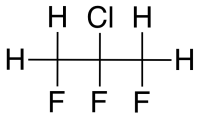
HCFC-253ba

Molecular Formula:	$CH_2FCClFCH_2F$
Name:	2-Chloro-1,2,3-trifluoropropane
CAS number:	151771-11-8
Molecular Weight:	132.51



Global Atmospheric Lifetime (years):	3.66
Tropospheric Atmospheric Lifetime (years):	3.86
Stratospheric Atmospheric Lifetime (years):	72.9
Ozone Depletion Potential (ODP):	0.017

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.146	0.131
Global Warming Potential (GWP_H):		
GWP_{20}	904	814
GWP_{100}	246	221
Global Temperature Potentials (GTP_H)		
GTP_{20}		381
GTP_{50}		42
GTP_{100}		31

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 1.52 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 0.971 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 3.73$ years

$\tau^{OH}_{Trop} = 3.86$ years

$\tau^{OH}_{Strat} = 113.8$ years

Fractional Atmospheric Loss: 0.982

O(^{1}D) Reactivity

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

$k_{Est}(T) = 1.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 370$ years

Fractional Atmospheric Loss: 0.010

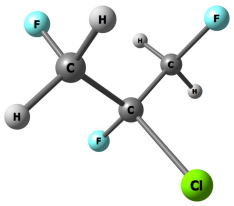
UV Photolysis

UV Spectrum: *No Recommendation*

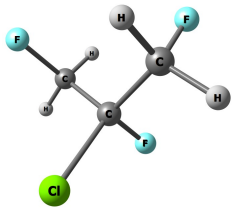
$\tau_{hv} = 450$ years

Fractional Atmospheric Loss: 0.008

Molecular Structure and Infrared Spectrum (5 conformers)



E = 0
Population = 0.447



E = 0
Population = 0.447

Optimized Coordinates (Angstroms)

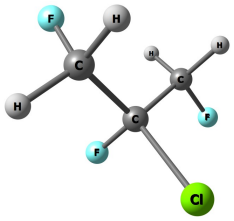
Atom	X	Y	Z
C	0.084262073720	1.212248529072	0.736986278869
C	-0.028565431397	-0.230435705826	0.253006018350
C	0.960287599926	-0.584049584706	-0.850637125689
F	-0.108635010014	2.068053598728	-0.315547253157
H	-0.661957838922	1.399346164337	1.514612803816
H	1.093133664219	1.351853195509	1.140061853671
Cl	-1.689069725908	-0.549196006761	-0.390843209819
F	0.181103828906	-1.029225638967	1.330864969608
H	0.869669541553	-1.645294047723	-1.100051975765
H	0.762414391686	0.032554112258	-1.731135803507
F	2.229726906233	-0.328494615921	-0.384094556377

Atom	X	Y	Z
C	-0.953342243722	-0.595804326090	-0.848375257462
C	0.034361659205	-0.230916390195	0.252623646697
C	-0.097191195966	1.208815165726	0.740652665434
F	-2.224592088713	-0.359466157751	-0.376660426152
H	-0.767417304730	0.025729720730	-1.728011100447
H	-0.848566418850	-1.655032665786	-1.100796561034
Cl	1.696892578075	-0.524458121116	-0.397951512659
F	-0.160060595415	-1.035274297775	1.329199111009
H	-1.106484413485	1.333074327560	1.147676351449
H	0.649094131667	1.404565341426	1.516083418291
F	0.079743891934	2.069881403272	-0.310393335126

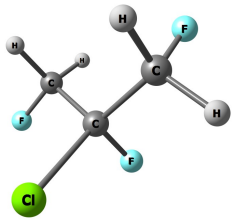
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
89.7410	0.278
141.5898	0.873
175.9357	0.147
239.5240	1.94
305.2306	0.581
329.9552	0.0830
394.3548	0.350
452.9704	3.31
522.8091	0.955
709.5459	11.1
864.0966	5.20
973.7858	3.50
1075.9496	16.8
1091.5208	5.50
1121.3949	15.5
1188.8932	4.66
1226.0868	5.84
1278.2510	1.47
1298.0055	1.87
1405.5795	0.101
1430.2522	0.866
1487.8314	0.417
1499.0500	1.34
3053.4671	2.58
3065.4978	1.71
3114.4412	1.97
3129.0046	1.63

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
89.7415	0.278
141.5902	0.873
175.9358	0.147
239.5242	1.94
305.2308	0.581
329.9552	0.0830
394.3548	0.350
452.9704	3.31
522.8090	0.955
709.5460	11.1
864.0968	5.20
973.7857	3.50
1075.9495	16.8
1091.5204	5.50
1121.3944	15.5
1188.8931	4.66
1226.0868	5.84
1278.2509	1.47
1298.0054	1.87
1405.5794	0.101
1430.2520	0.866
1487.8313	0.417
1499.0499	1.34
3053.4667	2.58
3065.4979	1.71
3114.4408	1.97
3129.0047	1.63



$\Delta E = 1.53$ kcal mol^{-1}
Population = 0.034



$\Delta E = 1.53$ kcal mol^{-1}
Population = 0.034

Optimized Coordinates (Angstroms)

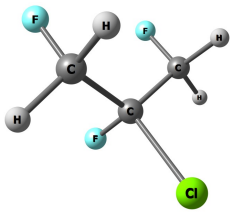
Atom	X	Y	Z
C	-0.310170797214	1.232606591845	-0.555258009301
C	0.084566636000	-0.078883499492	0.114412614088
C	1.415673381464	-0.631170452059	-0.384555501059
F	-1.513315773848	1.662124789595	-0.073977873355
H	0.462979278603	1.972299728995	-0.320384544950
H	-0.370934281127	1.093037956105	-1.639864729522
Cl	-1.172335489264	-1.346091541020	-0.199673208909
F	0.156449594445	0.120085706788	1.454087506394
H	1.685094539111	-1.506350974785	0.214255510487
H	1.340995046082	-0.911524595684	-1.439545728174
F	2.378055865747	0.342362289710	-0.236158035699

Atom	X	Y	Z
C	-1.413758190012	-0.637705888066	-0.381302148488
C	-0.084687436559	-0.078468685519	0.115344204002
C	0.307438869849	1.229321961843	-0.563039511169
F	-2.378843267539	0.334330239488	-0.240859660319
H	-1.337094238993	-0.925247236807	-1.434213551309
H	-1.681616908169	-1.509370105673	0.223310546185
Cl	1.175874698655	-1.344567165272	-0.188377437815
F	-0.158683915825	0.129693058404	1.453506355804
H	0.369855425862	1.082316440306	-1.646569374420
H	-0.467909221749	1.968624982377	-0.334262885708
F	1.508890184480	1.665336398919	-0.083372536765

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
98.1999	0.880
116.8889	0.509
178.9112	0.215
213.5276	0.366
329.0541	0.179
333.1576	0.294
367.5104	0.239
412.5603	0.372
592.4939	7.09
697.6921	8.52
896.0432	14.1
952.4044	2.31
1057.8407	12.5
1095.4086	2.74
1133.2743	13.0
1187.1671	5.30
1205.8715	4.81
1278.9953	2.49
1315.8441	4.91
1414.3069	0.708
1430.3071	0.707
1493.5709	0.697
1498.9572	0.515
3045.4662	2.53
3058.2002	1.71
3101.5236	2.15
3118.2701	2.51

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
98.1991	0.880
116.8884	0.509
178.9109	0.215
213.5274	0.366
329.0541	0.179
333.1573	0.294
367.5104	0.239
412.5604	0.372
592.4940	7.09
697.6920	8.52
896.0431	14.1
952.4049	2.31
1057.8410	12.5
1095.4084	2.74
1133.2749	13.0
1187.1681	5.30
1205.8715	4.81
1278.9960	2.49
1315.8446	4.91
1414.3077	0.708
1430.3076	0.707
1493.5715	0.697
1498.9580	0.515
3045.4664	2.53
3058.1999	1.71
3101.5239	2.15
3118.2699	2.51



$\Delta E = 1.91$ kcal mol^{-1}
Population = 0.018

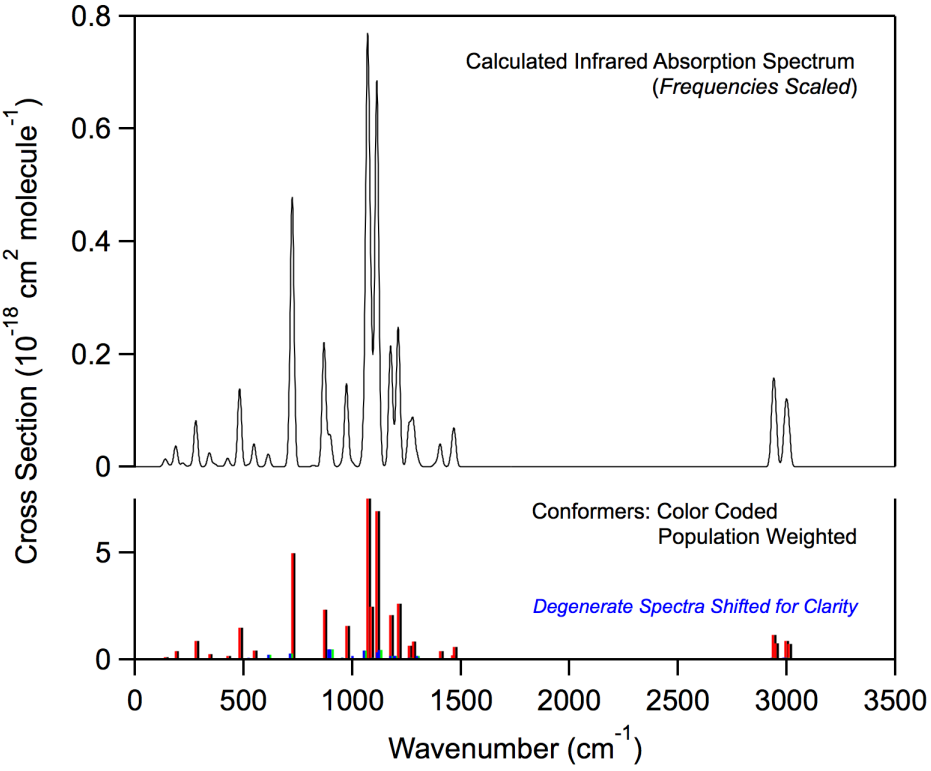
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	0.367299052161	1.301210568533	-0.402026075840
C	-0.201295571624	-0.000691959821	0.159926544829
C	0.371225641042	-1.295137115564	-0.415114506937
F	1.707978598435	1.369103320211	-0.132806037814
H	0.203405794551	1.340511518460	-1.484004768632
H	-0.144154631090	2.142631160589	0.076907311681
Cl	-1.980782271471	-0.001462749451	-0.221066901640
F	-0.043152591359	-0.007226291370	1.503627626607
H	-0.137669002845	-2.142886680513	0.055308361469
H	0.207429731055	-1.324026076688	-1.497436000132
F	1.712110251144	-1.361681694386	-0.146579553592

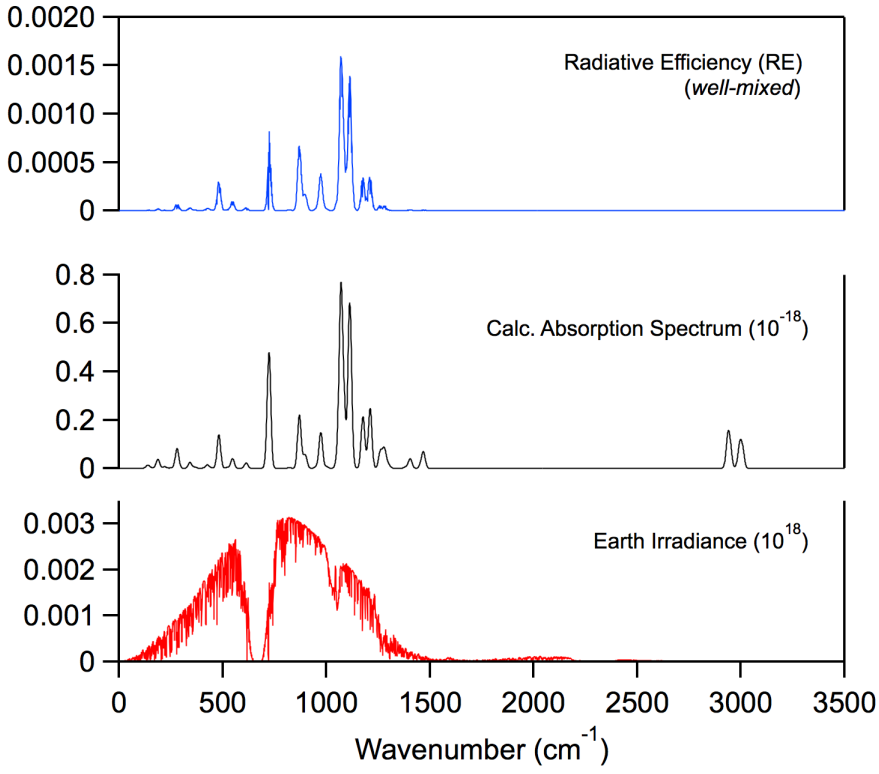
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
73.5940	0.372
138.2305	0.617
197.6720	0.538
216.3397	0.999
316.9933	0.337
327.5996	0.0437
360.5616	0.186
420.5775	0.774
495.3136	4.42
813.2408	3.09
884.6129	26.5
954.4692	0.440
1001.6162	9.28
1096.5551	0.669
1123.1617	19.6
1211.2560	8.77
1213.7957	0.0505
1300.8279	0.642
1324.9302	4.81
1407.3825	0.296
1440.1752	2.33
1488.9918	0.688
1500.0607	0.259
3046.6440	1.45
3050.7919	3.05
3103.5869	1.15
3107.8407	4.28

Infrared Spectrum

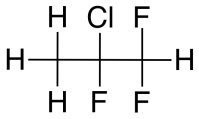


Radiative Efficiency



HCFC-253bb

Molecular Formula:	$CH_3CClFCHF_2$
Name:	2-Chloro-1,1,2-trifluoropropane
CAS number:	69202-10-4
Molecular Weight:	132.51



Global Atmospheric Lifetime (years): 7.85
- Tropospheric Atmospheric Lifetime (years): 8.46
- Stratospheric Atmospheric Lifetime (years): 108.1

Ozone Depletion Potential (ODP): 0.024

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.195	0.184
Global Warming Potential (GWP_H):		
GWP_{20}	2397	2265
GWP_{100}	704	665
Global Temperature Potentials (GTP_H)		
GTP_{20}		1547
GTP_{50}		195
GTP_{100}		94

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 6.93 \times 10^{-15}$; $k_{SAR}(272\ K) \approx 4.42 \times 10^{-15}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 8.16$ years

$\tau^{OH}_{Trop} = 8.46$ years

$\tau^{OH}_{Strat} = 231.0$ years

Fractional Atmospheric Loss: 0.962

O(^{1}D) Reactivity

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

$k_{Est}(T) = 1.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 370$ years

Fractional Atmospheric Loss: 0.021

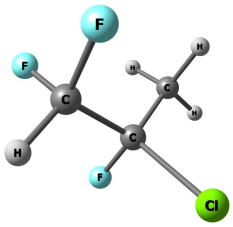
UV Photolysis

UV Spectrum: *No Recommendation*

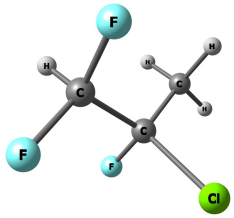
$\tau_{hv} = 450$ years

Fractional Atmospheric Loss: 0.017

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.828



$\Delta E = 1.27$ kcal mol^{-1}
Population = 0.097

Optimized Coordinates (Angstroms)

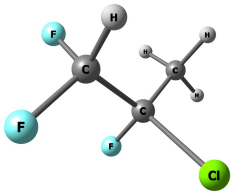
Atom	X	Y	Z
C	0.137691961668	0.911422326248	1.451574458449
C	0.249565811794	0.408945901511	0.028828308834
C	-0.954623737931	-0.432240971516	-0.429534557873
H	1.015697053602	1.508699401378	1.700911636909
H	-0.760166181355	1.529508116069	1.532282298608
H	0.059373667156	0.070639912991	2.141591722546
Cl	1.732619123033	-0.613455371382	-0.181404656955
F	0.340932900346	1.451974175582	-0.837748545381
H	-0.838161483134	-0.770373200777	-1.464779975757
F	-1.110667368079	-1.495241840836	0.384900001491
F	-2.063368747098	0.339076550733	-0.333840690872

Atom	X	Y	Z
C	1.031517929947	1.519211135781	0.569282578717
C	0.410498305709	0.371872239682	-0.200632196301
C	-1.125779540208	0.355432727747	-0.117871829581
H	2.115282237006	1.495925014806	0.446075354274
H	0.650110523186	2.467188307597	0.175607754653
H	0.782623160794	1.443178388566	1.627977580584
Cl	1.049155781062	-1.208086032863	0.401096449508
F	0.718663189334	0.476740377221	-1.522699280299
H	-1.525925299568	1.267248569344	-0.582818422101
F	-1.624519090047	-0.713819767610	-0.759526510366
F	-1.513736197215	0.311156039729	1.174793520912

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
83.3491	0.266
185.8556	0.123
225.8369	0.194
247.9593	0.977
311.5763	0.131
317.9710	0.179
394.4670	0.611
442.2874	2.12
500.9973	1.36
596.0065	2.04
725.3151	8.47
867.3692	7.84
985.2594	3.96
1101.5050	21.9
1127.8769	8.79
1155.6346	19.2
1200.0148	17.5
1254.9709	3.05
1385.7333	1.42
1385.9868	1.51
1415.5538	4.31
1477.2285	0.162
1487.1958	1.47
3065.7966	0.440
3080.0169	3.89
3147.6992	0.596
3164.1801	0.419

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
78.6906	0.137
194.8767	0.187
214.1448	0.304
233.7051	0.00661
308.4100	0.182
336.1278	0.143
379.2967	0.0960
490.3598	0.0467
532.5613	2.43
600.8648	9.93
649.0265	4.80
924.5602	2.04
946.0023	4.32
1117.7466	10.9
1148.1024	13.4
1169.7175	25.2
1194.3171	14.5
1240.0510	3.53
1382.1489	3.07
1404.1261	2.95
1410.6369	3.52
1480.8259	0.582
1484.1638	0.874
3035.6999	4.61
3054.0045	2.02
3134.9322	1.09
3165.9667	0.363



$\Delta E = 1.42$ kcal mol^{-1}
Population = 0.075

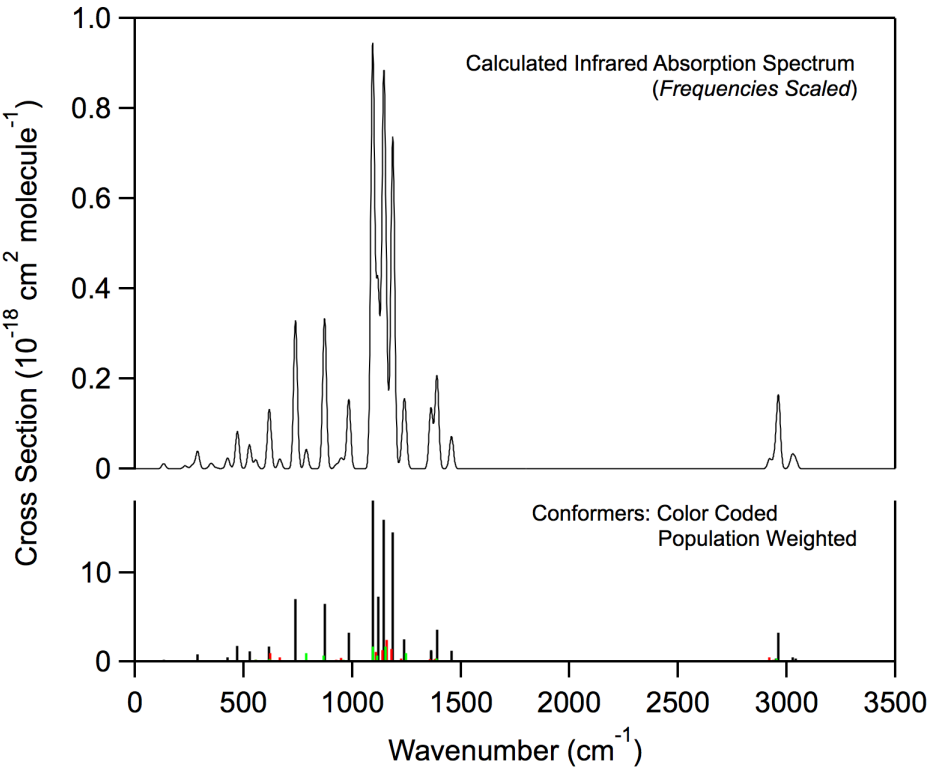
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	0.465572683315	1.780880937669	0.444549273262
C	0.259033642321	0.384799954641	-0.104987209604
C	-0.969670062562	-0.331012016768	0.486669773726
H	0.604534595730	1.755052934247	1.527235479500
H	1.349397624246	2.224429056281	-0.016440664501
H	-0.413379241480	2.384800039079	0.206731100550
Cl	1.705550958239	-0.654649677889	0.252738256835
F	0.098725895815	0.434217516255	-1.449551953171
H	-0.850694352894	-0.515721344878	1.560242172298
F	-2.052554408615	0.461093451557	0.287910118559
F	-1.178129334114	-1.493265850193	-0.153212347455

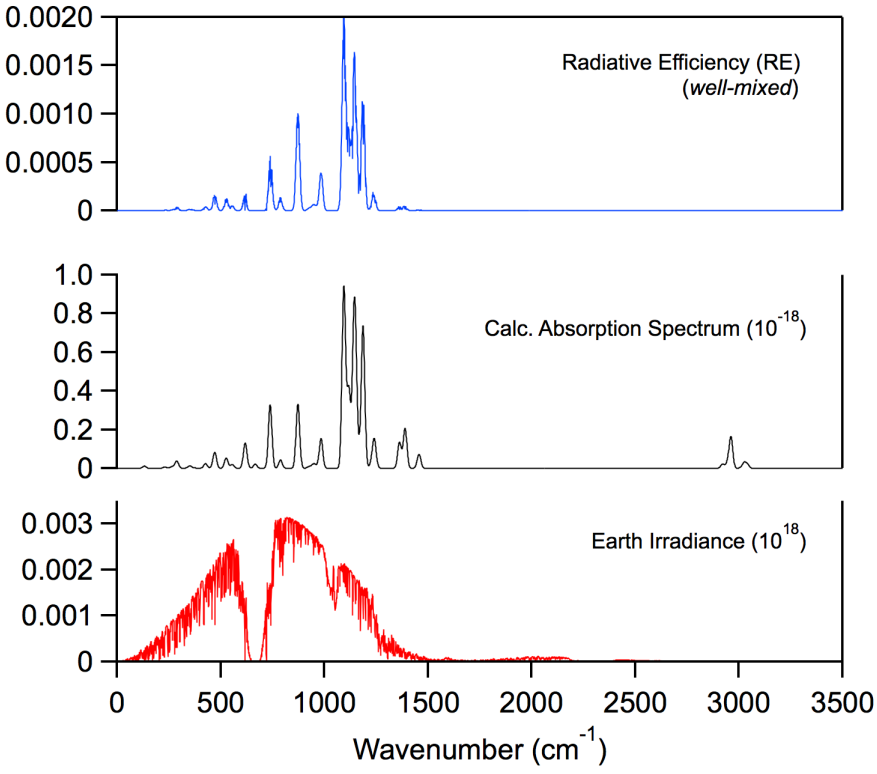
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
76.4264	0.123
190.8905	0.306
224.6283	0.0805
256.2181	0.132
299.8337	0.237
339.3547	0.415
363.6642	0.0849
420.7386	0.603
530.7116	2.54
598.8579	3.16
778.0474	12.2
862.5774	9.15
959.9185	3.10
1101.1968	22.2
1123.8277	9.44
1163.1743	22.6
1182.3799	1.43
1262.3367	12.7
1388.5792	1.86
1409.5280	0.856
1412.8963	4.53
1480.1103	0.547
1484.4838	1.05
3062.2883	0.432
3069.7482	4.25
3145.5196	0.852
3154.0830	0.614

Infrared Spectrum

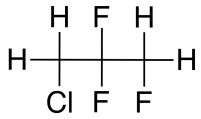


Radiative Efficiency



HCFC-253ca

Molecular Formula:	$CH_2ClCF_2CH_2F$
Name:	1-Chloro-2,2,3-trifluoropropane
CAS number:	56758-54-4
Molecular Weight:	132.51



Global Atmospheric Lifetime (years):	4.23
Tropospheric Atmospheric Lifetime (years):	4.47
Stratospheric Atmospheric Lifetime (years):	79.3
Ozone Depletion Potential (ODP):	0.018

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.148	0.135
Global Warming Potential (GWP_H):		
GWP_{20}	1058	964
GWP_{100}	289	263
Global Temperature Potentials (GTP_H)		
GTP_{20}		485
GTP_{50}		52
GTP_{100}		37

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 1.31 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 0.837 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 4.32$ years

$\tau^{OH}_{Trop} = 4.47$ years

$\tau^{OH}_{Strat} = 130.1$ years

Fractional Atmospheric Loss: 0.979

$O(^1D)$ Reactivity

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

$k_{Est}(T) = 1.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 370$ years

Fractional Atmospheric Loss: 0.011

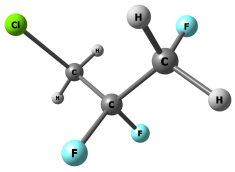
UV Photolysis

UV Spectrum: *No Recommendation*

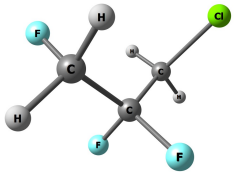
$\tau_{hv} = 450$ years

Fractional Atmospheric Loss: 0.010

Molecular Structure and Infrared Spectrum (6 conformers)



E = 0
Population = 0.397



E = 0
Population = 0.397

Optimized Coordinates (Angstroms)

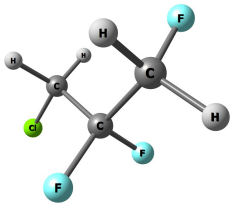
Atom	X	Y	Z
C	0.667884646565	0.268234051788	-0.870871193995
C	-0.538471873070	0.486750201643	0.035961734037
C	-1.072810211286	-0.755956736519	0.736820031666
Cl	2.114902781910	-0.265310871892	0.047445024736
H	0.430740192705	-0.502043317505	-1.602674889330
H	0.911632097769	1.206438736455	-1.368220340921
F	-1.518262762854	0.998004746168	-0.761844847002
F	-0.263746100647	1.412079029693	0.986898672589
H	-0.334262089709	-1.126508340954	1.452965829815
H	-2.000115637635	-0.491312441329	1.255575195105
F	-1.328330043747	-1.720552057549	-0.207504216701

Atom	X	Y	Z
C	0.669398279888	0.268711207972	0.869990391770
C	-0.535746889292	0.489141011394	-0.037989319644
C	-1.073832558091	-0.753397346099	-0.736273639008
Cl	2.115123545899	-0.271741948421	-0.046320485603
H	0.915994698037	1.207243200331	1.365313499202
H	0.429311523423	-0.499090642683	1.603434362147
F	-0.257451224484	1.411363088067	-0.990903917167
F	-1.514257784858	1.005475592029	0.758114911252
H	-1.999983547267	-0.486878728470	-1.256130188776
H	-0.336138603968	-1.128040069149	-1.451170258768
F	-1.333042439288	-1.714965364970	0.210130644596

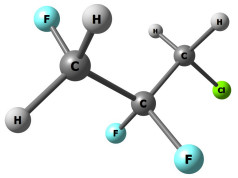
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
66.9198	0.234
133.7072	0.974
178.6206	0.242
226.8249	1.46
329.4913	0.475
360.8508	0.330
440.7158	1.11
521.6654	2.73
580.1214	0.789
760.6594	3.54
823.1863	4.25
889.2198	2.43
969.6027	5.89
1106.4388	18.2
1115.3432	0.177
1163.5749	16.1
1230.5470	10.3
1273.7152	5.53
1296.6559	5.20
1333.3662	2.69
1430.4523	0.455
1461.5277	2.20
1497.1244	1.27
3057.8892	2.59
3108.3003	0.941
3119.8225	2.51
3179.4157	0.0222

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
66.9202	0.234
133.7080	0.974
178.6209	0.242
226.8263	1.46
329.4917	0.475
360.8509	0.330
440.7159	1.11
521.6652	2.73
580.1215	0.789
760.6595	3.54
823.1865	4.25
889.2199	2.43
969.6028	5.89
1106.4386	18.2
1115.3429	0.177
1163.5749	16.1
1230.5473	10.3
1273.7152	5.53
1296.6561	5.20
1333.3662	2.69
1430.4523	0.455
1461.5276	2.20
1497.1241	1.27
3057.8895	2.59
3108.3002	0.941
3119.8229	2.51
3179.4156	0.0222



$\Delta E = 0.92$ kcal mol^{-1}
Population = 0.083



$\Delta E = 0.92$ kcal mol^{-1}
Population = 0.083

Optimized Coordinates (Angstroms)

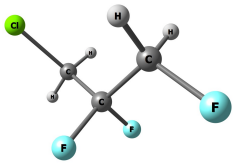
Atom	X	Y	Z
C	0.561993743795	-0.698752545530	0.471762552666
C	-0.412031124148	0.381245109073	0.020261826109
C	-1.857125205831	0.081068406287	0.420183531742
Cl	2.238248481744	-0.341903632223	-0.047450271377
H	0.557228085292	-0.765789379393	1.560049226874
H	0.264095432955	-1.653168623033	0.040412186938
F	-0.350528371427	0.524498665011	-1.324678882360
F	-0.090054008027	1.578113392041	0.576317596930
H	-1.953912081985	0.103258149793	1.510915069865
H	-2.502975349413	0.845944552495	-0.023525606628
F	-2.214971602955	-1.158727094523	-0.049412230758

Atom	X	Y	Z
C	0.561390866447	-0.699413678902	-0.470716526835
C	-0.411274282529	0.382126707031	-0.019977975492
C	-1.856778571350	0.083366264777	-0.419474559655
Cl	2.238139746750	-0.344162937034	0.047996534018
H	0.262395433739	-1.653116907296	-0.038549329119
H	0.556408419762	-0.767333884073	-1.558947454694
F	-0.087924593613	1.578150771755	-0.577052845500
F	-0.349430566934	0.526405570418	1.324837397153
H	-2.501650628293	0.849384182009	0.023687122088
H	-1.953674005015	0.104778599524	-1.510212041984
F	-2.216060818963	-1.155611688210	0.051181680020

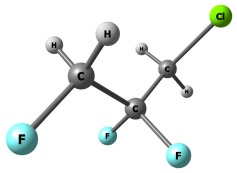
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
78.1696	0.488
99.3880	0.770
168.6157	0.0910
215.0067	0.457
327.7493	0.203
352.8858	0.121
444.5405	0.338
543.4511	2.22
594.9117	7.49
771.0242	1.49
822.9463	1.54
902.1786	1.59
959.5959	4.78
1105.3814	12.6
1110.4266	13.3
1181.8763	5.65
1221.1139	4.53
1254.6239	9.38
1314.3922	7.29
1338.1618	3.39
1422.6366	0.652
1464.8270	1.53
1498.8721	0.729
3047.8275	3.01
3100.7557	1.20
3107.1562	3.19
3169.7364	0.104

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
78.1695	0.488
99.3887	0.770
168.6157	0.0910
215.0068	0.457
327.7495	0.203
352.8859	0.121
444.5409	0.338
543.4511	2.22
594.9119	7.49
771.0241	1.49
822.9466	1.54
902.1787	1.59
959.5963	4.78
1105.3814	12.6
1110.4262	13.3
1181.8771	5.65
1221.1138	4.53
1254.6240	9.38
1314.3923	7.29
1338.1620	3.39
1422.6367	0.652
1464.8270	1.53
1498.8720	0.729
3047.8273	3.01
3100.7556	1.20
3107.1562	3.19
3169.7364	0.104



$\Delta E = 1.98$ kcal mol^{-1}
Population = 0.014



$\Delta E = 1.98$ kcal mol^{-1}
Population = 0.014

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	0.975851007470	0.740263832630	-0.488266696301
C	-0.425733331199	0.398876394934	0.012901974223
C	-0.994159992325	-0.929846777089	-0.473244097757
Cl	2.204946964392	-0.465379771545	0.022402407361
H	0.985290595779	0.789020739177	-1.576846630955
H	1.261188369351	1.706180724793	-0.071816191797
F	-1.234119737290	1.406972104700	-0.423392468228
F	-0.448826444905	0.426742919040	1.365619651910
H	-0.996496665507	-0.945653712928	-1.569582506827
H	-0.383633335485	-1.754552585645	-0.094867352913
F	-2.275688430282	-1.051162868067	-0.010106088717

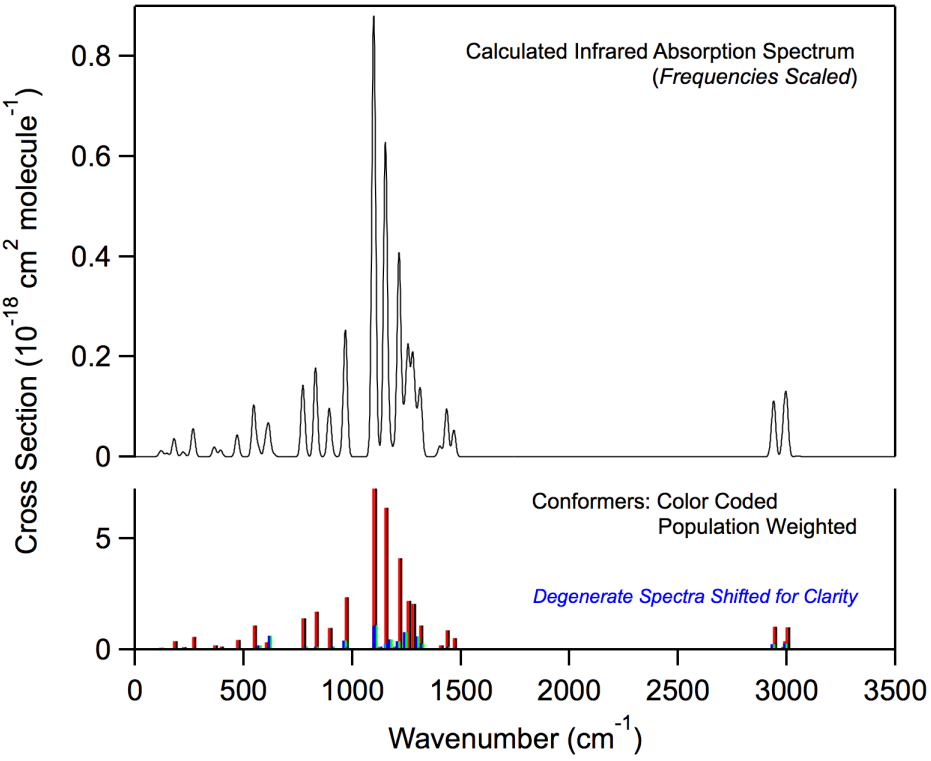
Atom	X	Y	Z
C	0.976257273690	0.741527949364	0.487859682599
C	-0.425314589185	0.399090457382	-0.012627073171
C	-0.993534645916	-0.928865762255	0.475850299778
Cl	2.205479181211	-0.464834352172	-0.020805118670
H	1.261440241321	1.706761326807	0.069722040364
H	0.985761037540	0.792167207970	1.576353116767
F	-0.448499287433	0.424617233209	-1.365389423265
F	-1.233805729234	1.407831710233	0.421977998617
H	-0.382924494397	-1.754143689318	0.098858252054
H	-0.995797473904	-0.942779630994	1.572214532127
F	-2.275077513694	-1.051149450225	0.013006692799

Infrared Absorption Spectrum (unscaled frequencies)

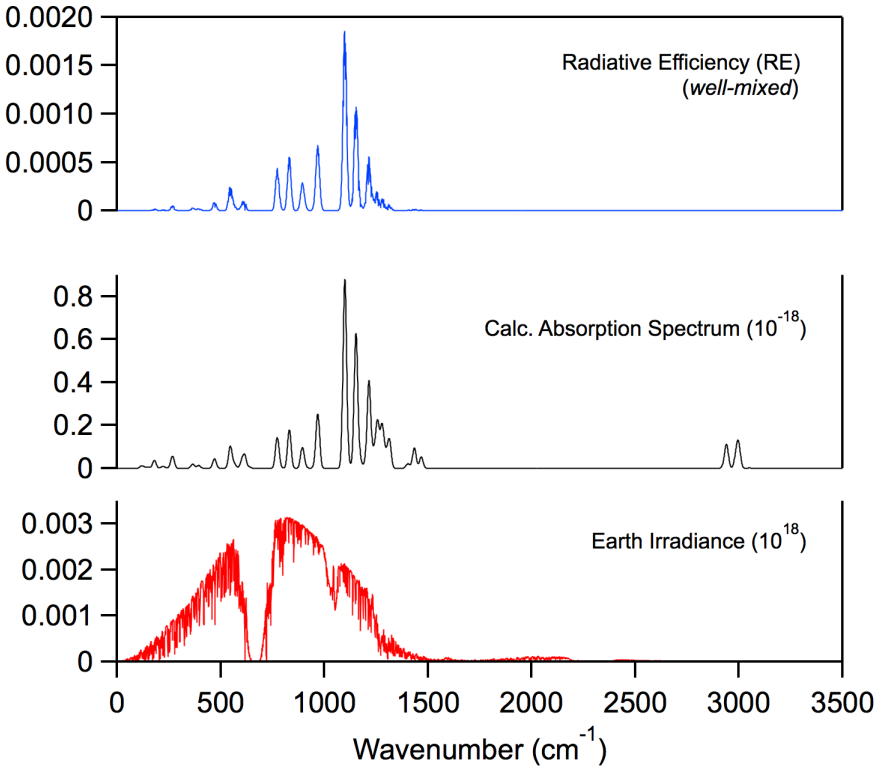
Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
75.4507	1.05
100.8370	0.360
164.5328	0.130
228.8262	0.154
328.8581	0.0969
349.3251	0.397
408.6450	0.113
537.8823	1.61
618.2028	4.47
767.5085	4.75
822.2269	5.17
893.7649	1.18
967.6070	9.24
1096.2822	6.45
1132.9352	8.92
1161.1869	19.1
1203.6320	9.07
1274.6476	3.41
1316.4909	0.448
1326.4899	8.38
1441.6584	0.523
1467.1252	2.02
1498.1104	0.296
3044.0201	3.29
3100.1493	0.775
3109.6222	2.83
3167.1282	0.182

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
75.4508	1.05
100.8371	0.360
164.5327	0.130
228.8264	0.154
328.8582	0.0969
349.3251	0.397
408.6450	0.113
537.8824	1.61
618.2028	4.47
767.5085	4.75
822.2270	5.17
893.7649	1.18
967.6070	9.24
1096.2823	6.45
1132.9351	8.92
1161.1868	19.1
1203.6320	9.07
1274.6475	3.41
1316.4908	0.448
1326.4899	8.38
1441.6584	0.523
1467.1252	2.02
1498.1103	0.296
3044.0200	3.29
3100.1493	0.775
3109.6222	2.83
3167.1282	0.182

Infrared Spectrum

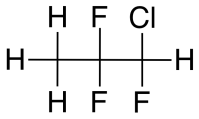


Radiative Efficiency



HCFC-253cb

Molecular Formula:	CH_3CF_2CHClF
Name:	1-Chloro-1,2,2-trifluoropropane
CAS number:	70192-76-6
Molecular Weight:	132.51



Global Atmospheric Lifetime (years):	3.48
Tropospheric Atmospheric Lifetime (years):	3.66
Stratospheric Atmospheric Lifetime (years):	70.8
Ozone Depletion Potential (ODP):	0.017

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.204	0.183
Global Warming Potential (GWP_H):		
GWP_{20}	1201	1077
GWP_{100}	326	293
Global Temperature Potentials (GTP_H)		
GTP_{20}		492
GTP_{50}		56
GTP_{100}		41

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 1.60 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 1.02 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

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

$\tau^{OH}_{Trop} = 3.66$ years

$\tau^{OH}_{Strat} = 108.7$ years

Fractional Atmospheric Loss: 0.983

O(^{1}D) Reactivity

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

$k_{Est}(T) = 1.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 370$ years

Fractional Atmospheric Loss: 0.009

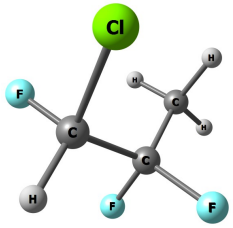
UV Photolysis

UV Spectrum: *No Recommendation*

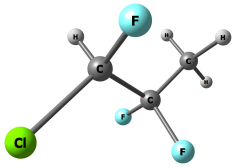
$\tau_{hv} = 450$ years

Fractional Atmospheric Loss: 0.008

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.771



$\Delta E = 0.88$ kcal mol^{-1}
Population = 0.173

Optimized Coordinates (Angstroms)

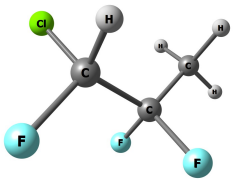
Atom	X	Y	Z
C	1.085544936687	-0.387262151479	1.429731687277
C	0.855864867927	-0.185073724110	-0.049513810925
C	-0.460373078167	0.514099705814	-0.438626212454
H	2.082853787326	-0.808371325463	1.571783288163
H	1.018594208331	0.571685404771	1.945965848429
H	0.340180184310	-1.071071277357	1.837808766585
F	0.907659529728	-1.364095372348	-0.716863320865
F	1.840561377481	0.606399699999	-0.565647583001
H	-0.493936641914	0.667814454647	-1.519143775647
Cl	-1.890571922588	-0.478846828903	-0.003838140869
F	-0.527232249121	1.704166414429	0.198346253307

Atom	X	Y	Z
C	2.116198175443	0.517966863928	-0.345269170012
C	0.841006853409	-0.226004157592	0.000304932998
C	-0.428248951235	0.504138751439	-0.476921411255
H	2.965273267825	-0.063159075139	0.020386674111
H	2.205789604338	0.638489246393	-1.427413251247
H	2.113635283447	1.500028073034	0.129030127832
F	0.768984940704	-0.410213329052	1.339379088443
F	0.844522415380	-1.452205856342	-0.584801671939
H	-0.457408115737	0.543615993923	-1.568035804443
Cl	-1.908429107447	-0.349248264800	0.052429452753
F	-0.424727366128	1.762115754208	0.025403032759

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
75.4025	0.270
182.3844	0.0806
205.1199	0.0796
239.4361	1.06
311.1519	0.167
347.1971	0.0683
414.1183	0.130
478.7975	2.85
488.0665	1.07
603.8937	1.59
764.2630	4.34
836.6709	14.9
965.1513	5.34
979.8936	2.80
1128.9361	18.2
1175.0795	19.2
1216.8178	20.6
1275.6761	7.04
1295.3591	1.08
1370.9865	1.90
1418.6639	7.02
1478.7015	0.274
1488.7173	0.166
3070.8488	0.244
3109.1566	1.57
3154.6971	0.807
3161.8873	0.541

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
65.9383	0.133
183.1284	0.213
208.6930	0.0508
241.0858	0.242
300.1038	0.269
356.0730	0.0419
386.6352	0.0274
467.1014	0.423
541.5618	4.09
613.4691	4.57
787.8279	7.84
834.2597	7.11
958.7390	4.69
978.8167	4.23
1122.0244	19.2
1172.4110	13.9
1220.4187	18.8
1275.0323	12.5
1307.6556	1.08
1371.0771	1.15
1409.9323	3.04
1481.0918	0.307
1486.8812	0.192
3064.4836	0.364
3101.1110	1.98
3144.5863	1.23
3160.8097	0.607



$\Delta E = 1.55$ kcal mol^{-1}
Population = 0.056

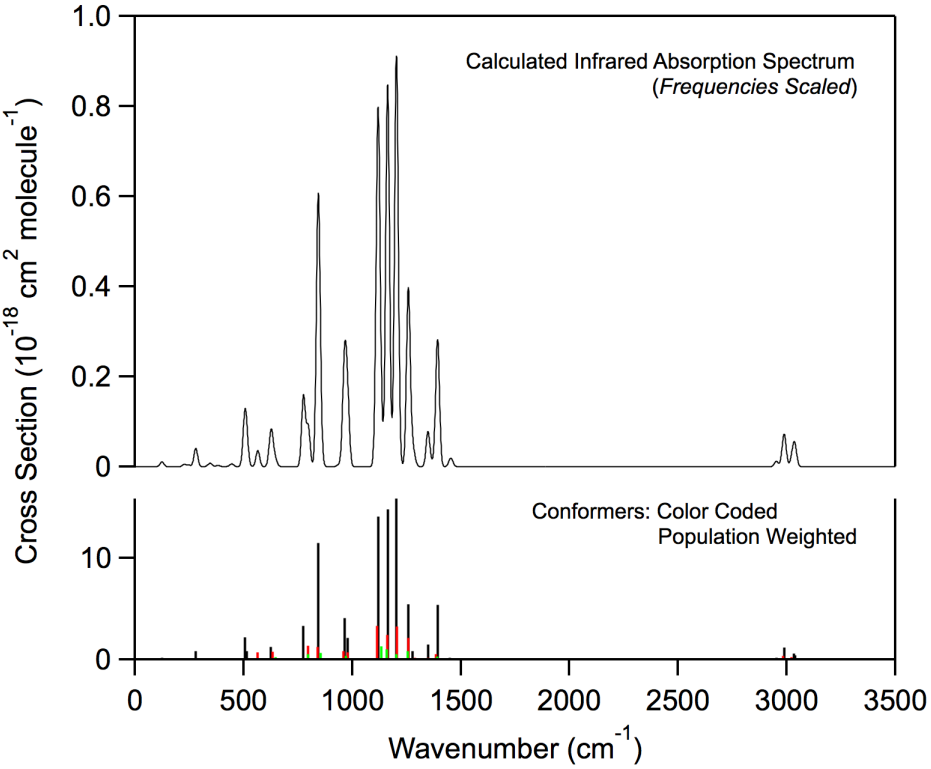
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.202738801108	1.529735085622	0.403286393030
C	0.863274246149	0.120861977745	-0.029519278992
C	-0.463899066504	-0.448055667867	0.510294760902
H	1.200955011528	1.604779745547	1.493380566727
H	2.203148973621	1.766395907675	0.034346154774
H	0.486091589139	2.239868708046	-0.009610838532
F	1.823986931743	-0.737919574468	0.421998564575
F	0.851721714784	0.028987624823	-1.379483441815
H	-0.467957773521	-0.447182039217	1.602536382366
Cl	-1.866339435815	0.544993271171	-0.018779416245
F	-0.613325992231	-1.706079039079	0.054043153213

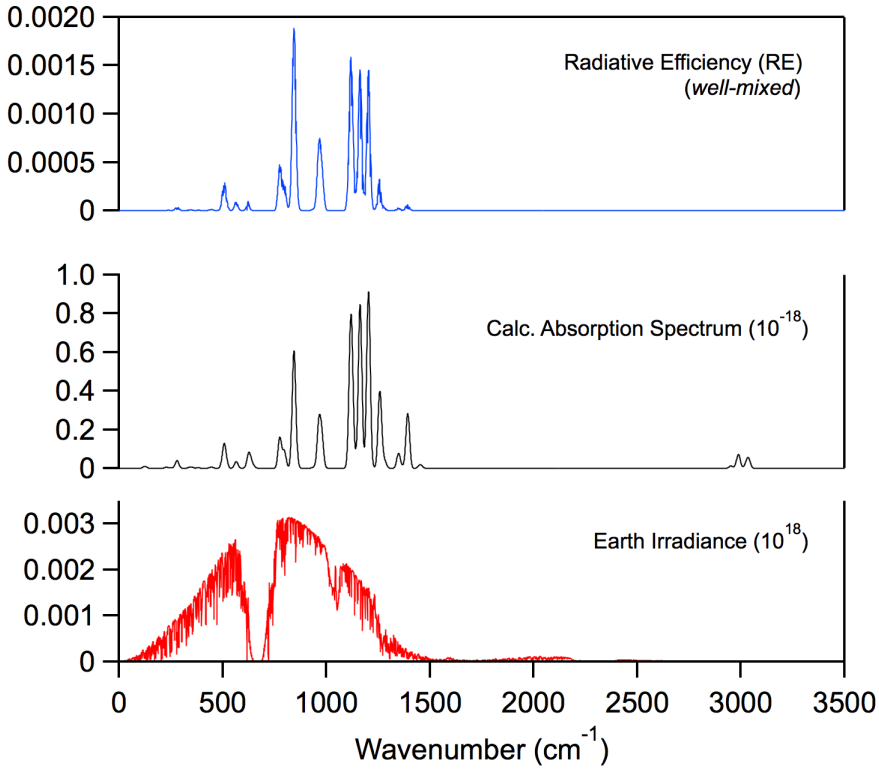
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
68.9652	0.105
189.7450	0.209
201.7760	0.112
239.2286	0.113
319.2273	0.249
344.1715	0.0948
402.1587	0.245
420.1612	0.559
543.0110	1.03
629.2221	4.68
786.4205	9.55
848.7939	11.9
934.5440	1.48
971.4369	6.39
1142.2586	22.9
1170.5671	18.0
1216.8143	9.56
1273.6964	14.7
1289.4232	1.61
1390.0263	2.31
1415.4974	5.11
1481.7139	0.257
1485.2590	0.271
3064.9849	0.272
3100.8282	1.95
3142.4386	1.23
3163.6476	0.652

Infrared Spectrum

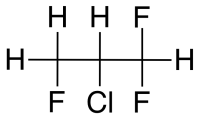


Radiative Efficiency



HCFC-253da

Molecular Formula:	$CH_2FCHClCHF_2$
Name:	2-Chloro-1,1,3-trifluoropropane
CAS number:	–
Molecular Weight:	132.51



Global Atmospheric Lifetime (years):	1.67
Tropospheric Atmospheric Lifetime (years):	1.74
Stratospheric Atmospheric Lifetime (years):	43.6
Ozone Depletion Potential (ODP):	0.012

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.144	0.118
Global Warming Potential (GWP_H):		
GWP_{20}	408	335
GWP_{100}	111	91
Global Temperature Potentials (GTP_H)		
GTP_{20}		118
GTP_{50}		16
GTP_{100}		13

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

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

OH Reactivity

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

k_{SAR}(298 K) = 3.38×10^{-14}; k_{SAR}(272 K) ≈ 2.15×10^{-14} cm^3 $molecule^{-1}$ s^{-1}

τ^{OH}_{Global} = 1.68 years

τ^{OH}_{Trop} = 1.74 years

τ^{OH}_{Strat} = 55.5 years

Fractional Atmospheric Loss: 0.992

O(^{1}D) Reactivity

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

$k_{Est}(T) = 1.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)}$ = 370 years

Fractional Atmospheric Loss: 0.004

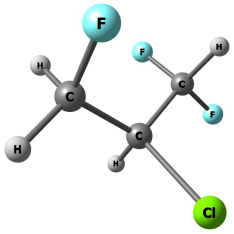
UV Photolysis

UV Spectrum: *No Recommendation*

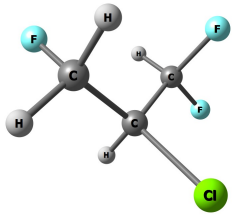
τ_{hv} = 450 years

Fractional Atmospheric Loss: 0.004

Molecular Structure and Infrared Spectrum (8 conformers)



E = 0
Population = 0.365



$\Delta E = 0.19$ kcal mol^{-1}
Population = 0.265

Optimized Coordinates (Angstroms)

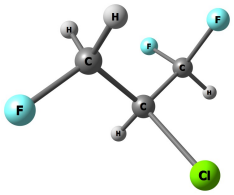
Atom	X	Y	Z
C	0.941713285233	-1.256848555654	-0.549764448014
C	0.157869586526	0.044340847203	-0.562862419204
C	-1.094033810449	-0.032265478594	0.312120637668
F	1.265798098714	-1.596224090192	0.743297110416
H	0.316933127490	-2.049887116215	-0.977049636241
H	1.860219608202	-1.155078110584	-1.135889098679
H	-0.149475271048	0.280871918039	-1.584299244017
Cl	1.180705903288	1.414600122843	0.011142453481
H	-0.856360357281	-0.180966872417	1.369706948380
F	-1.831438231417	1.087610693361	0.171707883100
F	-1.842224939257	-1.081226357791	-0.126215186890

Atom	X	Y	Z
C	1.549226097308	0.562799447909	0.192737150173
C	0.194005528844	0.310824263117	-0.460548661768
C	-0.333768465580	-1.083947571701	-0.138497927300
F	2.433306576476	-0.390214296048	-0.275973865619
H	1.920068105937	1.558067225687	-0.067791082654
H	1.467634825735	0.472519364252	1.280076021188
H	0.270139078288	0.406005890481	-1.545417222527
Cl	-0.957401258614	1.573293623417	0.100433002099
H	0.379177449400	-1.843287630237	-0.483153931890
F	-0.503743195560	-1.226183317260	1.196797524100
F	-1.522390742233	-1.291349999617	-0.743541005803

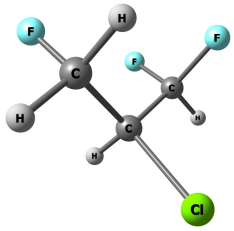
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
73.7740	0.317
101.2806	0.374
170.8336	0.0473
227.5563	1.05
305.5071	0.369
391.6030	0.224
419.0575	2.78
560.4340	1.21
635.3447	4.60
760.0814	3.78
920.9618	0.664
1004.2959	3.59
1103.1921	21.8
1116.4397	8.66
1141.4452	3.61
1153.1875	20.7
1236.3235	1.45
1279.0436	2.03
1299.4362	0.785
1390.4806	1.05
1411.1725	5.07
1432.7133	3.76
1499.2762	0.999
3043.7667	3.23
3088.7367	1.70
3100.3305	2.61
3104.7485	2.38

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
73.3558	0.297
122.5783	0.751
188.1059	0.260
201.2937	0.497
238.9607	0.524
371.5700	0.0839
480.1521	3.00
547.3115	0.632
659.3360	6.46
741.9678	2.49
941.5542	1.36
1018.2209	6.14
1072.5347	13.3
1102.0235	1.08
1155.0639	18.6
1176.2652	14.8
1236.9990	0.805
1259.2236	1.89
1341.1671	0.933
1394.0211	6.81
1411.1582	1.96
1421.9456	3.05
1510.5686	0.546
3056.7407	3.30
3060.2198	2.66
3103.5239	1.22
3122.7738	2.48



$\Delta E = 0.57$ kcal mol^{-1}
Population = 0.140



$\Delta E = 0.91$ kcal mol^{-1}
Population = 0.079

Optimized Coordinates (Angstroms)

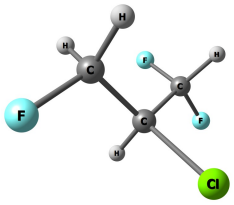
Atom	X	Y	Z
C	-0.625897464170	1.209557865544	0.376759941102
C	-0.152817795709	0.040480207735	-0.475276567996
C	1.328455395869	-0.260346568548	-0.261944314289
F	-1.902907779629	1.556084181963	0.018106722785
H	-0.604427526536	0.945635415789	1.437796061606
H	0.042076955421	2.061294216289	0.199509025995
H	-0.313220573751	0.263465279698	-1.531550194760
Cl	-1.110275505819	-1.447530753039	-0.122644120254
H	1.655608564331	-1.160558157639	-0.792799780391
F	2.045167793961	0.803779052606	-0.713427752860
F	1.594602936031	-0.406648740398	1.056190979062

Atom	X	Y	Z
C	0.235031967882	1.398477594233	0.404116108223
C	-0.274607541149	0.276723228002	-0.499214006420
C	0.418657336840	-1.067477129631	-0.261399573790
F	1.550005205354	1.656266497279	0.096651221086
H	-0.359115632919	2.302698507953	0.239558523712
H	0.159224755225	1.098021950705	1.453341730112
H	-0.154892005151	0.546268002441	-1.549726354519
Cl	-2.043203649547	0.072342618999	-0.203850058452
H	-0.087773470794	-1.888220202005	-0.782262969293
F	1.695152395091	-0.986322196130	-0.703413966386
F	0.449442639168	-1.348811871845	1.062005345727

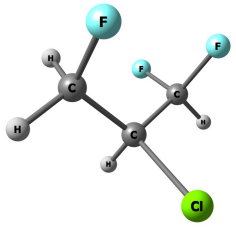
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
77.3706	0.342
99.7593	0.500
177.1987	0.455
203.2833	0.944
281.1056	0.145
353.0960	0.245
445.2163	2.00
545.7290	1.41
698.9157	4.02
722.1359	5.65
928.8155	1.09
1010.4564	5.38
1096.6778	21.0
1114.6696	10.5
1125.6133	2.70
1172.5930	16.5
1242.0183	1.06
1287.5238	1.06
1312.8181	5.31
1385.9617	3.88
1409.7327	4.19
1434.8599	0.640
1507.3978	0.659
3041.5328	2.85
3077.0113	4.64
3100.8051	0.583
3116.8124	2.19

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
55.0034	0.0833
129.9595	0.726
187.4705	0.301
219.7569	0.274
281.9797	1.73
358.1518	2.21
395.3823	0.190
534.5218	1.24
657.0593	0.965
835.7934	8.54
892.0710	1.73
1010.0113	4.03
1088.6528	5.87
1117.7374	17.5
1134.6769	17.0
1174.8870	12.7
1220.1762	1.03
1263.3828	1.15
1354.8611	0.147
1385.2647	4.88
1411.3048	2.40
1438.9080	2.35
1509.3043	0.577
3055.8093	3.43
3064.6377	4.46
3105.4867	1.34
3121.4475	1.92



$\Delta E = 1.17$ kcal mol^{-1}
Population = 0.051



$\Delta E = 1.27$ kcal mol^{-1}
Population = 0.043

Optimized Coordinates (Angstroms)

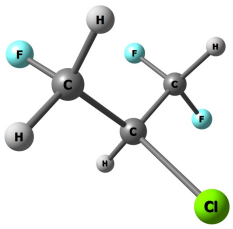
Atom	X	Y	Z
C	1.066214374580	-1.144484923786	0.271118938381
C	0.145831361953	-0.054314194564	-0.259092235909
C	-1.272887666807	-0.176271898142	0.292866238354
F	2.299372271524	-1.034617901070	-0.315504583587
H	1.178039007771	-1.062839268796	1.358934285278
H	0.635103116118	-2.120882245282	0.022913400091
H	0.100082499689	-0.098752381857	-1.349235701069
Cl	0.788796546574	1.576226657199	0.162737691935
H	-1.323321660624	0.002072989050	1.373792559808
F	-2.090748863480	0.692155028649	-0.332917919255
F	-1.724325987298	-1.434663861400	0.035818325972

Atom	X	Y	Z
C	-0.213393701281	1.399675615194	-0.615974744692
C	-0.245159167808	-0.121015530537	-0.684022546069
C	0.965857338015	-0.794668463875	-0.034594729303
F	-0.288813998589	1.843603104423	0.676320918425
H	0.729708554348	1.742398348125	-1.060172000371
H	-1.053605476307	1.810887297794	-1.185773683574
H	-0.260957008314	-0.419514680920	-1.735161196300
Cl	-1.748386346841	-0.778662896271	0.061551140180
H	0.921672391684	-1.886786776414	-0.117362617808
F	2.077358670634	-0.352301557941	-0.686590904895
F	1.083209744458	-0.458672459578	1.262558364407

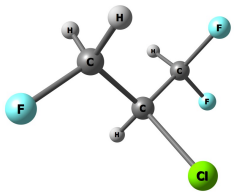
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
71.7808	0.132
104.4829	0.791
174.5631	0.524
206.3395	0.547
332.1446	0.629
358.2433	0.426
420.0244	0.342
529.6071	4.38
576.6067	1.28
734.9798	5.40
1005.5028	3.95
1067.0336	4.87
1089.1718	11.2
1116.9618	11.2
1124.5240	17.3
1158.0563	10.6
1243.4581	1.08
1265.2876	0.860
1310.7066	3.67
1388.8030	2.22
1425.3874	4.01
1432.6141	4.49
1507.2188	0.533
3034.0880	3.15
3058.9356	4.62
3086.0605	1.72
3111.8611	2.14

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
60.3332	0.213
122.3616	0.285
193.1538	0.241
206.1726	0.373
272.2042	0.943
372.4846	0.160
440.6161	2.94
557.3416	1.90
722.4984	5.58
787.9435	1.31
888.4298	0.691
996.0298	1.04
1042.8672	4.42
1103.2582	23.5
1144.2379	13.4
1193.4066	11.5
1236.8541	2.41
1287.1512	2.87
1344.4421	2.13
1380.5588	2.68
1419.6854	1.41
1437.1642	4.94
1499.8335	1.08
3033.5060	3.44
3063.8250	5.37
3086.3558	3.12
3095.7013	1.13



$\Delta E = 1.36$ kcal mol^{-1}
Population = 0.037



$\Delta E = 1.90$ kcal mol^{-1}
Population = 0.015

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-0.690884158569	-1.471457706275	0.146807695504
C	0.148934146217	-0.289794736253	-0.337338411934
C	-0.195296979364	1.033240787603	0.346261255947
F	-1.985122195362	-1.323964053828	-0.285980016952
H	-0.277868204635	-2.399548770121	-0.260525113637
H	-0.678511683866	-1.530604446762	1.242210921325
H	0.041586730125	-0.164450085406	-1.416576177128
Cl	1.881551801064	-0.665232838135	-0.006228017470
H	0.001992593827	1.004159900677	1.425637113416
F	0.524064217594	2.035161359756	-0.203033993091
F	-1.506394267030	1.302076588744	0.144415744020

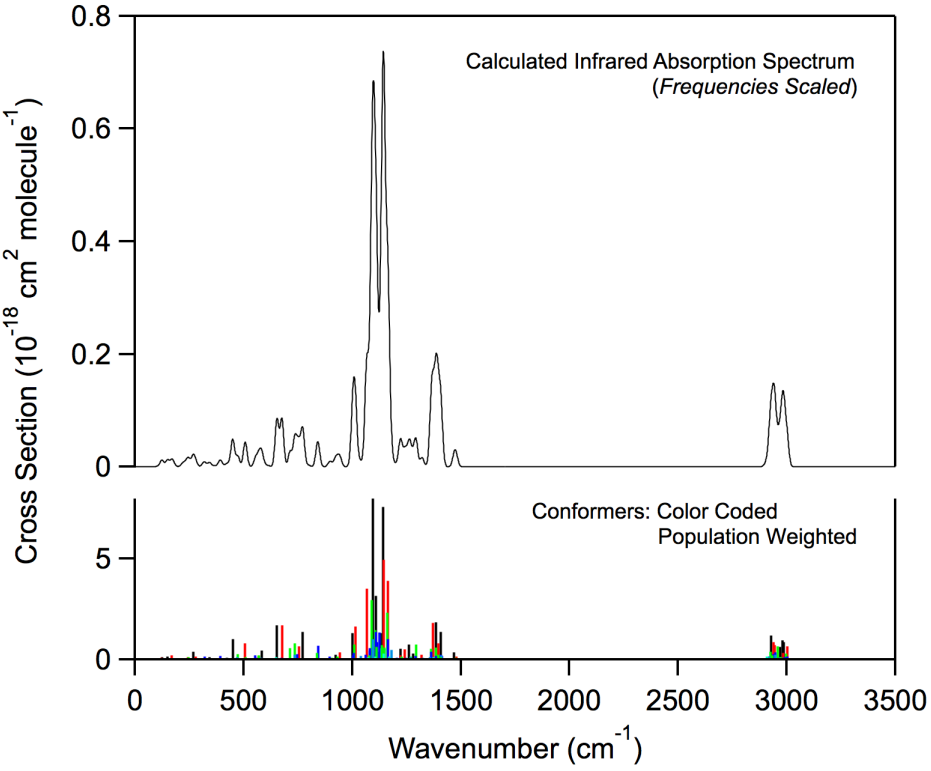
Atom	X	Y	Z
C	1.278651774237	-1.019251929103	0.065144354749
C	0.203007839944	-0.089220127837	-0.478686617316
C	-1.190569115165	-0.671196035142	-0.265983355067
F	2.516110729274	-0.571340591529	-0.314469726265
H	1.224501809715	-1.065943127016	1.156896927172
H	1.127629847092	-2.028068293744	-0.345358160897
H	0.354386392077	0.062910059423	-1.549648695100
Cl	0.329553730628	1.535693874187	0.285732018554
H	-1.297384932479	-1.622665307497	-0.807763977637
F	-1.405347202561	-0.906803081558	1.050501278301
F	-2.138062872763	0.178461559814	-0.707942046495

Infrared Absorption Spectrum (unscaled frequencies)

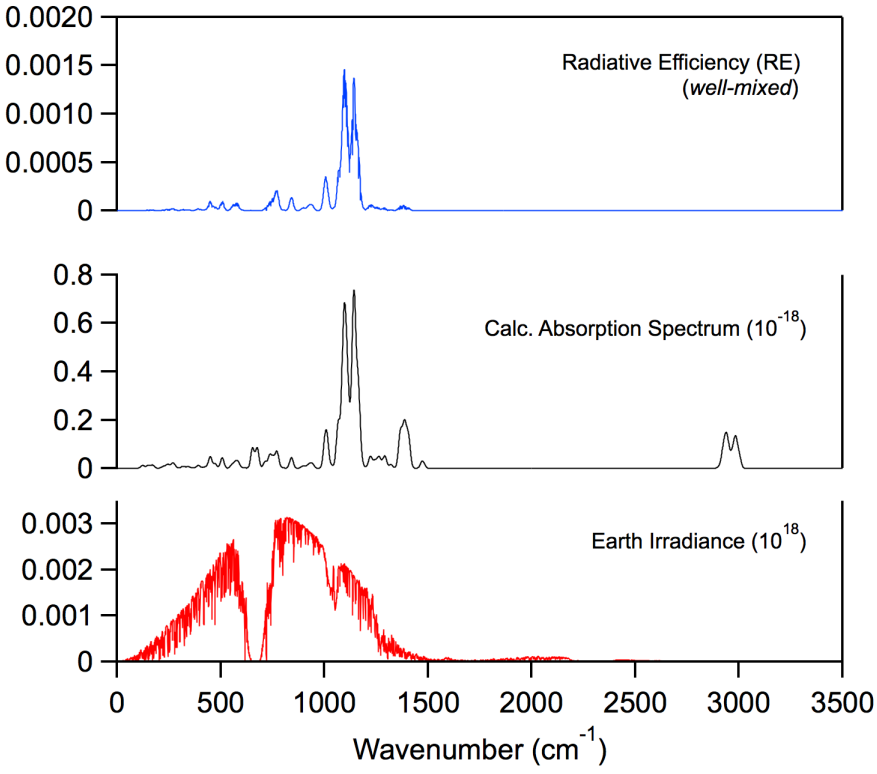
Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
53.4997	0.127
130.2622	0.878
183.2232	0.149
216.3831	0.614
312.6738	0.782
363.4843	0.592
396.8125	0.848
482.6540	3.14
594.4583	0.906
830.1752	8.53
903.2874	2.08
1085.4712	5.35
1097.8758	1.26
1119.1368	17.2
1145.9476	19.1
1157.3160	16.3
1218.5130	0.551
1257.9920	0.222
1329.6352	0.282
1392.1491	1.42
1421.3959	6.10
1432.8949	3.20
1511.6825	0.587
3036.0030	2.36
3048.5878	5.71
3091.8554	2.95
3114.7252	1.36

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
73.2315	0.165
105.5614	0.736
174.7513	0.493
195.1469	0.219
279.8320	0.0873
363.4487	0.112
478.2911	2.04
549.7868	1.22
631.0853	7.08
769.1187	3.66
921.1618	0.941
1033.6662	1.57
1079.5491	7.99
1113.4762	9.56
1154.4703	20.5
1181.1334	9.11
1247.9273	0.538
1283.0525	2.05
1312.2193	3.10
1397.1770	8.40
1410.5865	3.63
1434.4941	2.66
1503.5016	0.598
3009.6375	1.23
3021.8345	10.1
3090.6314	0.674
3107.7865	2.75

Infrared Spectrum

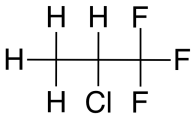


Radiative Efficiency



HCFC-253db

Molecular Formula:	$CH_3CHClCF_3$
Name:	2-Chloro-1,1,1-trifluoropropane
CAS number:	421-47-6
Molecular Weight:	132.51



Global Atmospheric Lifetime (years):	1.02
Tropospheric Atmospheric Lifetime (years):	1.06
Stratospheric Atmospheric Lifetime (years):	30.2
Ozone Depletion Potential (ODP):	0.009

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.132	0.12
Global Warming Potential (GWP_H):		
GWP_{20}	230	209
GWP_{100}	62	57
Global Temperature Potentials (GTP_H)		
GTP_{20}		68
GTP_{50}		10
GTP_{100}		8

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

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

OH Reactivity

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

k_{SAR}(298 K) = 5.54×10^{-14}; k_{SAR}(272 K) ≈ 3.54×10^{-14} cm^3 $molecule^{-1}$ s^{-1}

τ^{OH}_{Global} = 1.03 years
τ^{OH}_{Trop} = 1.06 years
τ^{OH}_{Strat} = 35.5 years

Fractional Atmospheric Loss: 0.990

O(^{1}D) Reactivity

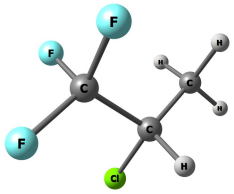
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 1.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)}$ = 370 years
Fractional Atmospheric Loss: 0.005

UV Photolysis

UV Spectrum: *No Recommendation*
τ_{hv} = 450 years
Fractional Atmospheric Loss: 0.005

Molecular Structure and Infrared Spectrum (1 conformer)



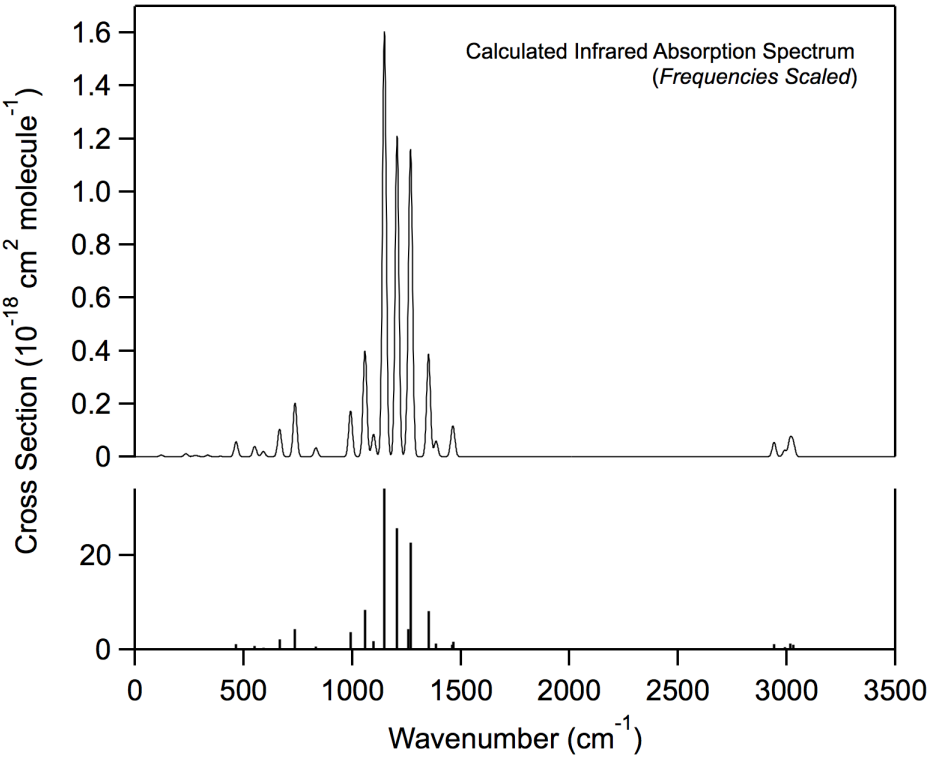
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-0.636221296777	1.865165294983	0.038814493250
C	-0.451301934601	0.448058417693	-0.482894622114
C	0.864401066687	-0.174259260294	-0.010163077871
H	-1.570796617535	2.283537385810	-0.337785737093
H	-0.659863610557	1.871644571291	1.130436729922
H	0.194382168161	2.490376768563	-0.300944865192
H	-0.442467523960	0.418390871847	-1.573534942041
Cl	-1.819756166737	-0.613022987568	0.030979854029
F	1.030884171108	-1.410359016631	-0.480920272658
F	1.885994174025	0.575415445772	-0.462615928141
F	0.950115570186	-0.217695491467	1.321402367911

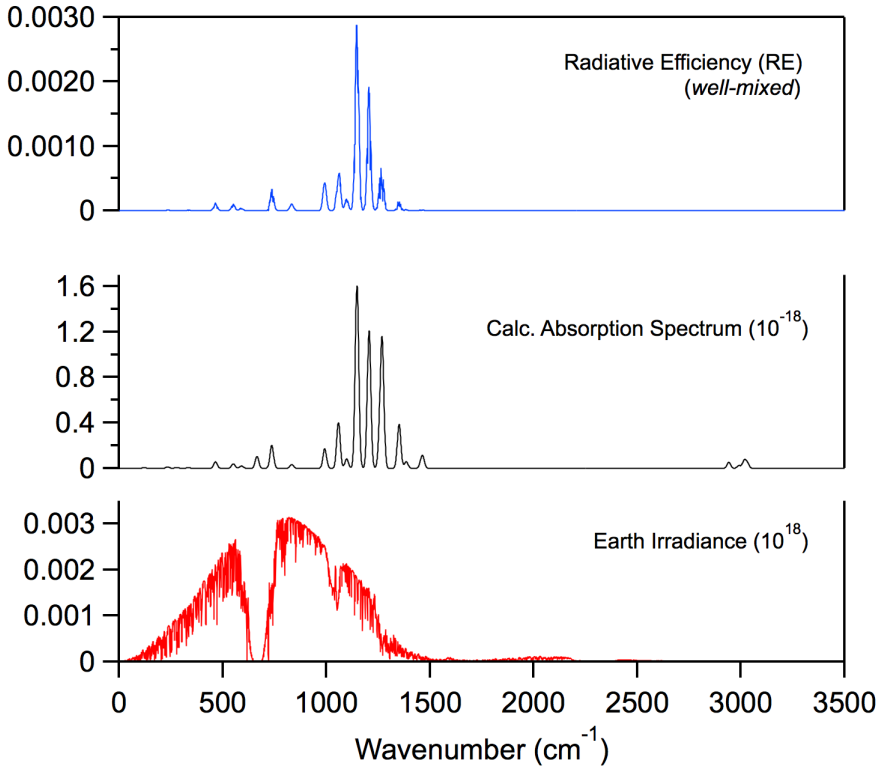
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
70.8098	0.128
191.1483	0.244
230.2767	0.0654
246.7777	0.0615
297.6701	0.127
359.4050	0.0338
435.8770	1.19
526.5409	0.837
568.5593	0.426
647.8669	2.21
723.2860	4.31
825.1993	0.713
993.8710	3.67
1063.8873	8.51
1105.7691	1.78
1158.6081	34.2
1220.3953	25.7
1275.5057	4.40
1287.2273	22.7
1373.8178	8.25
1410.3040	1.26
1487.8784	1.04
1495.2559	1.63
3058.2081	1.15
3109.6936	0.500
3136.0886	1.33
3151.6360	1.03

Infrared Spectrum

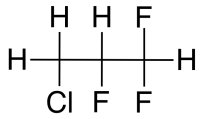


Radiative Efficiency



HCFC-253ea

Molecular Formula:	$CH_2ClCHFCHF_2$
Name:	3-Chloro-1,1,2-trifluoropropane
CAS number:	121612-65-5
Molecular Weight:	132.51



Global Atmospheric Lifetime (years):	1.44
Tropospheric Atmospheric Lifetime (years):	1.50
Stratospheric Atmospheric Lifetime (years):	39.1
Ozone Depletion Potential (ODP):	0.011

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.142	0.113
Global Warming Potential (GWP_H):		
GWP_{20}	347	277
GWP_{100}	94	75
Global Temperature Potentials (GTP_H)		
GTP_{20}		95
GTP_{50}		13
GTP_{100}		10

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 3.92 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 2.50 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 1.45$ years

$\tau^{OH}_{Trop} = 1.50$ years

$\tau^{OH}_{Strat} = 48.5$ years

Fractional Atmospheric Loss: 0.993

$O(^1D)$ Reactivity

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

$k_{Est}(T) = 1.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 370$ years

Fractional Atmospheric Loss: 0.004

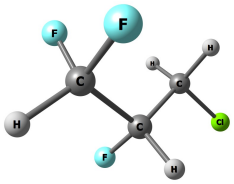
UV Photolysis

UV Spectrum: *No Recommendation*

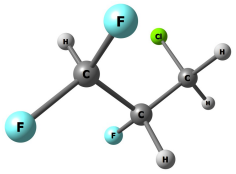
$\tau_{hv} = 450$ years

Fractional Atmospheric Loss: 0.003

Molecular Structure and Infrared Spectrum (7 conformers)



E = 0
Population = 0.359



$\Delta E = 0.07$ kcal mol^{-1}
Population = 0.319

Optimized Coordinates (Angstroms)

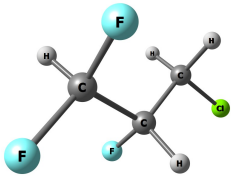
Atom	X	Y	Z
C	0.713414602503	-0.514409803739	0.411974426091
C	-0.158129963469	0.306213979936	-0.521176908220
C	-1.644560036279	0.046945770629	-0.269170596885
Cl	2.454061613532	-0.350187288454	-0.012148473713
H	0.592408087277	-0.175767183204	1.439884078033
H	0.450950238792	-1.569560198733	0.335359737230
H	0.060234354285	0.063139797628	-1.567344895329
F	0.060176053348	1.648878953702	-0.324810503066
H	-2.276752716719	0.737611809176	-0.839770007932
F	-1.934839126624	-1.228265557201	-0.630101553096
F	-1.927783106648	0.187361720259	1.047275696886

Atom	X	Y	Z
C	1.055448078240	-0.016556531191	-0.961817633410
C	-0.286128811138	0.573225417874	-0.568297015604
C	-1.136107125316	-0.338912661902	0.314450185562
Cl	2.101763107254	-0.363241671104	0.468094214302
H	0.908802114957	-0.955045365513	-1.495564004990
H	1.603486784899	0.688022453598	-1.586910869397
H	-0.858405450934	0.761714810016	-1.488406936498
F	-0.114978355778	1.761472619978	0.095805451045
H	-0.695728937515	-0.505068324960	1.302618636949
F	-2.359703752911	0.214194005182	0.463934107000
F	-1.282215651757	-1.531447751979	-0.319240134960

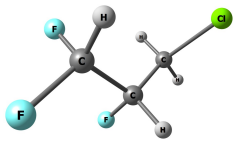
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
77.7003	0.199
81.1316	0.644
165.1341	0.841
213.1823	0.433
261.7628	0.0193
391.8928	1.28
481.1244	2.02
563.3610	1.69
645.9564	7.29
812.7025	0.819
856.2806	1.10
930.7479	2.92
1064.7008	2.67
1125.6732	26.9
1138.1008	4.67
1172.5293	12.7
1223.1587	2.29
1272.3041	1.89
1346.6088	1.37
1368.0053	6.94
1407.9340	1.69
1425.1889	3.65
1466.5253	1.10
3058.3264	2.77
3067.1701	5.69
3104.0307	0.969
3171.2313	0.126

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
60.8173	0.343
99.8472	0.273
167.9643	0.118
220.3666	0.823
325.7459	0.295
414.6347	3.71
456.9320	0.156
555.2777	2.66
635.3624	2.53
704.0547	2.11
881.2253	0.541
970.9035	2.00
1092.3034	4.77
1126.7139	14.7
1149.2570	22.7
1151.7700	14.8
1226.2511	1.84
1295.2860	2.33
1321.2597	2.26
1356.4504	4.35
1398.4734	0.686
1440.7111	1.79
1459.9445	2.31
3022.4948	1.96
3089.1477	3.89
3102.2273	1.61
3167.2894	0.145



$\Delta E = 0.55$ kcal mol^{-1}
Population = 0.143



$\Delta E = 0.84$ kcal mol^{-1}
Population = 0.87

Optimized Coordinates (Angstroms)

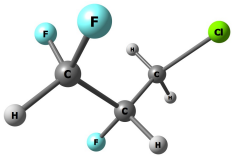
Atom	X	Y	Z
C	0.915830210880	-0.621589235506	0.387207255926
C	-0.165317594620	0.287089486238	-0.169275683816
C	-1.560338816105	-0.156825028861	0.275272846825
Cl	2.538833205568	-0.150737430857	-0.229295629799
H	0.956082543894	-0.554029209675	1.475850865467
H	0.732588957656	-1.652460658747	0.087177528769
H	-0.140244722763	0.294841037753	-1.265269937684
F	0.010583432894	1.569924244493	0.289181001304
H	-1.702135115971	-0.059152003285	1.359342812342
F	-2.486163449903	0.596677362365	-0.352758555783
F	-1.750600651531	-1.452866563919	-0.082682503550

Atom	X	Y	Z
C	1.077587134618	0.792993654086	0.344678919888
C	-0.238056406695	0.639951112574	-0.409332157161
C	-0.961670215820	-0.669319924743	-0.103935508581
Cl	2.312380012398	-0.365339675724	-0.274927513013
H	1.468807220884	1.799031466769	0.199417186456
H	0.938467856899	0.594254028607	1.406777389841
H	-0.076706835464	0.708984708570	-1.491219422715
F	-1.055188144954	1.674184322559	-0.010863522335
H	-0.377456886497	-1.545902709427	-0.405542929420
F	-1.211270219587	-0.744349954229	1.226855598402
F	-2.145398515783	-0.679782029042	-0.756718041362

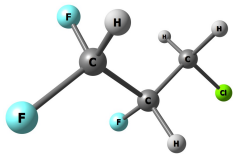
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
73.9023	0.166
79.9302	0.581
151.8425	0.654
218.5645	0.353
314.3858	0.166
400.7561	2.40
450.6737	0.0640
517.1302	4.74
601.0129	0.618
763.9935	6.97
867.8393	0.654
1044.4380	2.39
1091.2931	2.22
1131.6392	26.2
1135.4545	4.82
1153.4582	18.9
1215.6293	2.68
1265.3937	2.46
1332.7501	0.157
1371.1677	4.71
1401.8693	0.113
1435.5398	6.37
1467.4201	0.592
3047.0515	3.05
3064.7598	4.24
3091.9988	2.06
3162.7411	0.293

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
61.8121	0.369
103.1698	0.624
186.6335	0.618
239.5277	0.534
250.3440	0.208
372.8874	0.506
472.0485	2.43
546.2966	0.718
726.8838	2.81
764.6620	5.80
844.7160	7.59
967.0705	4.43
1078.2507	2.10
1103.4576	7.20
1130.7160	17.0
1173.4182	13.9
1186.8664	11.5
1278.0179	0.816
1348.2866	0.986
1380.6670	0.291
1414.3695	3.58
1430.3306	1.96
1482.0157	1.55
3060.0110	1.64
3072.6834	5.06
3105.1738	1.25
3173.0600	0.151



$\Delta E = 1.24$ kcal mol^{-1}
Population = 0.044



$\Delta E = 1.62$ kcal mol^{-1}
Population = 0.023

Optimized Coordinates (Angstroms)

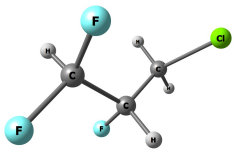
Atom	X	Y	Z
C	0.724620344055	0.997760680652	0.351924016550
C	-0.449597463645	0.672879159817	-0.565290212039
C	-1.183927976269	-0.628771015316	-0.236242968511
Cl	2.167525923742	-0.006906945755	-0.025900693528
H	1.004343072834	2.040864310639	0.208217522710
H	0.460323460662	0.823639330797	1.393782163372
H	-0.131818926415	0.644260747858	-1.613029829422
F	-1.377909342131	1.685957860518	-0.405531257361
H	-2.159134809529	-0.654825121774	-0.738694034207
F	-0.452899894118	-1.695034555970	-0.625898228660
F	-1.389952389185	-0.718346451466	1.100280521096

Atom	X	Y	Z
C	0.939083786697	-0.726970074023	-0.146481124117
C	-0.146317044002	0.324717302371	-0.297863334381
C	-1.526877736207	-0.323711103690	-0.417043401612
Cl	2.575106267717	0.019649526160	-0.162189185619
H	0.823652531741	-1.249005794263	0.802928670606
H	0.903316922982	-1.445229873969	-0.967489648506
H	0.025583632583	0.934481692036	-1.193352058146
F	-0.155374494551	1.146224608698	0.799128885378
H	-1.612813136818	-0.938557287380	-1.323564241797
F	-1.761611690099	-1.108644317150	0.662947085273
F	-2.470810040041	0.639744321210	-0.453322647078

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
43.4274	0.110
107.1276	0.283
185.6681	0.755
247.7660	0.0473
293.9491	2.91
344.4828	1.42
452.9349	0.309
563.3235	1.05
659.0006	1.56
779.7192	6.90
882.3589	1.78
957.9312	4.54
1080.5678	5.52
1094.7198	9.81
1148.1751	20.3
1179.0346	8.21
1185.8994	5.59
1281.6303	2.10
1336.5235	1.86
1378.2892	0.787
1416.1028	2.20
1424.0305	2.52
1481.4426	1.84
3052.2484	6.09
3070.9093	2.78
3105.0962	1.37
3172.4604	0.143

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
73.5645	0.104
84.9603	0.647
151.5347	0.518
244.4038	0.211
255.8778	0.0157
342.6827	0.101
493.3821	2.07
542.5945	1.77
746.9987	13.8
794.9446	1.33
867.7070	2.83
900.9800	3.07
1053.8269	0.399
1122.6009	15.2
1145.2451	9.89
1173.0925	14.4
1226.8401	5.07
1266.0141	3.18
1349.1335	1.21
1391.4403	3.78
1415.2599	3.88
1422.9033	4.64
1465.7314	0.656
3031.9217	5.27
3053.5139	3.97
3090.1424	1.91
3159.6299	0.331



$\Delta E = 1.90$ kcal mol^{-1}
Population = 0.015

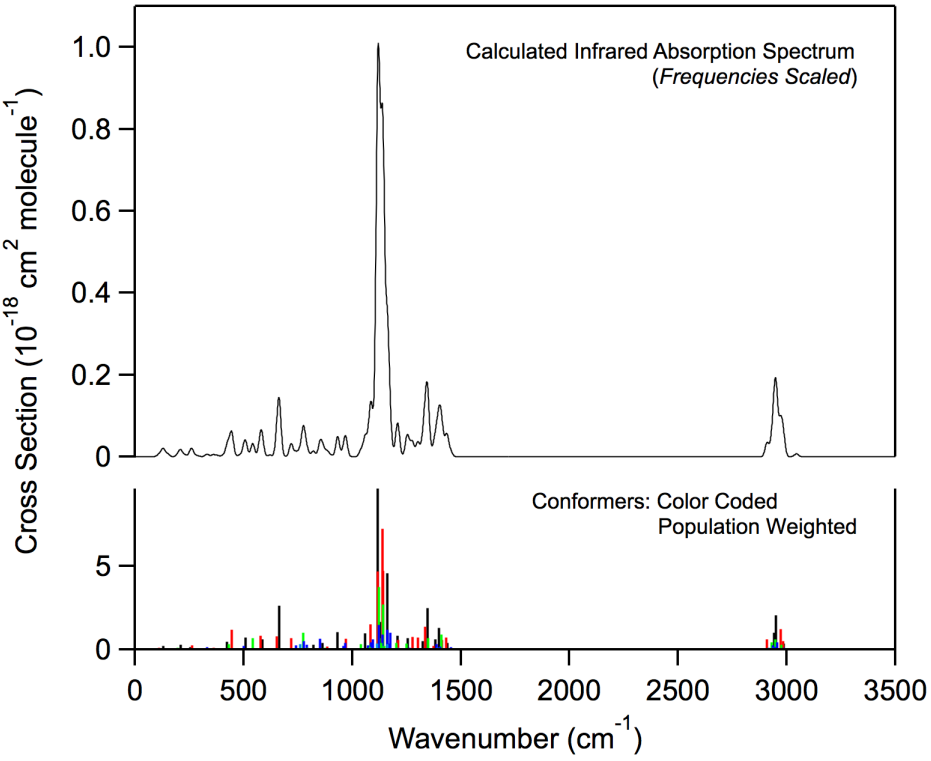
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.018930065688	0.938782436941	0.224277589764
C	-0.377851434939	0.664188366396	-0.327785680809
C	-1.127730413626	-0.468519309076	0.370380893047
Cl	2.248175003670	-0.200993688493	-0.422299047093
H	1.314410613539	1.943183990590	-0.078483057204
H	1.045046379246	0.870603074120	1.313280129637
H	-0.339627311531	0.460068844483	-1.403265969399
F	-1.127760648145	1.804537953115	-0.110994764748
H	-1.306472327039	-0.235765398209	1.429240114418
F	-2.320383978518	-0.643435039913	-0.240822325002
F	-0.430383948344	-1.621800229956	0.280582117389

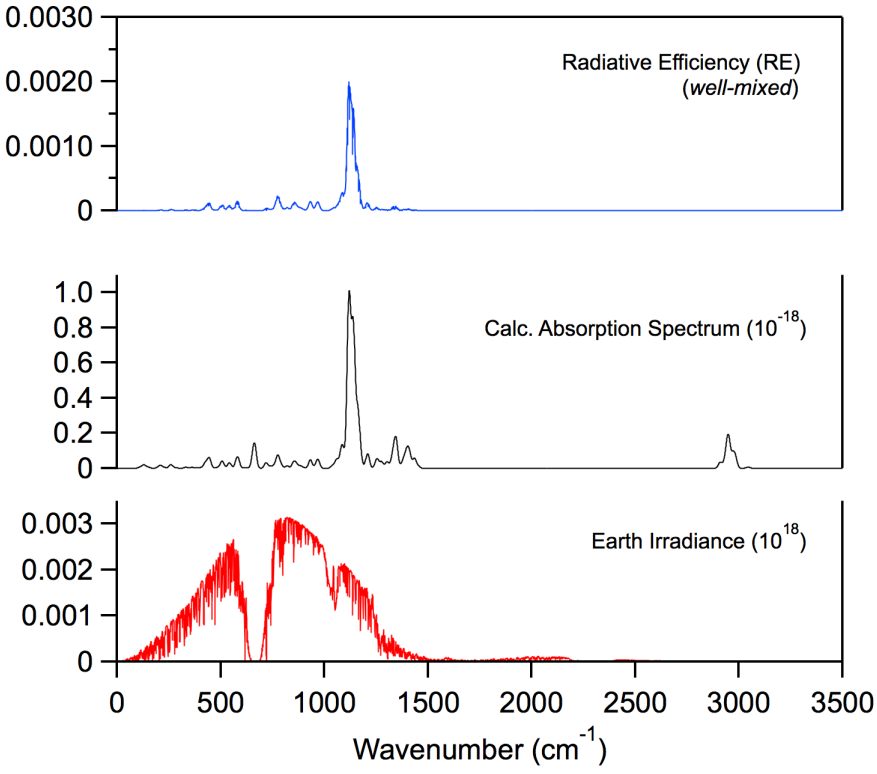
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
44.0901	0.157
100.1006	0.367
180.6956	0.432
225.5306	0.940
326.0447	0.113
371.3568	2.24
441.0002	2.13
505.8056	1.43
596.5994	0.131
782.6525	6.69
859.9574	1.51
1058.3005	0.526
1087.5542	10.0
1112.4949	4.94
1144.7539	28.6
1157.8434	14.5
1199.4307	1.20
1277.4682	2.23
1329.3435	2.09
1360.9594	0.411
1399.0373	2.11
1441.4946	2.60
1485.0064	1.77
3036.2150	4.90
3072.9020	1.72
3089.0258	2.94
3152.1811	0.450

Infrared Spectrum

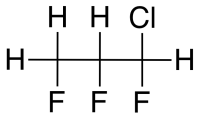


Radiative Efficiency



HCFC-253eb

Molecular Formula:	$CH_2FCHFCHClF$
Name:	1-Chloro-1,2,3-trifluoropropane
CAS number:	151771-12-9
Molecular Weight:	132.51



Global Atmospheric Lifetime (years):	1.50
Tropospheric Atmospheric Lifetime (years):	1.56
Stratospheric Atmospheric Lifetime (years):	40.4
Ozone Depletion Potential (ODP):	0.011

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.155	0.125
Global Warming Potential (GWP_H):		
GWP_{20}	397	320
GWP_{100}	108	87
Global Temperature Potentials (GTP_H)		
GTP_{20}		111
GTP_{50}		15
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) = 3.75×10^{-14}; k_{SAR}(272 K) ≈ 2.40×10^{-14} cm^3 $molecule^{-1}$ s^{-1}

τ^{OH}_{Global} = 1.52 years

τ^{OH}_{Trop} = 1.56 years

τ^{OH}_{Strat} = 50.4 years

Fractional Atmospheric Loss: 0.993

O(^{1}D) Reactivity

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

$k_{Est}(T) = 1.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)}$ = 370 years

Fractional Atmospheric Loss: 0.004

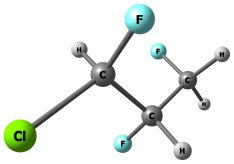
UV Photolysis

UV Spectrum: *No Recommendation*

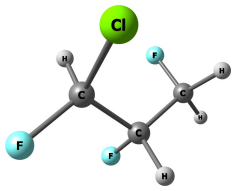
τ_{hv} = 450 years

Fractional Atmospheric Loss: 0.003

Molecular Structure and Infrared Spectrum (11 conformers)



E = 0
Population = 0.335



$\Delta E = 0.23$ kcal mol^{-1}
Population = 0.228

Optimized Coordinates (Angstroms)

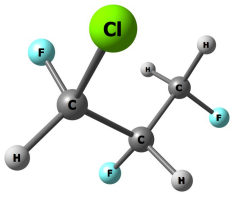
Atom	X	Y	Z
C	-1.897582450459	0.206079129593	-0.486631842294
C	-0.499299600085	-0.383539413073	-0.571842189613
C	0.496004001262	0.423743554569	0.261443185995
H	-1.919073303114	1.186458880989	-0.974117134378
H	-2.605269485880	-0.468061049733	-0.981828549477
F	-2.263236655952	0.347117266213	0.834053335812
H	-0.169934490526	-0.389320213724	-1.618608736906
F	-0.515330769198	-1.670534352781	-0.093752490807
H	0.236800905414	0.412344986966	1.320378145223
Cl	2.150157909984	-0.261503700412	0.121791354543
F	0.499792938553	1.701641911393	-0.197020078098

Atom	X	Y	Z
C	-1.445075757957	0.837437670728	-0.504504405362
C	-0.590526892596	-0.414352006514	-0.573674307809
C	0.604002617250	-0.400298785566	0.379456341968
H	-0.917029679383	1.689435516326	-0.943174338053
H	-2.376642177198	0.659431367098	-1.053278361824
F	-1.748232743509	1.118634908776	0.810258775037
H	-0.230612128225	-0.567327084748	-1.598644922623
F	-1.357288802432	-1.500792162506	-0.204846568858
H	0.298474136040	-0.209818341835	1.408507398935
F	1.246802402336	-1.584315349589	0.304335202572
Cl	1.749328025673	0.918585267830	-0.079833813983

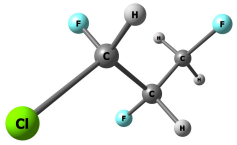
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
63.4541	0.313
104.6939	0.465
174.2518	0.225
222.4288	0.533
304.2873	1.21
376.4623	0.351
397.0990	2.41
497.3919	0.296
620.6678	10.8
818.9767	6.84
888.6095	1.87
963.8268	7.92
1090.8595	6.08
1113.6872	19.5
1144.0177	3.07
1154.3334	11.2
1242.5959	1.45
1281.8550	1.98
1335.2040	2.50
1365.2654	1.13
1399.4515	0.285
1426.1387	1.33
1493.6466	0.912
3040.6855	1.06
3053.3644	4.87
3100.4644	3.03
3128.8688	1.18

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
61.8158	0.354
108.1314	0.323
184.8339	0.269
231.5401	1.24
314.5002	0.343
390.0085	0.0789
397.3661	1.32
444.7407	2.05
663.9780	4.52
793.2518	17.0
898.5000	4.77
944.9227	1.74
1086.4773	6.50
1127.5940	16.1
1143.2886	8.04
1148.4674	12.9
1243.3975	1.57
1278.0902	2.11
1329.0525	0.911
1368.3892	0.368
1407.7516	1.67
1428.8502	1.48
1495.6399	1.22
3045.3495	1.38
3057.3328	3.86
3106.1578	3.07
3130.6495	1.09



$\Delta E = 0.73$ kcal mol^{-1}
Population = 0.097



$\Delta E = 0.85$ kcal mol^{-1}
Population = 0.080

Optimized Coordinates (Angstroms)

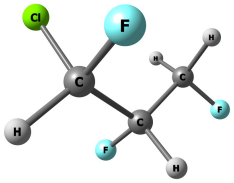
Atom	X	Y	Z
C	-1.224419448252	0.678950056127	0.542736496205
C	-0.581089016748	-0.191426584626	-0.523802990213
C	0.856004595035	-0.589040834802	-0.198647721188
H	-1.368670721601	0.093211185147	1.455919473421
H	-0.592607328816	1.546560776788	0.760036770859
F	-2.445772356649	1.108044362156	0.082131175213
H	-0.605298348657	0.321039795977	-1.491404287580
F	-1.296741943674	-1.367281317850	-0.634915807380
H	1.203590981213	-1.376983490530	-0.869554889260
Cl	1.969764080380	0.812774295520	-0.425759878485
F	0.943909507770	-1.022827243907	1.081639658408

Atom	X	Y	Z
C	-1.956823084523	-0.215194145984	0.068114124042
C	-0.527831093323	-0.562059894240	-0.347796604062
C	0.441969542344	0.543485093847	0.052496020803
H	-2.631341180517	-1.029746584473	-0.214656590848
H	-2.004018296668	-0.057631142990	1.150033614772
F	-2.332422029874	0.941199586008	-0.582043734414
H	-0.471969971482	-0.700270046396	-1.433589055230
F	-0.186294941120	-1.732495613744	0.280357085717
H	0.190616885645	1.478682354568	-0.451260402206
F	0.397751223941	0.726120533919	1.395354280092
Cl	2.123964945578	0.124942859485	-0.427565738666

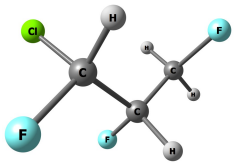
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
77.6883	0.317
85.8115	0.618
188.1006	1.08
206.7608	0.383
305.6605	0.140
323.5716	0.505
406.2728	0.485
483.7512	2.37
670.8419	3.67
793.6979	17.8
891.8887	6.55
947.6648	2.83
1105.0351	18.6
1109.8444	8.06
1128.5261	7.29
1160.3994	8.97
1256.7704	2.05
1281.8147	1.14
1310.5815	0.111
1377.9772	1.35
1397.3023	1.84
1444.2272	0.922
1502.1894	0.609
3051.7922	2.33
3071.5916	1.24
3108.8880	2.80
3109.6243	2.20

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
61.0774	0.210
107.4924	0.826
195.6635	0.330
208.3100	0.484
243.4981	0.101
379.2183	1.20
429.6042	3.13
474.4799	2.25
692.5343	4.89
775.7883	6.40
868.2237	9.44
1017.6597	4.74
1092.9815	16.6
1098.1986	3.35
1123.6163	5.36
1172.3916	14.1
1243.9915	0.259
1267.9123	2.88
1342.4167	0.116
1382.9530	0.338
1392.7818	2.71
1425.6657	0.611
1514.3693	0.516
3053.0976	3.24
3060.8529	2.41
3111.0886	1.14
3112.6583	3.83



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



$\Delta E = 1.14$ kcal mol^{-1}
Population = 0.049

Optimized Coordinates (Angstroms)

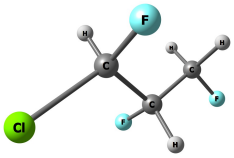
Atom	X	Y	Z
C	-1.320666919871	-0.313539381282	-0.703600002328
C	-0.615639065442	-0.050957600167	0.615296828888
C	0.872903462968	-0.393046247940	0.607150601748
H	-1.068305840512	0.465389797683	-1.428987152567
H	-1.018541848155	-1.291831838405	-1.093521268678
F	-2.679018804950	-0.306897451273	-0.488381662492
H	-1.080782665298	-0.676332976228	1.390054720041
F	-0.751644329442	1.265359301530	0.981307126045
H	1.344797392898	-0.117566387011	1.552151323995
F	1.014364352824	-1.724687147516	0.395089719636
Cl	1.770228264980	0.509916930610	-0.670018234288

Atom	X	Y	Z
C	-1.736110571854	0.184646003948	0.366360543004
C	-0.601446485041	-0.764408656530	-0.002321729487
C	0.585714473363	-0.061558199469	-0.651341233827
H	-2.559987459954	-0.385862139988	0.807817443226
H	-1.392773750990	0.939667039343	1.080545391401
F	-2.172261763901	0.806550548881	-0.784910303343
H	-0.958946082213	-1.499724078045	-0.736616926340
F	-0.205310132583	-1.429163642111	1.128647441217
H	0.251096639736	0.575079681906	-1.472577201759
Cl	1.441269351278	1.011454348116	0.516669345106
F	1.459462782159	-0.986000906051	-1.113579769199

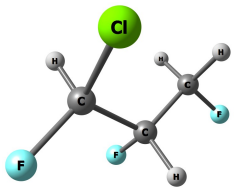
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
76.6213	0.293
89.9600	0.513
166.6883	0.456
212.5288	0.898
286.5990	0.470
355.2166	0.331
440.8669	1.70
518.0478	0.724
620.3790	9.49
712.2651	6.52
901.9028	3.07
1016.4005	5.34
1104.1631	14.3
1113.3494	14.5
1146.5824	14.0
1155.9086	1.36
1271.6075	2.18
1282.2111	0.751
1333.2109	3.66
1342.7727	2.94
1399.7275	1.03
1440.8581	0.714
1500.4130	0.529
3031.7323	2.06
3050.7816	2.62
3107.6136	2.04
3111.3445	2.57

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
59.1698	0.224
111.8859	0.744
199.5620	0.139
203.7799	0.670
247.6653	0.621
382.0730	0.998
451.3137	0.366
518.5856	2.09
594.5575	8.30
769.2550	6.05
862.8664	5.98
1049.4950	1.58
1093.0281	14.5
1117.2317	8.51
1139.4734	8.94
1163.9137	12.1
1242.6155	0.274
1287.5092	3.21
1325.5756	0.890
1368.7003	2.56
1402.8185	2.15
1429.7948	0.195
1515.7490	0.862
3030.4779	2.42
3051.5859	3.60
3108.7520	3.62
3110.9638	1.16



$\Delta E = 1.29$ kcal mol^{-1}
Population = 0.038



$\Delta E = 1.65$ kcal mol^{-1}
Population = 0.021

Optimized Coordinates (Angstroms)

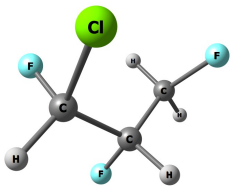
Atom	X	Y	Z
C	-1.795285847613	0.517790861038	0.231857704980
C	-0.537624183558	-0.231713917662	-0.183336065726
C	0.721679044684	0.446968092744	0.353655230868
H	-1.937540820227	0.436776237519	1.316898242883
H	-1.711565837009	1.572758288218	-0.048894587317
F	-2.876368555790	-0.041065906552	-0.402525558628
H	-0.484284078588	-0.282786393164	-1.277195547791
F	-0.584116014784	-1.507836393229	0.320825858791
H	0.753282968391	0.449641589603	1.446175595924
Cl	2.194758102271	-0.425455871353	-0.187108937590
F	0.763065222222	1.724607412836	-0.104078936393

Atom	X	Y	Z
C	-1.402214930285	0.817367910148	0.309529138578
C	-0.575627512574	-0.339668217034	-0.226812499160
C	0.843921064045	-0.418264800736	0.330424606014
H	-1.537804487768	0.709210629082	1.393190797837
H	-0.918231841722	1.774685951622	0.095880314095
F	-2.633798676123	0.783779475362	-0.297384327296
H	-0.527162574884	-0.295297799583	-1.321224089478
F	-1.190760269362	-1.519416031480	0.136062866819
H	0.859116027416	-0.479084057535	1.421480218329
F	1.456170202773	-1.505566034937	-0.182892600502
Cl	1.790361998484	1.052317975089	-0.119079425236

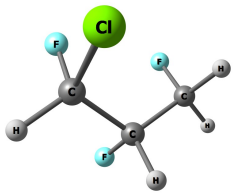
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
64.2432	0.0787
94.0911	0.757
152.0480	0.596
245.7478	0.815
289.4416	0.598
375.4225	0.163
403.9916	1.61
479.2499	1.36
550.5655	3.22
781.5800	19.3
906.2420	3.13
1091.3291	9.19
1096.7080	4.84
1117.3688	7.28
1126.8718	13.2
1146.8114	9.38
1241.6668	1.99
1285.1394	0.622
1327.1582	3.26
1354.6635	1.80
1405.0023	0.250
1435.8881	1.76
1504.0609	0.405
3032.3489	3.04
3060.6253	0.949
3092.1233	0.940
3098.6626	5.81

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
70.6581	0.385
92.0746	0.586
163.0750	0.521
239.8320	0.924
307.2997	0.295
372.7460	0.593
411.1652	0.915
440.6924	0.513
557.0159	3.96
786.7283	16.6
907.5707	5.57
1070.8015	13.7
1107.4265	6.50
1118.9799	3.22
1125.1721	5.86
1147.8973	20.9
1235.3665	1.76
1282.5835	0.0616
1306.5500	1.23
1372.2997	0.290
1411.9577	2.17
1441.0171	1.06
1502.5738	0.453
3033.6628	2.96
3061.9439	1.12
3095.8426	1.65
3105.0158	4.55



ΔE = 1.66 kcal mol^{-1}
Population = 0.020



ΔE = 1.77 kcal mol^{-1}
Population = 0.017

Optimized Coordinates (Angstroms)

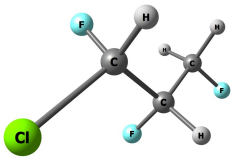
Atom	X	Y	Z
C	-1.314817951332	0.976824679771	0.318197365634
C	-0.833606441348	-0.147123264861	-0.599182095263
C	0.416786639490	-0.881575363044	-0.120427705458
H	-2.363600519636	1.179414969172	0.074705862752
H	-1.237979606584	0.675187362351	1.367293364250
F	-0.568926838749	2.109692072911	0.110263688271
H	-0.663357337426	0.239591521273	-1.609498206804
F	-1.836098451273	-1.099286069285	-0.638489660942
H	0.595684044272	-1.773502740692	-0.724671966154
Cl	1.878110265548	0.154894925763	-0.276858158231
F	0.264030197038	-1.251864093358	1.174036511944

Atom	X	Y	Z
C	-1.204306162376	1.007628399723	-0.509703514740
C	-0.574360644134	-0.354321933944	-0.751650561461
C	0.632454485426	-0.704023510999	0.120569425697
H	-0.475575313127	1.798500930619	-0.719432939595
H	-2.059268390860	1.116841430930	-1.187836235267
F	-1.647844185966	1.119122898350	0.782369459139
H	-0.257082404604	-0.411886085198	-1.800601948130
F	-1.515577178081	-1.335788655275	-0.515716051344
H	0.953936997382	-1.730693656179	-0.069781011697
Cl	2.034789123023	0.352509803677	-0.320399439297
F	0.358339673318	-0.560031621705	1.429903816694

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
43.0719	0.150
109.5694	0.407
184.3197	0.805
243.7791	0.0668
295.0738	1.80
333.3802	2.81
388.8818	0.337
484.9342	0.236
647.1726	1.80
803.0080	16.8
886.4924	1.29
1010.6127	5.41
1085.5682	11.0
1113.8305	8.40
1121.7943	12.3
1161.7092	10.8
1247.0602	2.25
1268.6560	0.669
1333.9689	0.652
1374.2307	2.14
1390.3698	0.816
1442.7205	0.0475
1515.2711	0.658
3047.9857	3.87
3071.2936	1.73
3101.9219	1.61
3107.3733	3.81

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
47.1278	0.253
132.5675	0.407
194.8342	0.718
213.7852	0.322
286.8229	0.383
345.3277	0.324
393.2982	1.09
482.4789	3.55
769.7606	10.4
821.5981	4.54
831.0091	10.5
963.5160	1.41
1005.9389	2.77
1112.1286	6.59
1147.1357	25.2
1178.7150	6.53
1253.6793	3.58
1287.3926	0.568
1360.3937	0.866
1377.7744	0.500
1411.6262	1.26
1436.4501	3.00
1496.9696	1.20
3034.0305	1.81
3049.4022	4.51
3089.2599	3.34
3098.1203	2.29



$\Delta E = 1.88$ kcal mol^{-1}
Population = 0.014

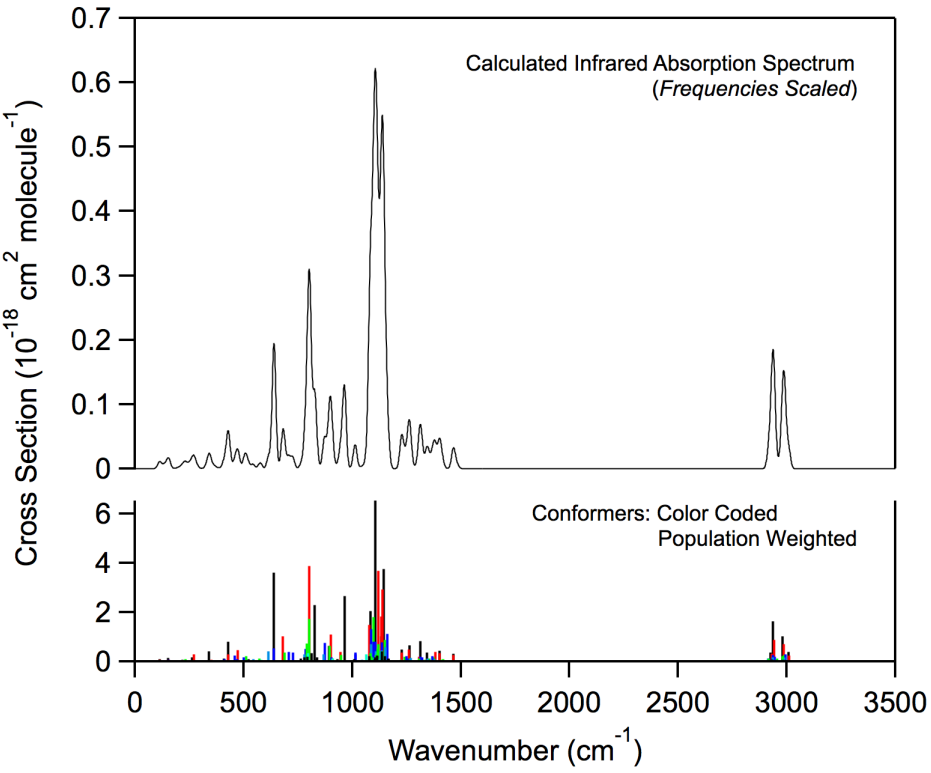
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.798332213539	0.512407392196	-0.286843639926
C	-0.536061373685	-0.337289970668	-0.219426355445
C	0.710897266814	0.525556760129	-0.380816117608
H	-1.872556489179	1.127094942469	0.615791157942
H	-1.776211429067	1.165301622583	-1.168895349702
F	-2.890523097574	-0.314280056642	-0.367394125989
H	-0.553610817811	-1.085670701312	-1.021096103636
F	-0.501452277917	-0.985199517088	0.988213232144
H	0.773596590904	0.945221638430	-1.388403516192
F	0.690764513300	1.539269739605	0.522332076473
Cl	2.203703327753	-0.444266849703	-0.143733258060

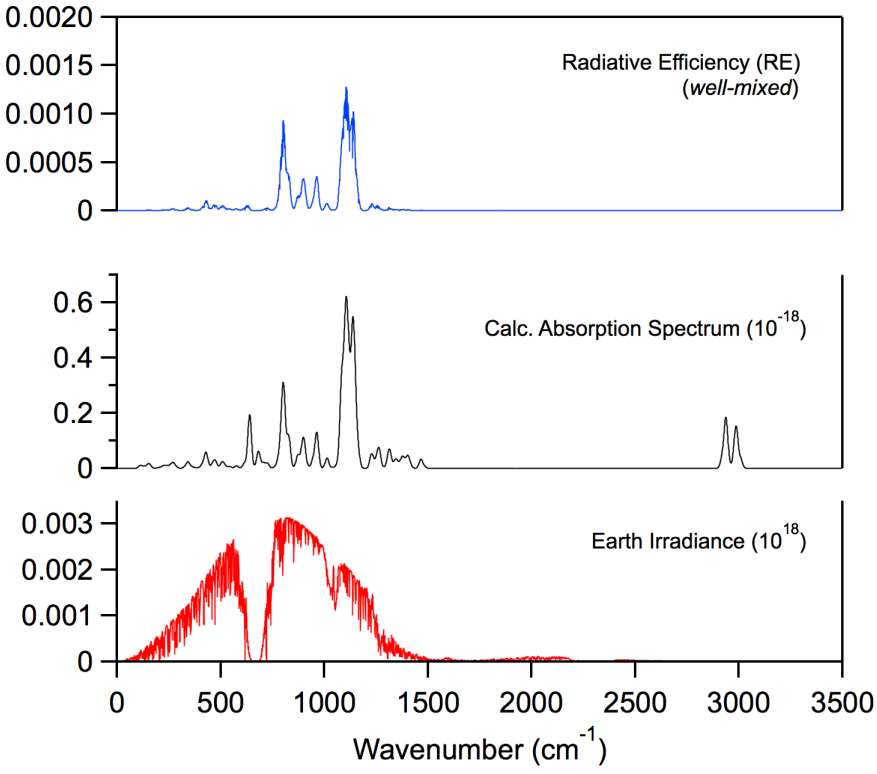
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
67.2862	0.0333
99.6589	0.882
153.8396	0.617
229.3576	0.131
300.8055	0.180
313.9357	0.286
397.4664	0.188
490.5618	3.33
752.3134	9.57
782.6292	13.9
893.2293	3.65
929.6972	6.39
1084.4507	5.67
1114.9785	5.66
1124.3586	16.2
1179.0548	9.15
1262.3664	0.795
1283.5354	1.67
1320.8561	2.21
1375.0665	0.881
1405.5032	1.83
1436.4766	1.88
1499.5365	0.464
3030.0086	3.84
3053.0638	1.26
3086.2595	1.54
3099.5153	5.05

Infrared Spectrum

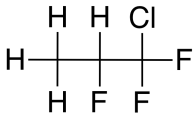


Radiative Efficiency



HCFC-253ec

Molecular Formula:	$CH_3CHFCClF_2$
Name:	1-Chloro-1,1,2-trifluoropropane
CAS number:	134251-05-1
Molecular Weight:	132.51



Global Atmospheric Lifetime (years):	1.13
Tropospheric Atmospheric Lifetime (years):	1.17
Stratospheric Atmospheric Lifetime (years):	32.7
Ozone Depletion Potential (ODP):	0.009

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.240	0.183
Global Warming Potential (GWP_H):		
GWP_{20}	462	352
GWP_{100}	125	95
Global Temperature Potentials (GTP_H)		
GTP_{20}		116
GTP_{50}		16
GTP_{100}		13

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

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

OH Reactivity

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

k_{SAR}(298 K) = 5.00×10^{-14}; k_{SAR}(272 K) ≈ 3.19×10^{-14} cm^3 $molecule^{-1}$ s^{-1}

τ^{OH}_{Global} = 1.14 years
τ^{OH}_{Trop} = 1.17 years
τ^{OH}_{Strat} = 38.9 years

Fractional Atmospheric Loss: 0.994

O(^{1}D) Reactivity

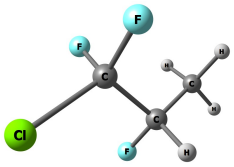
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 1.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)}$ = 370 years
Fractional Atmospheric Loss: 0.003

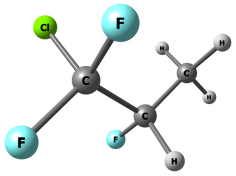
UV Photolysis

UV Spectrum: *No Recommendation*
τ_{hv} = 450 years
Fractional Atmospheric Loss: 0.003

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.398



$\Delta E = 0.11$ kcal mol^{-1}
Population = 0.329

Optimized Coordinates (Angstroms)

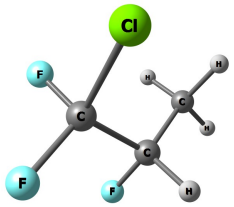
Atom	X	Y	Z
C	-2.253816397265	0.331599522690	-0.205304807384
C	-0.945853252830	-0.400639811911	-0.459381745161
C	0.257800030417	0.393993752405	0.066640062473
H	-3.082091630858	-0.269863871408	-0.585897674031
H	-2.393403436053	0.492397860137	0.865916646964
H	-2.255033247487	1.297883958281	-0.714722559574
H	-0.780357027564	-0.571287539738	-1.528914393487
F	-0.958931416816	-1.614415735702	0.183182903819
Cl	1.800856101927	-0.498364428242	-0.178141865735
F	0.335837316707	1.561955974835	-0.587799608796
F	0.127482959823	0.656597318653	1.370323040912

Atom	X	Y	Z
C	-1.807434714164	0.696284559466	-0.842528785163
C	-1.123219609699	-0.346907318127	0.018174184392
C	0.399171837022	-0.417712854267	-0.166704114221
H	-2.886370926867	0.644461755112	-0.679344425467
H	-1.458554876649	1.697980731097	-0.582453257187
H	-1.602218224458	0.509680657000	-1.899127598713
H	-1.483068510973	-1.356787132144	-0.223692780470
F	-1.369777549898	-0.113804499388	1.348531866547
Cl	1.230594831925	1.099612713272	0.330595026801
F	0.901655247212	-1.420920699150	0.557869569975
F	0.678771496548	-0.657047912871	-1.455879686495

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
71.5873	0.196
182.7102	0.220
217.1518	0.00307
247.3913	0.0979
304.6336	0.389
348.1468	0.257
413.0500	0.106
436.8915	1.80
484.7425	2.44
616.6564	1.46
728.7908	5.05
897.1719	8.51
975.7231	34.5
1034.2205	7.39
1128.6971	1.70
1160.8871	13.1
1171.2444	24.5
1260.2298	14.7
1365.7399	0.799
1382.6794	0.390
1405.4252	1.35
1485.6409	0.783
1496.8019	0.523
3060.6611	1.02
3062.9996	2.45
3142.0324	1.27
3146.2271	1.49

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
77.9324	0.212
192.4387	0.0550
211.9807	0.170
221.7086	0.185
328.3432	0.0958
339.0830	0.171
413.9239	0.0608
481.0917	0.887
509.4138	0.948
586.5570	9.19
662.7796	2.23
895.1520	10.8
957.2773	11.6
1108.3544	14.5
1133.4137	6.37
1163.0694	23.6
1192.5787	23.4
1223.5173	7.48
1365.4365	1.08
1381.2281	4.44
1411.1319	2.43
1485.6397	0.589
1496.6912	0.644
3028.5020	3.54
3060.5227	0.718
3139.2620	1.45
3146.3136	1.23



$\Delta E = 0.22$ kcal mol^{-1}
Population = 0.273

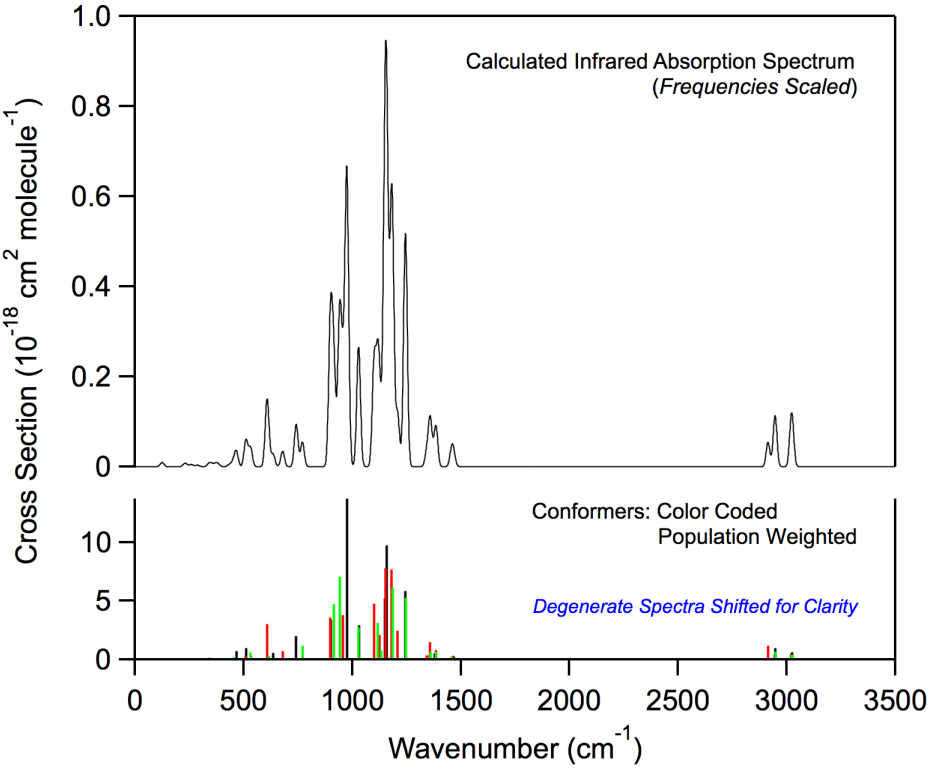
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.355136454849	1.570004233120	0.164285595429
C	-0.976774228968	0.260844897262	-0.501703925534
C	0.281206439025	-0.399008060383	0.082295477170
H	-0.597742863094	2.334907055197	-0.016426633870
H	-2.306667269429	1.912277264803	-0.248598693794
H	-1.467835254727	1.424981408418	1.241052176101
H	-0.813876544777	0.378519772987	-1.578620430678
F	-1.990017261827	-0.657839275909	-0.314653376490
Cl	1.749334662935	0.599455755028	-0.269632030984
F	0.177536318020	-0.548613311385	1.405186557582
F	0.462184457690	-1.605400739139	-0.456236714933

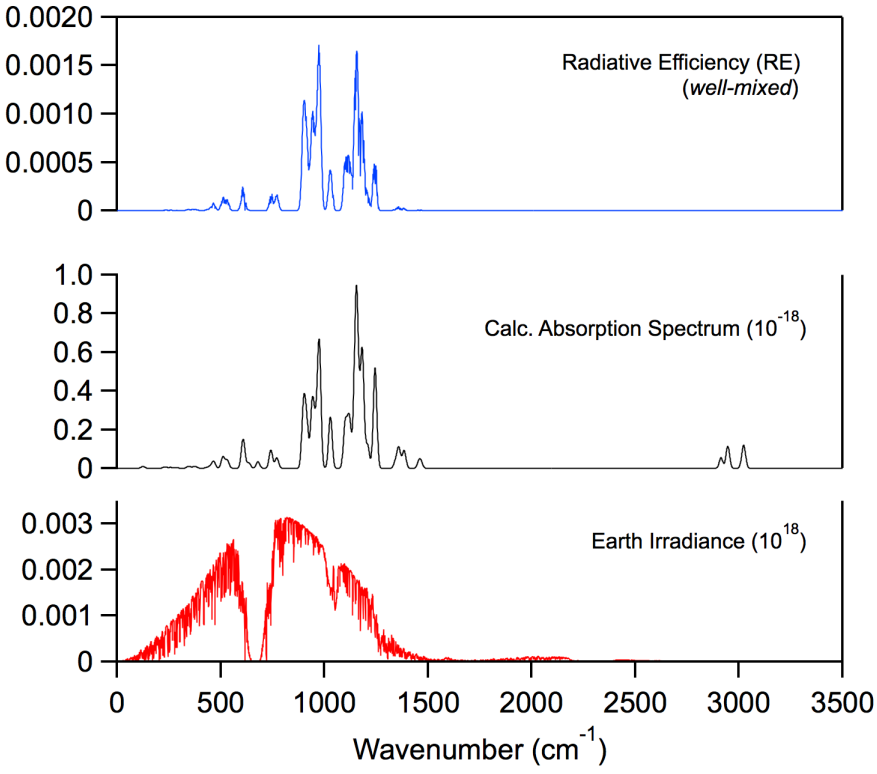
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
76.5120	0.220
191.9238	0.286
213.7243	0.00269
248.5989	0.126
316.3374	0.362
335.4938	0.234
401.0540	0.289
422.5944	0.719
504.5282	2.20
596.1097	1.17
759.2100	4.25
911.9821	17.3
940.5148	25.9
1031.7381	10.2
1125.4371	11.5
1145.0412	2.86
1198.7214	22.4
1262.3225	19.3
1363.8735	0.0523
1383.8986	2.40
1410.6191	2.50
1487.2940	0.880
1496.0540	0.379
3062.9362	0.608
3065.3727	2.48
3142.1891	1.50
3150.2474	1.28

Infrared Spectrum

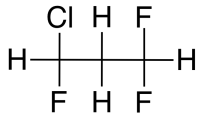


Radiative Efficiency



HCFC-253fa

Molecular Formula:	$CHClFCH_2CHF_2$
Name:	1-Chloro-1,3,3-trifluoropropane
CAS number:	149329-30-6
Molecular Weight:	132.51



Global Atmospheric Lifetime (years):	1.83
Tropospheric Atmospheric Lifetime (years):	1.90
Stratospheric Atmospheric Lifetime (years):	46.4
Ozone Depletion Potential (ODP):	0.012

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.210	0.175
Global Warming Potential (GWP_H):		
GWP_{20}	652	542
GWP_{100}	177	147
Global Temperature Potentials (GTP_H)		
GTP_{20}		196
GTP_{50}		26
GTP_{100}		20

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 3.08 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 1.97 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

τ^{OH}_{Global} = 1.84 years
τ^{OH}_{Trop} = 1.90 years
τ^{OH}_{Strat} = 60.2 years

Fractional Atmospheric Loss: 0.991

O(^{1}D) Reactivity

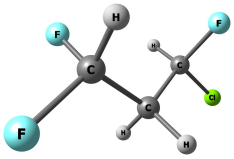
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 1.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)}$ = 370 years
Fractional Atmospheric Loss: 0.005

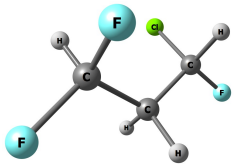
UV Photolysis

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

Molecular Structure and Infrared Spectrum (7 conformers)



E = 0
Population = 0.506



$\Delta E = 0.38$ kcal mol^{-1}
Population = 0.268

Optimized Coordinates (Angstroms)

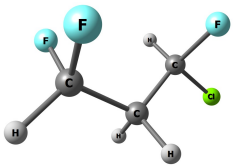
Atom	X	Y	Z
C	0.820687833654	-0.344328124089	0.177552741849
C	-0.298482285207	0.613405712960	-0.183214232088
C	-1.646193137890	-0.093496862173	-0.189511936109
F	0.862211203446	-1.361042530394	-0.725373513425
Cl	2.415413685176	0.503445144739	0.169226989926
H	0.709596431893	-0.768027174444	1.176583439776
H	-0.110470859298	1.039154876705	-1.172323734487
H	-0.338846370710	1.427522113997	0.544881877340
H	-1.706892419025	-0.901497949695	-0.927094847381
F	-1.886392718212	-0.624210891063	1.040913161671
F	-2.623045363827	0.807044683457	-0.452259947072

Atom	X	Y	Z
C	0.942680052802	-0.476098747107	0.354667730944
C	-0.353189983787	-0.755851464320	-0.382916329910
C	-1.439646213267	0.269165679431	-0.110223989250
F	1.810260549674	-1.494572305563	0.149234507865
Cl	1.715949432220	1.057455476438	-0.234677398486
H	0.797467562758	-0.334375004537	1.426475796141
H	-0.722498522628	-1.731001953404	-0.046272012320
H	-0.160666729684	-0.810331369426	-1.457365542569
H	-1.193040728276	1.276125038319	-0.463674031156
F	-2.586200150509	-0.131261383503	-0.711709243085
F	-1.672327269303	0.335222033672	1.229858511826

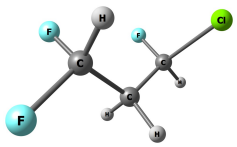
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
64.5394	0.192
100.3602	0.935
141.0367	0.385
259.7812	0.219
344.7607	0.168
394.2437	0.140
493.2072	4.78
506.8511	1.69
568.5319	0.499
772.5440	17.7
880.2400	3.20
956.8971	3.02
1106.4162	10.0
1118.0186	18.3
1133.4236	18.4
1151.5206	19.2
1229.3892	2.09
1271.2315	0.608
1337.2899	3.50
1391.2959	1.14
1417.3497	8.36
1423.3716	8.68
1462.5527	0.719
3068.4078	4.97
3077.2984	0.396
3114.3431	0.853
3137.0659	1.34

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
60.1112	0.202
108.1606	0.851
146.5161	0.288
297.5786	0.522
337.6073	0.204
408.7984	0.718
468.9706	1.86
534.3106	2.55
569.4854	1.45
671.0167	11.1
900.7539	2.26
1031.1515	8.75
1081.9594	7.62
1112.6825	22.2
1140.0925	20.9
1155.7094	16.1
1220.6940	2.99
1293.1348	1.61
1320.1435	4.80
1389.2999	0.567
1416.3671	4.37
1431.0710	9.19
1465.7568	0.740
3058.8611	0.102
3074.7376	4.63
3112.2079	0.367
3128.3414	1.76



$\Delta E = 0.92$ kcal mol^{-1}
Population = 0.107



$\Delta E = 1.47$ kcal mol^{-1}
Population = 0.042

Optimized Coordinates (Angstroms)

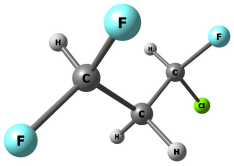
Atom	X	Y	Z
C	0.679559054339	-0.068362461737	0.346170042491
C	-0.227955305257	0.590251521530	-0.680322830559
C	-1.704556874705	0.392858672751	-0.362073329922
F	0.561908724853	-1.414634333816	0.292634211131
Cl	2.407620715323	0.373103485080	0.018986775461
H	0.475247537578	0.267535883864	1.363617741495
H	-0.013750868469	0.180256894355	-1.671026019650
H	-0.022279550361	1.663276263824	-0.702225065666
H	-2.351212740064	0.953435426907	-1.049173649043
F	-2.046958883477	-0.914712903355	-0.427152802983
F	-1.960735809760	0.823919550595	0.904601927246

Atom	X	Y	Z
C	0.999023185858	0.367218730741	-0.661764859181
C	-0.407001676406	-0.113313413479	-0.975750786461
C	-1.309738319287	-0.306356108881	0.234661408507
F	0.976371900076	1.537884220917	0.013224496817
Cl	1.909850110234	-0.853487700285	0.334954215475
H	1.597191745871	0.489040068600	-1.566990426451
H	-0.344075860955	-1.058092265621	-1.521026883529
H	-0.880989904266	0.629043657842	-1.628026932115
H	-0.886219397836	-0.975596099043	0.991456498915
F	-1.574812377335	0.887405744888	0.816789722138
F	-2.488917405953	-0.830406835680	-0.191683454114

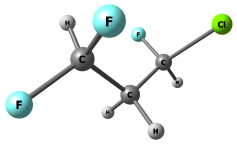
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
40.9112	0.260
115.4218	0.146
166.9247	0.443
250.8918	0.0646
352.8035	0.766
385.3564	0.154
458.9304	2.11
515.8835	2.40
639.4134	10.6
823.3232	7.18
854.3197	3.24
943.9062	1.82
1010.1198	3.86
1117.3288	9.77
1144.6926	17.2
1172.2389	29.6
1233.3344	3.47
1282.6228	0.171
1365.5383	14.1
1387.3795	3.30
1415.6226	4.00
1422.4394	3.61
1454.3606	1.36
3043.9369	7.66
3078.4602	0.869
3114.7988	0.796
3133.3506	1.09

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
41.8066	0.210
112.4804	0.271
167.1982	0.218
306.5156	0.388
321.7367	0.623
387.2428	0.201
451.4357	2.41
549.6033	2.72
635.7505	6.16
712.4470	5.44
875.5797	4.49
974.8969	6.05
1042.2238	3.02
1125.1841	13.2
1136.4845	13.6
1166.4249	36.4
1251.8878	0.626
1283.5998	8.51
1336.2672	0.960
1389.8044	2.95
1418.0389	4.86
1435.6690	5.08
1454.9021	1.71
3056.6232	0.0652
3073.9183	4.47
3099.8662	2.85
3122.8680	0.789



$\Delta E = 1.62$ kcal mol^{-1}
Population = 0.033



$\Delta E = 1.86$ kcal mol^{-1}
Population = 0.022

Optimized Coordinates (Angstroms)

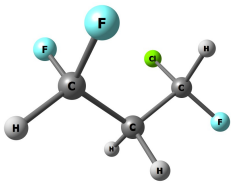
Atom	X	Y	Z
C	0.849657374273	-0.223268657649	0.408600304857
C	-0.283525927498	0.646814667444	-0.104690327257
C	-1.655079857821	0.151440607068	0.335215233545
F	0.779583875155	-1.465842334801	-0.120567260906
Cl	2.446879362642	0.506513171070	-0.038597602348
H	0.867340846024	-0.305834408103	1.498920154172
H	-0.256383235604	0.673938358711	-1.197648568585
H	-0.150878110645	1.664369708932	0.270394795371
H	-1.746996275256	0.045614039967	1.425436042436
F	-2.592459743408	1.039293900659	-0.082546815972
F	-1.935302307860	-1.046039053296	-0.229708955312

Atom	X	Y	Z
C	0.990030335086	0.758506855724	-0.338596845493
C	-0.462681603487	0.637711652281	-0.767844851784
C	-1.392283623031	0.050444905093	0.286338843292
F	1.062152795416	1.434265587105	0.841003666627
Cl	1.802654586339	-0.841596466027	-0.131197929613
H	1.588096602095	1.288748629042	-1.081999550062
H	-0.538982262857	0.045147858477	-1.682772568717
H	-0.817308318335	1.651427295504	-0.984585160808
H	-1.238449408365	0.489355130849	1.278478038300
F	-2.675493869793	0.285413908551	-0.095070864976
F	-1.233257233068	-1.290171356598	0.379556223233

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
41.7192	0.0343
113.2389	0.557
156.8628	0.772
262.1749	0.149
315.8264	0.163
396.8245	0.137
478.8672	2.01
500.7701	4.10
589.2269	0.676
765.0559	17.6
882.4405	3.33
970.4004	3.38
1099.7307	3.68
1119.8014	1.34
1134.5778	20.1
1169.2702	37.9
1235.7850	3.97
1275.2468	0.571
1338.4812	3.97
1399.3558	1.11
1417.2613	6.16
1427.6463	12.4
1458.0572	0.646
3025.6890	7.44
3075.4229	0.502
3081.7656	2.74
3135.0540	0.865

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
37.3739	0.171
107.9201	0.168
168.9021	0.418
261.6534	0.319
363.5793	0.519
389.0738	0.0278
449.6342	2.65
561.4100	0.998
650.3271	8.64
696.0545	4.28
896.2847	0.394
933.5902	5.43
1085.5662	13.1
1115.0755	9.05
1124.2900	20.6
1154.2307	25.5
1242.7716	1.50
1292.9613	7.95
1340.5696	2.23
1374.5849	3.17
1421.1360	3.37
1437.1732	5.46
1456.8830	1.47
3059.0166	0.464
3069.2362	4.51
3101.6393	2.77
3124.5773	0.806



$\Delta E = 1.88$ kcal mol^{-1}
Population = 0.021

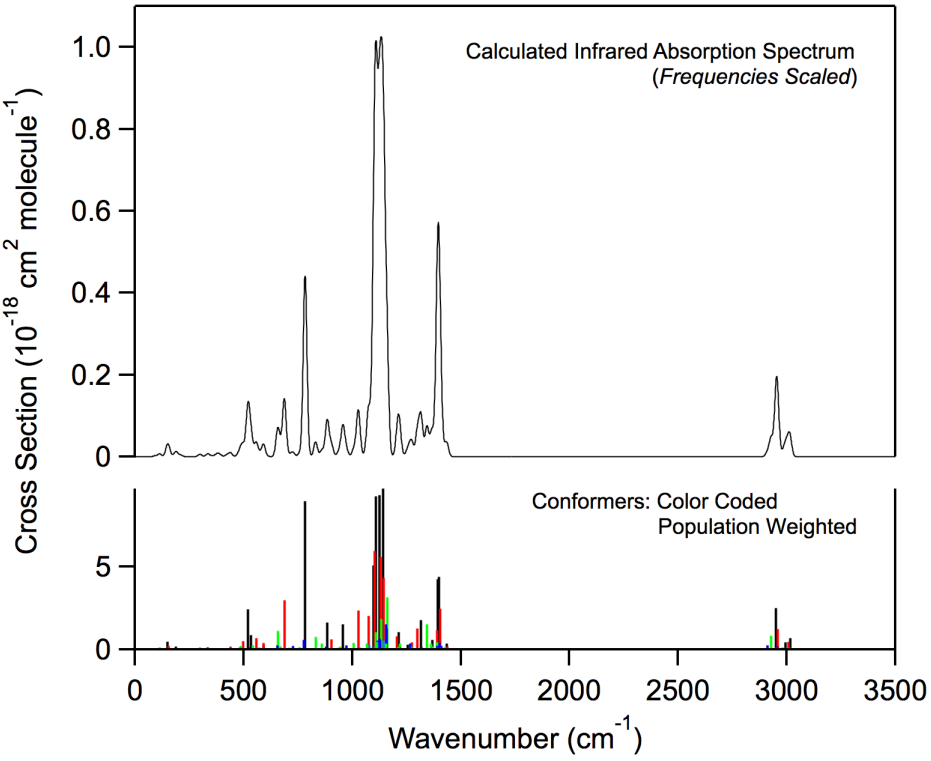
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	0.850843016947	-0.550916171319	0.289536541006
C	-0.290273292135	-0.886867208694	-0.660484370646
C	-1.621365617608	-0.243164945698	-0.305631966002
F	1.868593671487	-1.424873287345	0.078699366519
Cl	1.484591343584	1.120179390659	0.036296252834
H	0.547982027992	-0.600214298811	1.336078212219
H	-0.426067927545	-1.973058965320	-0.611343244164
H	-0.017697868525	-0.626144380973	-1.686223729986
H	-2.439700141860	-0.640900946116	-0.919247371105
F	-1.915017823490	-0.493965434800	1.001200965576
F	-1.588306388846	1.099222248418	-0.467298656250

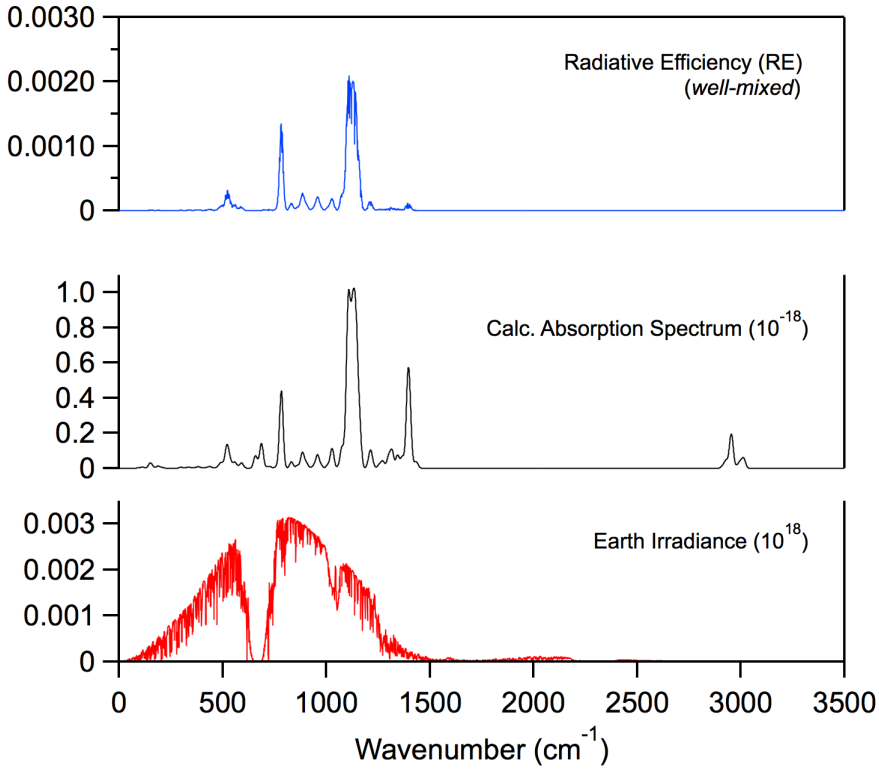
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
38.6534	0.242
117.2536	0.0593
162.4528	0.522
281.9926	0.528
362.3708	1.08
386.4863	0.257
439.4103	1.26
531.3757	0.848
652.6183	7.80
745.1392	7.67
888.5414	1.09
935.8020	2.29
1072.1516	16.5
1106.1622	5.13
1120.8189	20.6
1167.2712	17.1
1228.2318	9.25
1316.9593	4.06
1336.7329	3.47
1395.9469	8.33
1418.9291	4.72
1422.7380	0.468
1460.8979	1.26
3042.6569	6.28
3061.6638	3.04
3112.2855	0.187
3126.2036	1.59

Infrared Spectrum

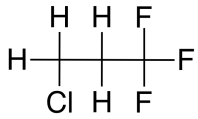


Radiative Efficiency



HCFC-253fb

Molecular Formula: $CH_2ClCH_2CF_3$
Name: 3-Chloro-1,1,1-trifluoropropane
CAS number: 460-35-5
Molecular Weight: 132.51



Global Atmospheric Lifetime (years): 1.05
  Tropospheric Atmospheric Lifetime (years): 1.09
  Stratospheric Atmospheric Lifetime (years): 30.8
Ozone Depletion Potential (ODP): 0.009

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.162	0.121
Global Warming Potential (GWP_H):		
GWP_{20}	288	216
GWP_{100}	78	58
Global Temperature Potentials (GTP_H)		
GTP_{20}		70
GTP_{50}		10
GTP_{100}		8

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

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

OH Reactivity

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

k_{SAR}(298 K) = 5.40×10^{-14}; k_{SAR}(272 K) ≈ 3.45×10^{-14} cm^3 $molecule^{-1}$ s^{-1}

τ^{OH}_{Global} = 1.05 years
τ^{OH}_{Trop} = 1.09 years
τ^{OH}_{Strat} = 36.3 years

Fractional Atmospheric Loss: 0.995

O(^{1}D) Reactivity

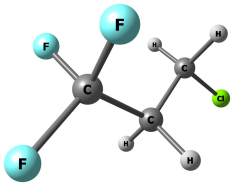
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 1.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)}$ = 370 years
Fractional Atmospheric Loss: 0.003

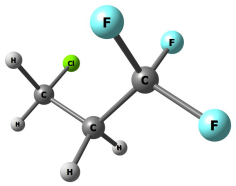
UV Photolysis

UV Spectrum: *No Recommendation*
τ_{hv} = 450 years
Fractional Atmospheric Loss: 0.002

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.695



$\Delta E = 0.90$ kcal mol^{-1}
Population = 0.153

Optimized Coordinates (Angstroms)

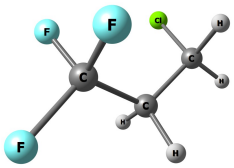
Atom	X	Y	Z
C	1.208913092137	-0.177358271154	0.000000000000
C	-0.106779636159	0.591888845563	0.000000000000
C	-1.299141305612	-0.347264299668	0.000000000000
Cl	2.609868512190	0.959865336234	0.000000000000
H	1.307106471395	-0.800079545439	0.888668156740
H	1.307106471395	-0.800079545439	-0.888668156740
H	-0.181523354805	1.229333118574	-0.884364439515
H	-0.181523354805	1.229333118574	0.884364439515
F	-2.450332399160	0.335531569379	0.000000000000
F	-1.299045748361	-1.144504663248	-1.081588127798
F	-1.299045748361	-1.144504663248	1.081588127798

Atom	X	Y	Z
C	1.187420528811	1.059721904817	0.164319402403
C	-0.145955497990	0.977732640590	-0.568039163594
C	-1.123991379582	-0.033160540655	0.006794479052
Cl	2.270985591931	-0.347226828018	-0.172272181575
H	1.736046113581	1.945505845526	-0.153656137566
H	1.043451258020	1.094434511982	1.244004971474
H	-0.001829936023	0.752989893731	-1.627451383415
H	-0.636207428357	1.954913196226	-0.496154417261
F	-2.322872702027	0.096646979582	-0.583163043102
F	-0.726930445668	-1.297347460206	-0.163465938833
F	-1.300824102697	0.160803856426	1.325995412416

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
74.4851	0.805
95.8168	0.00452
147.1820	0.733
256.9133	0.0477
360.6912	0.110
382.2784	0.655
539.1639	0.0906
551.0078	0.201
638.5787	6.85
763.7215	5.39
779.8351	0.0292
852.8752	0.682
988.2681	6.40
1061.0144	0.254
1111.9297	7.76
1183.6876	28.3
1240.8130	15.6
1261.1686	28.9
1298.0117	7.38
1327.8070	8.48
1389.9423	17.0
1477.5113	1.21
1493.7511	0.350
3079.0693	0.490
3102.1726	1.55
3128.2306	0.294
3166.0493	0.548

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
45.0268	0.288
112.9155	0.133
219.9707	0.298
258.0295	0.206
368.8912	0.194
445.0510	1.58
535.5759	0.302
547.0861	1.31
621.5374	0.897
674.0464	4.41
800.8901	0.206
913.2495	0.681
946.7718	3.38
1051.3980	3.74
1120.2796	11.8
1171.8475	26.6
1225.4436	17.5
1261.6069	23.7
1308.6260	21.3
1341.5031	2.19
1405.7848	7.35
1462.5688	1.89
1481.1654	1.23
3060.5188	0.734
3099.1038	1.43
3121.7565	0.803
3160.5432	0.402



$\Delta E = 0.90$ kcal mol^{-1}
Population = 0.153

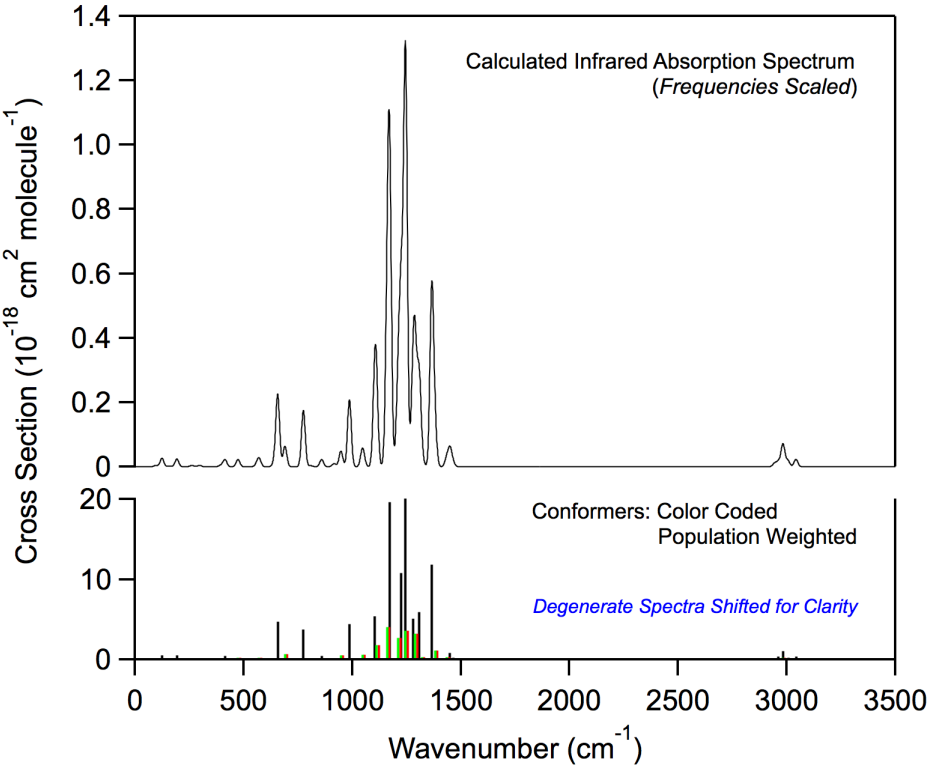
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.187634980341	1.059477405852	-0.163976201550
C	-0.145655761902	0.977336787906	0.568520538132
C	-1.123964464654	-0.033048199051	-0.006741956113
Cl	2.270975146227	-0.347867338012	0.171682715602
H	1.043523458405	1.094818721157	-1.243622407815
H	1.736475065122	1.944978501921	0.154416687110
H	-0.635729744763	1.954651420327	0.497247724065
H	-0.001427544676	0.751976051738	1.627787490629
F	-2.322740164205	0.096660677299	0.583451803753
F	-1.300940245949	0.161684845787	-1.325810456122
F	-0.727122723946	-1.297405874924	0.162760062309

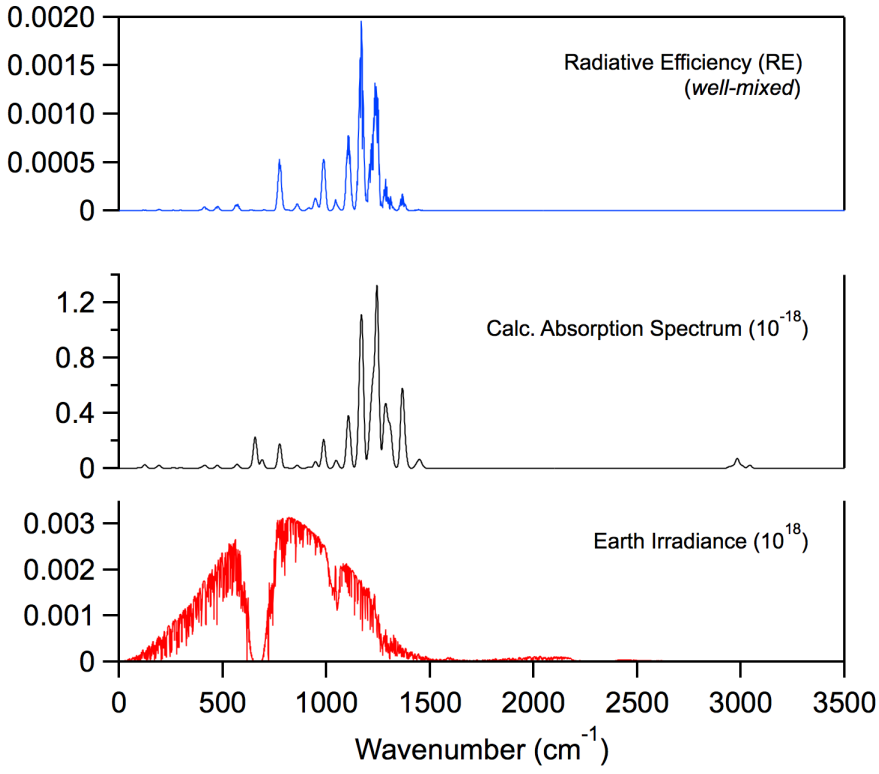
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
45.0273	0.288
112.9161	0.133
219.9713	0.298
258.0297	0.206
368.8916	0.194
445.0511	1.58
535.5760	0.302
547.0861	1.31
621.5374	0.897
674.0464	4.41
800.8902	0.206
913.2495	0.681
946.7718	3.38
1051.3980	3.74
1120.2795	11.8
1171.8479	26.6
1225.4438	17.5
1261.6068	23.7
1308.6262	21.3
1341.5030	2.19
1405.7847	7.35
1462.5684	1.89
1481.1658	1.23
3060.5188	0.734
3099.1038	1.43
3121.7566	0.803
3160.5431	0.402

Infrared Spectrum

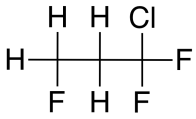


Radiative Efficiency



HCFC-253fc

Molecular Formula:	$CH_2FCH_2CClF_2$
Name:	1-Chloro-1,1,3-trifluoropropane
CAS number:	83124-56-5
Molecular Weight:	132.51



Global Atmospheric Lifetime (years): 1.48
- Tropospheric Atmospheric Lifetime (years): 1.54
- Stratospheric Atmospheric Lifetime (years): 39.9

Ozone Depletion Potential (ODP): 0.011

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.242	0.194
Global Warming Potential (GWP_H):		
GWP_{20}	607	487
GWP_{100}	164	132
Global Temperature Potentials (GTP_H)		
GTP_{20}		168
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*

$k_{SAR}(298\ K) = 3.82 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 2.44 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 1.49$ years

$\tau^{OH}_{Trop} = 1.54$ years

$\tau^{OH}_{Strat} = 49.6$ years

Fractional Atmospheric Loss: 0.993

O(^{1}D) Reactivity

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

$k_{Est}(T) = 1.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 370$ years

Fractional Atmospheric Loss: 0.004

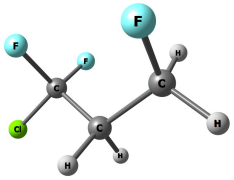
UV Photolysis

UV Spectrum: *No Recommendation*

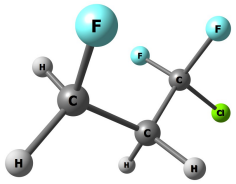
$\tau_{hv} = 450$ years

Fractional Atmospheric Loss: 0.003

Molecular Structure and Infrared Spectrum (9 conformers)



E = 0
Population = 0.190



E = 0
Population = 0.190

Optimized Coordinates (Angstroms)

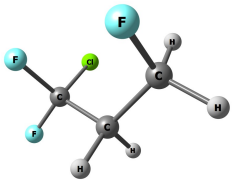
Atom	X	Y	Z
C	-1.990824469071	-0.661460159985	0.235272740588
C	-0.557737685988	-0.982164588783	-0.178405204881
C	0.408912803349	0.146170322162	0.143835987820
F	-2.494191682294	0.364801406357	-0.531024256208
H	-2.618222147835	-1.548944676892	0.090947541353
H	-2.034063871646	-0.366958809702	1.289847253239
H	-0.509168530341	-1.181988828907	-1.251511456854
H	-0.221110607156	-1.877531305128	0.350874598973
Cl	2.116435632876	-0.328966901691	-0.251122065127
F	0.126390899430	1.255265473211	-0.542829798416
F	0.366296658677	0.455630069358	1.449583659513

Atom	X	Y	Z
C	-1.990642317771	-0.661210604833	-0.236363101667
C	-0.557523286193	-0.982373078486	0.176847520252
C	0.408984415168	0.146596421245	-0.143594307348
F	-2.494166777820	0.363777666366	0.531533123767
H	-2.033893900331	-0.365057602769	-1.290474477823
H	-2.617924865324	-1.549004894930	-0.093449565197
H	-0.220762619533	-1.876861566078	-0.353830399229
H	-0.508955103747	-1.183877524533	1.249639583064
Cl	2.116560651790	-0.328932495121	0.250660802804
F	0.366360563088	0.458102775720	-1.448854992146
F	0.126296240674	1.254572903418	0.544806813524

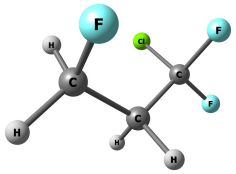
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
47.2562	0.405
135.7982	0.297
203.2913	0.146
265.2836	0.214
328.8114	0.282
404.4205	0.105
422.7452	0.209
461.1539	6.06
554.5028	1.46
730.2051	4.03
868.8435	7.16
946.9299	31.3
975.9674	1.30
1040.3524	2.70
1108.7148	15.5
1172.4018	22.5
1238.8865	20.5
1273.6366	2.98
1306.3278	7.40
1382.1595	3.25
1430.3299	3.50
1453.8311	1.14
1513.6402	0.574
3035.0446	5.51
3075.0325	0.792
3087.1803	3.43
3131.8601	0.812

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
47.2562	0.405
135.7982	0.297
203.2913	0.146
265.2836	0.214
328.8114	0.282
404.4205	0.105
422.7452	0.209
461.1539	6.06
554.5028	1.46
730.2051	4.03
868.8435	7.16
946.9299	31.3
975.9673	1.30
1040.3524	2.70
1108.7148	15.5
1172.4018	22.5
1238.8865	20.5
1273.6366	2.98
1306.3277	7.40
1382.1595	3.25
1430.3299	3.50
1453.8311	1.14
1513.6402	0.574
3035.0446	5.51
3075.0325	0.792
3087.1803	3.43
3131.8601	0.812



$\Delta E = 0.30$ kcal mol^{-1}
Population = 0.114



$\Delta E = 0.30$ kcal mol^{-1}
Population = 0.114

Optimized Coordinates (Angstroms)

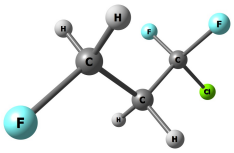
Atom	X	Y	Z
C	-1.809063274151	-0.399665788196	-0.578774724638
C	-0.646151280345	0.513121595718	-0.939399123335
C	0.556464174291	0.425795315953	-0.013037657463
F	-2.366355676145	-0.011603171883	0.618602944516
H	-2.575632641250	-0.333190014490	-1.360003777014
H	-1.483404901266	-1.442232039934	-0.494644526545
H	-0.979353655778	1.556716935602	-0.911585664987
H	-0.304165922773	0.293260252315	-1.954135992111
Cl	1.331999635231	-1.219213713419	-0.058220527102
F	1.488018503037	1.314493440695	-0.385561059186
F	0.230293039149	0.684845187641	1.254514107865

Atom	X	Y	Z
C	-1.809304664302	0.400113666453	-0.578445108368
C	-0.646600032718	-0.512798766505	-0.939421310038
C	0.556189283012	-0.425816959286	-0.013253183786
F	-2.366452246651	0.011941214580	0.618964351963
H	-1.483466084098	1.442614201056	-0.494198383180
H	-2.576019285161	0.333889135622	-1.359552952581
H	-0.304754975934	-0.292823794351	-1.954180829982
H	-0.979963483841	-1.556345732703	-0.911723038204
Cl	1.331978721158	1.219076118982	-0.058298247244
F	0.230195956926	-0.685024390943	1.254312103280
F	1.487537811609	-1.314601692906	-0.386084401859

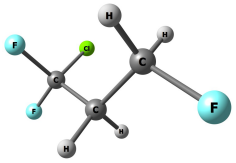
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
49.3395	0.347
142.8725	0.284
203.5420	0.288
285.7022	0.101
337.7879	0.143
386.8919	0.405
414.2726	0.806
497.6491	2.96
568.9552	3.58
658.8554	5.91
867.1685	8.91
922.8085	14.4
984.8907	2.85
1103.0141	9.04
1119.9889	14.8
1174.4739	27.7
1220.5694	16.9
1266.8867	6.77
1302.1102	6.13
1390.2297	4.38
1433.6011	2.59
1454.1682	0.797
1514.1591	0.878
3035.7259	5.16
3057.0706	0.235
3087.1799	4.29
3118.4849	0.918

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
49.3395	0.347
142.8724	0.284
203.5420	0.288
285.7022	0.101
337.7879	0.143
386.8919	0.405
414.2726	0.806
497.6491	2.96
568.9552	3.58
658.8554	5.91
867.1685	8.91
922.8086	14.4
984.8908	2.85
1103.0141	9.04
1119.9889	14.8
1174.4739	27.7
1220.5695	16.9
1266.8867	6.77
1302.1102	6.13
1390.2298	4.38
1433.6011	2.59
1454.1682	0.797
1514.1591	0.878
3035.7259	5.16
3057.0706	0.235
3087.1799	4.29
3118.4849	0.918



$\Delta E = 0.31$ kcal mol^{-1}
Population = 0.112



$\Delta E = 0.48$ kcal mol^{-1}
Population = 0.084

Optimized Coordinates (Angstroms)

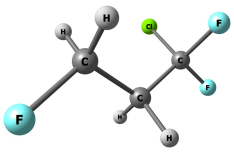
Atom	X	Y	Z
C	-1.043196208814	-1.687145991034	0.000000000000
C	0.256531861479	-0.880602832407	0.000000000000
C	-0.013205670941	0.610497477954	0.000000000000
F	-0.723368092996	-3.025694602671	0.000000000000
H	-1.640558073893	-1.464909415352	0.890794940835
H	-1.640558073893	-1.464909415352	-0.890794940835
H	0.847997482111	-1.127247864949	-0.884725956773
H	0.847997482111	-1.127247864949	0.884725956773
Cl	1.521923527893	1.567432025619	0.000000000000
F	-0.721994616220	0.973772241250	-1.080759521241
F	-0.721994616220	0.973772241250	1.080759521241

Atom	X	Y	Z
C	-1.742209522632	-0.310183907439	0.333302696594
C	-0.755459058466	0.505833255923	-0.495995898821
C	0.674750864770	0.432917093031	-0.000443315382
F	-3.007933004555	-0.084136518237	-0.161514793917
H	-1.524745175853	-1.381271452039	0.269860411782
H	-1.712584799331	-0.004348960718	1.384737970752
H	-1.041119655322	1.562942945004	-0.458172413597
H	-0.779279647071	0.184938570310	-1.539861693028
Cl	1.363559633963	-1.242977140535	-0.125587875584
F	1.463404811694	1.244253636387	-0.713733579826
F	0.761463552804	0.808082478315	1.284881491028

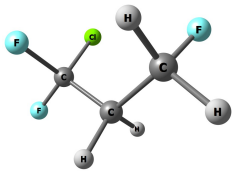
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
82.6513	0.803
98.0973	0.143
141.9640	0.534
296.3068	0.846
325.8518	0.102
363.5291	1.03
419.2808	1.44
424.2978	0.00332
581.9229	1.54
793.8201	13.5
799.2736	0.0633
930.9877	31.1
1025.7167	8.31
1059.0193	15.4
1108.3447	10.8
1193.0570	14.1
1234.0671	18.3
1262.8432	3.71
1320.9886	2.59
1331.9259	6.01
1435.7506	4.52
1476.6409	0.720
1527.6152	0.133
3042.5497	4.23
3082.8940	0.596
3090.2565	3.24
3137.6804	1.31

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
78.2421	0.780
100.2682	0.0590
161.4572	0.615
294.6303	0.439
334.4581	0.388
350.7310	0.196
417.3751	0.849
460.0689	0.798
607.3707	1.89
671.0435	13.3
807.4082	0.610
946.7919	20.4
1065.0609	0.227
1082.2744	18.9
1125.7199	24.0
1182.1896	19.3
1220.2039	11.8
1255.2799	6.39
1314.4841	2.11
1342.0856	6.20
1440.0761	3.63
1476.2582	0.614
1526.8305	0.235
3045.1595	3.24
3061.0700	1.30
3093.8701	2.57
3127.4149	1.76



$\Delta E = 0.48$ kcal mol^{-1}
Population = 0.084



$\Delta E = 0.71$ kcal mol^{-1}
Population = 0.057

Optimized Coordinates (Angstroms)

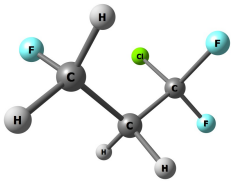
Atom	X	Y	Z
C	-1.742240375841	0.311189469023	0.333489182203
C	-0.755953937282	-0.505767900443	-0.495435469266
C	0.674376337412	-0.433053119897	-0.000200406801
F	-3.008141991139	0.085279814117	-0.160935412842
H	-1.712532668187	0.006064320426	1.385128331157
H	-1.524384670040	1.382151214208	0.269271389792
H	-0.779849264480	-0.185578988160	-1.539516252163
H	-1.042007523171	-1.562743207252	-0.456834515685
Cl	1.363795269420	1.242494412720	-0.126620550337
F	0.761187492094	-0.807371175462	1.285364840037
F	1.462590331213	-1.245175839281	-0.713082136095

Atom	X	Y	Z
C	-1.884390241054	0.616411970359	0.082323706723
C	-0.581775888463	0.956913224205	-0.630131203196
C	0.675510221899	0.402290559783	0.021866725012
F	-2.241496780942	-0.693443470894	-0.137893769962
H	-1.788955045342	0.780459421824	1.161566084318
H	-2.683190908777	1.261726022547	-0.301561859308
H	-0.455843844648	2.046173501490	-0.629558164224
H	-0.618044444743	0.621565402854	-1.669201576300
Cl	0.787719107155	-1.396516673857	-0.056137238301
F	1.762594731098	0.902681455722	-0.583882845550
F	0.734638093817	0.760560585966	1.315453140790

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
78.2420	0.780
100.2680	0.0590
161.4573	0.615
294.6302	0.439
334.4582	0.388
350.7311	0.196
417.3752	0.849
460.0689	0.798
607.3707	1.89
671.0435	13.3
807.4082	0.610
946.7918	20.4
1065.0611	0.227
1082.2743	18.9
1125.7198	24.0
1182.1897	19.3
1220.2038	11.8
1255.2797	6.39
1314.4840	2.11
1342.0855	6.20
1440.0761	3.63
1476.2581	0.614
1526.8305	0.235
3045.1596	3.24
3061.0700	1.30
3093.8703	2.57
3127.4150	1.76

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
49.5158	0.459
127.3970	0.281
221.0114	0.371
260.4967	0.148
330.7150	0.158
394.5910	0.148
427.1190	0.405
498.3839	3.34
584.7055	1.31
651.4275	7.25
861.9911	9.68
912.1114	4.00
1008.9098	8.22
1093.3843	5.91
1122.0378	28.6
1174.9139	24.3
1210.9035	16.5
1264.3963	5.91
1298.8813	2.28
1388.0161	4.02
1435.5323	1.88
1455.4506	0.806
1515.1686	0.595
3034.6043	4.92
3054.7748	1.38
3083.6716	4.03
3123.5456	0.924



$\Delta E = 0.71$ kcal mol^{-1}
Population = 0.057

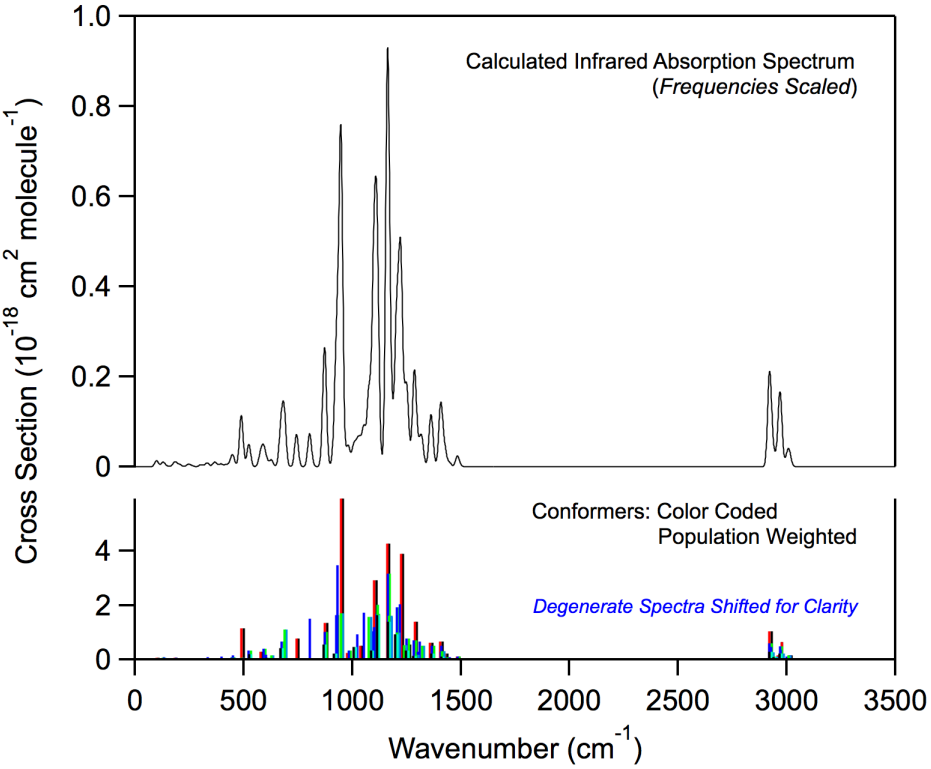
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.883646127344	-0.618615101704	0.081978012085
C	-0.580495806719	-0.957543008236	-0.630247424985
C	0.676005947372	-0.401421575604	0.021986074877
F	-2.242283494419	0.690814347917	-0.138285470020
H	-2.681603467411	-1.264881125877	-0.302059892089
H	-1.788208361891	-0.782562801743	1.161235279276
H	-0.616979423463	-0.622222524859	-1.669319033065
H	-0.453256538450	-2.046651315026	-0.629668751945
Cl	0.786070281758	1.397520336093	-0.055973212172
F	0.735329001954	-0.759637969311	1.315578390882
F	1.763799988612	-0.900499261652	-0.583572972844

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
49.5157	0.459
127.3973	0.281
221.0118	0.371
260.4968	0.148
330.7150	0.158
394.5910	0.148
427.1189	0.405
498.3839	3.34
584.7055	1.31
651.4274	7.25
861.9909	9.68
912.1111	4.00
1008.9095	8.22
1093.3840	5.91
1122.0376	28.6
1174.9140	24.3
1210.9035	16.5
1264.3961	5.91
1298.8809	2.28
1388.0157	4.02
1435.5321	1.88
1455.4506	0.806
1515.1686	0.595
3034.6046	4.92
3054.7753	1.38
3083.6719	4.03
3123.5461	0.924

Infrared Spectrum



Radiative Efficiency