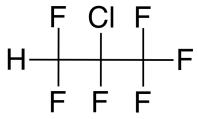
HCFC-226ba

Molecular Formula:	$CHF_2CClFCF_3$
Name:	2-Chloro-1,1,1,2,3,3-hexafluoropropane
CAS number:	51346-64-6
Molecular Weight:	186.48



Global Atmospheric Lifetime (years):	17.0
Tropospheric Atmospheric Lifetime (years):	19.0
Stratospheric Atmospheric Lifetime (years):	161.2
Ozone Depletion Potential (ODP):	0.019

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.276	0.267
Global Warming Potential (GWP_H):		
GWP_{20}	3914	3792
GWP_{100}	1528	1480
Global Temperature Potentials (GTP_H)		
GTP_{20}		3314
GTP_{50}		1020
GTP_{100}		265

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

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

OH Reactivity

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

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

$\tau^{OH}_{Global} = 18.3$ years

$\tau^{OH}_{Trop} = 19.0$ years

$\tau^{OH}_{Strat} = 478.6$ years

Fractional Atmospheric Loss: 0.930

$O(^1D)$ Reactivity

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

$k_{Est}(T) = 0.7 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 529$ years

Fractional Atmospheric Loss: 0.032

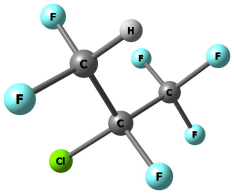
UV Photolysis

UV Spectrum: *No Recommendation*

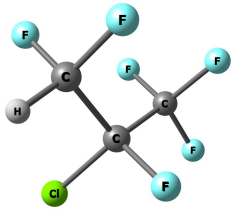
$\tau_{hv} = 450$ years

Fractional Atmospheric Loss: 0.038

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.515



$\Delta E = 0.29$ kcal mol^{-1}
Population = 0.313

Optimized Coordinates (Angstroms)

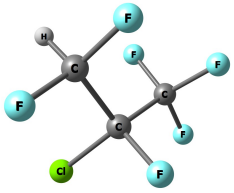
Atom	X	Y	Z
C	1.209206115625	-0.888522170711	0.213374689601
C	0.155058146700	0.234015646115	0.336263160384
C	-1.267057419385	-0.245951511470	-0.052088916808
F	1.269129420033	-1.323904795672	-1.057605935524
F	2.408004605651	-0.401640978055	0.571217774016
H	0.941927697045	-1.719714890546	0.876287497994
Cl	0.609084887991	1.638076556824	-0.657749020864
F	0.103883701126	0.589233666468	1.640717038198
F	-2.166159634026	0.679272316374	0.256331201420
F	-1.354866133640	-0.528498004913	-1.344729346308
F	-1.544356387121	-1.356911834415	0.646374857890

Atom	X	Y	Z
C	1.562074224795	0.047407298809	0.093184177524
C	0.079406933260	0.339304973103	0.422016158889
C	-0.939764917709	-0.651722140174	-0.203608533167
F	1.879149768233	-1.178940521536	0.551593419502
F	1.761467354833	0.078392543521	-1.235031066802
H	2.195912928479	0.794810538146	0.584686334789
Cl	-0.301300122713	1.999641821751	-0.118782459953
F	-0.055746422264	0.257494147187	1.763407243577
F	-2.174467213171	-0.321567079457	0.163509468597
F	-0.863151608077	-0.639609405897	-1.529834755540
F	-0.687997925666	-1.884902175452	0.232151012584

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
54.0861	0.0976
81.2236	0.102
154.8657	0.126
184.0597	0.0490
206.7407	0.405
256.7533	0.245
308.9474	0.149
333.0301	0.0408
359.6524	0.0546
387.6170	0.150
495.7344	0.823
550.3952	1.39
583.7671	0.597
608.3416	0.877
679.5424	11.3
739.4055	5.01
969.3243	20.8
1079.2158	7.53
1149.6724	8.23
1167.0296	19.4
1200.1147	13.7
1221.4975	30.8
1266.9155	39.3
1305.2513	20.2
1388.3808	7.33
1400.4876	4.65
3071.2123	3.05

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
33.7595	0.0367
98.6025	0.144
168.1618	0.0316
183.2569	0.0144
206.6087	0.203
270.2283	0.430
306.5658	0.0697
319.2914	0.184
358.4317	0.0267
412.6048	0.161
497.8980	0.624
533.3581	2.86
570.0126	1.11
588.9873	2.73
663.9872	6.17
778.7403	2.45
937.5868	26.0
1101.2606	4.33
1143.4673	7.49
1167.1079	20.3
1189.8569	5.48
1241.2883	42.2
1254.2953	37.1
1292.0071	27.5
1390.1148	2.81
1412.7223	5.98
3068.8444	3.37



$\Delta E = 0.65$ kcal mol^{-1}
Population = 0.172

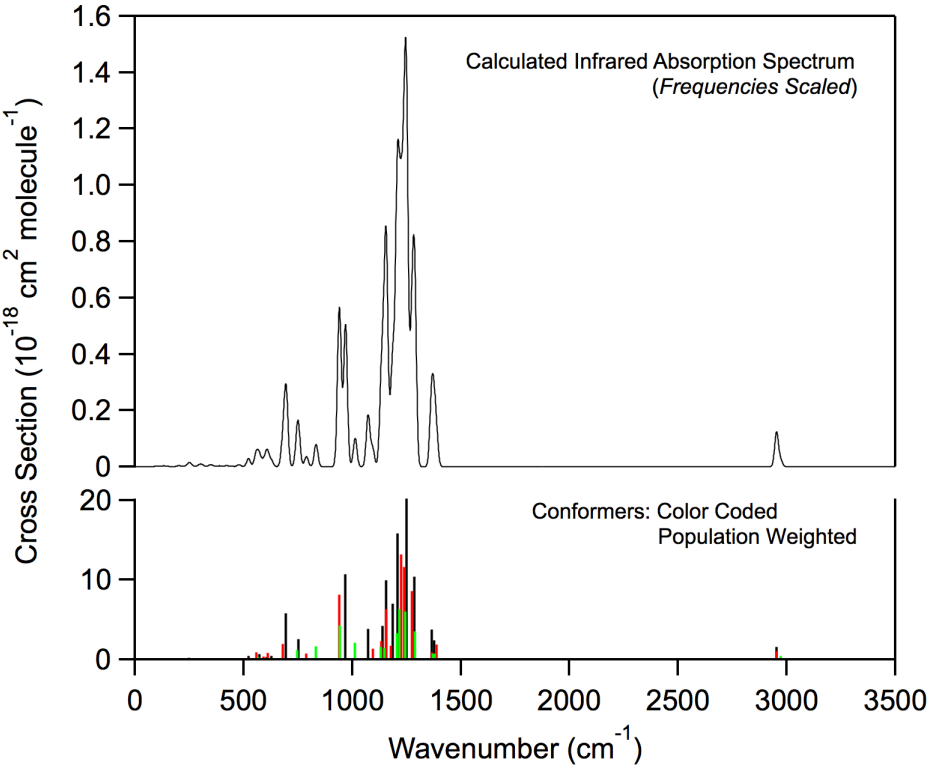
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.305069364763	-0.526651390550	-0.505636329680
C	0.184280776574	0.214591498746	0.260592877733
C	-1.231850087716	-0.321803506076	-0.079005687531
F	2.491690012141	-0.058551069941	-0.085713419066
F	1.234483184712	-1.840080020796	-0.206917957039
H	1.208126498493	-0.388023082601	-1.586806156279
Cl	0.268471023654	1.950796758325	-0.162659193224
F	0.375449124732	0.054221245638	1.583293116826
F	-2.172356801813	0.439716442814	0.464870884320
F	-1.399027810265	-0.341103351817	-1.404954267298
F	-1.370725285275	-1.559171523741	0.387490131239

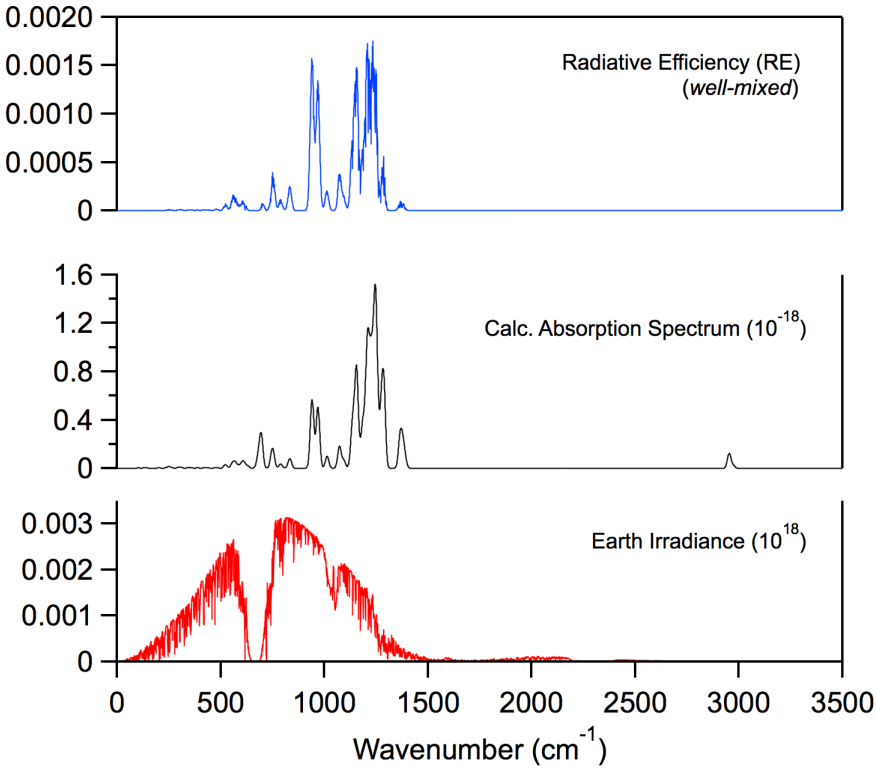
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
50.0322	0.0796
75.2354	0.0635
158.4086	0.0884
190.5508	0.0678
218.8035	0.553
260.5626	0.0583
311.6539	0.0680
312.8458	0.0859
351.6246	0.219
395.5921	0.0743
449.9234	0.905
542.5574	1.64
572.6186	0.628
589.1330	0.580
732.3987	6.90
825.7692	9.86
942.7244	25.2
1016.1279	12.5
1141.7364	9.26
1158.0541	8.28
1218.8222	19.2
1231.9320	37.0
1261.4165	35.1
1306.2423	20.6
1395.9373	4.57
1405.5892	4.26
3090.4013	2.87

Infrared Spectrum

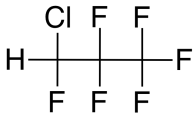


Radiative Efficiency



HCFC-226ca

Molecular Formula:	$CHClFCF_2CF_3$
Name:	3-Chloro-1,1,1,2,2,3-hexafluoropropane
CAS number:	422-57-1
Molecular Weight:	186.48



Global Atmospheric Lifetime (years):	5.47
Tropospheric Atmospheric Lifetime (years):	5.80
Stratospheric Atmospheric Lifetime (years):	98.0
Ozone Depletion Potential (ODP):	0.013

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.285	0.261
Global Warming Potential (GWP_H):		
GWP_{20}	1813	1681
GWP_{100}	504	467
Global Temperature Potentials (GTP_H)		
GTP_{20}		967
GTP_{50}		103
GTP_{100}		66

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 1.01 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 0.646 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 5.60$ years

$\tau^{OH}_{Trop} = 5.80$ years

$\tau^{OH}_{Strat} = 164.3$ years

Fractional Atmospheric Loss: 0.978

O(^{1}D) Reactivity

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

$k_{Est}(T) = 0.7 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 529$ years

Fractional Atmospheric Loss: 0.010

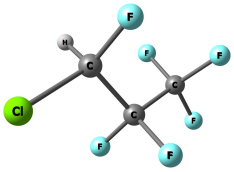
UV Photolysis

UV Spectrum: *No Recommendation*

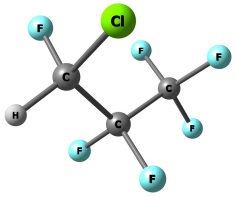
$\tau_{hv} = 450$ years

Fractional Atmospheric Loss: 0.012

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.777



$\Delta E = 1.05$ kcal mol^{-1}
Population = 0.131

Optimized Coordinates (Angstroms)

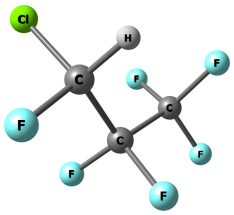
Atom	X	Y	Z
C	1.025289588200	0.481253374257	0.445589127126
C	-0.062237979656	-0.430828986540	-0.151739336464
C	-1.499379605866	0.111731464192	0.080558474306
Cl	2.641634960701	-0.198642030514	0.109800481083
F	0.916537002893	1.709463793610	-0.103446712744
H	0.912851492184	0.543252780525	1.528989045033
F	0.011464640360	-1.634804644584	0.445085675305
F	0.111565957975	-0.577588394752	-1.472774938247
F	-2.386151923175	-0.812636360903	-0.269645996877
F	-1.662944549359	0.397392671249	1.377409373577
F	-1.715431584257	1.209935333459	-0.632715192098

Atom	X	Y	Z
C	1.214558620366	-0.692775267118	0.017239099016
C	-0.239239084175	-0.556281540569	-0.480795099036
C	-1.158801097519	0.455064086358	0.254410307239
Cl	2.192804420979	0.765852392074	-0.304548892110
F	1.208726217274	-0.966363967343	1.336986309827
H	1.675659688570	-1.517559100577	-0.532211469924
F	-0.806652641058	-1.774399122372	-0.337369340349
F	-0.227234066826	-0.239789181001	-1.786129387823
F	-2.374954642810	0.388595988334	-0.283836941374
F	-1.244749201499	0.154748198451	1.546673537409
F	-0.702788213302	1.696916513764	0.125591877125

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
44.6780	0.0804
68.8399	0.0232
137.9882	0.113
210.7665	0.562
226.1761	0.109
237.3484	0.109
294.3417	0.260
338.4026	0.00971
371.5956	0.0174
409.7505	0.243
471.1526	0.636
535.9819	0.960
585.2571	0.219
638.4842	2.10
720.5672	16.2
797.7810	9.25
812.6763	6.86
1051.3061	12.2
1129.8914	10.5
1188.5214	19.8
1228.6014	46.1
1245.9645	22.1
1270.6172	26.7
1294.5558	2.56
1348.2889	17.5
1375.5202	1.00
3120.2820	0.892

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
20.7622	0.0269
90.3621	0.0831
154.8696	0.0651
188.5816	0.126
216.7164	0.130
268.1091	0.639
310.7440	0.139
344.9904	0.00923
360.0664	0.0377
427.0095	0.297
487.2217	0.442
520.3505	2.82
587.8938	3.16
602.0376	2.39
679.5340	3.30
770.5929	2.13
836.8134	15.2
1109.7481	17.4
1139.5661	11.6
1177.1889	24.5
1213.5563	20.5
1236.9355	24.9
1252.9543	48.0
1280.9354	7.94
1335.7027	7.29
1409.6999	1.63
3095.8538	1.28



$\Delta E = 1.26$ kcal mol^{-1}
Population = 0.092

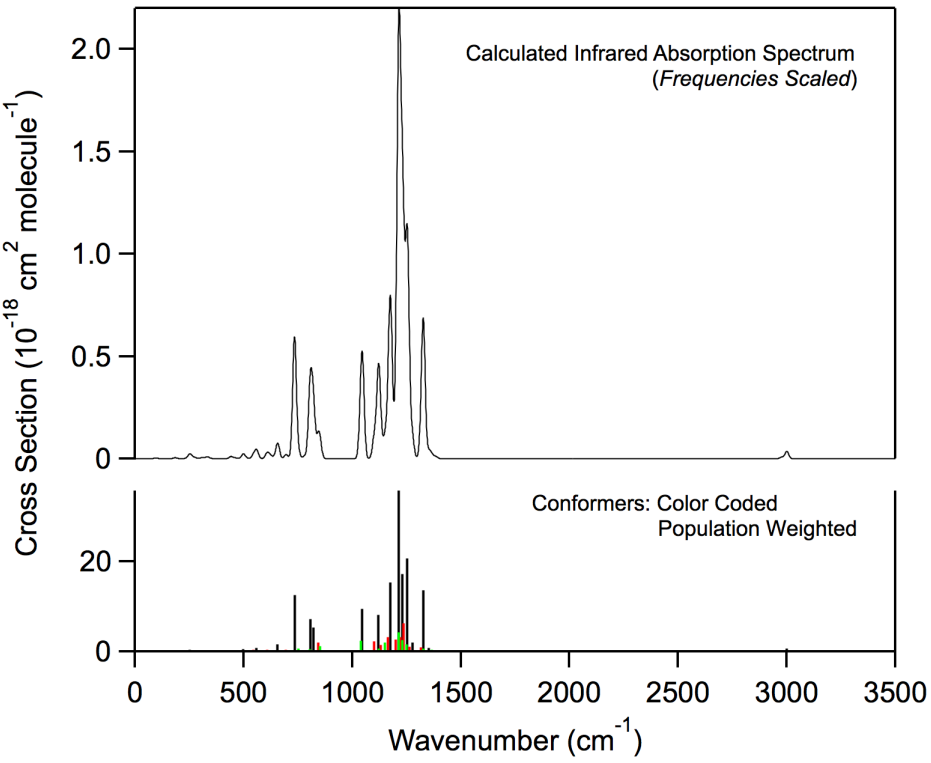
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.175114645404	-0.318439615577	-0.545556925866
C	-0.149968295497	-0.623738237582	0.184027831679
C	-1.303467488087	0.377119069183	-0.088616067123
Cl	1.919577048437	1.200402996815	0.027774119439
F	2.009158975816	-1.349932044998	-0.304867218061
H	1.002292523602	-0.218330293598	-1.618004565031
F	0.044415768479	-0.702931262172	1.507374149329
F	-0.564506019271	-1.828122194334	-0.266298564092
F	-2.451195606515	-0.147071380534	0.326358916560
F	-1.107051014489	1.528716375615	0.540573934884
F	-1.386296537879	0.610581587182	-1.403866611719

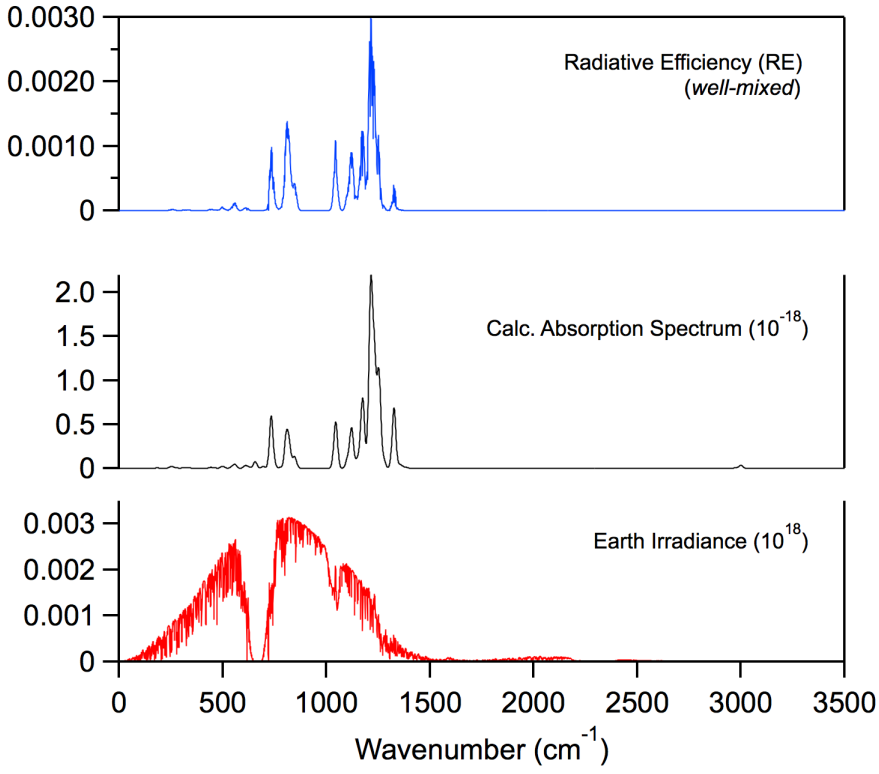
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
37.6340	0.0467
76.4687	0.0345
140.6506	0.105
201.5971	0.526
222.6430	0.109
269.5005	0.247
305.9015	0.185
333.0890	0.0407
369.0947	0.00729
418.3385	0.518
438.8280	0.628
534.5973	1.48
585.1759	0.0210
617.3181	1.06
738.6815	7.48
794.7110	6.17
845.4019	12.4
1043.2276	26.8
1133.0453	7.58
1160.5213	22.1
1227.8811	46.6
1246.9674	28.2
1265.8547	18.0
1292.3455	3.24
1349.2850	7.74
1389.9983	4.27
3120.8167	0.890

Infrared Spectrum

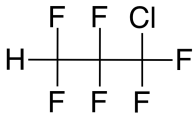


Radiative Efficiency



HCFC-226cb

Molecular Formula:	$CHF_2CF_2CClF_2$
Name:	1-Chloro-1,1,2,2,3,3-hexafluoropropane
CAS number:	422-55-9
Molecular Weight:	186.48



Global Atmospheric Lifetime (years): 21.6
- Tropospheric Atmospheric Lifetime (years): 24.7
- Stratospheric Atmospheric Lifetime (years): 173.6

Ozone Depletion Potential (ODP): 0.022

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.350	0.341
Global Warming Potential (GWP_H):		
GWP_{20}	5515	5370
GWP_{100}	2453	2388
Global Temperature Potentials (GTP_H)		
GTP_{20}		4920
GTP_{50}		1976
GTP_{100}		539

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 2.37 \times 10^{-15}$; $k_{SAR}(272\ K) \approx 1.51 \times 10^{-15}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 23.8$ years

$\tau^{OH}_{Trop} = 24.7$ years

$\tau^{OH}_{Strat} = 607.2$ years

Fractional Atmospheric Loss: 0.911

$O(^1D)$ Reactivity

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

$k_{Est}(T) = 0.7 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 529$ years

Fractional Atmospheric Loss: 0.041

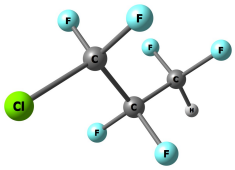
UV Photolysis

UV Spectrum: *No Recommendation*

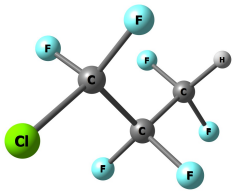
$\tau_{hv} = 450$ years

Fractional Atmospheric Loss: 0.048

Molecular Structure and Infrared Spectrum (9 conformers)



E = 0
Population = 0.303



$\Delta E = 0.19$ kcal mol^{-1}
Population = 0.221

Optimized Coordinates (Angstroms)

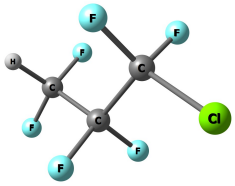
Atom	X	Y	Z
C	1.800320455328	-0.244971702271	-0.001831920850
C	0.312575222102	-0.664522807751	-0.002728529238
C	-0.710090381115	0.503845591134	0.002072940939
F	2.070239715787	0.489736481008	-1.095383982305
F	2.071218664756	0.481580022606	1.096915250128
H	2.417863737211	-1.152401780069	-0.005483792369
F	0.107054465737	-1.420115930644	1.090610374047
F	0.106076295784	-1.411963207454	-1.101473621915
Cl	-2.383297182879	-0.133818290080	0.000450485242
F	-0.527841383969	1.251776835582	1.088158037218
F	-0.528810608742	1.259832787940	-1.078583240898

Atom	X	Y	Z
C	1.688787380893	0.222417248207	0.378116548353
C	0.367947884366	-0.458522720923	-0.050540770211
C	-0.876669896993	0.445226904396	0.151352122200
F	2.691517898564	-0.631827438886	0.108654801273
F	1.868164957756	1.348951768224	-0.336784526936
H	1.680788265732	0.457335838337	1.447626786168
F	0.223360019631	-1.562383732066	0.705497014681
F	0.441265354441	-0.809645330194	-1.341337667205
Cl	-2.383992959335	-0.463357938890	-0.142654868205
F	-0.869098243061	0.898477120065	1.412447504805
F	-0.820915661994	1.485436281732	-0.674419944922

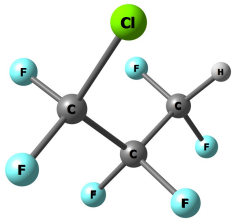
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
22.9897	0.0333
92.8689	0.199
153.0803	0.0116
208.0093	0.341
214.9264	0.210
220.6138	0.00261
326.6117	0.0312
334.1660	0.00809
370.5061	0.0299
421.7853	0.0600
432.3080	0.0113
558.3364	1.49
567.8971	0.00
573.8183	18.2
632.3604	5.23
710.1257	0.578
952.9580	21.7
1125.9424	3.67
1161.6667	5.02
1169.9092	50.2
1202.8223	1.72
1227.5610	69.6
1228.1992	0.655
1288.1378	1.83
1388.8981	2.96
1421.0853	6.79
3055.6338	4.31

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
42.0270	0.108
72.3998	0.0792
139.8211	0.151
212.6384	0.518
218.0861	0.0720
246.2930	0.208
297.8046	0.437
327.4627	0.0445
355.0571	0.0620
406.0496	0.166
428.5255	0.0547
523.0772	0.260
558.4208	4.24
608.7883	1.41
686.0290	0.887
806.6662	32.3
888.7975	16.0
1110.1117	19.6
1154.6534	7.04
1165.4547	16.4
1191.2827	9.48
1212.2732	53.1
1251.9105	16.8
1305.4545	6.71
1398.5888	3.41
1414.4215	4.24
3082.8277	3.52



$\Delta E = 0.19$ kcal mol^{-1}
Population = 0.221



$\Delta E = 1.03$ kcal mol^{-1}
Population = 0.053

Optimized Coordinates (Angstroms)

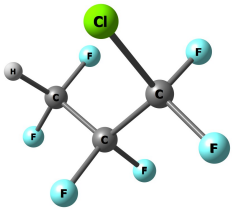
Atom	X	Y	Z
C	1.690178693285	0.220364083547	-0.376742495255
C	0.368182220382	-0.461153762850	0.047406079965
C	-0.875068068262	0.445489566478	-0.149884258420
F	1.870805740417	1.342539165123	0.344670643474
F	2.691580469575	-0.636819306016	-0.111708041068
H	1.683010950223	0.461404466704	-1.444895574354
F	0.440402523486	-0.819757150950	1.336206586531
F	0.222394414884	-1.560467059848	-0.715000742390
Cl	-2.383805293381	-0.462637157104	0.138225449403
F	-0.818236825996	1.480877323321	0.681852270428
F	-0.866268824612	0.905936831597	-1.408361918313

Atom	X	Y	Z
C	1.405112851802	0.695414020443	0.190162936197
C	0.429920875269	-0.500086574672	0.194526241476
C	-1.003293860265	-0.207250465582	-0.328722983606
F	2.617686963434	0.223443577660	0.532823973627
F	1.470530399285	1.215154014697	-1.050332134809
H	1.096522237235	1.467793068454	0.901496973840
F	0.329241584485	-0.952971279603	1.457286304522
F	0.930887160556	-1.477971516726	-0.581393279412
Cl	-1.777801017431	1.113396429286	0.610774282615
F	-0.961746966508	0.133352619257	-1.612011091695
F	-1.731544227862	-1.313019893214	-0.201128222754

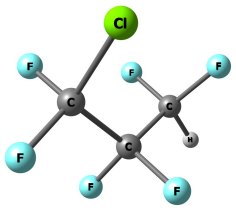
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
42.0273	0.108
72.3997	0.0792
139.8211	0.151
212.6386	0.518
218.0861	0.0720
246.2930	0.208
297.8047	0.437
327.4628	0.0445
355.0572	0.0620
406.0496	0.166
428.5255	0.0547
523.0771	0.260
558.4208	4.24
608.7883	1.41
686.0291	0.887
806.6660	32.3
888.7977	16.0
1110.1116	19.6
1154.6533	7.04
1165.4548	16.4
1191.2825	9.48
1212.2732	53.1
1251.9107	16.8
1305.4547	6.71
1398.5888	3.41
1414.4213	4.24
3082.8279	3.52

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
38.9462	0.117
79.7260	0.0643
143.9080	0.126
190.2731	0.207
238.0633	0.285
270.4998	0.231
300.3379	0.244
318.0637	0.181
364.9331	0.311
395.2629	0.227
423.1629	0.260
475.9183	1.48
569.6484	1.89
625.7832	1.17
668.8823	2.14
805.5071	11.8
941.1332	41.5
1068.5333	22.3
1156.3179	8.04
1163.5635	10.1
1197.5164	24.6
1224.2588	38.6
1256.6961	9.15
1300.4023	17.2
1399.3894	2.28
1417.5547	2.28
3089.6766	3.25



$\Delta E = 1.03$ kcal mol^{-1}
Population = 0.053



$\Delta E = 1.15$ kcal mol^{-1}
Population = 0.043

Optimized Coordinates (Angstroms)

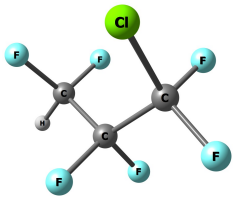
Atom	X	Y	Z
C	1.405745679556	0.690979614115	-0.211045538244
C	0.432622050822	-0.505891381357	-0.183309064766
C	-1.001932260044	-0.200994621126	0.329271372001
F	1.468275213120	1.245508151980	1.014444275694
F	2.619679336329	0.211702930035	-0.538410214020
H	1.096969240222	1.442506284142	-0.944297423713
F	0.934027023300	-1.460689324782	0.620575996048
F	0.334747825780	-0.994274638166	-1.432991647904
Cl	-1.777203646106	1.091352303942	-0.648183838966
F	-1.728071796514	-1.311198281817	0.231678615121
F	-0.963031666465	0.175617963035	1.602540468749

Atom	X	Y	Z
C	1.659799357560	0.302881572013	0.085142845837
C	0.443788495161	-0.581997623262	0.428734862712
C	-0.903995089689	-0.286427611989	-0.289984439671
F	1.847503561339	0.324696432053	-1.246904905574
F	1.468601751806	1.558273464839	0.524578972357
H	2.543715610147	-0.126264478530	0.574582838871
F	0.244790927074	-0.523355685429	1.756212959583
F	0.779031071775	-1.848550315707	0.097981656777
Cl	-1.559975905203	1.321525734423	0.124643872189
F	-0.735894722489	-0.372390216469	-1.607474572994
F	-1.777568057480	-1.219851271942	0.089197909915

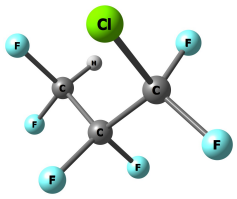
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
38.9469	0.117
79.7257	0.0643
143.9076	0.126
190.2729	0.207
238.0639	0.285
270.5001	0.231
300.3379	0.244
318.0639	0.181
364.9334	0.311
395.2628	0.227
423.1628	0.260
475.9184	1.48
569.6483	1.89
625.7834	1.17
668.8822	2.14
805.5070	11.8
941.1335	41.5
1068.5337	22.3
1156.3181	8.04
1163.5634	10.1
1197.5161	24.6
1224.2592	38.6
1256.6964	9.15
1300.4023	17.2
1399.3894	2.28
1417.5547	2.28
3089.6771	3.25

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
20.1650	0.0613
96.9255	0.174
154.0526	0.0571
192.9768	0.0738
212.1956	0.124
271.8407	0.568
308.9704	0.254
335.1137	0.219
360.9967	0.00888
413.3658	0.778
427.7395	0.0922
527.4105	0.682
559.9578	2.62
586.2508	6.33
676.4874	1.21
720.6945	6.68
949.9851	33.8
1131.5115	10.6
1150.9792	12.0
1168.6095	17.5
1188.6367	18.7
1215.8206	60.7
1236.2689	1.37
1293.1011	11.4
1391.3328	2.72
1426.4661	2.07
3054.6146	4.60



$\Delta E = 1.15$ kcal mol^{-1}
Population = 0.043



$\Delta E = 1.34$ kcal mol^{-1}
Population = 0.031

Optimized Coordinates (Angstroms)

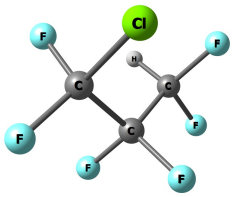
Atom	X	Y	Z
C	1.658624656799	0.308995578537	-0.090935800620
C	0.444897432314	-0.581290380527	-0.428582438227
C	-0.902012106262	-0.288408720762	0.292872306040
F	1.461708793679	1.562364103913	-0.533610696520
F	1.849841313289	0.335489254998	1.240527277994
H	2.542762010765	-0.118430501879	-0.581480422912
F	0.785597585268	-1.845622243533	-0.094923195165
F	0.242128608818	-0.527374063870	-1.755690399388
Cl	-1.564918522477	1.315901024798	-0.124844027690
F	-1.773217436441	-1.226125312313	-0.081128936220
F	-0.730064335753	-0.369766739362	1.610158332707

Atom	X	Y	Z
C	1.466056732390	0.398415554470	0.536004260959
C	0.466923396213	-0.499583893448	-0.223925825720
C	-1.023621576938	-0.314246772970	0.182519352846
F	2.697933814466	0.094794364922	0.088221225842
F	1.214164394929	1.693691014563	0.272688534195
H	1.410627448054	0.220702617480	1.615101889151
F	0.783305496287	-1.778398340323	0.075037832404
F	0.596827457984	-0.318711605844	-1.543966628596
Cl	-1.731759012410	1.196556659782	-0.441152205983
F	-1.723477974370	-1.346072083616	-0.281506032598
F	-1.093988176604	-0.319221515017	1.521335597500

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
20.1639	0.0613
96.9248	0.174
154.0518	0.0571
192.9756	0.0738
212.1950	0.124
271.8408	0.568
308.9703	0.254
335.1139	0.219
360.9966	0.00888
413.3663	0.778
427.7395	0.0922
527.4103	0.682
559.9572	2.62
586.2511	6.33
676.4878	1.21
720.6939	6.68
949.9848	33.8
1131.5115	10.6
1150.9797	12.0
1168.6096	17.5
1188.6378	18.7
1215.8200	60.7
1236.2687	1.37
1293.1008	11.4
1391.3329	2.72
1426.4665	2.07
3054.6140	4.60

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
35.9966	0.136
73.6460	0.0634
149.0659	0.0697
186.9059	0.179
235.0245	0.542
266.3389	0.357
311.9857	0.283
313.8701	0.0854
344.3239	0.162
424.5530	0.0669
438.8695	0.423
469.4340	0.615
575.9635	2.07
624.6027	1.81
651.6182	1.67
826.5118	16.0
934.6242	29.9
1079.8805	28.8
1145.9813	10.1
1165.3708	19.7
1179.6963	16.6
1204.1930	27.0
1262.2972	22.3
1302.9770	9.95
1399.5978	1.80
1419.1607	2.55
3083.0189	3.40



$\Delta E = 1.34$ kcal mol^{-1}
Population = 0.031

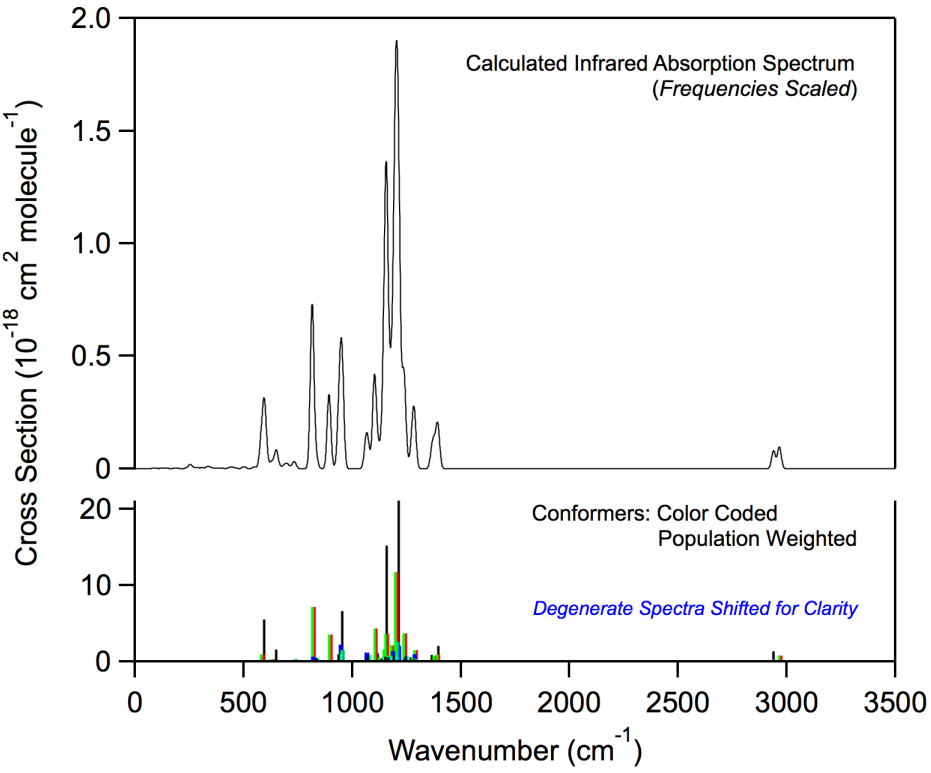
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.468104074618	0.400198903451	-0.532216866469
C	0.468393569219	-0.501907966207	0.222066899357
C	-1.021529585510	-0.316456698381	-0.186599843242
F	1.214326367573	1.694134494793	-0.264164933042
F	2.699399982849	0.096048183872	-0.083196611274
H	1.415021255907	0.226800590820	-1.612133957890
F	0.595478787303	-0.326259610143	1.543087132541
F	0.786699774975	-1.779171794609	-0.081448377948
Cl	-1.732472575915	1.191069480021	0.441793029868
F	-1.089224498574	-0.316060351618	-1.525562630095
F	-1.721238152445	-1.350880232000	0.271830158193

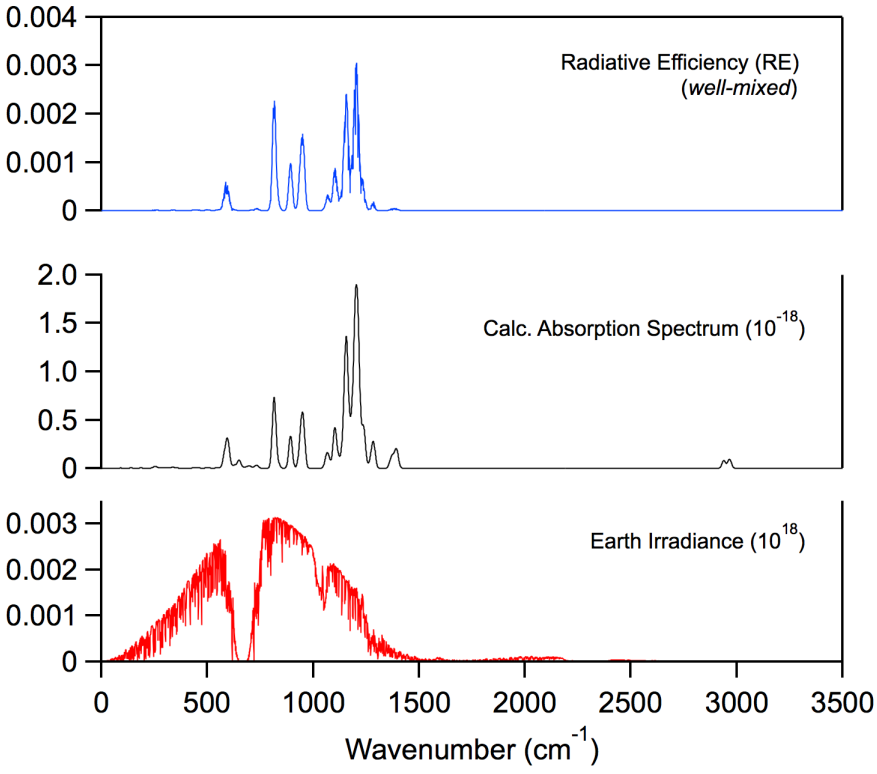
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
35.9974	0.136
73.6464	0.0634
149.0672	0.0697
186.9069	0.179
235.0253	0.542
266.3391	0.357
311.9857	0.283
313.8697	0.0854
344.3238	0.162
424.5527	0.0669
438.8697	0.423
469.4332	0.615
575.9633	2.07
624.6034	1.81
651.6186	1.67
826.5116	16.0
934.6239	29.9
1079.8811	28.8
1145.9819	10.1
1165.3698	19.7
1179.6965	16.6
1204.1937	27.0
1262.2975	22.3
1302.9771	9.95
1399.5971	1.80
1419.1603	2.55
3083.0201	3.40

Infrared Spectrum

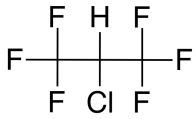


Radiative Efficiency



HCFC-226da

Molecular Formula:	$CF_3CHClCF_3$
Name:	2-Chloro-1,1,1,3,3,3-hexafluoropropane
CAS number:	431-87-8
Molecular Weight:	186.48



Global Atmospheric Lifetime (years):	27.7
Tropospheric Atmospheric Lifetime (years):	32.6
Stratospheric Atmospheric Lifetime (years):	185.2
Ozone Depletion Potential (ODP):	0.025

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.257	0.251
Global Warming Potential (GWP_H):		
GWP_{20}	4421	4323
GWP_{100}	2267	2216
Global Temperature Potentials (GTP_H)		
GTP_{20}		4111
GTP_{50}		2081
GTP_{100}		667

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 1.80 \times 10^{-15}$; $k_{SAR}(272\ K) \approx 1.15 \times 10^{-15}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 31.3$ years

$\tau^{OH}_{Trop} = 32.6$ years

$\tau^{OH}_{Strat} = 778.8$ years

Fractional Atmospheric Loss: 0.886

$O(^1D)$ Reactivity

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

$k_{Est}(T) = 0.7 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 529$ years

Fractional Atmospheric Loss: 0.052

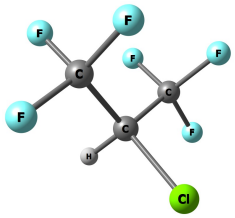
UV Photolysis

UV Spectrum: *No Recommendation*

$\tau_{hv} = 450$ years

Fractional Atmospheric Loss: 0.062

Molecular Structure and Infrared Spectrum (1 conformer)



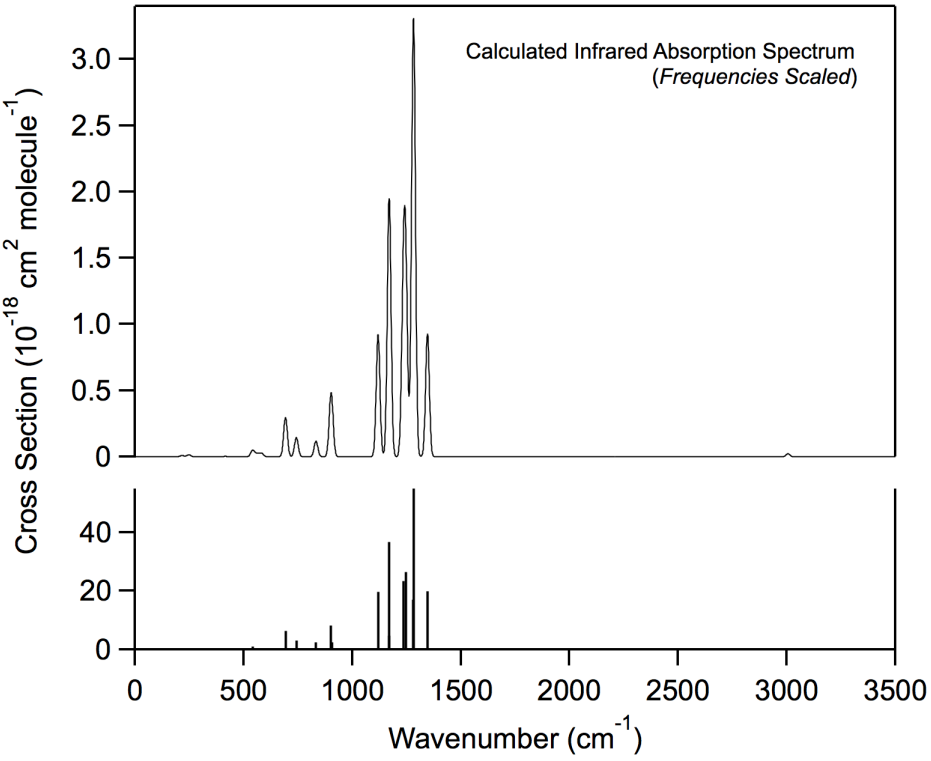
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.288565558957	-0.379259823402	-0.032513405519
C	0.000026457324	0.309335583499	-0.518454114482
C	-1.288613125436	-0.379080876828	-0.032526128644
F	2.354293957916	0.258216584990	-0.517601787721
F	1.374728285555	-0.398839210853	1.294570410804
F	1.325470052095	-1.639790647191	-0.477019938324
H	0.000029898742	0.281200639636	-1.608703668447
Cl	0.000142961427	2.020219127579	-0.011211111362
F	-2.354248207578	0.258544128387	-0.517624218526
F	-1.325688664042	-1.639606252637	-0.477033909772
F	-1.374791174960	-0.398649253180	1.294556871993

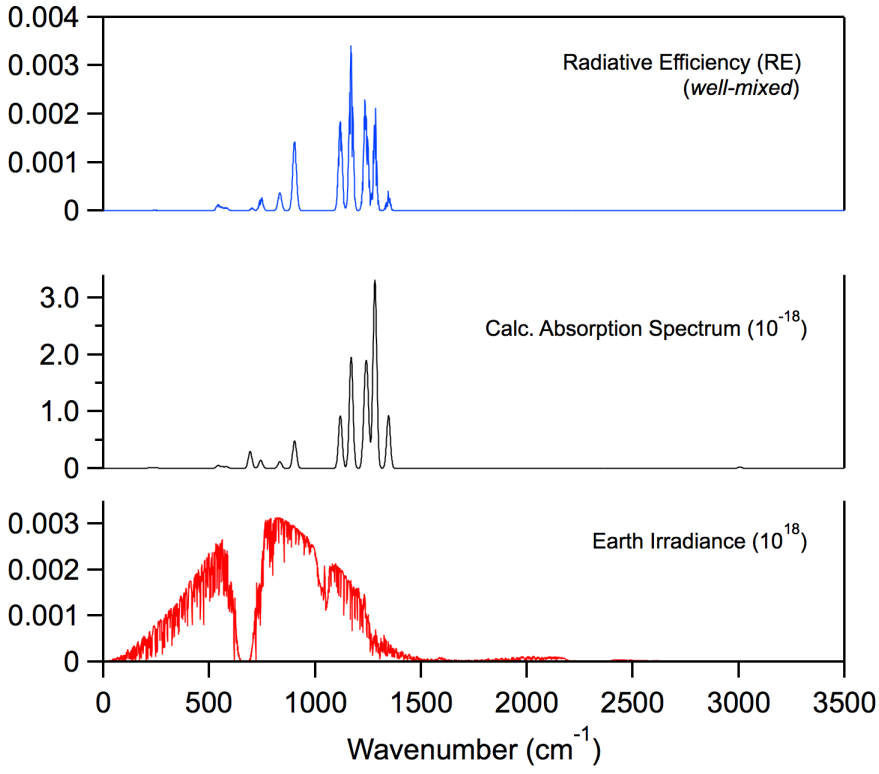
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
32.6422	0.000
82.3476	0.000
172.3244	0.176
193.2789	0.0627
206.3645	0.269
296.1155	0.0233
311.4212	0.0286
328.3218	0.0319
383.2284	0.0569
516.4329	1.07
537.6884	0.476
551.5634	0.111
560.3245	0.509
676.8139	6.32
729.6496	3.06
825.3378	2.51
897.9629	8.13
903.5081	2.53
1127.9251	19.6
1181.9978	36.8
1182.9213	4.76
1251.0437	23.4
1262.6936	26.4
1297.3800	17.0
1301.6892	54.9
1368.7776	19.8
3125.9592	0.495

Infrared Spectrum

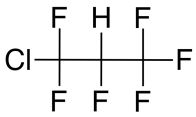


Radiative Efficiency



HCFC-226ea

Molecular Formula:	$CClF_2CHFCF_3$
Name:	1-Chloro-1,1,2,3,3,3-hexafluoropropane
CAS number:	359-58-0
Molecular Weight:	186.48



Global Atmospheric Lifetime (years):	24.9
Tropospheric Atmospheric Lifetime (years):	28.8
Stratospheric Atmospheric Lifetime (years):	180.2
Ozone Depletion Potential (ODP):	0.023

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.315	0.307
Global Warming Potential (GWP_H):		
GWP_{20}	5219	5095
GWP_{100}	2512	2452
Global Temperature Potentials (GTP_H)		
GTP_{20}		4771
GTP_{50}		2193
GTP_{100}		649

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 2.03 \times 10^{-15}$; $k_{SAR}(272\ K) \approx 1.30 \times 10^{-15}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 27.7$ years

$\tau^{OH}_{Trop} = 28.8$ years

$\tau^{OH}_{Strat} = 697.4$ years

Fractional Atmospheric Loss: 0.898

$O(^1D)$ Reactivity

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

$k_{Est}(T) = 0.7 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 529$ years

Fractional Atmospheric Loss: 0.047

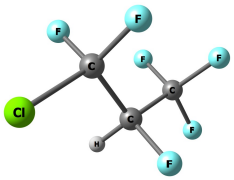
UV Photolysis

UV Spectrum: *No Recommendation*

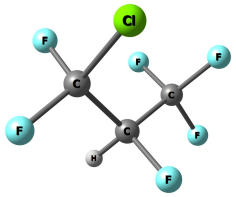
$\tau_{hv} = 450$ years

Fractional Atmospheric Loss: 0.055

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.633



$\Delta E = 0.62$ kcal mol^{-1}
Population = 0.223

Optimized Coordinates (Angstroms)

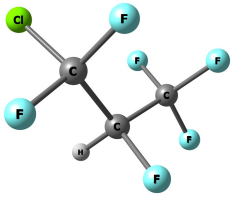
Atom	X	Y	Z
C	0.972759117106	-0.362578920410	0.087506335122
C	-0.177341117468	0.527487781655	-0.417770735779
C	-1.577688644861	-0.027985472974	-0.092237565719
Cl	2.551703565722	0.408331209106	-0.290641211514
F	0.894710990117	-0.549071931460	1.403511223710
F	0.920403181795	-1.551881182430	-0.516953308593
H	-0.092016264201	0.619843133408	-1.504818859465
F	-0.078510818835	1.750087358236	0.171285978352
F	-2.495240577535	0.804217328856	-0.589832451161
F	-1.749673572171	-1.227562320591	-0.652184162275
F	-1.775966859668	-0.133444983395	1.218676757322

Atom	X	Y	Z
C	1.110632020531	0.225477075015	-0.377377851292
C	-0.271934717011	0.828056550935	-0.061898236071
C	-1.463868060642	-0.143019756264	-0.098327600423
Cl	1.693570077660	-0.904558692494	0.878530915294
F	1.072139830134	-0.402124516004	-1.555467209054
F	1.983532256047	1.235157612283	-0.470273662063
H	-0.453656201971	1.594476514160	-0.825482673421
F	-0.229179864993	1.405421298383	1.168397701789
F	-2.577001320696	0.548240108951	0.162550772947
F	-1.583039082042	-0.689920074226	-1.309934475324
F	-1.359174937016	-1.115018120739	0.802497317618

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
25.2375	0.000
86.1991	0.0172
148.0813	0.162
216.9951	0.123
220.6668	0.478
258.0759	0.150
298.5388	0.159
324.2309	0.0368
393.6322	0.142
421.0229	0.110
480.2478	0.580
530.8361	0.545
573.9145	1.77
633.6344	2.24
691.5061	13.9
831.1074	18.7
865.4304	4.87
983.8071	18.8
1154.2234	6.29
1165.5227	9.70
1208.1823	15.9
1232.4757	56.6
1257.4988	17.8
1296.8605	43.8
1369.3128	2.34
1382.6725	11.1
3089.3582	0.888

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
22.5504	0.00218
91.7033	0.0381
158.0530	0.211
191.0529	0.119
229.2554	0.248
267.9039	0.303
308.9452	0.144
332.1338	0.0476
392.3876	0.164
423.1390	0.0112
491.9526	0.449
522.8035	1.83
591.2680	0.195
639.2842	3.24
686.2465	15.2
729.1226	3.76
892.6035	3.96
1064.5565	23.9
1151.2782	17.1
1171.3312	33.3
1187.8374	9.76
1221.8270	13.3
1242.1154	54.6
1303.9814	23.3
1365.9482	4.12
1391.8602	8.16
3060.8024	1.14



$\Delta E = 0.88$ kcal mol^{-1}
Population = 0.144

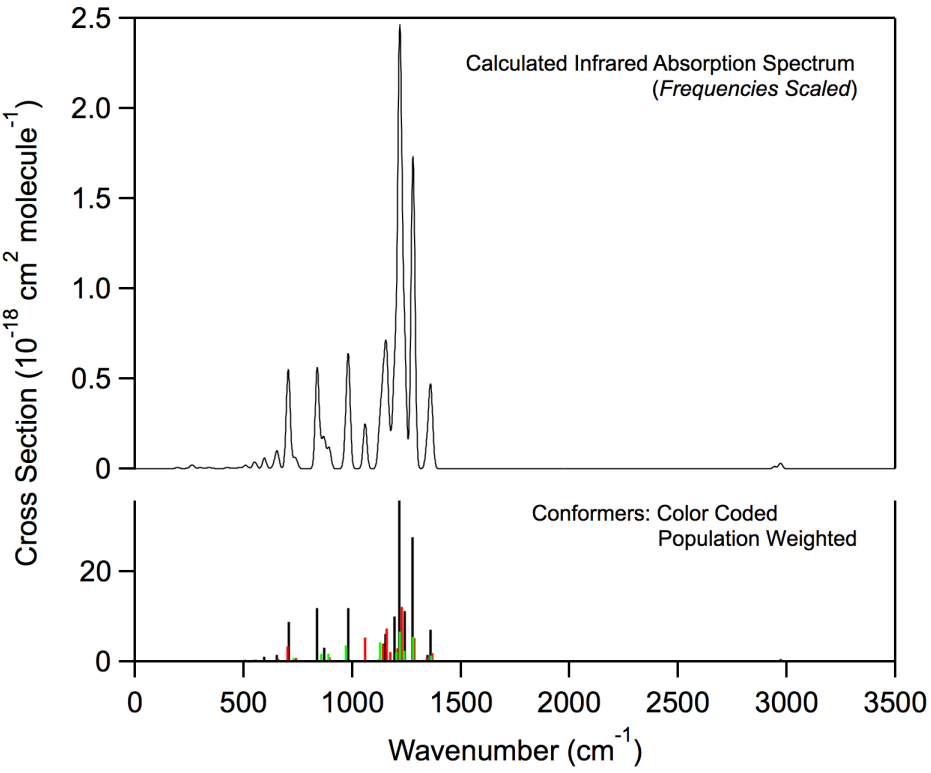
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.116149805530	0.346658960457	0.053468821799
C	-0.270185411913	0.549706303291	-0.589290792427
C	-1.421861799733	-0.279238135955	0.007397139576
Cl	1.790968654412	-1.275339555581	-0.317031785768
F	1.940823136833	1.269190398800	-0.448350982835
F	1.065143762957	0.508467223127	1.374174684153
H	-0.196600187586	0.327206657788	-1.657983536640
F	-0.598080137214	1.863705469533	-0.407615074289
F	-2.551766549482	0.062683845280	-0.617303703747
F	-1.225470494305	-1.586019378207	-0.171191224720
F	-1.575447779498	-0.042327788532	1.307367454898

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
22.0067	0.00
92.8017	0.0176
151.3520	0.0818
205.6585	0.362
232.6350	0.399
280.6341	0.0271
308.7445	0.240
320.1444	0.0694
390.0355	0.272
418.7497	0.0739
451.1376	1.01
527.8880	0.871
573.0119	0.849
619.7819	2.22
717.1356	5.62
851.5094	12.3
887.3254	11.6
971.9919	25.0
1131.0598	3.51
1137.6504	30.0
1217.8459	14.7
1234.2578	46.5
1253.4305	17.0
1300.0598	37.7
1366.7882	1.84
1387.2316	9.54
3091.9244	0.693

Infrared Spectrum



Radiative Efficiency