		
GWP_{20}	582	483
GWP_{100}	158	131
Global Temperature Potentials (GTP_H)		
GTP_{20}		173
GTP_{50}		23
GTP_{100}		18

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

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

OH Reactivity

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

k_{SAR}(298 K) = 3.05×10^{-14}; k_{SAR}(272 K) ≈ 1.95×10^{-14} cm^3 $molecule^{-1}$ s^{-1}

τ^{OH}_{Global} = 1.86 years
τ^{OH}_{Trop} = 1.92 years
τ^{OH}_{Strat} = 60.7 years

Fractional Atmospheric Loss: 0.965

O(^{1}D) Reactivity

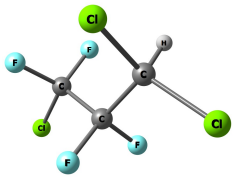
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 1.9 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)}$ = 195 years
Fractional Atmospheric Loss: 0.009

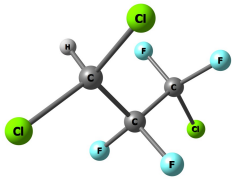
UV Photolysis

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

Molecular Structure and Infrared Spectrum (5 conformers)



E = 0
Population = 0.352



E = 0
Population = 0.352

Optimized Coordinates (Angstroms)

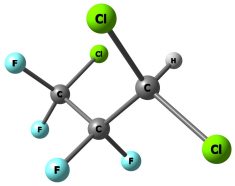
Atom	X	Y	Z
C	1.272481590017	-0.070171740477	0.467895529398
C	-0.043706128665	0.482733237091	-0.134897299937
C	-1.306708177331	-0.353191743470	0.250940751322
Cl	1.679625007883	-1.679497845092	-0.176254085743
Cl	2.590099204101	1.094864829246	0.164658475312
H	1.159275299327	-0.162924393038	1.544822461620
F	0.027609948123	0.552871176468	-1.467950580123
F	-0.221728470628	1.719928672558	0.365539743907
Cl	-2.799310123786	0.530489396827	-0.175729672237
F	-1.308275095922	-1.523542300158	-0.376049225082
F	-1.285237053118	-0.572165289955	1.571950901561

Atom	X	Y	Z
C	1.273480771292	0.074348204253	0.476646605321
C	-0.041731431276	-0.491595654096	-0.116091384123
C	-1.303950696992	0.358261567632	0.240784392641
Cl	2.589023464129	-1.102336042756	0.211805393013
Cl	1.687951915242	1.663885187364	-0.210528220707
H	1.155994607140	0.197524895254	1.550059101656
F	-0.225403834596	-1.713809820572	0.417985812931
F	0.034998582096	-0.599204192358	-1.446343325918
Cl	-2.797261517576	-0.532908535393	-0.167430233926
F	-1.287435346259	0.614043816417	1.555235071592
F	-1.299514513199	1.510614574255	-0.418686212480

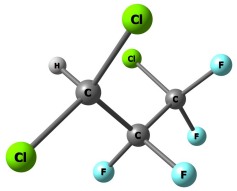
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
31.5589	0.0253
66.2219	0.0267
128.0872	0.107
190.7087	0.197
208.1149	0.170
229.0142	0.0986
239.9181	0.105
294.0024	0.101
337.0833	0.121
359.1701	0.120
380.1490	0.298
427.1812	0.0376
520.0155	0.197
573.9911	2.44
661.8111	3.78
711.7133	29.5
755.4042	1.13
821.2374	14.9
909.5775	19.2
1095.3368	20.4
1162.2141	15.5
1205.0070	34.7
1220.1662	5.91
1231.9504	5.96
1266.2007	1.84
1319.4405	4.59
3160.8910	0.362

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
31.5570	0.0253
66.2215	0.0267
128.0872	0.107
190.7084	0.197
208.1141	0.170
229.0142	0.0986
239.9178	0.105
294.0024	0.101
337.0830	0.121
359.1700	0.120
380.1491	0.298
427.1812	0.0376
520.0157	0.197
573.9912	2.44
661.8112	3.78
711.7133	29.5
755.4040	1.13
821.2376	14.9
909.5773	19.2
1095.3364	20.4
1162.2146	15.5
1205.0079	34.7
1220.1665	5.91
1231.9506	5.96
1266.2004	1.84
1319.4408	4.59
3160.8925	0.362



$\Delta E = 0.62$ kcal mol^{-1}
Population = 0.124



$\Delta E = 0.62$ kcal mol^{-1}
Population = 0.124

Optimized Coordinates (Angstroms)

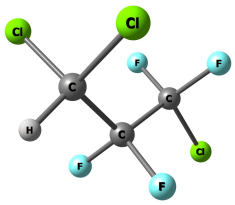
Atom	X	Y	Z
C	1.090103700679	-0.148028792692	0.497717331129
C	0.003525027711	0.576792602023	-0.325957347080
C	-1.432100328862	-0.045479178430	-0.298527728372
Cl	1.359993079574	-1.812029226037	-0.075757686555
Cl	2.595645144139	0.810040683756	0.432651312496
H	0.785056012367	-0.201088065087	1.539062655821
F	0.359491110627	0.648395922081	-1.618178340585
F	-0.119564680431	1.826534308554	0.159451797929
Cl	-2.011369534344	-0.284097196013	1.384542028652
F	-2.247975436763	0.804406418845	-0.916824643116
F	-1.463812094696	-1.203960477001	-0.944320380318

Atom	X	Y	Z
C	1.091233152997	-0.171425324523	-0.498138661562
C	0.011158454908	0.600657515816	0.290406899878
C	-1.427345916436	-0.015448166716	0.300896358638
Cl	2.601312843716	0.781652235856	-0.488945767655
Cl	1.355885991311	-1.804351498812	0.160745489753
H	0.781854780274	-0.277541335087	-1.534137353355
F	-0.108201802283	1.823809475691	-0.259396058280
F	0.372484546728	0.738212959492	1.575782235021
Cl	-2.014256098253	-0.339166775674	-1.365223535813
F	-1.461735135207	-1.138357777194	1.006607107545
F	-2.236968817756	0.869467691150	0.876813285830

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
34.9273	0.0225
75.9504	0.0200
132.8010	0.0796
176.3512	0.152
208.4785	0.0526
234.7522	0.173
265.5079	0.122
313.3683	0.298
320.1107	0.0366
337.6165	0.237
392.3110	0.191
424.0871	0.244
469.0640	1.12
595.9849	2.38
643.9123	4.53
738.0127	5.99
764.5627	13.1
816.7225	12.8
936.1904	36.8
1068.3429	12.1
1166.6351	21.5
1214.7072	13.7
1227.6634	21.2
1228.6754	4.32
1267.5603	12.9
1314.1477	5.17
3165.9501	0.455

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
34.9233	0.0225
75.9496	0.0200
132.8023	0.0797
176.3504	0.152
208.4731	0.0526
234.7494	0.173
265.5051	0.122
313.3675	0.298
320.1091	0.0367
337.6149	0.237
392.3101	0.191
424.0876	0.244
469.0627	1.12
595.9848	2.38
643.9139	4.53
738.0077	5.99
764.5648	13.1
816.7235	12.8
936.1899	36.8
1068.3422	12.1
1166.6344	21.5
1214.7050	13.7
1227.6659	21.2
1228.6787	4.33
1267.5601	12.9
1314.1526	5.17
3165.9515	0.455



$\Delta E = 1.17$ kcal mol^{-1}
Population = 0.049

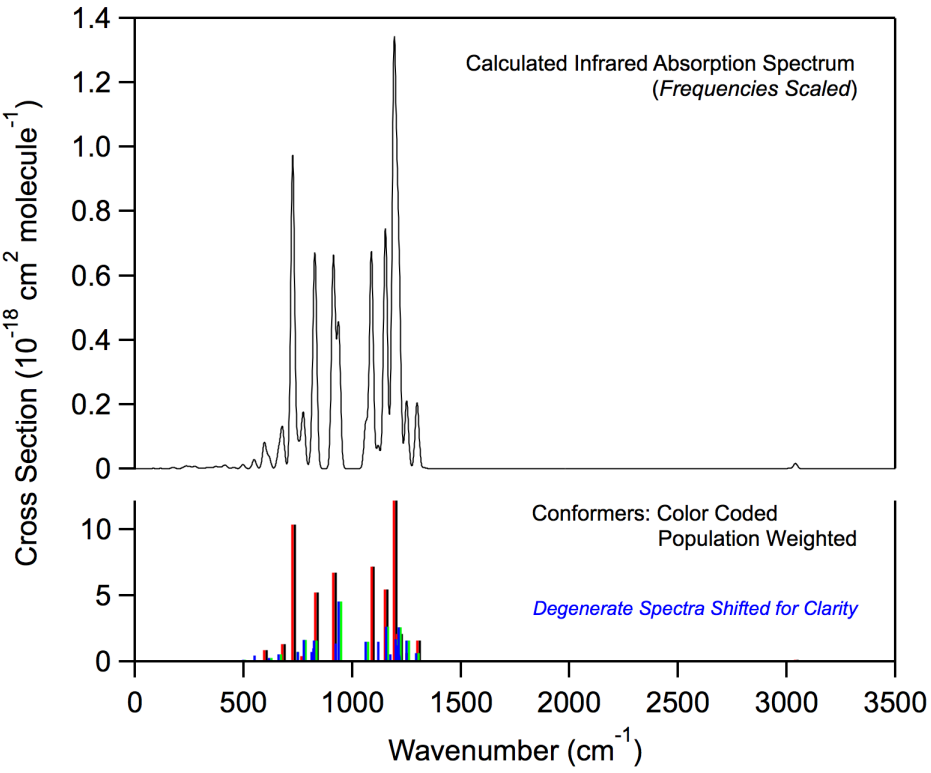
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.393445054005	-0.017806704701	-0.535348410668
C	-0.146116895812	-0.055682349367	-0.731583409778
C	-1.062524696725	0.038179176707	0.526225916109
Cl	1.960903323717	1.529776553675	0.139225795860
Cl	2.001547948014	-1.413801213160	0.388493414962
H	1.810603066304	-0.096968001157	-1.538176031380
F	-0.431140682069	-1.209609024668	-1.362454135452
F	-0.461201911183	0.967498493659	-1.546817011076
Cl	-2.782260698820	-0.028270927501	0.022045806006
F	-0.816718324744	-0.974444252093	1.352132697538
F	-0.846498182687	1.181605248606	1.169544367879

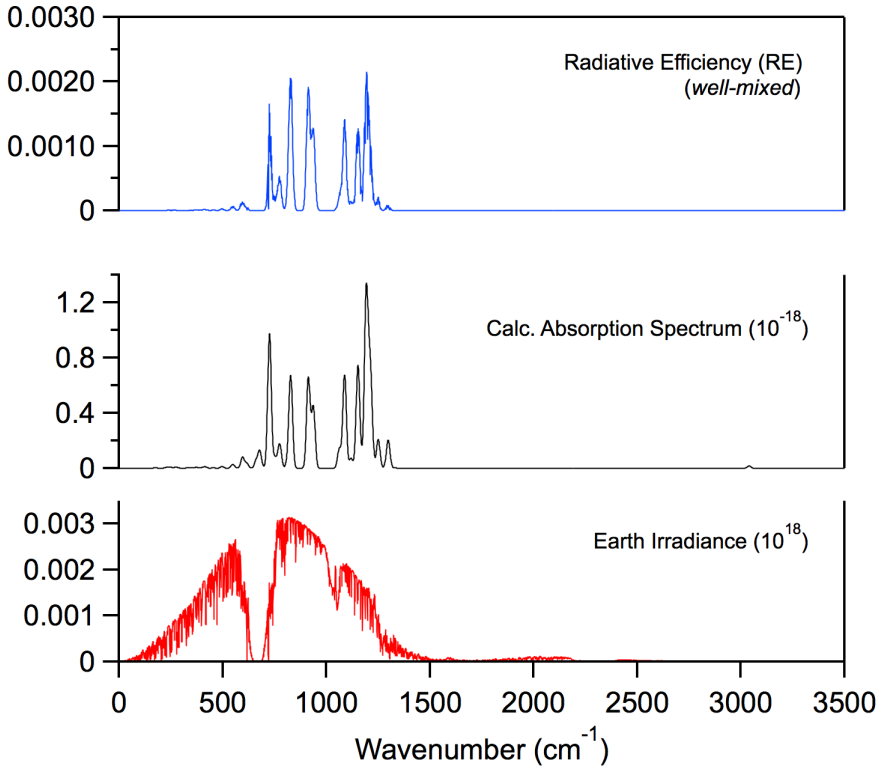
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
19.7999	0.00686
84.0544	0.0479
139.2864	0.0177
182.0367	0.160
193.1338	0.0984
220.2082	0.0743
255.9502	0.0247
314.9362	0.0222
343.9923	0.0270
374.9975	0.0374
383.2435	0.317
421.4417	0.0671
525.0553	9.77
539.9608	0.245
595.7723	3.27
684.3334	0.736
804.4957	14.5
814.0290	20.0
922.0698	28.0
1128.3493	31.1
1168.3000	2.90
1186.0860	11.6
1219.3632	25.1
1230.1766	6.54
1232.4850	9.22
1353.8462	1.32
3132.5222	0.613

Infrared Spectrum

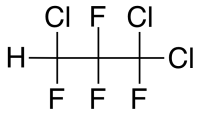


Radiative Efficiency



HCFC-224cb

Molecular Formula:	$CHClFCF_2CCl_2F$
Name:	1,1,3-Trichloro-1,2,2,3-tetrafluoropropane
CAS number:	422-53-7
Molecular Weight:	219.39



Global Atmospheric Lifetime (years):	1.57
Tropospheric Atmospheric Lifetime (years):	1.64
Stratospheric Atmospheric Lifetime (years):	35.0
Ozone Depletion Potential (ODP):	0.022

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.306	0.248
Global Warming Potential (GWP_H):		
GWP_{20}	493	400
GWP_{100}	134	108
Global Temperature Potentials (GTP_H)		
GTP_{20}		139
GTP_{50}		19
GTP_{100}		15

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 3.57 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 2.28 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

τ^{OH}_{Global} = 1.59 years
τ^{OH}_{Trop} = 1.64 years
τ^{OH}_{Strat} = 52.8 years

Fractional Atmospheric Loss: 0.985

O(^{1}D) Reactivity

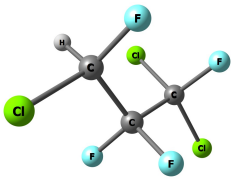
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 1.9 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)}$ = 195 years
Fractional Atmospheric Loss: 0.008

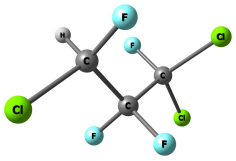
UV Photolysis

UV Spectrum: *No Recommendation*
τ_{hv} = 225 years
Fractional Atmospheric Loss: 0.007

Molecular Structure and Infrared Spectrum (5 conformers)



E = 0
Population = 0.579



$\Delta E = 0.49$ kcal mol^{-1}
Population = 0.253

Optimized Coordinates (Angstroms)

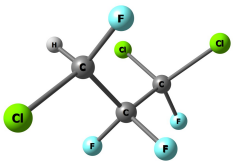
Atom	X	Y	Z
C	-1.435205463360	0.587816753716	0.029864862362
C	-0.284652324360	-0.436573665786	-0.110063391466
C	1.125201541771	0.142445022115	0.248074455069
Cl	-2.989320522530	-0.212688723959	-0.347088137332
F	-1.458976435958	1.061744022959	1.291337481334
H	-1.314110672630	1.406256140730	-0.679372701507
F	-0.255728447205	-0.875043711610	-1.377006622863
F	-0.502138301332	-1.470431949576	0.716846940760
Cl	2.361151605305	-1.119068947053	-0.000655012874
Cl	1.488156634372	1.571335986189	-0.770992261525
F	1.134748385927	0.509864072275	1.528756388041

Atom	X	Y	Z
C	-1.450402886034	-0.388957729052	0.473660792221
C	-0.295194867493	0.444310244125	-0.133704144919
C	1.124370932628	-0.051363087364	0.307999764010
Cl	-3.015034497120	0.364120184475	0.044632498014
F	-1.414179256320	-1.647846541325	-0.002784746508
H	-1.377403541060	-0.394259938952	1.561746386254
F	-0.428069886448	1.702786690687	0.325825813397
F	-0.365623907086	0.449015941847	-1.467548900838
Cl	1.539766146170	-1.624025524043	-0.410176900459
Cl	2.347798276304	1.165972280859	-0.143554381159
F	1.105261486459	-0.171223521256	1.646944819987

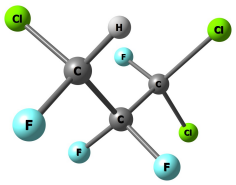
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
34.7215	0.0753
73.6966	0.0248
124.7976	0.0924
183.1035	0.134
211.5537	0.126
231.7691	0.163
252.5654	0.0761
283.5784	0.0357
317.6551	0.261
348.2126	0.143
388.0783	0.137
415.2294	0.328
471.2220	0.959
512.0481	0.651
640.9159	2.34
700.8340	37.9
778.3893	2.59
865.9090	33.9
908.6464	7.77
1109.3496	1.31
1134.8805	11.7
1186.6573	30.1
1213.3458	14.8
1252.4740	8.62
1298.7866	2.05
1372.1103	0.609
3133.7681	0.757

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
29.6581	0.0855
67.6001	0.0438
130.0600	0.0603
189.2767	0.110
221.0776	0.436
223.4694	0.0396
236.3046	0.123
280.8864	0.0250
316.6481	0.124
367.5328	0.0679
385.8896	0.0450
415.7622	0.437
468.0713	0.544
536.3716	0.539
616.1555	2.49
705.0676	39.2
793.4982	2.05
870.0443	33.6
905.4320	2.32
1101.5514	16.6
1142.5767	19.9
1149.2640	4.10
1200.4972	20.0
1265.8673	9.80
1301.7539	1.50
1375.4050	1.02
3125.0435	0.640



ΔE = 1.18 kcal mol^{-1}
Population = 0.078



ΔE = 1.35 kcal mol^{-1}
Population = 0.059

Optimized Coordinates (Angstroms)

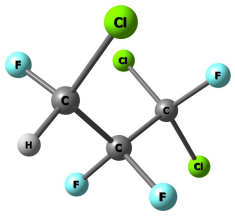
Atom	X	Y	Z
C	-1.268997537322	-0.156504594195	0.662023486142
C	-0.333537132611	0.299037071629	-0.477695317568
C	1.206216739987	0.144106563233	-0.215013961609
Cl	-2.967004820464	0.133743199572	0.178290640383
F	-1.086973438270	-1.468476082393	0.908093484256
H	-1.086828547359	0.425717564833	1.565259306444
F	-0.545126308969	1.610712170051	-0.692710938121
F	-0.610384917422	-0.373855587423	-1.603961751381
Cl	1.660990912138	0.982449670284	1.303281577199
Cl	1.716848638196	-1.557545657842	-0.171264507718
F	1.826948412097	0.747711682249	-1.231962018028

Atom	X	Y	Z
C	-1.553764606398	0.056971311307	-0.574538542089
C	-0.217647677586	0.686174626828	-0.101448637489
C	0.956068792564	-0.298384458277	0.202341037043
Cl	-2.306254871477	-0.974916979550	0.672295139169
F	-2.377247630848	1.087589263899	-0.857921183405
H	-1.402786933310	-0.553518297934	-1.464367952103
F	-0.436281965656	1.411474038153	1.005115039374
F	0.177321303093	1.511002081692	-1.089675216380
Cl	1.252149222177	-1.365002437198	-1.207123834130
Cl	2.424061301325	0.643553800416	0.579942359723
F	0.650005066115	-1.050344949335	1.258148790286

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
30.8016	0.0817
74.3528	0.0313
133.5609	0.0655
176.0083	0.145
201.8995	0.0929
236.1015	0.129
252.8919	0.0382
301.9726	0.315
325.8037	0.173
353.0318	0.306
381.2395	0.0235
407.7555	0.548
474.0029	1.55
486.0669	0.626
611.1695	2.61
754.5652	20.8
791.0165	13.9
861.7496	38.0
917.4800	9.82
1084.0900	8.69
1140.8043	18.5
1169.4185	8.87
1201.6860	24.8
1260.0554	10.1
1297.9291	0.974
1376.5983	0.790
3131.7406	0.756

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
32.5393	0.0416
82.2173	0.0289
132.6412	0.134
179.0607	0.176
195.3376	0.0737
243.8397	0.0594
278.9003	0.172
293.6946	0.151
326.6463	0.173
327.9613	0.275
386.3906	0.0994
417.8510	0.820
439.5550	0.903
513.8748	0.629
609.4995	3.62
764.7487	13.2
802.3761	30.8
836.1311	17.4
900.3630	19.0
1118.8206	9.88
1132.4137	7.13
1173.2073	39.8
1205.1497	2.39
1253.7359	12.8
1289.4489	1.53
1377.8178	2.39
3134.0386	0.738



$\Delta E = 1.75$ kcal mol^{-1}
Population = 0.030

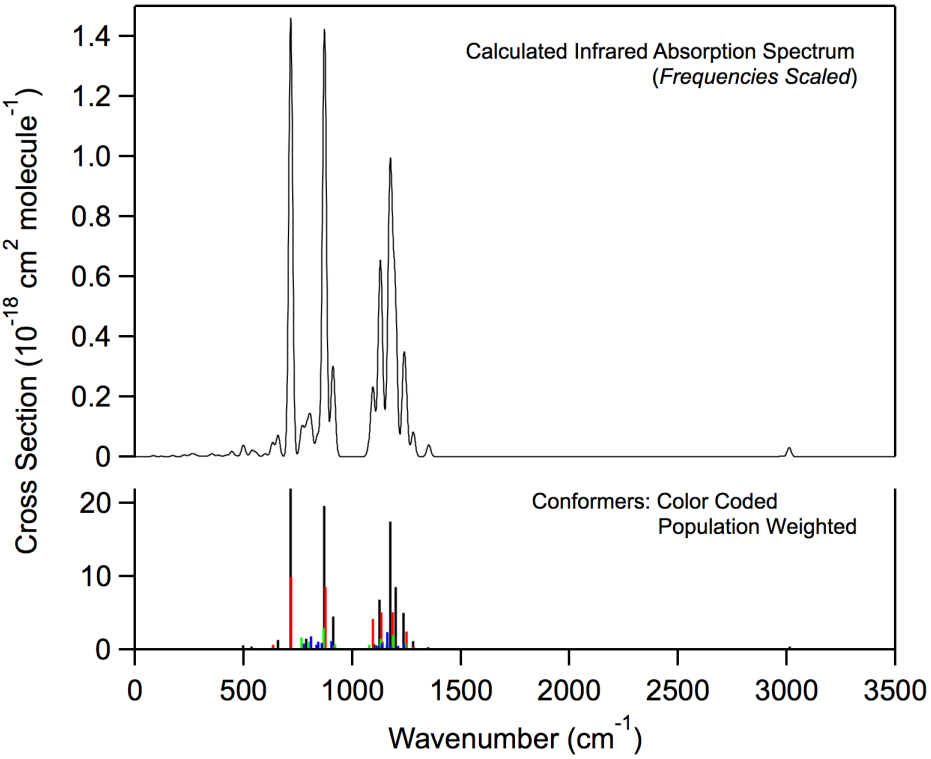
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.611078344194	-0.069143884493	-0.645153432263
C	-0.143253285753	-0.569073632454	-0.605380859829
C	0.863728024555	0.077350575655	0.398581923583
Cl	-2.443512842590	-0.179367565274	0.930445299400
F	-1.669345750486	1.189629057281	-1.114489008860
H	-2.137456214922	-0.741207520532	-1.328246698953
F	0.334630073300	-0.404991841517	-1.852639565581
F	-0.190166754453	-1.886148112202	-0.329049641270
Cl	2.475087660122	-0.661631129611	0.138781386762
Cl	0.960233297629	1.842939231103	0.187127675442
F	0.473104136791	-0.196122177955	1.644138921569

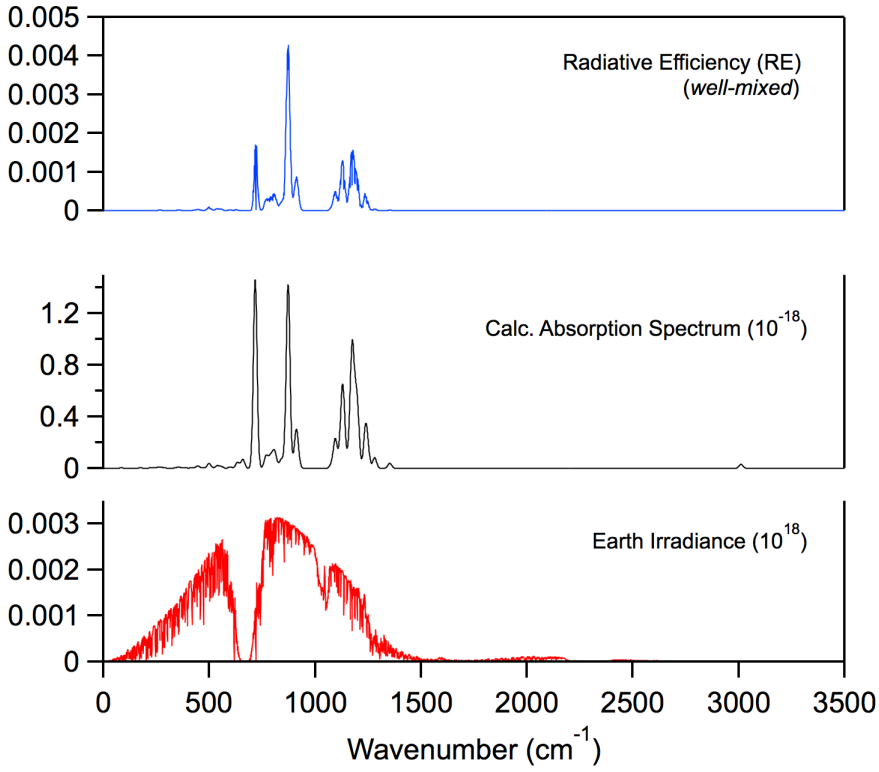
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
27.4317	0.0241
92.2949	0.0974
146.3219	0.0532
179.2549	0.0637
198.2622	0.0362
216.9204	0.202
272.8353	0.112
303.8445	0.154
322.5118	0.0319
360.1775	0.0906
383.9459	0.0706
427.1957	0.301
478.1409	0.378
528.8412	6.34
577.2849	6.83
637.4940	5.53
827.0471	21.1
853.1243	29.3
917.4087	9.09
1145.8752	26.7
1147.7420	12.8
1180.0087	3.35
1188.7483	16.1
1224.8615	15.1
1307.1237	3.79
1382.3376	2.64
3092.3700	1.18

Infrared Spectrum

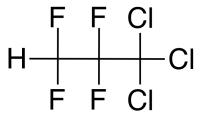


Radiative Efficiency



HCFC-224cc

Molecular Formula: $CHF_2CF_2CCl_3$
Name: 1,1,1-Trichloro-2,2,3,3-tetrafluoropropane
CAS number: 422-51-5
Molecular Weight: 219.39



Global Atmospheric Lifetime (years): 12.5
  Tropospheric Atmospheric Lifetime (years): 19.0
  Stratospheric Atmospheric Lifetime (years): 36.7
Ozone Depletion Potential (ODP): 0.174

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.326	0.314
Global Warming Potential (GWP_H):		
GWP_{20}	3342	3213
GWP_{100}	1134	1090
Global Temperature Potentials (GTP_H)		
GTP_{20}		2598
GTP_{50}		549
GTP_{100}		165

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 3.09 \times 10^{-15}$; $k_{SAR}(272\ K) \approx 1.97 \times 10^{-15}$ cm^3 $molecule^{-1}$ s^{-1}

τ_{OH} = 19.0 years

τ^{OH}_{Global} = 18.3 years

τ^{OH}_{Trop} = 19.0 years

τ^{OH}_{Strat} = 478.6 years

Fractional Atmospheric Loss: 0.686

$O(^1D)$ Reactivity

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

$k_{Est}(T) = 1.9 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)}$ = 195 years

Fractional Atmospheric Loss: 0.064

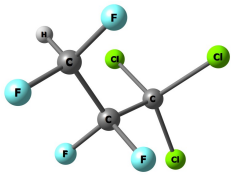
UV Photolysis

UV Spectrum: *No Recommendation*

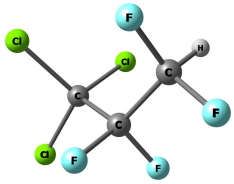
τ_{hv} = 50 years

Fractional Atmospheric Loss: 0.250

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.411



E = 0
Population = 0.411

Optimized Coordinates (Angstroms)

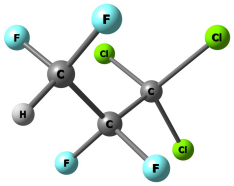
Atom	X	Y	Z
C	1.827504944169	0.192111158268	0.448158841591
C	0.617339568330	-0.545356437419	-0.185566899471
C	-0.796834348191	0.089429901412	0.040214743642
F	2.913257701023	-0.557437102052	0.178304161323
F	1.990185042666	1.400749031941	-0.116741689821
H	1.715669113808	0.298015197079	1.530914441105
F	0.601445140509	-1.779939359064	0.352564914056
F	0.825776943218	-0.652912995151	-1.505958036996
Cl	-2.015263144459	-1.021544694883	-0.645158187258
Cl	-1.077358067220	0.271640489704	1.800949515061
Cl	-0.918404893853	1.670893810165	-0.762642803232

Atom	X	Y	Z
C	1.829517723369	0.198126764178	-0.443007161146
C	0.618343015100	-0.552638860615	0.172924749588
C	-0.795478302814	0.086820447016	-0.041592410811
F	1.991235284992	1.394488119154	0.147712266979
F	2.914851398559	-0.556989756863	-0.187365052138
H	1.719448791098	0.327013266928	-1.523449354319
F	0.824642527276	-0.688260254911	1.491065482371
F	0.603350925162	-1.775495269188	-0.391373005036
Cl	-2.014988514714	-1.038476131812	0.618007869352
Cl	-0.918389322530	1.650841942145	0.794538891800
Cl	-1.073153525498	0.306457733967	-1.798503276640

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
30.1237	0.122
84.4422	0.0588
143.5492	0.0783
175.0950	0.0693
206.6784	0.106
244.7066	0.114
251.9008	0.190
266.3109	0.0128
285.7820	0.211
332.6075	0.127
365.7175	0.574
413.6989	0.0660
453.1693	0.918
562.8048	4.31
615.8524	1.83
758.1975	22.4
789.0663	9.23
827.1946	21.8
886.4794	10.2
1115.5439	13.6
1163.8512	12.5
1167.8406	5.95
1187.8294	26.0
1262.2931	15.4
1398.4895	2.09
1408.6997	2.48
3097.5119	2.81

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
30.1236	0.122
84.4424	0.0588
143.5490	0.0783
175.0955	0.0693
206.6784	0.106
244.7070	0.114
251.9008	0.190
266.3116	0.0128
285.7819	0.211
332.6073	0.127
365.7186	0.574
413.6993	0.0660
453.1681	0.918
562.8046	4.31
615.8536	1.83
758.1966	22.4
789.0669	9.23
827.1957	21.8
886.4801	10.2
1115.5459	13.6
1163.8514	12.5
1167.8409	5.95
1187.8285	26.0
1262.2929	15.4
1398.4893	2.09
1408.6990	2.48
3097.5134	2.81



$\Delta E = 0.49$ kcal mol^{-1}
Population = 0.179

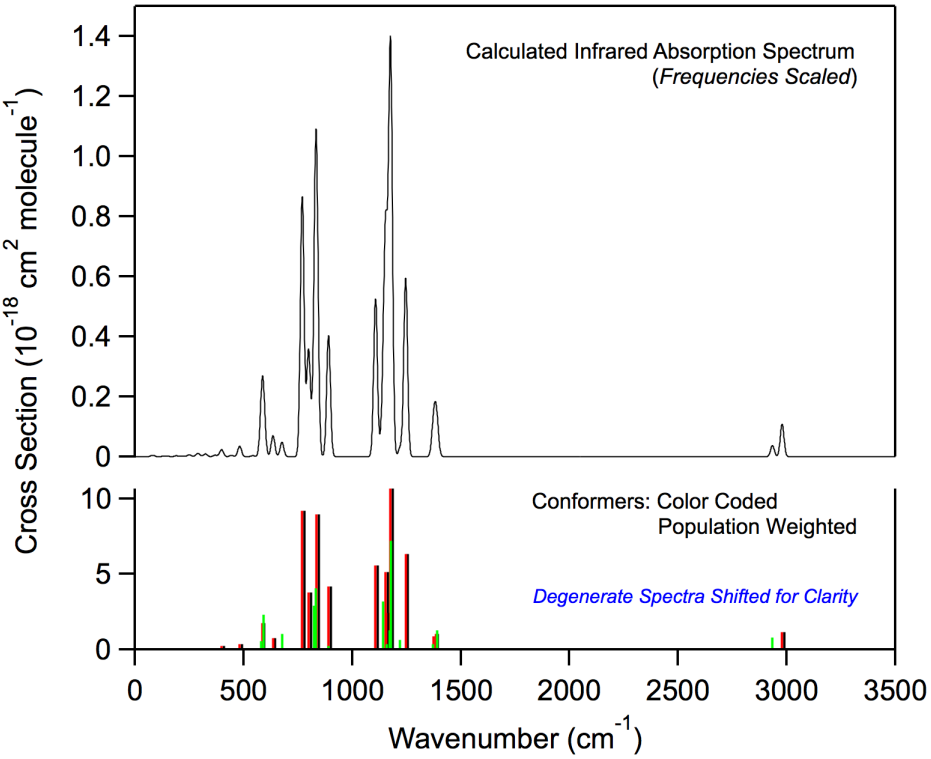
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.959363612047	-0.164983069607	-0.225013549998
C	0.503831985062	-0.508941842690	-0.641432648992
C	-0.701713342100	0.109561264034	0.143345732912
F	2.198951998259	1.151789665994	-0.332704499616
F	2.211807037095	-0.557306889973	1.034052479371
H	2.616179876177	-0.711562184834	-0.914670341803
F	0.405449428814	-1.850563170526	-0.568425806631
F	0.392588281224	-0.143681557220	-1.933394696899
Cl	-2.204080711411	-0.508133921848	-0.614824702110
Cl	-0.655731992874	-0.395506938367	1.850699728408
Cl	-0.672977172291	1.886524645038	0.025666305358

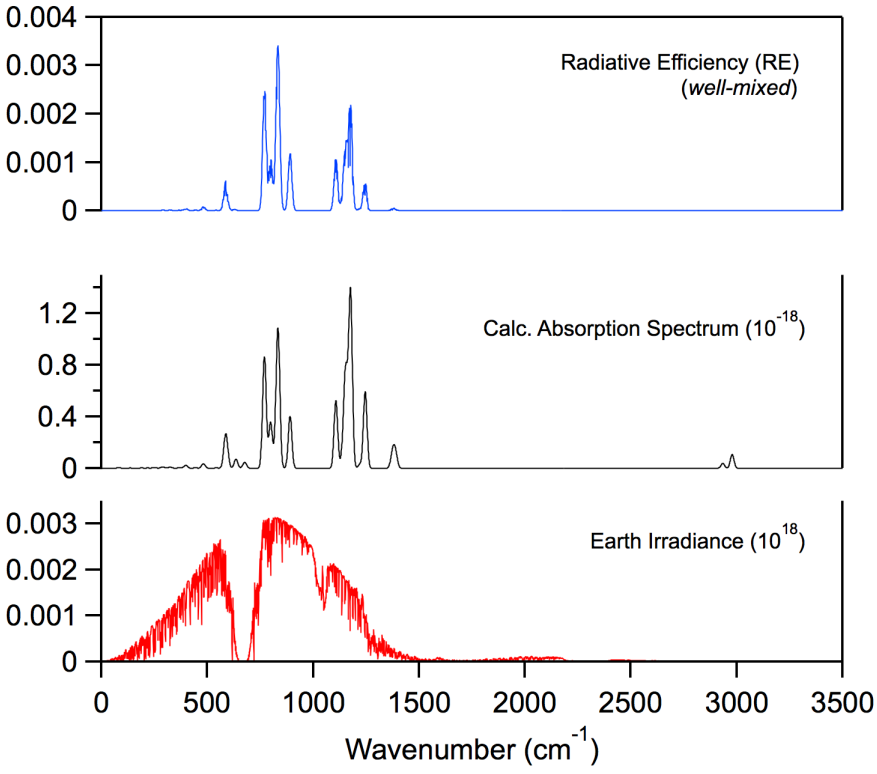
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
18.7713	0.0613
103.3008	0.171
153.8370	0.0451
179.1455	0.00108
202.9285	0.203
216.8116	0.153
259.0825	0.00922
267.4073	0.0121
293.1950	0.154
353.3118	0.264
363.7581	0.0656
412.6764	0.260
517.3625	0.423
558.4110	3.21
570.9068	12.9
659.5608	5.70
816.3395	16.2
823.0480	22.8
886.8990	1.44
1151.8227	17.8
1170.6949	2.09
1183.9480	7.17
1191.5664	40.3
1235.6487	3.50
1394.0051	2.00
1416.9056	7.21
3050.2988	4.44

Infrared Spectrum

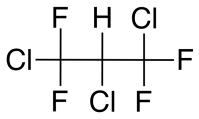


Radiative Efficiency



HCFC-224da

Molecular Formula:	$CClF_2CHClCClF_2$
Name:	1,2,3-Trichloro-1,1,3,3-tetrafluoropropane
CAS number:	431-85-6
Molecular Weight:	219.39



Global Atmospheric Lifetime (years):	10.4
Tropospheric Atmospheric Lifetime (years):	12.3
Stratospheric Atmospheric Lifetime (years):	67.1
Ozone Depletion Potential (ODP):	0.096

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.366	0.349
Global Warming Potential (GWP_H):		
GWP_{20}	3325	3176
GWP_{100}	1053	1006
Global Temperature Potentials (GTP_H)		
GTP_{20}		2418
GTP_{50}		405
GTP_{100}		146

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 4.78 \times 10^{-15}$; $k_{SAR}(272\ K) \approx 3.05 \times 10^{-15}$ cm^3 $molecule^{-1}$ s^{-1}

τ^{OH}_{Global} = 11.8 years

τ^{OH}_{Trop} = 12.3 years

τ^{OH}_{Strat} = 322.7 years

Fractional Atmospheric Loss: 0.878

O(^{1}D) Reactivity

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

$k_{Est}(T) = 1.9 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)}$ = 195 years

Fractional Atmospheric Loss: 0.053

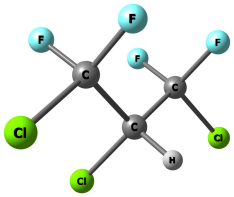
UV Photolysis

UV Spectrum: *No Recommendation*

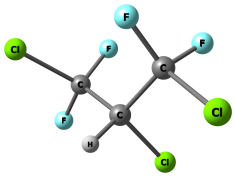
τ_{hv} = 150 years

Fractional Atmospheric Loss: 0.069

Molecular Structure and Infrared Spectrum (8 conformers)



E = 0
Population = 0.221



$\Delta E = 0.11$ kcal mol^{-1}
Population = 0.184

Optimized Coordinates (Angstroms)

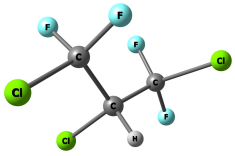
Atom	X	Y	Z
C	1.287647339921	-0.485656682094	0.046109738915
C	0.000052064211	0.268699342220	-0.377562247730
C	-1.287892574333	-0.485047035277	0.046130837930
Cl	2.754375342249	0.344479658535	-0.583027912092
F	1.377229090653	-0.578766010241	1.369911181608
F	1.276971991524	-1.721346185085	-0.461966879853
H	0.000064562058	0.355213340067	-1.463297579663
Cl	0.000441672263	1.906865224974	0.321279588415
Cl	-2.754233886496	0.345765499248	-0.583016429066
F	-1.277799163843	-1.720751297113	-0.461921576568
F	-1.377511438208	-0.578087855233	1.369934278104

Atom	X	Y	Z
C	1.036025023422	-0.573771967724	0.233339630347
C	0.052028936382	0.395301052781	-0.468920887190
C	-1.420517784889	0.232079074676	-0.006638170539
Cl	2.649949596551	-0.516171328523	-0.561577131377
F	1.179894011983	-0.267371697208	1.518579120086
F	0.587689074204	-1.829149390231	0.153216678237
H	0.094788404821	0.223490861973	-1.542668935250
Cl	0.572119892513	2.080109074072	-0.164621586005
Cl	-2.163430881147	-1.249607834855	-0.714740820458
F	-1.505151430375	0.166066323604	1.320761751251
F	-2.143052843467	1.269958831436	-0.424516649103

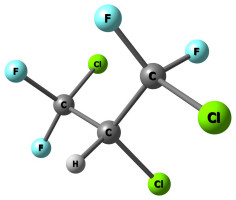
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
30.9553	0.000
69.2007	0.00935
149.5946	0.0881
185.6345	0.0430
207.5775	0.200
232.3909	0.101
257.8101	0.0155
289.5077	0.0131
354.9587	0.0387
410.5368	0.00118
425.7680	0.0766
427.8702	0.143
429.5317	0.478
601.2408	5.50
604.7363	3.04
700.9550	29.8
818.7635	2.14
887.5843	5.82
965.6530	29.7
978.5306	13.2
1141.4350	0.328
1174.6509	37.4
1208.5280	9.52
1235.0344	43.6
1272.4995	16.6
1332.3216	6.41
3140.9042	0.545

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
34.1103	0.00392
71.6529	0.00237
152.7555	0.108
173.9490	0.0698
208.5944	0.126
245.9031	0.102
261.8614	0.201
301.7555	0.0417
336.4246	0.0982
391.3374	0.346
421.6267	0.125
423.7394	0.195
436.9742	0.0654
588.3068	5.36
611.9654	1.87
762.1260	29.9
810.7144	4.87
845.1807	12.8
950.4835	15.9
966.8998	23.2
1166.7168	22.8
1183.2000	11.9
1215.3740	17.4
1235.2319	27.8
1268.9214	17.6
1336.3868	8.49
3149.9035	0.612



$\Delta E = 0.11$ kcal mol^{-1}
Population = 0.184



$\Delta E = 0.29$ kcal mol^{-1}
Population = 0.136

Optimized Coordinates (Angstroms)

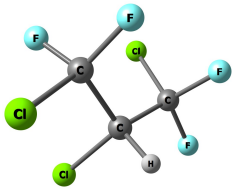
Atom	X	Y	Z
C	1.420486817193	0.231790786491	-0.006914579770
C	-0.052045492138	0.395299533459	-0.469141981312
C	-1.036236239269	-0.573436909936	0.233310058580
Cl	2.163006996819	-1.250175436579	-0.714844827527
F	2.143248259721	1.269437547242	-0.424980126291
F	1.505175557872	0.165947692205	1.320490265443
H	-0.094903579233	0.223345718484	-1.542863105273
Cl	-0.571716387158	2.080275726621	-0.165056355816
Cl	-2.650189287031	-0.515563944683	-0.561529112866
F	-0.588205217423	-1.828933169098	0.153343603136
F	-1.179963429353	-0.266817544206	1.518513161696

Atom	X	Y	Z
C	1.113200019105	-0.557673446040	0.101536617730
C	0.066816158016	0.392211652643	-0.527769418173
C	-1.387778851787	-0.145339476142	-0.523477761378
Cl	2.776172941059	-0.052088828949	-0.371585995308
F	1.038546590778	-0.573539921962	1.427455182729
F	0.919163111422	-1.801911916082	-0.345197046782
H	0.321302804738	0.512655087573	-1.582152759838
Cl	0.144153647714	1.997789169834	0.234939869694
Cl	-2.023877026071	-0.548344311846	1.098918146209
F	-2.180763730719	0.776227800896	-1.074018834266
F	-1.444998664255	-1.238646809924	-1.291601000618

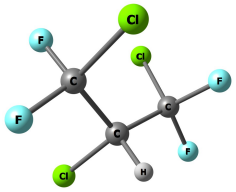
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
34.1102	0.00392
71.6528	0.00237
152.7555	0.108
173.9490	0.0698
208.5944	0.126
245.9031	0.102
261.8614	0.201
301.7555	0.0417
336.4246	0.0982
391.3374	0.346
421.6267	0.125
423.7394	0.195
436.9743	0.0654
588.3068	5.36
611.9653	1.87
762.1260	29.9
810.7144	4.87
845.1808	12.8
950.4835	15.9
966.8998	23.2
1166.7168	22.8
1183.2000	11.9
1215.3739	17.4
1235.2319	27.8
1268.9215	17.6
1336.3870	8.49
3149.9035	0.612

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
39.7663	0.000
75.8075	0.00834
146.2309	0.130
184.4730	0.0795
193.2551	0.0275
224.8396	0.0999
292.2291	0.0374
293.6094	0.0605
348.4449	0.0623
411.8750	0.157
418.5709	0.0162
428.2328	0.174
450.3293	0.407
600.4836	3.55
612.0279	10.3
659.6168	6.68
824.4167	15.7
867.2485	8.89
940.8432	11.9
1062.5833	50.4
1147.7997	1.06
1177.5613	28.8
1189.1608	21.9
1238.8423	23.8
1266.2679	14.0
1336.5838	6.39
3116.0397	0.539



$\Delta E = 0.29$ kcal mol^{-1}
Population = 0.136



$\Delta E = 0.75$ kcal mol^{-1}
Population = 0.062

Optimized Coordinates (Angstroms)

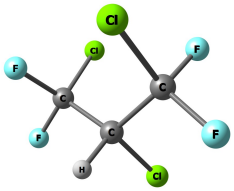
Atom	X	Y	Z
C	1.387706806111	-0.145069303495	-0.523577851334
C	-0.067012545846	0.392145617711	-0.527821039819
C	-1.113132473590	-0.557916456103	0.101656606526
Cl	2.024013284627	-0.547761663800	1.098813972796
F	1.445124441282	-1.238441797647	-1.291593586585
F	2.180439819683	0.776624800373	-1.074269327880
H	-0.321601894767	0.512422475982	-1.582198602617
Cl	-0.144666534388	1.997783348916	0.234729413945
Cl	-2.776255568657	-0.052764491926	-0.371400033100
F	-0.918839839577	-1.802155959146	-0.344963049295
F	-1.038381494879	-0.573629570865	1.427571497363

Atom	X	Y	Z
C	1.155342783891	-0.534883666166	-0.428971502528
C	0.008103555967	0.491958886019	-0.597541872856
C	-1.307649620553	0.253676950636	0.177299692740
Cl	1.691249391686	-0.778520008410	1.259388494032
F	0.777216789231	-1.713964967011	-0.932217024536
F	2.198571158409	-0.111417111957	-1.147576733175
H	-0.240100867960	0.485306539352	-1.660644214911
Cl	0.602995441769	2.132467823245	-0.201182473870
Cl	-2.061588429675	-1.326130403207	-0.238386487667
F	-1.132994294804	0.310240010633	1.493263585286
F	-2.172599907961	1.211201946867	-0.170465462514

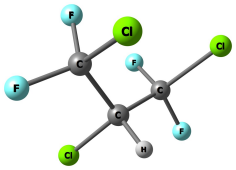
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
39.7663	0.000
75.8075	0.00834
146.2308	0.130
184.4730	0.0795
193.2551	0.0275
224.8396	0.0999
292.2291	0.0374
293.6094	0.0605
348.4449	0.0623
411.8750	0.157
418.5709	0.0162
428.2328	0.174
450.3293	0.407
600.4836	3.55
612.0279	10.3
659.6168	6.68
824.4167	15.7
867.2484	8.89
940.8432	11.9
1062.5833	50.4
1147.7997	1.06
1177.5613	28.8
1189.1607	21.9
1238.8423	23.8
1266.2679	14.0
1336.5838	6.39
3116.0397	0.539

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
28.2565	0.001
85.6535	0.00877
153.2179	0.0830
176.6110	0.0675
200.6139	0.0805
248.3343	0.202
269.1528	0.125
315.5200	0.0189
335.7666	0.139
382.3924	0.389
425.5716	0.175
427.4753	0.0639
444.2889	0.187
596.5701	3.28
656.5870	1.12
664.6045	10.3
790.8092	28.2
846.2108	5.01
969.1849	14.1
1045.7702	24.3
1150.8110	31.8
1169.2207	17.1
1196.4315	20.6
1232.1592	12.8
1261.3446	17.3
1341.9283	5.99
3113.9614	0.490



$\Delta E = 0.75$ kcal mol^{-1}
Population = 0.062



$\Delta E = 1.82$ kcal mol^{-1}
Population = 0.010

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.307529938197	0.254622134714	0.176917997319
C	-0.008385424393	0.491644716990	-0.598034325442
C	-1.155057217288	-0.535705802677	-0.428699392323
Cl	2.062310665368	-1.325066193477	-0.237690845404
F	2.171944352995	1.212373254176	-0.171556443363
F	1.132899620517	0.312014323630	1.492849297232
H	0.239778472508	0.484385530482	-1.661142172499
Cl	-0.604155419631	2.132105019199	-0.202794661436
Cl	-1.690756294405	-0.778461329544	1.259853326558
F	-2.198548133973	-0.113307624082	-1.147552188533
F	-0.776310559894	-1.714930029410	-0.931142592110

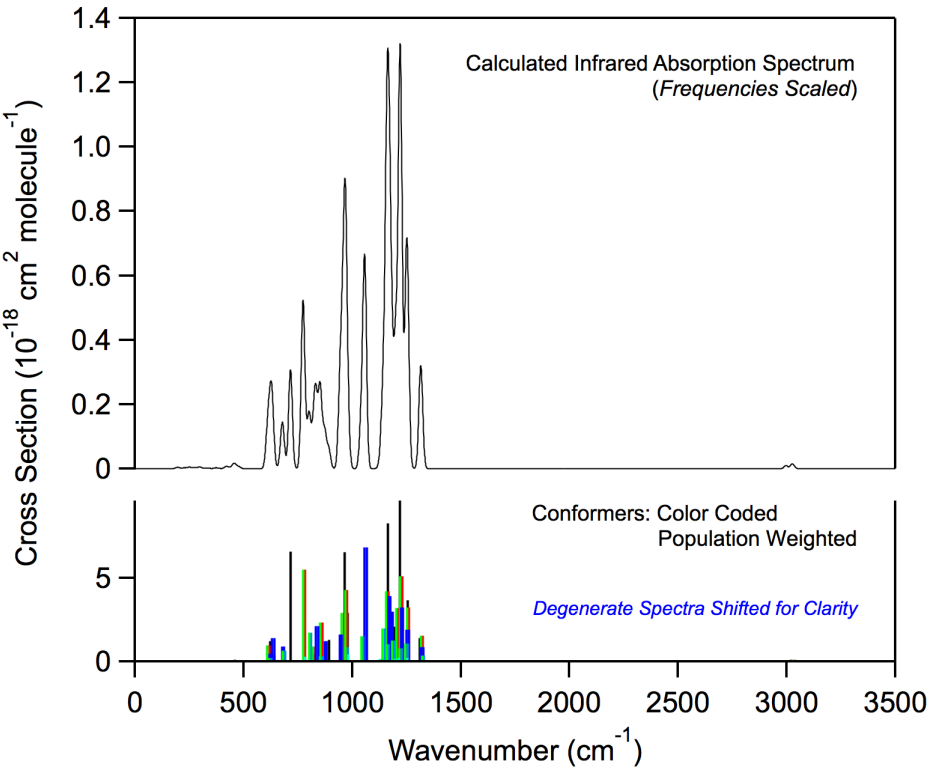
Atom	X	Y	Z
C	1.317490164164	0.073144697723	0.117657435006
C	0.000422266645	0.532584548521	-0.555384137684
C	-1.313852149719	-0.019599681922	0.068460889047
Cl	1.528547614772	-1.711142452947	0.097691560519
F	2.339294335841	0.601689098211	-0.561839885008
F	1.390524066485	0.491944260521	1.377625882658
H	0.038267948827	0.252811662843	-1.606208720047
Cl	-0.014820458313	2.329275141693	-0.486691227908
Cl	-1.755498372431	-1.614324143329	-0.648245381790
F	-1.201296964336	-0.155143576969	1.388521170675
F	-2.327827451935	0.805214445657	-0.181468585468

Infrared Absorption Spectrum (unscaled frequencies)

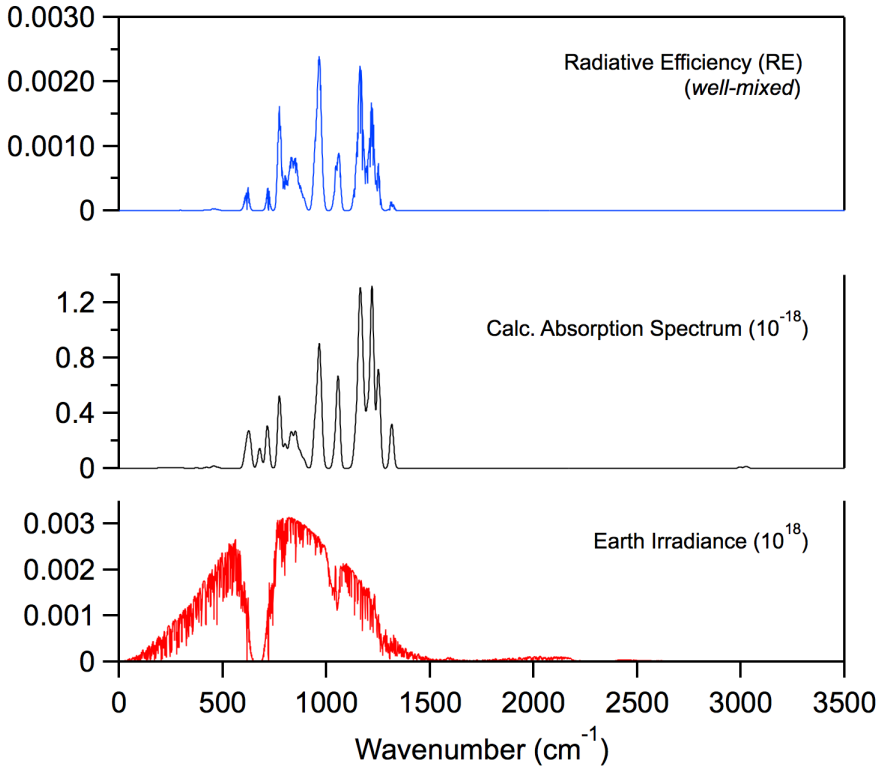
Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
28.2569	0.001
85.6533	0.00877
153.2176	0.0830
176.6110	0.0675
200.6142	0.0805
248.3343	0.202
269.1529	0.125
315.5200	0.0189
335.7665	0.139
382.3924	0.389
425.5717	0.175
427.4753	0.0639
444.2890	0.187
596.5701	3.28
656.5871	1.12
664.6046	10.3
790.8091	28.2
846.2109	5.01
969.1852	14.1
1045.7702	24.3
1150.8109	31.8
1169.2207	17.1
1196.4313	20.6
1232.1592	12.8
1261.3445	17.3
1341.9284	5.99
3113.9613	0.490

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
26.3416	0.00598
73.0043	0.00505
147.0714	0.0372
192.3347	0.139
210.0844	0.158
227.6137	0.0572
295.3613	0.0907
307.9695	0.357
323.0256	0.00626
397.7354	0.151
411.0546	0.309
425.0388	0.165
428.5911	0.112
585.4981	2.85
632.6391	2.35
770.8371	28.8
792.7598	9.16
823.1072	6.64
943.1390	2.80
983.5849	41.0
1134.1024	15.3
1203.9822	15.3
1215.0836	13.1
1229.6308	20.2
1270.3445	22.4
1336.3394	8.25
3151.5205	0.559

Infrared Spectrum

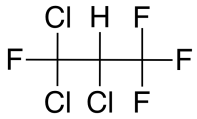


Radiative Efficiency



HCFC-224db

Molecular Formula:	$CCl_2FCHClCF_3$
Name:	1,1,2-Trichloro-1,3,3,3-tetrafluoropropane
CAS number:	431-84-5
Molecular Weight:	219.39



Global Atmospheric Lifetime (years):	9.39
Tropospheric Atmospheric Lifetime (years):	12.0
Stratospheric Atmospheric Lifetime (years):	43.4
Ozone Depletion Potential (ODP):	0.119

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.299	0.285
Global Warming Potential (GWP_H):		
GWP_{20}	2538	2416
GWP_{100}	780	743
Global Temperature Potentials (GTP_H)		
GTP_{20}		1775
GTP_{50}		266
GTP_{100}		107

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 4.89 \times 10^{-15}$; $k_{SAR}(272\ K) \approx 3.12 \times 10^{-15}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 11.6$ years

$\tau^{OH}_{Trop} = 12.0$ years

$\tau^{OH}_{Strat} = 316.1$ years

Fractional Atmospheric Loss: 0.814

$O(^1D)$ Reactivity

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

$k_{Est}(T) = 1.9 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 195$ years

Fractional Atmospheric Loss: 0.048

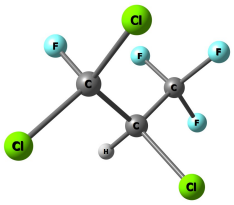
UV Photolysis

UV Spectrum: *No Recommendation*

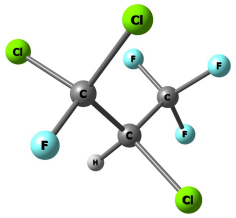
$\tau_{hv} = 68$ years

Fractional Atmospheric Loss: 0.138

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.377



$\Delta E = 0.07$ kcal mol^{-1}
Population = 0.333

Optimized Coordinates (Angstroms)

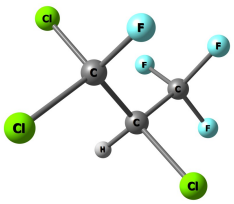
Atom	X	Y	Z
C	0.943477315907	-0.395364758693	-0.241967992909
C	-0.326543641695	0.469341461749	-0.447620224035
C	-1.666901958677	-0.267590308264	-0.209721763792
Cl	1.180895137563	-0.926846991257	1.443484013865
F	0.836153258961	-1.484544317466	-1.016892115596
Cl	2.386178360939	0.519305945034	-0.799784727657
H	-0.322891508143	0.768054252836	-1.497492821372
Cl	-0.292140165063	1.953796144667	0.534331650171
F	-2.670196940269	0.548514859233	-0.541015403814
F	-1.748236566827	-1.349185744620	-0.988678943843
F	-1.833427292697	-0.644325543219	1.053308328983

Atom	X	Y	Z
C	1.069303822778	0.173342057614	-0.269961477787
C	-0.436534162991	0.236219798167	-0.628517624117
C	-1.403229908364	-0.682558494827	0.152547382724
Cl	1.757084939394	-1.408768304937	-0.777649372344
F	1.699294307750	1.116875475322	-0.980545253879
Cl	1.405324106058	0.458077159987	1.458536465552
H	-0.512910581123	-0.040899745089	-1.681035708547
Cl	-1.022711208249	1.921723616518	-0.488457927222
F	-2.603873999771	-0.622509909467	-0.429994199924
F	-0.996652425123	-1.953060209741	0.117313184135
F	-1.538198890358	-0.322400443548	1.423968531410

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
30.1087	0.00149
82.0263	0.00830
156.9837	0.106
173.9886	0.0528
195.5479	0.0889
234.1259	0.0189
254.0273	0.126
301.0598	0.131
332.9225	0.00335
382.0332	0.0158
391.4947	0.123
493.9482	0.410
523.8519	1.20
551.8723	0.790
653.4654	8.79
677.2383	13.6
808.5325	13.9
851.1753	10.6
900.0949	5.49
1060.2559	10.8
1131.4687	3.61
1166.3217	30.7
1217.0006	33.4
1261.7288	17.0
1270.8174	32.3
1350.9932	10.3
3113.8255	0.520

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
32.8772	0.001
84.8700	0.00463
158.2881	0.142
168.9616	0.0399
206.3784	0.0465
226.4793	0.108
268.2305	0.144
297.5018	0.146
335.7258	0.0515
371.8643	0.0596
390.0343	0.0940
479.2980	0.664
523.6486	1.34
558.4850	0.619
660.6926	8.72
705.2990	5.19
779.7321	27.9
849.0872	8.30
894.5850	3.82
1049.8411	7.03
1133.2551	26.7
1172.0051	11.7
1220.2761	35.3
1260.6242	5.30
1277.6136	31.2
1352.4319	10.7
3119.3212	0.538



$\Delta E = 0.16$ kcal mol^{-1}
Population = 0.290

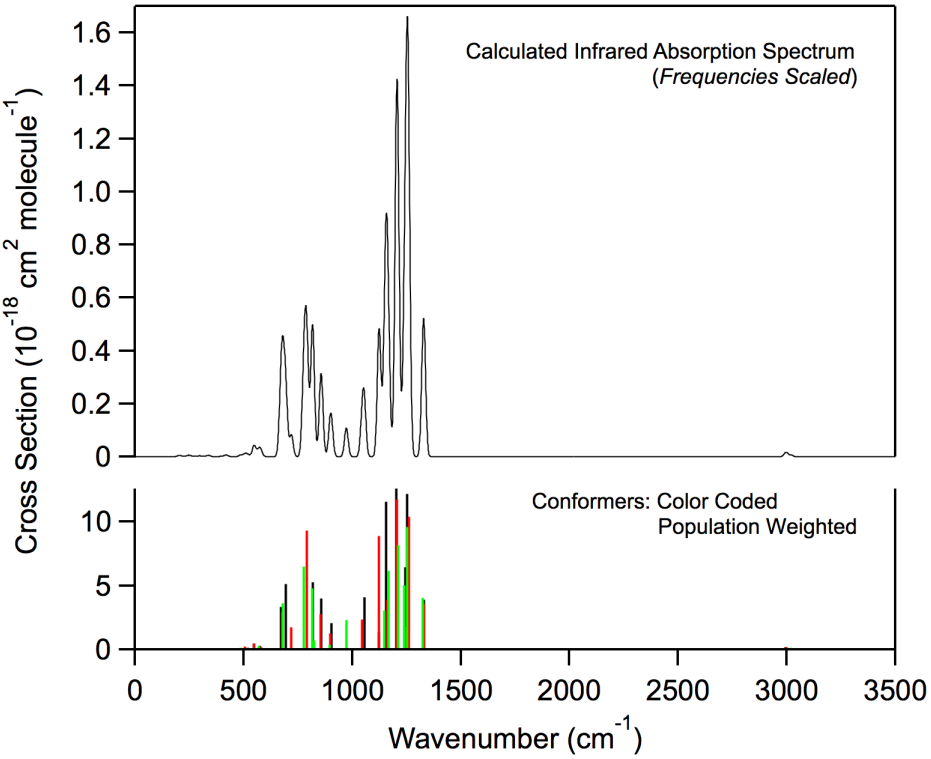
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	0.966209676926	-0.121042884358	0.223371600845
C	-0.327082183478	0.361697184567	-0.480344067779
C	-1.612429847146	-0.417179773806	-0.096483199558
Cl	2.376739901980	0.816071748807	-0.377184229585
F	0.871569539576	0.050946901460	1.541760338559
Cl	1.277081394774	-1.859718686322	-0.099975814651
H	-0.192585996308	0.272770633850	-1.557603024283
Cl	-0.593034949778	2.091567119834	-0.096817301932
F	-2.678927924300	0.198465486522	-0.606500761446
F	-1.586527000963	-1.651381068692	-0.606023779670
F	-1.763522611282	-0.506575661862	1.222110239500

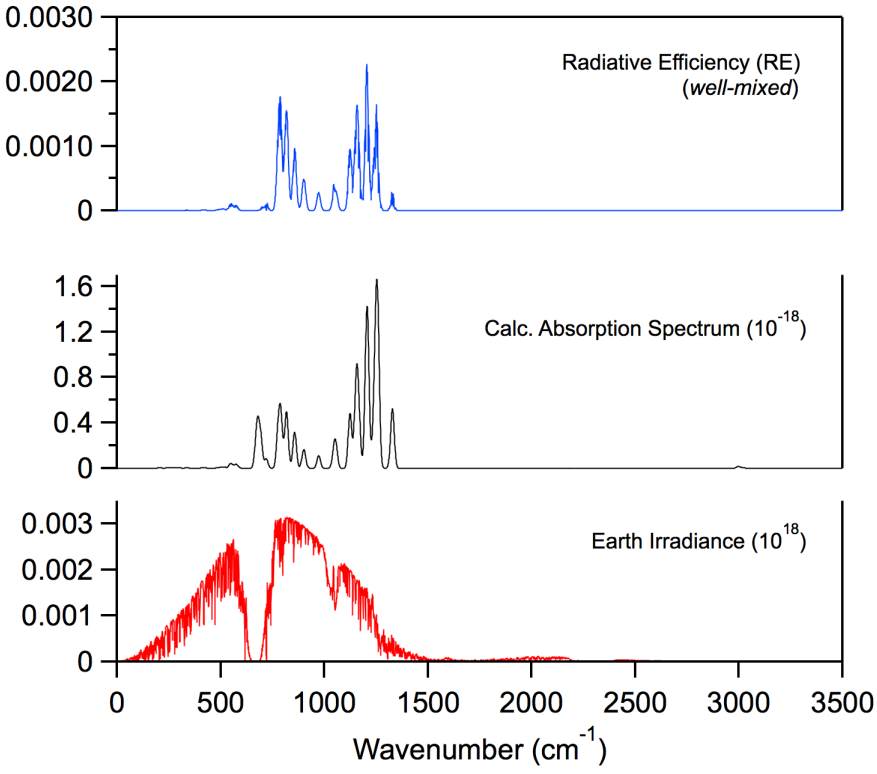
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
25.5963	0.00151
73.7216	0.00088
159.0940	0.0546
205.2110	0.106
206.4033	0.192
234.2962	0.0671
241.1971	0.0743
303.8442	0.0949
326.7552	0.00918
359.0748	0.0662
383.6377	0.201
457.9150	0.487
539.4559	0.310
547.3812	0.992
664.2518	12.5
766.3113	22.4
808.0750	16.5
815.5190	2.44
892.7484	1.30
973.1967	8.02
1158.4990	10.6
1179.0111	21.2
1225.7114	28.2
1254.6834	17.4
1270.8069	33.1
1346.8692	13.9
3140.9129	0.488

Infrared Spectrum

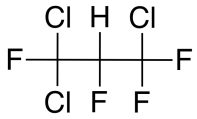


Radiative Efficiency



HCFC-224ea

Molecular Formula:	$CCl_2FCHFCClF_2$
Name:	1,1,3-Trichloro-1,2,3,3-tetrafluoropropane
CAS number:	53063-53-9
Molecular Weight:	219.39



Global Atmospheric Lifetime (years):	9.16
Tropospheric Atmospheric Lifetime (years):	11.6
Stratospheric Atmospheric Lifetime (years):	43.3
Ozone Depletion Potential (ODP):	0.117

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.328	0.312
Global Warming Potential (GWP_H):		
GWP_{20}	2735	2601
GWP_{100}	835	794
Global Temperature Potentials (GTP_H)		
GTP_{20}		1892
GTP_{50}		276
GTP_{100}		114

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 5.05 \times 10^{-15}$; $k_{SAR}(272\ K) \approx 3.22 \times 10^{-15}$ cm^3 $molecule^{-1}$ s^{-1}

τ^{OH}_{Global} = 11.2 years

τ^{OH}_{Trop} = 11.6 years

τ^{OH}_{Strat} = 307.5 years

Fractional Atmospheric Loss: 0.818

$O(^1D)$ Reactivity

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

$k_{Est}(T) = 1.9 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)}$ = 195 years

Fractional Atmospheric Loss: 0.047

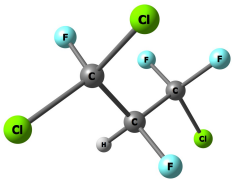
UV Photolysis

UV Spectrum: *No Recommendation*

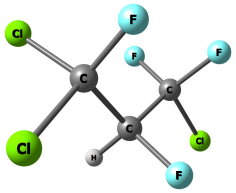
τ_{hv} = 68 years

Fractional Atmospheric Loss: 0.135

Molecular Structure and Infrared Spectrum (5 conformers)



E = 0
Population = 0.466



$\Delta E = 0.28$ kcal mol^{-1}
Population = 0.292

Optimized Coordinates (Angstroms)

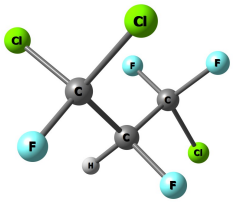
Atom	X	Y	Z
C	-1.192334291009	0.046416727285	-0.298829335100
C	0.170072184394	-0.638961787882	-0.018344244312
C	1.411788306304	0.266145771815	-0.201172594064
Cl	-1.580418728546	1.319625763084	0.885889699215
F	-1.174705732082	0.577857419225	-1.526209819651
Cl	-2.465673748333	-1.222417065019	-0.252272317468
H	0.262452530297	-1.461714544377	-0.734896106666
F	0.166367837864	-1.117435574120	1.249809231123
Cl	2.893380884160	-0.713622586764	0.098127950523
F	1.457119781826	0.731464534744	-1.450438048660
F	1.413609975125	1.295480342010	0.639352585060

Atom	X	Y	Z
C	-1.201471047332	0.009722268780	0.169566061320
C	0.161663030780	-0.511377626205	-0.356814805952
C	1.396132838973	0.275826057916	0.150376572449
Cl	-2.473411066033	-1.177023926589	-0.271058596054
F	-1.178989385601	0.127527862378	1.499155049934
Cl	-1.602571166651	1.598517762185	-0.550202200402
H	0.146453960828	-0.486321875721	-1.448917639651
F	0.314450096331	-1.789307192655	0.088728735791
Cl	2.883261130364	-0.461312712053	-0.549890827385
F	1.347528816494	1.553426025367	-0.223352401358
F	1.480975791846	0.220855356596	1.476493051309

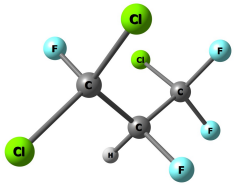
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
18.8324	0.00289
86.4062	0.0217
135.2923	0.139
186.6168	0.0746
208.0296	0.133
221.4382	0.109
244.9233	0.172
284.5698	0.0938
332.1651	0.0524
376.3704	0.00963
395.8270	0.126
419.8538	0.115
465.4500	0.874
553.7696	0.602
632.2318	17.0
638.4415	8.08
730.6555	32.5
885.3344	5.26
957.4442	22.5
1076.9100	19.8
1155.3903	7.55
1172.9807	7.66
1200.8098	40.3
1255.5852	20.1
1347.2034	0.874
1369.0240	1.71
3080.3670	0.593

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
19.7718	0.001
84.1029	0.00259
135.8243	0.0865
187.6068	0.105
220.9355	0.0929
230.4620	0.370
250.0854	0.0314
300.5076	0.144
325.6021	0.0362
362.9815	0.0698
384.2820	0.273
419.9187	0.140
459.8432	1.05
489.1498	0.988
625.2234	5.18
690.0560	33.5
840.2368	23.2
864.3043	12.3
958.7264	15.9
978.1740	14.8
1139.0352	8.42
1191.6311	10.2
1204.0175	27.7
1248.2464	29.6
1348.9173	2.90
1359.9904	0.673
3107.5123	0.405



$\Delta E = 0.99$ kcal mol^{-1}
Population = 0.088



$\Delta E = 1.07$ kcal mol^{-1}
Population = 0.076

Optimized Coordinates (Angstroms)

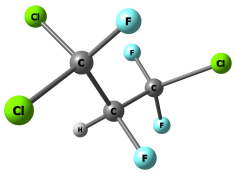
Atom	X	Y	Z
C	-1.270566847807	-0.104425467627	-0.359086756287
C	0.232569827382	-0.265887265233	-0.708916729153
C	1.277745768508	0.257707478260	0.301088012487
Cl	-1.736983776356	1.620003674999	-0.265814829195
F	-1.943686529554	-0.656516773259	-1.380927225346
Cl	-1.734906773634	-0.966105394473	1.130946502310
H	0.384692352675	0.260064040827	-1.657344192838
F	0.454319708854	-1.598060863989	-0.877107625425
Cl	2.923741433297	-0.034243391904	-0.373389525942
F	1.134896843978	1.566919672179	0.502665596345
F	1.189428992659	-0.366831709780	1.471120773045

Atom	X	Y	Z
C	-1.051564411891	0.307854457427	-0.135213914113
C	0.088497968743	-0.686832013301	-0.460497800464
C	1.512516579106	-0.349514430241	0.049963972750
Cl	-1.369711762962	0.436431481941	1.614095100821
F	-0.755888401097	1.518293395012	-0.616791723665
Cl	-2.534786453782	-0.278081099799	-0.969176126483
H	0.148812064758	-0.767467000960	-1.550771328244
F	-0.237271972891	-1.894762059024	0.075461090276
Cl	2.192733357266	1.104001611215	-0.753571198292
F	1.551903097634	-0.180135263059	1.367766112738
F	2.289282935114	-1.393773079212	-0.256428185325

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
17.3855	0.00138
90.9644	0.0133
143.1256	0.151
181.4738	0.147
192.9823	0.0278
240.6481	0.238
252.2901	0.0291
308.6369	0.267
329.6089	0.0396
365.6986	0.192
393.6429	0.217
418.8539	0.102
475.7743	1.16
488.3406	1.82
632.8726	2.16
653.2892	16.9
817.9681	34.6
867.6338	20.1
937.2296	11.5
1078.0344	28.5
1122.3212	4.91
1160.1299	19.2
1196.3770	24.7
1259.7135	17.7
1347.0500	2.07
1365.6113	1.16
3079.5293	0.485

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
13.4240	0.00241
93.9797	0.0243
142.8327	0.0879
180.4607	0.117
192.7613	0.128
242.3503	0.121
275.7978	0.305
289.1256	0.0202
319.2743	0.251
373.0893	0.175
383.6296	0.309
420.2842	0.0614
445.6073	0.818
550.6782	0.619
598.6595	5.99
670.9390	14.6
780.9691	32.6
870.9158	7.73
957.4710	23.7
1084.3716	17.4
1143.8499	12.3
1173.7072	26.8
1178.8760	15.6
1250.2296	24.8
1347.8799	0.795
1367.1472	2.72
3081.1335	0.471



$\Delta E = 1.10$ kcal mol^{-1}
Population = 0.073

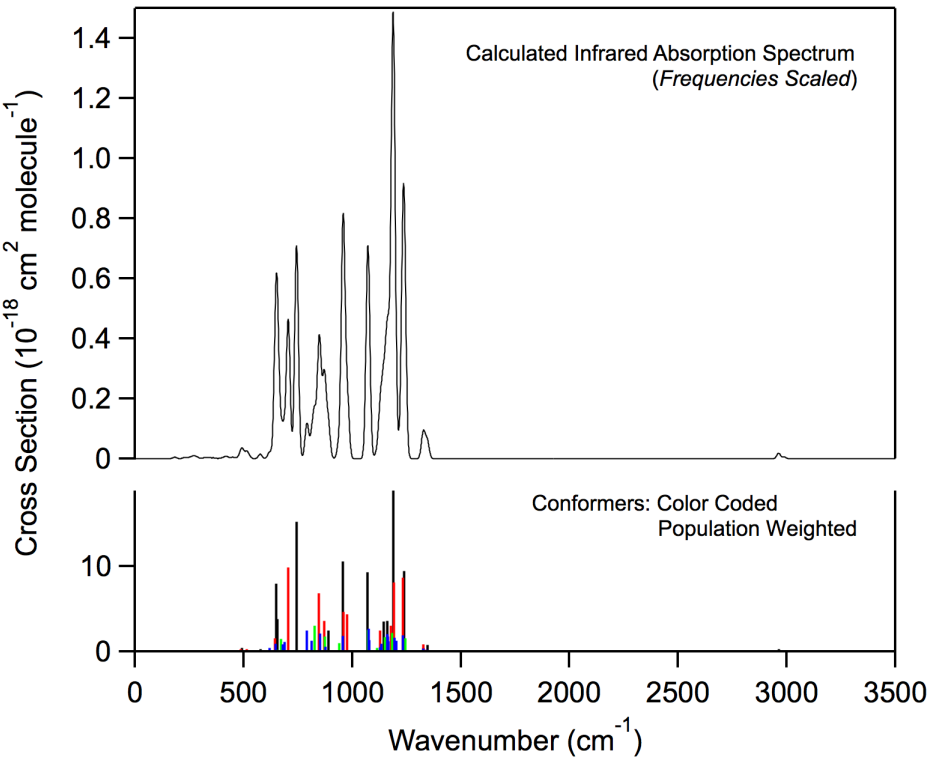
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.091184079746	0.068421838837	0.190556510932
C	0.069220050634	-0.563069237001	-0.615775966241
C	1.483048153619	0.045572641330	-0.423262032755
Cl	-2.547427126412	-0.961387731505	-0.015904052535
F	-0.804225213283	0.127398614701	1.491803609594
Cl	-1.448785896028	1.720189048298	-0.400621108112
H	-0.169020154658	-0.465679207135	-1.680185853647
F	0.165554327662	-1.879230197963	-0.284533035088
Cl	2.167983722716	-0.257396910408	1.200201257638
F	2.278251299452	-0.541326017638	-1.326579165703
F	1.484952916045	1.356170158485	-0.663604164083

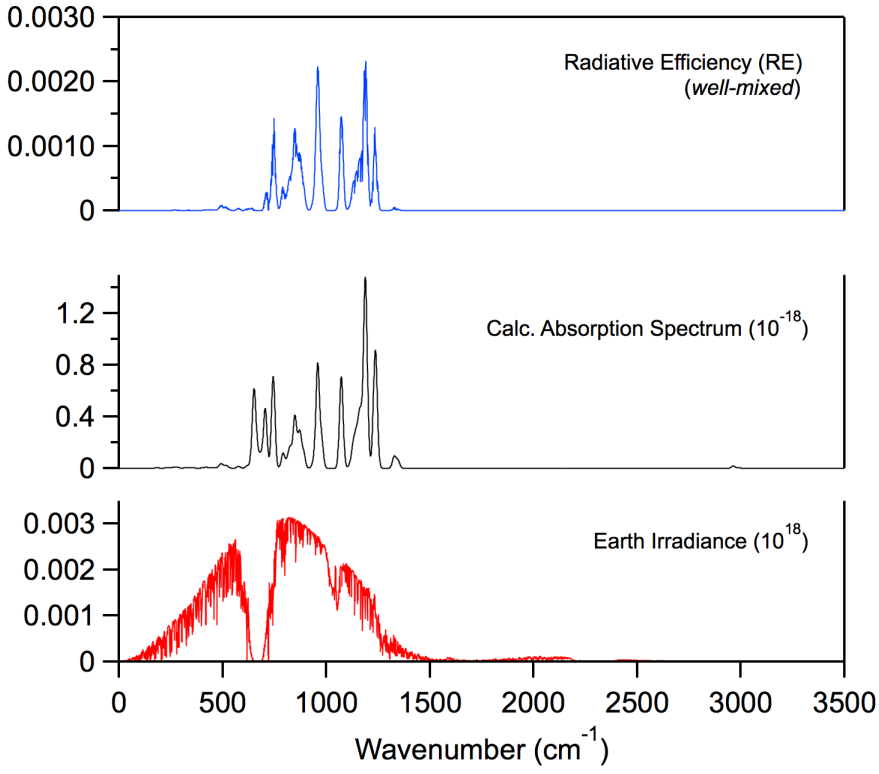
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
12.8382	0.00297
88.3848	0.0186
146.7346	0.0715
184.4954	0.0956
204.9988	0.157
225.1301	0.165
278.2591	0.134
297.2302	0.212
326.8745	0.163
357.9192	0.117
383.1345	0.255
423.6829	0.0121
469.2651	0.555
501.3301	1.34
629.6188	12.0
664.7935	11.9
803.7964	17.1
846.2566	28.6
951.3273	1.80
1082.3424	36.8
1137.1415	6.82
1175.4376	24.2
1208.5756	22.3
1216.2082	16.9
1347.2255	4.47
1364.8448	0.861
3079.9419	0.521

Infrared Spectrum

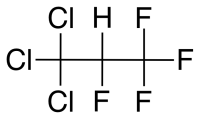


Radiative Efficiency



HCFC-224eb

Molecular Formula:	CCl_3CHFCF_3
Name:	1,1,1-Trichloro-2,3,3,3-tetrafluoropropane
CAS number:	53063-52-8
Molecular Weight:	219.39



Global Atmospheric Lifetime (years):	8.88
Tropospheric Atmospheric Lifetime (years):	11.9
Stratospheric Atmospheric Lifetime (years):	35.3
Ozone Depletion Potential (ODP):	0.126

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.247	0.235
Global Warming Potential (GWP_H):		
GWP_{20}	2016	1915
GWP_{100}	610	580
Global Temperature Potentials (GTP_H)		
GTP_{20}		1376
GTP_{50}		194
GTP_{100}		83

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 4.94 \times 10^{-15}$; $k_{SAR}(272\ K) \approx 3.15 \times 10^{-15}$ cm^3 $molecule^{-1}$ s^{-1}

τ^{OH}_{Global} = 11.4 years
τ^{OH}_{Trop} = 11.9 years
τ^{OH}_{Strat} = 313.3 years

Fractional Atmospheric Loss: 0.777

O(^{1}D) Reactivity

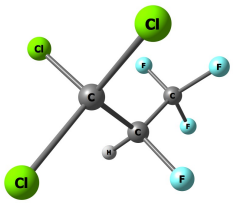
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 1.9 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)}$ = 195 years
Fractional Atmospheric Loss: 0.046

UV Photolysis

UV Spectrum: *No Recommendation*
τ_{hv} = 50 years
Fractional Atmospheric Loss: 0.177

Molecular Structure and Infrared Spectrum (1 conformer)



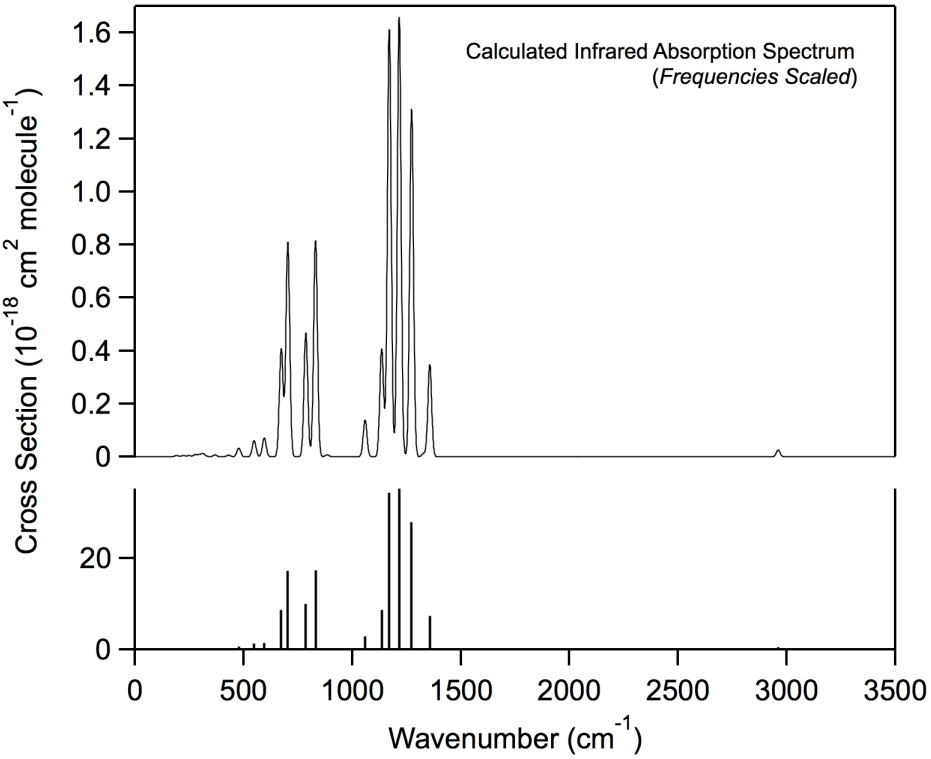
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-0.881778454877	0.072349233694	-0.027272569170
C	0.430673219641	-0.500345776888	-0.619800948783
C	1.780196732037	0.052014016676	-0.100008835693
Cl	-2.233574833320	-0.822617498571	-0.804985657371
Cl	-0.974163545378	-0.162319815659	1.736158667939
Cl	-1.034705061365	1.805629667238	-0.431113519722
H	0.401827830743	-0.318769547915	-1.699430848181
F	0.462364660164	-1.840540345636	-0.377820123253
F	2.746778119436	-0.547012535672	-0.804808097429
F	1.890875259671	1.366712386783	-0.283777438258
F	1.979265073248	-0.219197784050	1.185213369919

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
18.2671	0.000
97.1177	0.0121
146.3094	0.0921
178.9786	0.0975
206.0747	0.0933
236.3671	0.155
256.0113	0.144
274.4221	0.238
292.1829	0.0203
333.4335	0.135
399.3201	0.124
448.9309	0.686
523.9536	1.28
573.4055	1.51
655.8979	8.66
688.1343	17.3
775.9834	9.97
823.1985	17.4
879.5783	0.163
1064.6003	2.95
1145.6062	8.69
1182.6645	34.4
1230.9328	35.3
1291.3592	27.9
1350.7856	0.268
1379.9813	7.41
3078.2736	0.532

Infrared Spectrum



Radiative Efficiency