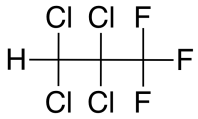
HCFC-223aa

Molecular Formula:	$CHCl_2CCl_2CF_3$
Name:	2,2,3,3-Tetrachloro-1,1,1-trifluoropropane
CAS number:	422-35-5
Molecular Weight:	235.85



Global Atmospheric Lifetime (years):	1.11
Tropospheric Atmospheric Lifetime (years):	1.17
Stratospheric Atmospheric Lifetime (years):	20
Ozone Depletion Potential (ODP):	0.024

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.257	0.195
Global Warming Potential (GWP_H):		
GWP_{20}	271	205
GWP_{100}	73	56
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*

$k_{SAR}(298\ K) = 5.01 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 3.20 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 1.14$ years

$\tau^{OH}_{Trop} = 1.17$ years

$\tau^{OH}_{Strat} = 38.9$ years

Fractional Atmospheric Loss: 0.972

$O(^1D)$ Reactivity

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

$k_{Est}(T) = 2.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 185$ years

Fractional Atmospheric Loss: 0.006

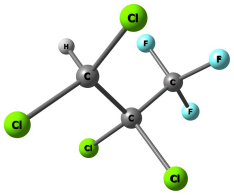
UV Photolysis

UV Spectrum: *No Recommendation*

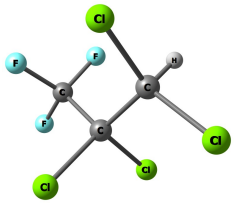
$\tau_{hv} = 50$ years

Fractional Atmospheric Loss: 0.022

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.460



E = 0
Population = 0.460

Optimized Coordinates (Angstroms)

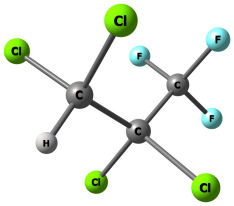
Atom	X	Y	Z
C	-1.021850528449	0.216081775804	-0.606796718160
C	0.232615312749	-0.344895676449	0.119733796492
C	1.523402657847	0.483713386411	-0.210177662820
Cl	-2.465847048073	-0.788571956100	-0.317279447677
Cl	-1.367260391801	1.915558643302	-0.175432020859
H	-0.824470677401	0.196673703286	-1.675663049178
Cl	0.524576759086	-1.996348501569	-0.529729898789
Cl	0.029671403139	-0.394150601395	1.884660255786
F	2.610149913218	-0.170756674965	0.176589426318
F	1.588395170327	0.681468823040	-1.531963989874
F	1.519172429357	1.665952078635	0.391888308761

Atom	X	Y	Z
C	-1.022318799379	-0.204019621300	-0.605887627273
C	0.237398031998	0.335516408647	0.127761676687
C	1.526507639384	-0.480062747204	-0.239099349788
Cl	-1.361823007518	-1.916953047487	-0.226149270649
Cl	-2.465207359005	0.788549379412	-0.272489348141
H	-0.833879726919	-0.150193316893	-1.675188211941
Cl	0.049091673599	0.328124495125	1.894979428264
Cl	0.521716670921	2.007311358342	-0.471078497392
F	2.615555053137	0.163483105480	0.159351528079
F	1.528881164157	-1.680914316770	0.324939592957
F	1.580758659623	-0.635435697351	-1.567017920802

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
55.2994	0.0250
78.2082	0.0117
144.3828	0.0596
165.7373	0.0195
200.9409	0.161
214.5676	0.0290
233.1845	0.0361
268.2271	0.0605
280.2706	0.165
340.2150	0.0234
363.6297	0.0617
385.0417	0.119
542.2746	1.34
557.9743	1.49
607.0034	2.16
698.3980	10.1
746.3375	17.4
782.9331	6.76
846.1428	11.4
927.6135	2.74
1039.1231	2.38
1210.7168	27.9
1223.0323	2.69
1245.6315	31.7
1252.0228	29.8
1281.1575	2.79
3157.3799	0.601

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
55.3012	0.0250
78.2102	0.0117
144.3835	0.0596
165.7379	0.0195
200.9417	0.161
214.5673	0.0290
233.1846	0.0361
268.2268	0.0605
280.2703	0.165
340.2147	0.0234
363.6306	0.0617
385.0418	0.119
542.2737	1.34
557.9750	1.49
607.0036	2.16
698.3982	10.1
746.3373	17.4
782.9334	6.76
846.1426	11.4
927.6152	2.74
1039.1242	2.38
1210.7155	27.9
1223.0309	2.69
1245.6327	31.7
1252.0239	29.8
1281.1550	2.79
3157.3820	0.601



$\Delta E = 1.04$ kcal mol^{-1}
Population = 0.08

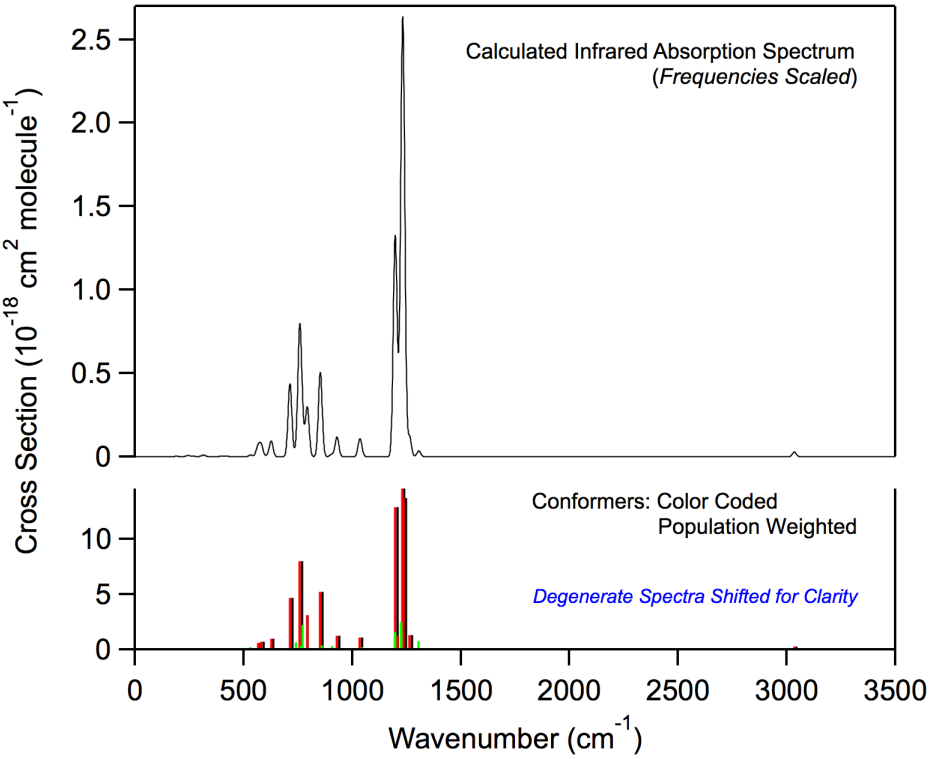
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.148619030958	-0.008575319649	0.579620407722
C	0.399741241937	-0.025831956294	0.407188536209
C	0.955461795957	0.055448886880	-1.052725874146
Cl	-1.906469689019	1.507013699455	0.007852564843
Cl	-1.959355861996	-1.412772984732	-0.174832812496
H	-1.345085211304	-0.071796317498	1.646931511811
Cl	1.014449355706	-1.543803377885	1.137338185473
Cl	1.067157532166	1.366154026651	1.319413000976
F	2.284429863053	0.029838197010	-1.028194578076
F	0.529110480724	-0.972972157055	-1.779199506157
F	0.568133523734	1.181089303117	-1.644417436159

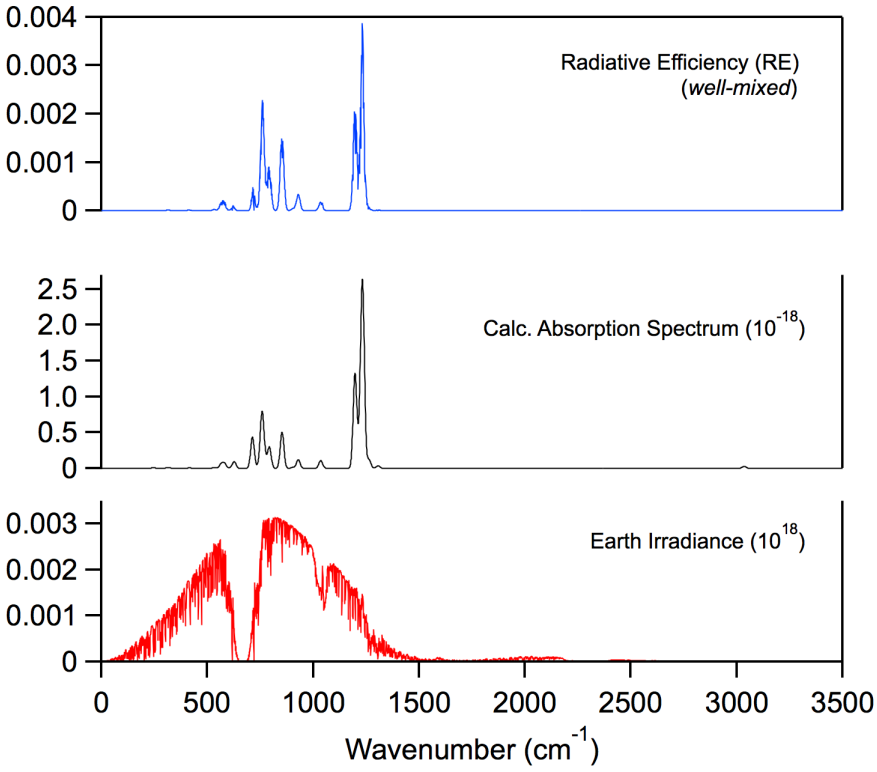
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
41.5813	0.00704
94.4719	0.0131
149.7846	0.00633
160.7473	0.00032
197.0069	0.0756
220.5742	0.00531
240.1645	0.0951
274.0190	0.283
276.0267	0.0279
324.6435	0.0171
359.7450	0.0420
397.0915	0.0434
506.6292	2.56
559.7661	1.05
588.7150	1.69
729.0382	8.10
750.5822	4.21
761.2676	27.6
852.4853	4.47
902.2258	3.79
1049.1063	2.52
1211.8506	19.6
1223.1324	0.419
1239.2332	26.8
1241.0392	31.6
1326.5059	9.33
3152.9781	0.596

Infrared Spectrum

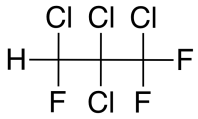


Radiative Efficiency



HCFC-223ab

Molecular Formula:	$CHClFCCl_2CClF_2$
Name:	1,2,2,3-Tetrachloro-1,1,3-trifluoropropane
CAS number:	144909-54-6
Molecular Weight:	235.85



Global Atmospheric Lifetime (years):	3.18
Tropospheric Atmospheric Lifetime (years):	3.54
Stratospheric Atmospheric Lifetime (years):	31.4
Ozone Depletion Potential (ODP):	0.059

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.317	0.282
Global Warming Potential (GWP_H):		
GWP_{20}	960	854
GWP_{100}	260	232
Global Temperature Potentials (GTP_H)		
GTP_{20}		374
GTP_{50}		43
GTP_{100}		32

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

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

OH Reactivity

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

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

τ^{OH}_{Global} = 3.42 years
τ^{OH}_{Trop} = 3.54 years
τ^{OH}_{Strat} = 105.3 years

Fractional Atmospheric Loss: 0.929

O(^{1}D) Reactivity

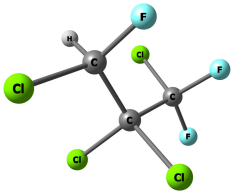
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 2.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)}$ = 185 years
Fractional Atmospheric Loss: 0.017

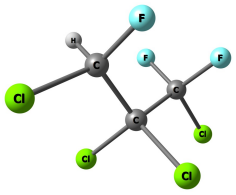
UV Photolysis

UV Spectrum: *No Recommendation*
τ_{hv} = 60 years
Fractional Atmospheric Loss: 0.054

Molecular Structure and Infrared Spectrum (7 conformers)



E = 0
Population = 0.390



$\Delta E = 0.35$ kcal mol^{-1}
Population = 0.217

Optimized Coordinates (Angstroms)

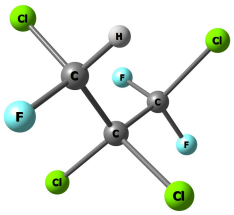
Atom	X	Y	Z
C	-0.988700712569	0.926260588858	0.215282385072
C	-0.119897468669	-0.317763693647	-0.109519841893
C	1.374789801326	-0.112710749883	0.333917878674
Cl	-2.707969087734	0.693786501510	-0.208471787880
F	-0.889287841624	1.197605960963	1.532684976605
H	-0.633498706999	1.777558744717	-0.366020758621
Cl	-0.150538877413	-0.604526889098	-1.868986003300
Cl	-0.716248486121	-1.748545062432	0.778545426481
Cl	2.082172215358	1.390436416840	-0.365150354319
F	1.455451731349	-0.028830642080	1.657026692872
F	2.105692433096	-1.145147175748	-0.068134613692

Atom	X	Y	Z
C	-1.302344537298	0.585654094474	-0.559366188258
C	-0.108395404779	-0.195853083179	0.067965662952
C	1.233300989582	0.518275745627	-0.338113516795
Cl	-2.882766001559	-0.160526528143	-0.192549654823
F	-1.300445054837	1.851696426459	-0.096419636641
H	-1.193356626904	0.588202070429	-1.644751014533
Cl	-0.106267483548	-1.840836601411	-0.623000623808
Cl	-0.235653813177	-0.220647188725	1.839122495474
Cl	2.692758764578	-0.378049007996	0.164553386663
F	1.245963553021	0.652698655765	-1.671766656079
F	1.282111614922	1.733341416699	0.198834745849

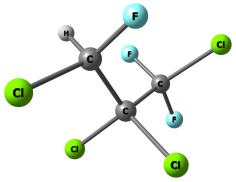
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
60.4338	0.0544
82.7731	0.0234
135.0438	0.0596
171.2918	0.0310
191.0193	0.0906
209.9706	0.0129
243.2230	0.0770
286.5473	0.105
304.0115	0.0697
316.1151	0.161
368.4450	0.236
424.5928	0.150
438.4344	0.0343
443.6533	0.450
604.7064	6.96
644.6195	4.42
763.9285	28.0
818.4642	13.1
882.8814	15.1
1001.3233	18.6
1054.5720	2.37
1131.2555	6.86
1197.3025	27.3
1224.0989	24.7
1284.3887	3.04
1360.5944	1.98
3127.3925	0.505

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
60.2284	0.0565
77.1962	0.0288
132.1748	0.0567
176.9569	0.0195
195.7905	0.0182
211.4137	0.251
239.0425	0.0270
255.5088	0.0426
300.3191	0.0141
336.1381	0.0458
389.2791	0.274
429.8930	0.0356
439.1772	0.172
452.8564	0.473
618.7996	11.7
631.2753	2.73
719.8551	22.3
869.5103	13.6
895.0238	5.82
996.1372	11.7
1052.6408	23.8
1130.9528	6.58
1166.5881	21.0
1204.9245	29.3
1281.9961	3.63
1359.9986	2.29
3121.3559	0.389



$\Delta E = 0.46$ kcal mol^{-1}
Population = 0.180



$\Delta E = 0.99$ kcal mol^{-1}
Population = 0.073

Optimized Coordinates (Angstroms)

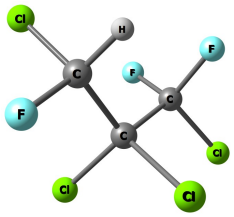
Atomi	X	Y	Z
C	1.136027646057	-0.182969421671	0.878701339902
C	0.093185312908	0.492487534994	-0.052200020510
C	-1.109325805957	-0.414620440097	-0.482421446420
Cl	1.872089526541	-1.653033033012	0.170062941120
F	2.111785409228	0.705594189145	1.140451110840
H	0.651240859366	-0.487384415464	1.806389820536
Cl	0.881735729061	1.083207518567	-1.540269508676
Cl	-0.567291388571	1.881111684868	0.876270893287
Cl	-1.871159886832	-1.222987565057	0.935537606849
F	-2.029273746526	0.326451987661	-1.089127001955
F	-0.708516655274	-1.354216039934	-1.331160734973

Atom	X	Y	Z
C	-1.009318701345	0.669331184268	-0.691546721520
C	-0.143036950186	-0.323192955795	0.132580482497
C	1.371079092688	-0.251039381347	-0.291518803391
Cl	-2.755224124904	0.506588963728	-0.349047003396
F	-0.636043000487	1.934836070710	-0.417432949536
H	-0.868830285363	0.462932040779	-1.753900342870
Cl	-0.675913642418	-1.988232179458	-0.276118233451
Cl	-0.291052388729	-0.024168945490	1.875301373687
Cl	2.180411322821	1.287135645870	0.122414584630
F	2.043791689485	-1.238806379832	0.287392323322
F	1.435729988439	-0.412356063433	-1.620712709973

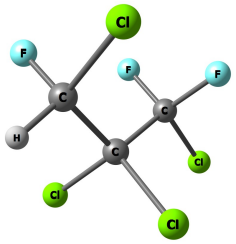
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
59.0666	0.0290
91.6130	0.0361
137.2246	0.0434
173.4969	0.0521
184.0657	0.132
228.5859	0.0152
236.9967	0.0277
273.6313	0.121
308.4011	0.163
333.2076	0.0196
352.4230	0.341
413.5154	0.341
425.8108	0.178
455.8106	0.230
618.1517	7.31
648.6357	1.39
764.8883	26.4
801.8655	29.6
855.8918	3.11
1012.8889	14.9
1050.4995	1.79
1149.1143	15.0
1204.3436	19.8
1219.8128	22.0
1280.2650	5.13
1363.5444	1.49
3129.4059	0.516

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
53.6569	0.0542
79.3414	0.0301
138.3707	0.0529
167.2463	0.0140
194.9942	0.127
210.5166	0.0579
243.4384	0.168
271.5960	0.0825
291.8796	0.135
334.8791	0.0259
370.6719	0.183
432.3106	0.0147
438.8127	0.315
448.6573	0.184
615.0916	4.84
640.5336	6.04
758.5525	28.2
817.9245	15.6
882.3958	7.04
1001.8201	16.1
1051.8596	6.08
1141.9867	19.8
1163.8644	18.6
1212.7795	22.4
1281.8861	3.81
1361.6962	2.11
3117.3532	0.404



ΔE = 1.03 kcal mol^{-1}
Population = 0.069



ΔE = 1.41 kcal mol^{-1}
Population = 0.036

Optimized Coordinates (Angstroms)

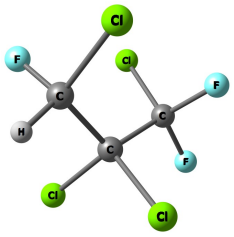
Atom	X	Y	Z
C	-1.460189168403	-0.202189103914	0.608853054180
C	-0.065713625824	-0.417265709672	-0.055963635697
C	0.944004071141	0.722140024139	0.316742563833
Cl	-2.287102404690	1.299603681436	0.094313852031
F	-2.248463322081	-1.246954010032	0.299002443024
H	-1.330476529551	-0.138033277340	1.689678373518
Cl	-0.218288592242	-0.543126826209	-1.818891669884
Cl	0.538592849055	-1.958962722240	0.641493974987
Cl	2.624438629344	0.366129941755	-0.171506754888
F	0.583250450365	1.865261705985	-0.257691853419
F	0.902924642887	0.891149296091	1.645668652316

Atom	X	Y	Z
C	-1.517213719642	-0.580728360840	-0.185301839853
C	-0.020127845330	-0.453156386531	0.244039017147
C	0.761772265283	0.702485461006	-0.471915313274
Cl	-2.519834847274	0.856236164313	0.191561578909
F	-1.592947568681	-0.823265046577	-1.507502193908
H	-1.948496512121	-1.413500257209	0.372223107738
Cl	0.728895932385	-2.019086081886	-0.207491570564
Cl	0.042746376897	-0.222973852161	2.007477512320
Cl	2.503154161790	0.723948733477	-0.050090743597
F	0.643998573415	0.556840584300	-1.790043425828
F	0.239419183279	1.877633042106	-0.129916129091

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
53.5479	0.0398
84.9241	0.0372
137.2722	0.0708
170.5613	0.0657
193.8135	0.0837
203.6941	0.0893
247.3825	0.118
263.4770	0.0334
309.5894	0.224
330.2934	0.00928
381.0353	0.347
415.0596	0.475
431.4180	0.243
451.2104	0.341
625.8191	5.27
637.8730	4.23
754.6445	28.3
826.7777	15.8
859.7322	8.95
998.1636	7.58
1065.9235	26.4
1144.2758	8.97
1176.5359	20.6
1203.9540	20.6
1280.6247	5.44
1362.7023	1.96
3124.6120	0.390

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
43.7338	0.00546
98.7069	0.0560
146.6929	0.0188
164.6420	0.0006
193.5166	0.0483
208.3883	0.0571
248.4287	0.0521
261.0906	0.0285
308.1653	0.00711
350.6584	0.0447
383.5579	0.107
423.1660	0.0619
436.7711	0.269
448.4816	0.514
534.6693	10.5
638.5776	2.88
762.0840	23.2
861.8510	11.5
901.4239	14.1
939.1118	9.34
1073.8376	23.9
1139.2526	10.6
1182.0431	14.8
1206.7972	24.0
1295.9243	8.19
1369.0571	1.93
3114.8923	0.541



$\Delta E = 1.44$ kcal mol^{-1}
Population = 0.034

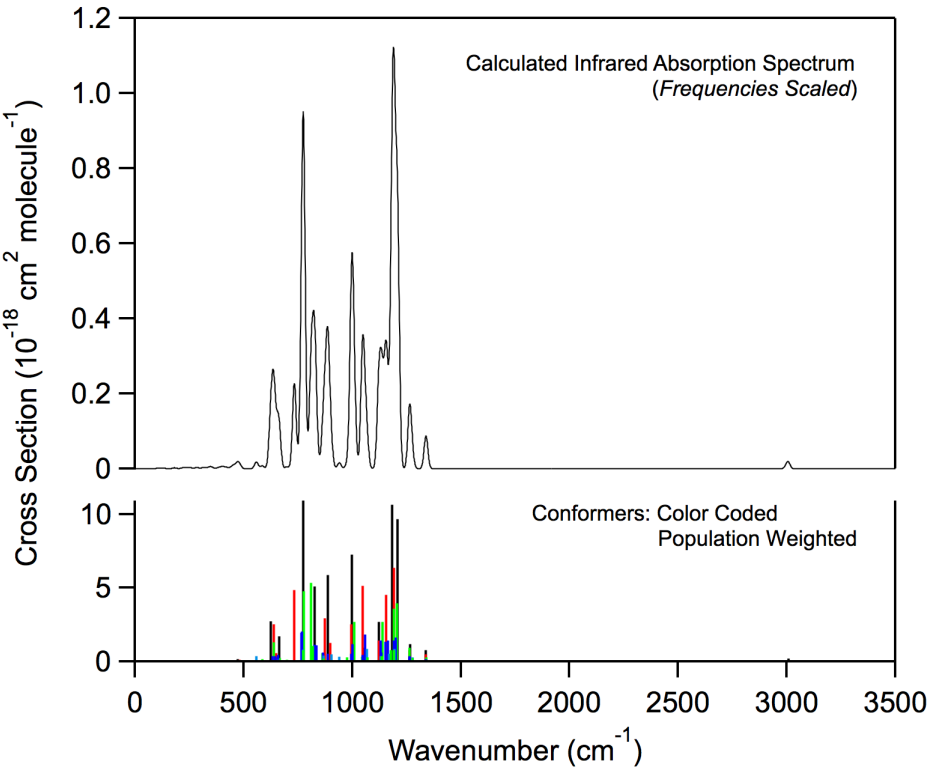
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.218712475269	0.172050046475	-0.876028540269
C	-0.029838287633	-0.569485730376	-0.197370741167
C	0.891369383336	0.250941056041	0.771021261998
Cl	-2.303775733170	0.999897000714	0.285602388147
F	-0.768858689148	1.075317256920	-1.766361133823
H	-1.822408047290	-0.579013225690	-1.387775863750
Cl	0.980694128180	-1.223971701292	-1.524186347323
Cl	-0.713793903401	-1.927418940206	0.753061301313
Cl	1.554400941473	1.728896577099	0.010497788802
F	0.211054768015	0.604834604765	1.858369123104
F	1.907489914908	-0.519960944450	1.153083762968

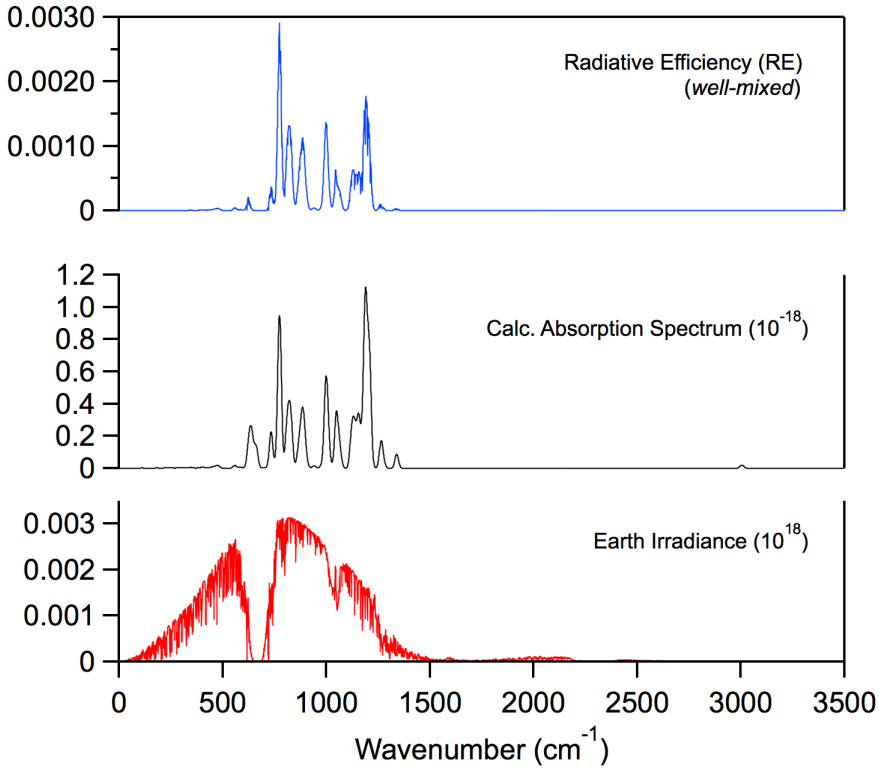
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
48.5476	0.0217
102.9597	0.0324
146.5101	0.0248
167.7136	0.0203
186.0674	0.0270
232.9892	0.0415
247.4514	0.0582
271.1867	0.376
290.3610	0.0378
343.5627	0.0444
366.2339	0.163
426.4644	0.636
432.4313	0.125
437.3972	0.167
563.4682	4.73
683.1579	3.32
763.1152	22.9
808.4929	30.3
861.4623	5.34
978.0761	8.62
1074.9943	8.28
1145.3327	10.6
1189.4242	22.0
1205.4286	22.4
1294.8625	6.68
1375.9751	0.268
3115.3022	0.521

Infrared Spectrum

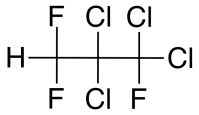


Radiative Efficiency



HCFC-223ac

Molecular Formula:	$CHF_2CCl_2CCl_2F$
Name:	1,1,2,2-Tetrachloro-1,3,3-trifluoropropane
CAS number:	422-29-7
Molecular Weight:	235.85



Global Atmospheric Lifetime (years):	9.29
Tropospheric Atmospheric Lifetime (years):	12.6
Stratospheric Atmospheric Lifetime (years):	35.2
Ozone Depletion Potential (ODP):	0.164

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.303	0.289
Global Warming Potential (GWP_H):		
GWP_{20}	2377	2262
GWP_{100}	728	693
Global Temperature Potentials (GTP_H)		
GTP_{20}		1654
GTP_{50}		245
GTP_{100}		99

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 4.65 \times 10^{-15}$; $k_{SAR}(272\ K) \approx 2.97 \times 10^{-15}$ cm^3 $molecule^{-1}$ s^{-1}

τ^{OH}_{Global} = 12.2 years
τ^{OH}_{Trop} = 12.6 years
τ^{OH}_{Strat} = 331.1 years

Fractional Atmospheric Loss: 0.764

O(^{1}D) Reactivity

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

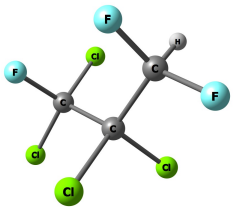
$k_{Est}(T) = 2.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)}$ = 185 years
Fractional Atmospheric Loss: 0.050

UV Photolysis

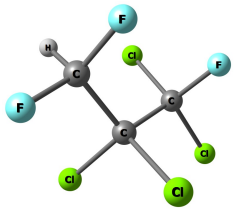
UV Spectrum: *No Recommendation*
τ_{hv} = 50 years
Fractional Atmospheric Loss: 0.186

Papanastasiou et al. (2018)

Molecular Structure and Infrared Spectrum (9 conformers)



E = 0
Population = 0.290



E = 0
Population = 0.290

Optimized Coordinates (Angstroms)

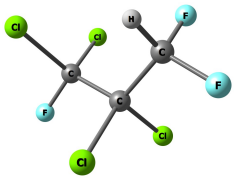
Atom	X	Y	Z
C	1.506833125128	-0.947738925631	0.014851785178
C	0.469035414403	0.210043978025	0.147488730829
C	-0.948311288479	-0.200877333791	-0.390105086923
F	1.589135155802	-1.339823952443	-1.269134487732
F	2.711346819300	-0.499407635117	0.401702284339
H	1.215230685866	-1.795724550805	0.640701321662
Cl	1.049674864041	1.595929424372	-0.816126939701
Cl	0.382028628870	0.631478144561	1.878360399862
Cl	-1.511279958089	-1.713328573313	0.408249477996
Cl	-2.160496354326	1.082973009259	-0.140258372565
F	-0.856355092515	-0.442308585116	-1.698166112944

Atom	X	Y	Z
C	1.506815517932	0.941612687168	0.030559413124
C	0.465973861396	-0.215374980692	0.145015625621
C	-0.951447255022	0.209141531628	-0.381708716887
F	2.710936618692	0.482985490714	0.406407694997
F	1.587200227200	1.356342478307	-1.246414518043
H	1.219174817348	1.779110587625	0.672166101157
Cl	0.381858940159	-0.667415740103	1.868291336909
Cl	1.040292886986	-1.585477817985	-0.844606248518
Cl	-2.166763523607	-1.075486235088	-0.151871116475
Cl	-1.508110430751	1.708702979672	0.444883622249
F	-0.861905660335	0.473629018753	-1.685471194134

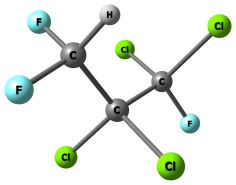
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
59.3934	0.0692
91.7599	0.0757
145.6930	0.0628
172.5305	0.0200
203.3899	0.0382
204.0915	0.117
235.3495	0.0500
259.4792	0.0303
298.0189	0.172
321.6268	0.217
352.6489	0.134
385.8066	0.0379
414.1492	0.335
496.0647	0.430
560.2394	3.41
656.5004	12.0
753.3052	17.6
814.9608	23.8
887.4617	16.5
1020.4781	1.11
1055.0271	8.49
1141.6381	1.40
1175.2964	22.2
1179.5759	30.7
1375.2858	6.02
1395.0217	1.47
3099.5032	1.86

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
59.3943	0.0692
91.7600	0.0757
145.6925	0.0628
172.5309	0.0200
203.3902	0.0381
204.0917	0.117
235.3494	0.0500
259.4795	0.0303
298.0187	0.172
321.6271	0.217
352.6493	0.134
385.8069	0.0379
414.1493	0.335
496.0647	0.430
560.2390	3.41
656.5009	12.0
753.3056	17.6
814.9605	23.8
887.4613	16.5
1020.4781	1.11
1055.0297	8.49
1141.6391	1.40
1175.2957	22.2
1179.5757	30.7
1375.2860	6.02
1395.0213	1.47
3099.5043	1.86



$\Delta E = 0.67$ kcal mol^{-1}
Population = 0.093



$\Delta E = 0.67$ kcal mol^{-1}
Population = 0.093

Optimized Coordinates (Angstroms)

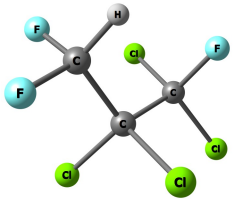
Atom	X	Y	Z
C	1.115387452317	-0.315612758995	-1.190498979431
C	0.528204680901	0.155897911421	0.170772243956
C	-1.039831699606	0.111724652507	0.260897852835
F	2.453124474438	-0.210240729887	-1.144178910958
F	0.802923011217	-1.604968072223	-1.411048222897
H	0.726899737806	0.301409556446	-2.006349298883
Cl	1.036999567229	1.863741265682	0.386410762389
Cl	1.210702266016	-0.837238932194	1.485793905241
Cl	-1.773462668552	1.052838101713	-1.088000392493
Cl	-1.689945330303	-1.549383455287	0.217112751143
F	-1.414136491463	0.671954460818	1.410195289098

Atom	X	Y	Z
C	1.111044038494	0.346835182124	-1.184833728984
C	0.530120665928	-0.157585704140	0.167296204629
C	-1.037545725804	-0.116952719750	0.265211384813
F	0.796608562138	1.640810713796	-1.373169934529
F	2.449051740050	0.241583634980	-1.146795290563
H	0.719526482945	-0.250869143997	-2.013515771587
Cl	1.217535818636	0.804450422535	1.502719435901
Cl	1.041166392541	-1.869645130246	0.339864703013
Cl	-1.689122241841	1.544157472955	0.263947316223
Cl	-1.776292260234	-1.026207291658	-1.102612927078
F	-1.406434472853	-0.704817436600	1.402393608163

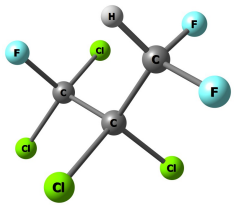
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
55.4506	0.0738
90.3316	0.0831
151.5356	0.0363
165.6456	0.0153
197.0352	0.150
220.9406	0.0134
236.0190	0.0233
257.5872	0.0772
287.3457	0.139
320.2841	0.327
345.5704	0.00956
388.0501	0.0808
410.6162	0.238
486.8609	0.616
579.8548	1.36
658.0134	11.9
752.6626	17.8
803.1235	37.6
877.6031	2.68
1017.2354	2.91
1053.8749	0.136
1155.0140	14.1
1175.2485	23.6
1180.7408	16.9
1380.1435	5.11
1393.4782	1.60
3092.8616	1.84

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
55.4514	0.0738
90.3311	0.0831
151.5345	0.0363
165.6469	0.0153
197.0353	0.150
220.9405	0.0134
236.0189	0.0233
257.5868	0.0772
287.3457	0.139
320.2835	0.327
345.5698	0.00956
388.0512	0.0808
410.6168	0.238
486.8612	0.616
579.8541	1.36
658.0133	11.9
752.6630	17.8
803.1257	37.6
877.6047	2.68
1017.2340	2.91
1053.8732	0.136
1155.0136	14.1
1175.2478	23.6
1180.7396	16.9
1380.1414	5.11
1393.4771	1.60
3092.8637	1.84



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



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

Optimized Coordinates (Angstroms)

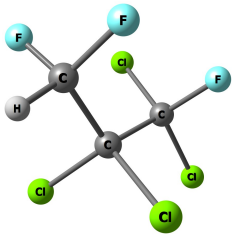
Atom	X	Y	Z
C	1.557209356902	0.637197611234	-0.627127756499
C	0.484299868821	-0.261614897121	0.068136685740
C	-0.972471544027	0.106143852331	-0.392700320473
F	1.473745172345	1.903632526556	-0.185633017552
F	2.779574805289	0.174816830138	-0.320956454592
H	1.413477564192	0.614100688863	-1.712309843349
Cl	0.653286096426	-0.143709829937	1.829150739967
Cl	0.823265727270	-1.933176335142	-0.495493074650
Cl	-2.185282370040	-1.038600507342	0.240105730431
Cl	-1.441398724430	1.764102036668	0.078571997496
F	-0.983203952748	0.043406023752	-1.736184686518

Atom	X	Y	Z
C	1.558011881887	-0.614128932489	-0.645852930574
C	0.480176611507	0.266373300701	0.065059248694
C	-0.975782723792	-0.114733026056	-0.387433416060
F	2.777265217952	-0.139892654684	-0.345462796876
F	1.492852274960	-1.884977260256	-0.214067512377
H	1.405461123159	-0.583975881205	-1.729656665764
Cl	0.795146406929	1.946304438268	-0.487496716877
Cl	0.664372392551	0.136230887190	1.823684890063
Cl	-1.421584863792	-1.781845503094	0.073885323859
Cl	-2.196870239955	1.010527928376	0.264122190483
F	-0.997821081405	-0.041260296752	-1.730235614570

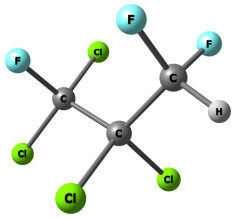
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
53.6766	0.0781
86.2050	0.0767
150.2282	0.0532
167.6194	0.00643
201.9237	0.125
211.6035	0.115
238.4082	0.149
260.6783	0.0241
275.5464	0.0867
321.0530	0.185
374.4443	0.0700
385.3244	0.00213
405.6304	0.345
499.0413	0.291
565.5326	3.84
673.8797	9.97
761.3004	18.7
801.7773	29.2
883.5892	5.01
1020.1301	5.52
1052.9910	8.42
1124.0884	13.6
1163.6237	21.1
1175.1906	18.4
1376.2779	6.35
1394.4989	1.90
3085.2923	1.88

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
53.6746	0.0781
86.2012	0.0767
150.2267	0.0532
167.6177	0.00643
201.9225	0.125
211.6015	0.115
238.4071	0.149
260.6782	0.0241
275.5455	0.0867
321.0523	0.185
374.4442	0.0700
385.3248	0.00213
405.6290	0.345
499.0415	0.291
565.5329	3.84
673.8788	9.97
761.2975	18.7
801.7759	29.2
883.5887	5.01
1020.1265	5.52
1052.9818	8.42
1124.0875	13.6
1163.6257	21.1
1175.1915	18.4
1376.2764	6.35
1394.4994	1.90
3085.2957	1.88



$\Delta E = 1.14$ kcal mol^{-1}
Population = 0.042



$\Delta E = 1.14$ kcal mol^{-1}
Population = 0.042

Optimized Coordinates (Angstroms)

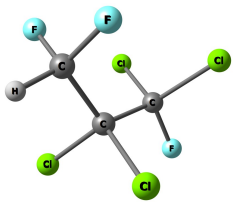
Atom	X	Y	Z
C	1.801349798736	0.407879538852	-0.049019510033
C	0.475099630463	-0.375015839566	0.230089341839
C	-0.805028668055	0.222809796436	-0.458685962492
F	1.955886672815	0.595734767986	-1.371189597405
F	1.795470224160	1.609414784476	0.550860647097
H	2.635608800666	-0.185523049837	0.340051623584
Cl	0.270787402872	-0.459847817364	1.995688443521
Cl	0.747445983048	-2.016080804201	-0.446544105544
Cl	-2.259836447129	-0.756559461697	-0.097299145060
Cl	-1.099935867804	1.912706841410	0.045615544006
F	-0.614058529770	0.210598243504	-1.780011279513

Atom	X	Y	Z
C	1.802292358814	-0.411493284529	-0.060241092847
C	0.478336490046	0.370746868180	0.231297683029
C	-0.805119208170	-0.217904729064	-0.459183025765
F	1.796358326241	-1.619071056029	0.527382717764
F	1.952075012204	-0.586118277906	-1.384769444142
H	2.638867935636	0.176507067914	0.332046584002
Cl	0.751213218977	2.018146300680	-0.429537510333
Cl	0.280121332126	0.437960551299	1.998349026359
Cl	-1.101201498553	-1.912347780511	0.028913731448
Cl	-2.257032846678	0.760165707832	-0.082947517147
F	-0.618574120644	-0.192579367865	-1.780954152368

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
46.1743	0.0292
105.7879	0.112
155.7176	0.0211
165.7760	0.0002
206.9591	0.0727
208.5475	0.0492
234.9221	0.0715
265.1401	0.0419
270.1386	0.0222
349.6123	0.0150
382.9701	0.121
388.6191	0.0893
401.7408	0.278
489.6650	1.45
547.9243	7.94
590.5588	4.71
781.3253	34.8
868.2748	10.3
885.7601	9.05
940.0394	3.52
1088.2812	9.49
1141.2484	1.12
1170.5052	28.2
1177.1260	24.9
1390.4559	5.59
1394.9928	2.51
3078.3855	2.44

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
46.1738	0.0292
105.7922	0.112
155.7217	0.0211
165.7750	0.0002
206.9640	0.0727
208.5471	0.0492
234.9225	0.0715
265.1403	0.0419
270.1386	0.0222
349.6127	0.0150
382.9716	0.121
388.6203	0.0894
401.7413	0.278
489.6653	1.45
547.9244	7.94
590.5589	4.71
781.3268	34.8
868.2769	10.3
885.7637	9.05
940.0430	3.52
1088.2842	9.49
1141.2502	1.12
1170.5031	28.2
1177.1263	24.9
1390.4589	5.59
1394.9941	2.51
3078.3781	2.44



$\Delta E = 1.65$ kcal mol^{-1}
Population = 0.018

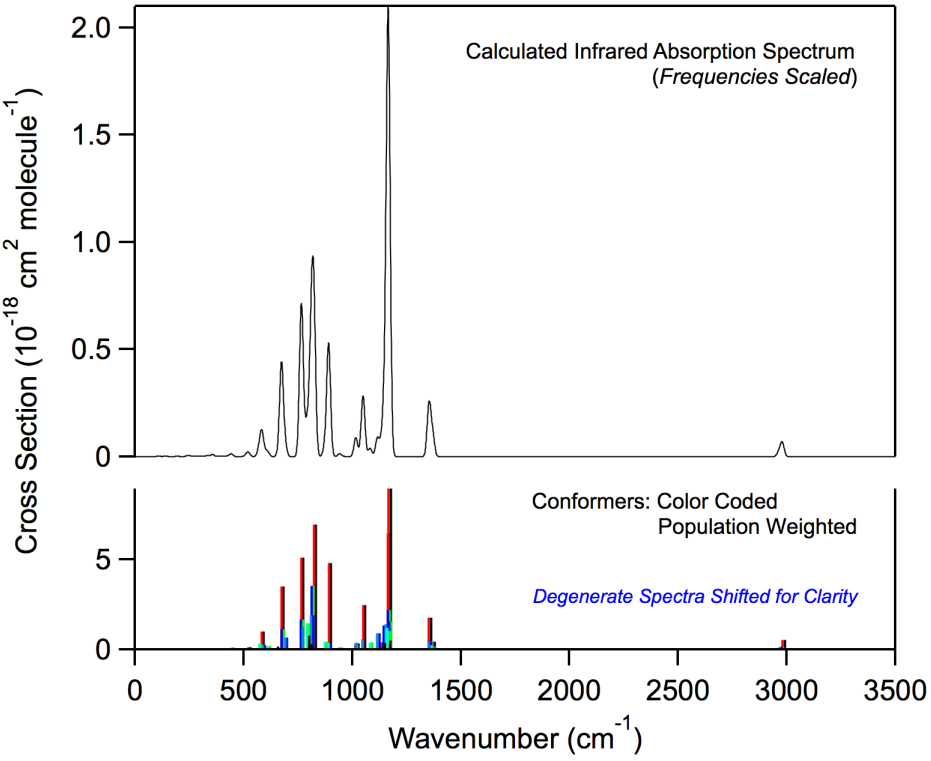
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.119129279634	0.040748715043	-1.328315223718
C	0.665250395724	-0.012839716597	0.162421184685
C	-0.877081375875	-0.004915090726	0.465716207570
F	0.646793223738	-1.015897096857	-2.010973746134
F	0.675042579070	1.160301743949	-1.924143638432
H	2.214219941710	0.027300350416	-1.347547045898
Cl	1.404949562782	1.404974763140	0.972876200357
Cl	1.367108541368	-1.509406432050	0.856590922052
Cl	-1.669269616725	1.485325680492	-0.125252736946
Cl	-1.707023443318	-1.422302155550	-0.241273266232
F	-1.031774088110	-0.055821761260	1.791848142695

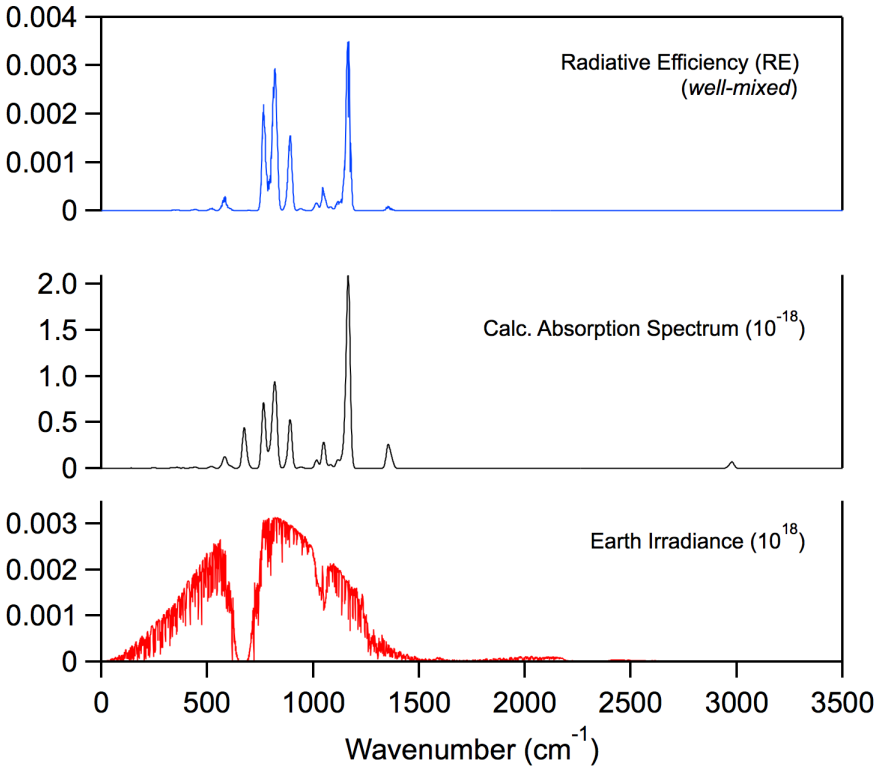
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
43.5205	0.0497
110.5979	0.0631
158.3825	0.00151
161.0362	0.0982
200.6843	0.00883
218.9468	0.00384
254.0187	0.0731
260.2990	0.148
263.3473	0.138
325.2938	0.218
384.6314	0.300
388.7001	0.165
392.5609	0.0827
459.3273	1.33
573.7092	1.10
640.7322	8.77
791.9148	43.2
804.2961	16.7
871.2539	0.528
959.1391	1.92
1097.8705	2.79
1147.8079	5.48
1161.2380	20.3
1187.3031	28.0
1394.4059	1.26
1399.7938	3.87
3077.2585	2.53

Infrared Spectrum

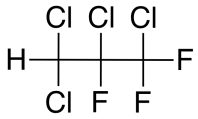


Radiative Efficiency



HCFC-223ba

Molecular Formula:	$CHCl_2CClFCClF_2$
Name:	1,2,3,3-Tetrachloro-1,1,2-trifluoropropane
CAS number:	422-41-3
Molecular Weight:	235.85



Global Atmospheric Lifetime (years):	1.39
Tropospheric Atmospheric Lifetime (years):	1.47
Stratospheric Atmospheric Lifetime (years):	23.1
Ozone Depletion Potential (ODP):	0.029

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.325	0.258
Global Warming Potential (GWP_H):		
GWP_{20}	430	341
GWP_{100}	116	92
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*

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

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

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

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

Fractional Atmospheric Loss: 0.969

O(^{1}D) Reactivity

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

$k_{Est}(T) = 2.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 185$ years

Fractional Atmospheric Loss: 0.007

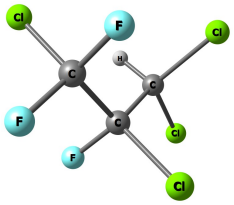
UV Photolysis

UV Spectrum: *No Recommendation*

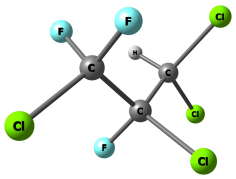
$\tau_{hv} = 60$ years

Fractional Atmospheric Loss: 0.024

Molecular Structure and Infrared Spectrum (5 conformers)



E = 0
Population = 0.437



$\Delta E = 0.04$ kcal mol^{-1}
Population = 0.411

Optimized Coordinates (Angstroms)

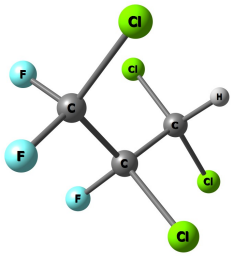
Atom	X	Y	Z
C	1.010668723986	-0.625152093597	0.356441037032
C	-0.021984912201	0.519864950028	0.208181180627
C	-1.464475380996	0.065913310250	-0.204543515970
Cl	1.302511522700	-1.504295653043	-1.161177147449
Cl	2.528114262599	0.005693698461	1.050808872922
H	0.616242983225	-1.341111300842	1.073439997446
Cl	0.507067835511	1.759621733319	-0.965112827593
F	-0.156461827537	1.092003250464	1.424178956075
F	-2.273287762065	1.116322022675	-0.115569124423
F	-1.502482632606	-0.399679140957	-1.444455817444
Cl	-2.076587812616	-1.206781776758	0.915876388776

Atom	X	Y	Z
C	1.257949824082	-0.273848227944	0.547531881697
C	-0.052358622074	0.431850733841	0.098573972020
C	-1.302027244403	-0.504226803505	0.254733655904
Cl	1.679465493425	-1.678838460508	-0.457831052703
Cl	2.596770156253	0.901164527678	0.620008890959
H	1.102164771772	-0.636581545216	1.560640631951
Cl	0.036895132466	1.048948831579	-1.565831597024
F	-0.237154525079	1.459267418090	0.956336440654
F	-1.328143070856	-1.442866588417	-0.681173884357
F	-1.220500035218	-1.103096072479	1.453129797655
Cl	-2.822988880368	0.429204186882	0.189897263243

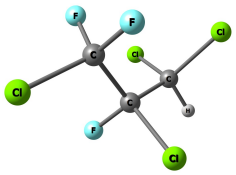
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
44.6639	0.0271
80.9984	0.0135
132.5649	0.0869
171.6190	0.0312
177.7106	0.0916
230.2956	0.0742
246.5772	0.151
266.4303	0.0509
319.1405	0.0292
336.6827	0.205
373.4784	0.153
399.4587	0.204
422.5414	0.151
536.7335	0.996
590.9791	5.47
647.0690	2.50
759.9374	19.6
803.7787	24.7
817.7021	21.2
1006.9184	4.75
1076.7752	12.6
1154.0166	14.8
1221.2765	12.0
1225.7528	14.9
1243.8938	14.6
1284.4107	2.27
3154.8228	0.447

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
46.7858	0.0318
73.0010	0.0150
129.8009	0.0924
170.5249	0.0354
189.9718	0.131
208.0193	0.0402
235.6920	0.127
292.1023	0.0850
313.7402	0.0891
340.2877	0.131
366.5779	0.304
424.8537	0.00309
443.7126	0.237
514.4141	1.17
597.6059	6.30
652.4895	2.24
713.1717	23.0
811.5538	12.9
870.1167	17.2
1003.2000	23.6
1084.6611	12.4
1135.3164	10.6
1188.0633	21.2
1223.5483	5.00
1242.4870	12.1
1282.9984	2.61
3154.8061	0.430



$\Delta E = 1.18$ kcal mol^{-1}
Population = 0.060



$\Delta E = 1.18$ kcal mol^{-1}
Population = 0.059

Optimized Coordinates (Angstroms)

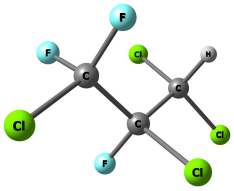
Atom	X	Y	Z
C	1.105320132531	-0.220705602691	-0.515114403198
C	0.008584326550	0.397829264736	0.386540960326
C	-1.399839745073	-0.300560781004	0.333310386108
Cl	2.656351441802	0.627049622379	-0.263967748862
Cl	1.316817747113	-1.968515692061	-0.201646266929
H	0.831102427815	-0.107924237298	-1.559516451818
Cl	-0.218180107294	2.112706145449	-0.098336868134
F	0.387747390214	0.346529029512	1.676300031190
F	-1.342629297386	-1.471203248852	0.959535832564
F	-2.282167817027	0.457872586874	0.976136433889
Cl	-1.966087499244	-0.557737087044	-1.349124905135

Atom	X	Y	Z
C	1.413725723774	0.156567879316	0.459698730143
C	-0.137861701624	0.229426216182	0.589837108860
C	-0.969443977391	-0.449645888070	-0.552434986895
Cl	2.030905603217	-1.484720741434	0.809825111770
Cl	2.019979661600	0.758596426084	-1.102375685073
H	1.820546877435	0.804768531410	1.232086971093
Cl	-0.596737047619	1.960673932246	0.695548794212
F	-0.460079522899	-0.370792630662	1.751143410875
F	-0.906934023568	0.262261199651	-1.671410249652
F	-0.474719585961	-1.663141678606	-0.795877385141
Cl	-2.685810006965	-0.621965246117	-0.068408820193

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
49.2847	0.0132
70.4991	0.0142
139.0540	0.0505
177.2878	0.0695
206.6608	0.0635
216.6965	0.0242
247.6362	0.0726
290.8134	0.0925
307.2432	0.0992
315.1963	0.191
363.2682	0.167
403.6142	0.328
432.5682	0.619
447.6117	0.664
628.3807	5.62
724.8911	4.81
745.0228	13.4
768.2926	16.5
877.8194	16.7
966.6750	27.5
1041.6092	10.6
1176.5912	2.21
1210.1967	15.0
1213.8590	20.8
1231.5399	15.3
1295.4566	1.55
3174.5600	0.596

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
39.1058	0.00329
79.5977	0.0289
141.8398	0.0125
168.6765	0.0329
194.5146	0.0758
203.8651	0.0600
244.5513	0.0170
297.7213	0.0610
314.1691	0.0765
343.5551	0.0338
360.9478	0.0964
422.8640	0.0512
440.8884	0.358
515.5854	0.668
520.6879	9.49
660.4302	1.19
741.9196	17.0
810.6707	17.3
879.0972	21.9
943.5181	19.8
1103.2491	17.0
1156.2304	9.82
1195.0969	11.1
1213.5629	14.7
1233.7193	7.28
1319.5562	2.95
3149.5748	0.669



$\Delta E = 1.53$ kcal mol^{-1}
Population = 0.033

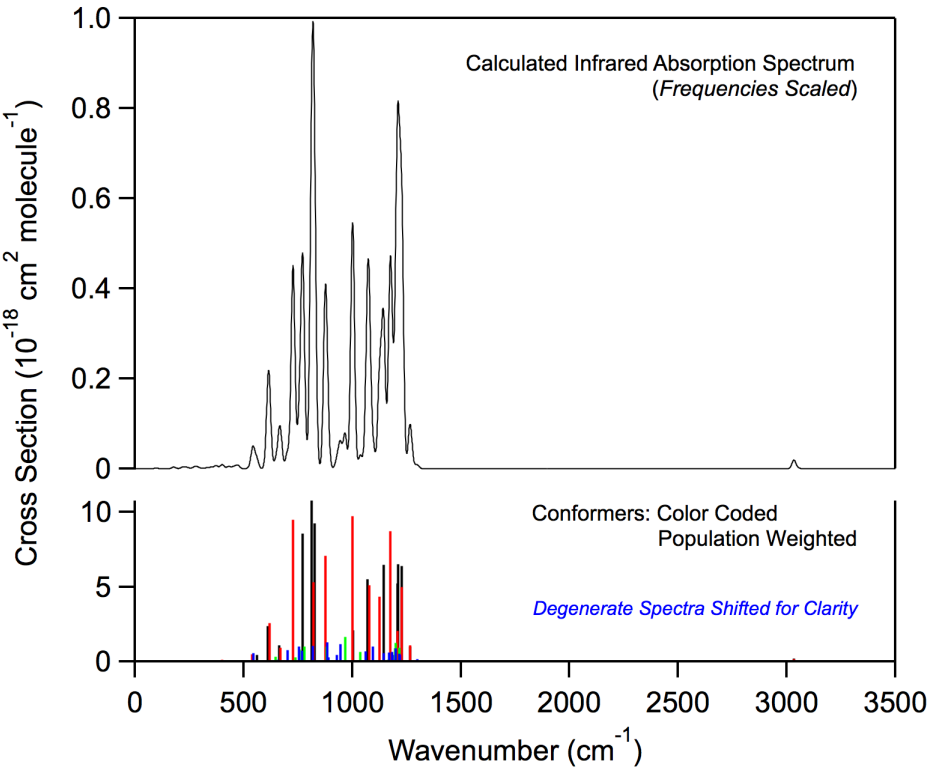
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.301007355760	-0.130432270896	-0.443369534205
C	-0.034451060708	0.329284621336	0.209842019040
C	-1.268678675683	-0.531987542558	-0.239128402891
Cl	2.646904377879	0.918380433557	0.083802888031
Cl	1.700685587806	-1.831453801459	-0.064077850704
H	1.216919714728	-0.048824768886	-1.523450307474
Cl	-0.325213052544	2.024320655953	-0.311301120036
F	0.046512005699	0.264646008900	1.545108745219
F	-1.291153878693	-0.585355958048	-1.573975753291
F	-1.157431883825	-1.769702954037	0.234752179274
Cl	-2.814386490419	0.132157576138	0.364409137037

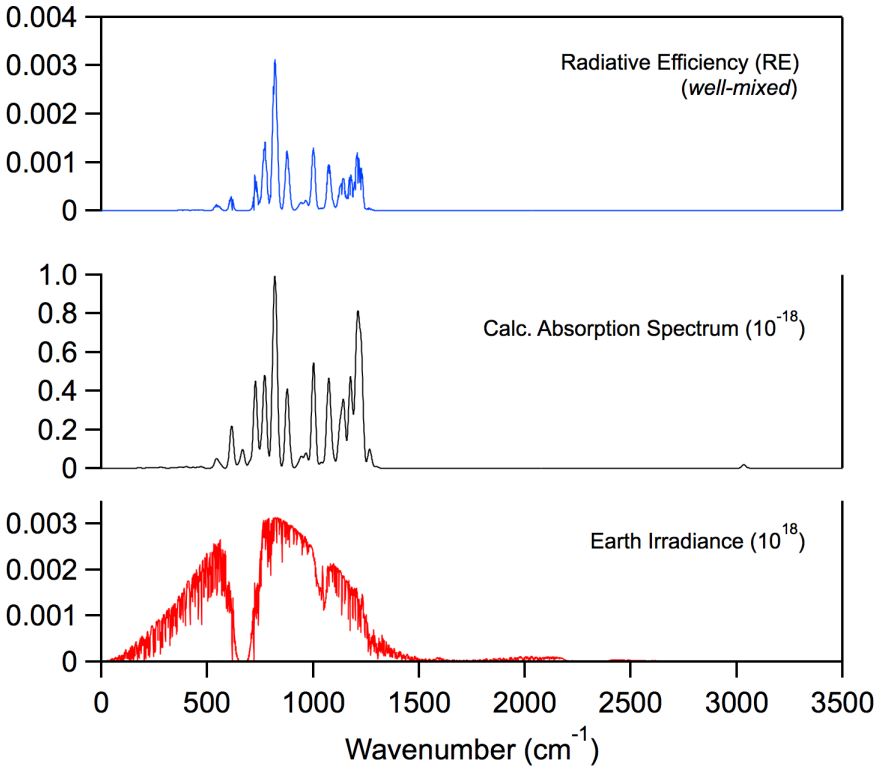
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
32.4434	0.0185
59.1142	0.0300
141.1510	0.0698
193.2654	0.0867
200.7983	0.160
221.8861	0.0533
231.4476	0.0244
253.9786	0.0646
309.7913	0.0556
325.5634	0.194
349.1834	0.185
419.2471	0.339
429.1818	0.00907
495.2115	0.593
638.8448	3.96
686.3356	23.2
744.8919	2.04
755.9115	21.8
886.0845	8.81
927.9575	12.8
1067.7587	20.2
1181.3872	18.1
1197.8559	13.5
1211.4752	3.90
1231.8641	15.7
1300.6842	2.15
3165.9747	0.492

Infrared Spectrum

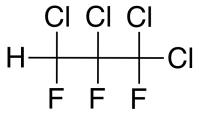


Radiative Efficiency



HCFC-223bb

Molecular Formula:	$CHClFCClFCCl_2F$
Name:	1,1,2,3-Tetrachloro-1,2,3-trifluoropropane
CAS number:	145599-91-3
Molecular Weight:	235.85



Global Atmospheric Lifetime (years):	3.18
Tropospheric Atmospheric Lifetime (years):	3.54
Stratospheric Atmospheric Lifetime (years):	31.4
Ozone Depletion Potential (ODP):	0.059

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.265	0.235
Global Warming Potential (GWP_H):		
GWP_{20}	802	713
GWP_{100}	218	193
Global Temperature Potentials (GTP_H)		
GTP_{20}		312
GTP_{50}		36
GTP_{100}		27

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

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

OH Reactivity

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

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

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

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

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

Fractional Atmospheric Loss: 0.929

$O(^1D)$ Reactivity

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

$k_{Est}(T) = 2.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 185$ years

Fractional Atmospheric Loss: 0.017

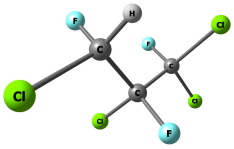
UV Photolysis

UV Spectrum: *No Recommendation*

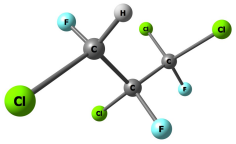
$\tau_{hv} = 59$ years

Fractional Atmospheric Loss: 0.054

Molecular Structure and Infrared Spectrum (6 conformers)



E = 0
Population = 0.514



$\Delta E = 0.85$ kcal mol^{-1}
Population = 0.122

Optimized Coordinates (Angstroms)

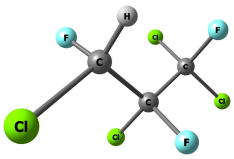
Atom	X	Y	Z
C	-1.344212868434	0.763522497206	-0.167574352381
C	-0.249734340931	-0.249741531115	0.263493981782
C	1.176388979525	0.169283771076	-0.244510531166
Cl	-2.920982970972	0.343911365397	0.560412917598
H	-1.089966184526	1.757392694739	0.201090558513
F	-1.440694718276	0.781828588539	-1.509456424335
Cl	-0.630474809934	-1.867712557137	-0.390759560075
F	-0.212666037541	-0.287442571934	1.605883973099
Cl	1.561580448561	1.831891058522	0.333610465579
Cl	2.419925609286	-0.950948604247	0.366908178510
F	1.196267893241	0.171934288954	-1.574681207124

Atom	X	Y	Z
C	-1.141764651104	0.677880054485	-0.561031175659
C	-0.291653576880	-0.115569620760	0.464396995776
C	1.260653417033	-0.025726182061	0.227145235895
Cl	-2.826657708710	0.836775734874	0.015668075082
H	-0.748557581984	1.691022953429	-0.659439091108
F	-1.128453946594	0.062727621163	-1.756820432985
Cl	-0.771966151944	-1.834909192018	0.487166539654
F	-0.497770292227	0.414844550129	1.687079456187
Cl	1.772919869376	-0.677117290801	-1.344676367726
Cl	1.778611324553	1.693595842135	0.371700272438
F	1.859554298481	-0.712249470576	1.199589492446

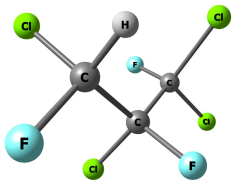
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
45.2718	0.0726
75.1530	0.0376
130.8342	0.0867
181.7622	0.0544
197.7637	0.0936
217.3148	0.0754
235.2808	0.0882
255.3625	0.0755
289.7629	0.0472
343.7046	0.0433
376.0531	0.0686
385.4220	0.204
425.1744	0.389
487.9531	0.320
599.4019	0.474
619.2002	11.5
702.5335	29.7
787.3422	29.2
873.9935	9.32
1020.2510	1.53
1091.9855	5.61
1147.3865	5.70
1182.0863	41.2
1201.4012	1.15
1291.1659	2.06
1361.0651	2.27
3129.0245	0.482

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
46.8525	0.0588
77.0327	0.0362
139.7391	0.0917
166.7352	0.0501
195.7430	0.0639
207.5767	0.0621
247.7062	0.0512
272.2289	0.125
317.0266	0.166
335.2636	0.103
367.8846	0.136
389.4487	0.161
427.7827	0.399
483.2130	1.08
540.3746	0.963
631.0364	8.72
753.1361	31.6
803.4434	23.7
868.4629	17.1
1014.4079	4.15
1082.0271	6.91
1150.9197	22.3
1176.7688	14.4
1179.7147	7.37
1289.6570	2.36
1363.4698	2.27
3117.6963	0.586



$\Delta E = 0.85$ kcal mol^{-1}
Population = 0.122



$\Delta E = 1.06$ kcal mol^{-1}
Population = 0.086

Optimized Coordinates (Angstroms)

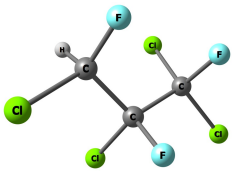
Atom	X	Y	Z
C	-1.385608364971	0.622833148942	0.465758423833
C	-0.268744934356	-0.399726656573	0.111858837385
C	1.160709689107	0.185295065855	0.409810980952
Cl	-2.976687261476	-0.187506791266	0.543402027117
H	-1.191877510428	1.034912032750	1.457373127523
F	-1.427227286718	1.611829801124	-0.443786046322
Cl	-0.411404123705	-0.947216066762	-1.570864833808
F	-0.406467609840	-1.447200821365	0.952175263788
Cl	2.396777424706	-1.090558342594	0.264792222239
Cl	1.579419707045	1.575279157251	-0.615950742154
F	1.134845270636	0.597376472637	1.692573739447

Atom	X	Y	Z
C	-1.467431130268	-0.444084458007	-0.618624390122
C	-0.199391727592	0.431034455428	-0.410012521455
C	1.004489595836	-0.274812188570	0.300295559613
Cl	-2.164701463423	-1.077905125520	0.895068543177
F	-2.379044785406	0.316309793609	-1.254638212862
H	-1.209771990926	-1.300641493472	-1.242018191905
Cl	-0.622346428324	1.915154822125	0.487089196033
F	0.206218195884	0.763954473811	-1.655369835495
Cl	1.326687900595	-1.860473253999	-0.489856870725
Cl	2.468368246772	0.738717449410	0.182319828558
F	0.729279586852	-0.489507474815	1.582627895185

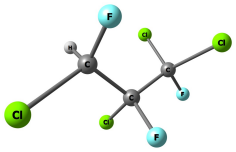
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
47.9362	0.0695
75.3914	0.0343
133.9402	0.0780
171.4147	0.0174
192.9285	0.104
217.1677	0.139
224.7640	0.126
273.0687	0.00751
314.3024	0.227
348.7410	0.0319
380.3462	0.0431
391.3364	0.0384
424.8112	0.618
497.0333	0.630
542.6258	0.874
628.8656	12.8
715.0509	25.3
863.1677	3.17
876.0288	34.8
1015.7539	14.5
1082.6332	5.18
1115.0154	6.84
1157.5629	30.9
1171.0697	2.91
1292.2174	2.61
1362.0502	2.57
3118.4327	0.413

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
51.1873	0.0401
83.1205	0.0371
136.4029	0.0691
180.1242	0.163
192.3046	0.0625
205.7040	0.0489
249.8822	0.0541
289.5713	0.0243
300.6112	0.252
322.4501	0.101
379.6291	0.0428
387.0933	0.203
420.1507	0.802
462.7881	0.519
565.6817	1.28
629.0656	9.17
765.6920	27.5
809.4960	36.5
830.5269	6.97
1025.1985	2.19
1099.0206	7.71
1144.7892	11.5
1156.2190	25.7
1197.4141	9.17
1278.5338	4.33
1366.8588	2.32
3127.2646	0.598



$\Delta E = 1.29$ kcal mol^{-1}
Population = 0.058



$\Delta E = 1.51$ kcal mol^{-1}
Population = 0.040

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.398868666159	-0.648924376122	0.258648358380
C	-0.265482456418	0.295276079798	-0.232385384080
C	1.151845089996	-0.387853238074	-0.190918093020
Cl	-3.000022513849	0.057339521169	-0.110151968673
F	-1.294906101309	-1.839895177608	-0.367111094976
H	-1.341762076243	-0.787244194706	1.337409623921
Cl	-0.286636818556	1.766249177759	0.779318724235
F	-0.475958255141	0.618108899055	-1.520959336612
Cl	2.421541949087	0.756387087604	-0.703266852277
Cl	1.511638490530	-1.034878764516	1.438612555910
F	1.144253358061	-1.400302014358	-1.060423532810

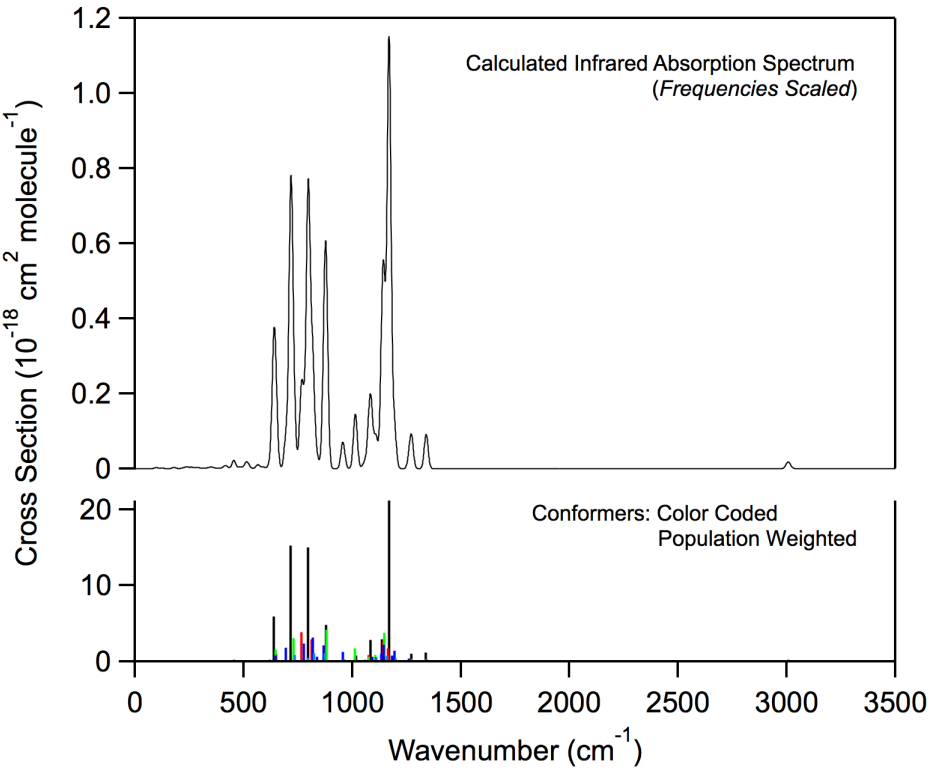
Atom	X	Y	Z
C	-1.173160664041	-0.514546260910	0.655203446415
C	-0.305814000557	0.230271132430	-0.392709285624
C	1.248639946255	0.080099182631	-0.183242798146
Cl	-2.883911330405	-0.542438170344	0.136821036969
F	-0.737974505959	-1.785097393995	0.790724842778
H	-1.129476435862	-0.003859119837	1.615918651870
Cl	-0.713943892632	1.976239541705	-0.304246844042
F	-0.573969937145	-0.217881676253	-1.630595245892
Cl	1.700830426550	0.411515791164	1.517629643358
Cl	1.806447150473	-1.544372359712	-0.667266058789
F	1.864651243323	0.964982333120	-0.968539388897

Infrared Absorption Spectrum (unscaled frequencies)

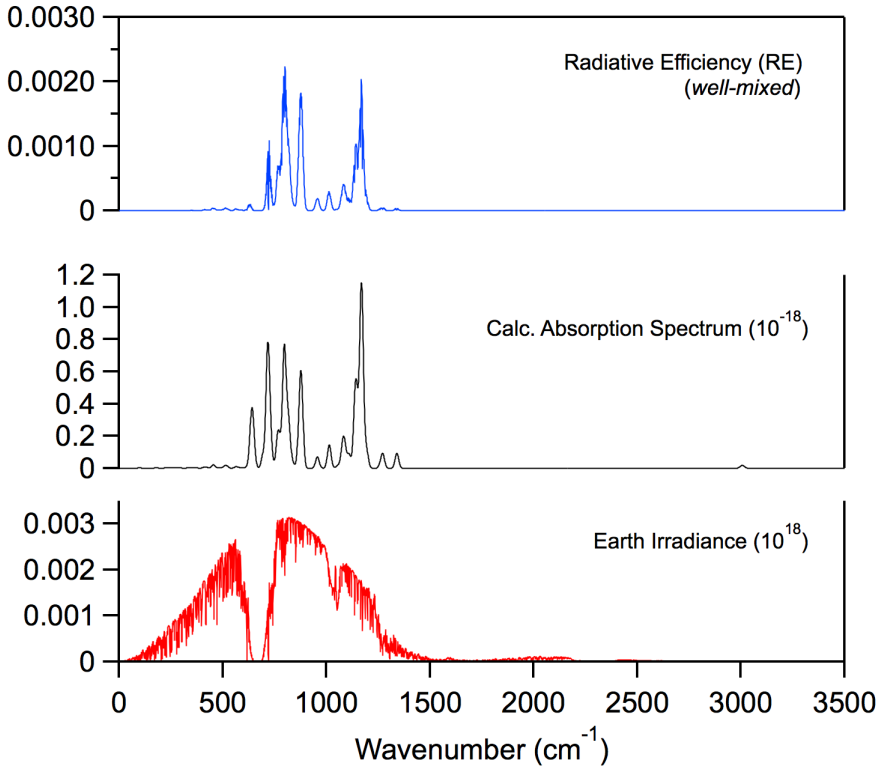
Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
49.9397	0.0524
70.5578	0.0221
133.1054	0.0491
177.1656	0.0265
193.2433	0.102
219.1750	0.0131
242.8634	0.0787
281.8617	0.0338
310.5898	0.213
322.8788	0.138
380.1009	0.0908
386.4813	0.0824
425.8214	0.915
451.4703	0.677
497.2019	0.822
679.1426	30.8
776.2650	3.26
862.2008	36.5
883.7081	3.07
954.8679	22.1
1064.4508	4.76
1118.7026	9.26
1155.1623	7.70
1206.8709	24.6
1284.1205	2.19
1369.9741	0.753
3140.6826	0.578

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
51.0002	0.0651
68.6710	0.0244
139.2166	0.0273
173.7553	0.0837
199.1438	0.0627
217.7161	0.0269
241.8404	0.0530
287.3460	0.0307
313.1695	0.436
333.0714	0.0959
345.3577	0.197
394.3313	0.0625
425.3842	0.693
455.1693	0.796
484.3099	1.16
721.3178	22.1
785.6296	11.2
814.9519	27.0
868.4775	27.7
962.8295	7.80
1055.9724	2.74
1120.8592	12.5
1171.3667	18.3
1212.6074	10.7
1285.3301	2.16
1374.3429	0.650
3142.4303	0.550

Infrared Spectrum

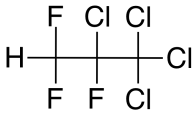


Radiative Efficiency



HCFC-223bc

Molecular Formula:	$CHF_2CClFCCl_3$
Name:	1,1,1,2-Tetrachloro-2,3,3-trifluoropropane
CAS number:	147728-32-3
Molecular Weight:	235.85



Global Atmospheric Lifetime (years):	10.6
Tropospheric Atmospheric Lifetime (years):	15.1
Stratospheric Atmospheric Lifetime (years):	35.7
Ozone Depletion Potential (ODP):	0.185

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.260	0.249
Global Warming Potential (GWP_H):		
GWP_{20}	2233	2135
GWP_{100}	713	682
Global Temperature Potentials (GTP_H)		
GTP_{20}		1638
GTP_{50}		282
GTP_{100}		99

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

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

OH Reactivity

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

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

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

Fractional Atmospheric Loss: 0.730

O(^{1}D) Reactivity

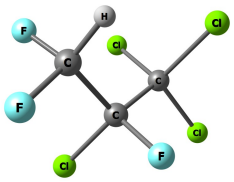
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 2.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)}$ = 185 years
Fractional Atmospheric Loss: 0.057

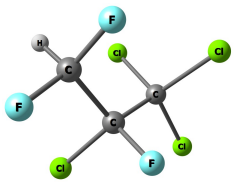
UV Photolysis

UV Spectrum: *No Recommendation*
τ_{hv} = 50 years
Fractional Atmospheric Loss: 0.212

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.777



$\Delta E = 1.02$ kcal mol^{-1}
Population = 0.139

Optimized Coordinates (Angstroms)

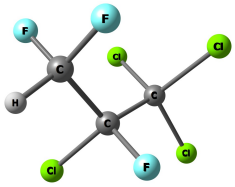
Atom	X	Y	Z
C	1.628922653125	0.875741634966	-0.223494993029
C	0.583811366868	-0.268661681927	-0.375482234685
C	-0.888121307138	0.109339910216	0.024648300577
F	1.817524912455	1.190109092173	1.067695612962
F	2.789534399603	0.430095377254	-0.735394127269
H	1.308651086123	1.763052328553	-0.777796315849
Cl	1.144230283515	-1.690525816221	0.546798318747
F	0.563735786841	-0.576340299987	-1.690638597807
Cl	-1.976190029055	-1.243382220025	-0.387517122163
Cl	-1.032670521260	0.500627359946	1.750432295479
Cl	-1.377752631078	1.543764315052	-0.951090136964

Atom	Z	Z	Z
C	1.712985934717	0.564279706626	0.450694621042
C	0.616468157005	-0.251217633670	-0.301249839696
C	-0.871602349424	0.122412457264	0.042873603740
F	2.906885857100	0.150134131099	-0.009228460127
F	1.595770030446	1.874273717585	0.168434584135
H	1.655192564918	0.410320992099	1.531161719753
Cl	0.923971907346	-1.976202123993	0.095515967127
F	0.786939030803	-0.066709807349	-1.621695378021
Cl	-1.983658456487	-0.991755777609	-0.799833461039
Cl	-1.130977963643	0.022987657194	1.810567376349
Cl	-1.227122712782	1.781260680755	-0.517326733263

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
47.3766	0.118
86.9209	0.0672
148.4151	0.0701
170.7770	0.0120
200.2633	0.146
208.8721	0.0599
236.4239	0.0588
257.2904	0.0638
282.4000	0.153
317.8081	0.197
335.1560	0.0542
381.3306	0.261
411.7556	0.0463
517.2958	1.64
580.6621	2.67
660.1187	15.5
735.5286	15.7
770.3543	14.5
836.7587	17.6
1024.4448	5.97
1084.5318	1.29
1153.1540	8.41
1173.1678	29.9
1188.7530	11.4
1383.0404	5.59
1396.5140	1.90
3093.2149	2.22

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
37.2734	0.0854
80.8366	0.0498
153.2299	0.0418
170.7203	0.0203
201.7563	0.0955
221.8968	0.0471
244.4194	0.0616
262.2753	0.102
280.7762	0.0878
301.4476	0.0387
343.7416	0.397
369.5356	0.258
408.5648	0.00247
445.9120	1.51
569.3987	3.30
735.6324	16.8
765.6894	27.6
793.1205	9.49
850.6456	12.2
942.0160	9.72
1067.4753	3.14
1152.0794	9.38
1161.1633	15.5
1219.6828	21.2
1394.4285	3.81
1397.1901	1.39
3105.6007	2.22



$\Delta E = 1.32$ kcal mol^{-1}
Population = 0.084

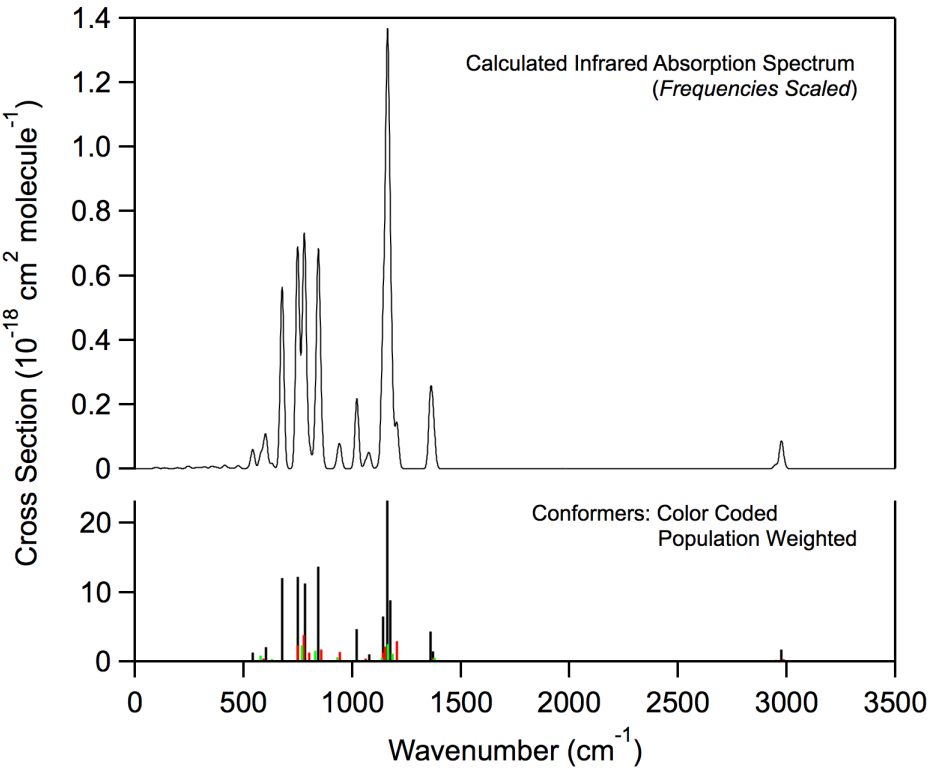
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.901027544186	0.336891891665	-0.183500632547
C	0.552825506762	-0.377720343012	-0.510561839266
C	-0.773222478440	0.180852366271	0.121390558529
F	1.880300447934	1.610262981593	-0.613071541964
F	2.160626424043	0.328741648920	1.132274932213
H	2.688291484472	-0.206617182434	-0.719309390289
Cl	0.786842170014	-2.097951483037	-0.051331335184
F	0.421242974233	-0.303453847551	-1.851856921362
Cl	-2.151291171853	-0.794443142831	-0.479658599494
Cl	-0.726344178517	0.119601173924	1.898431011581
Cl	-1.020811722833	1.871006936491	-0.412030242217

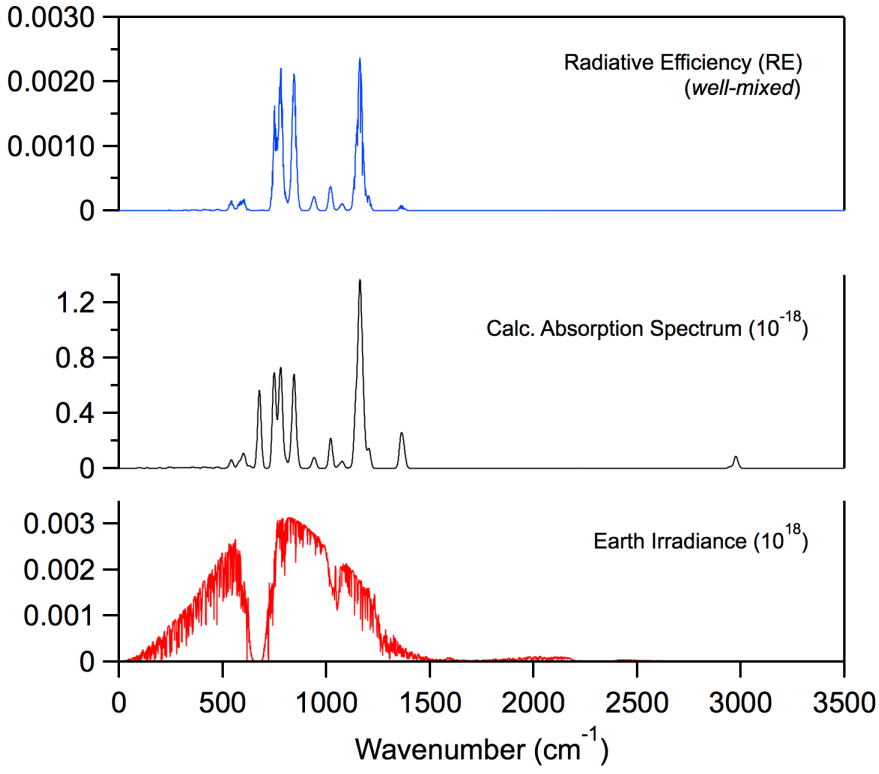
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
31.2542	0.0449
102.6869	0.120
160.2635	0.0464
171.2476	0.00961
202.5874	0.122
207.5492	0.0508
228.9301	0.0432
265.1129	0.0228
292.3467	0.0839
315.3821	0.148
331.7698	0.0935
394.0391	0.313
413.0397	0.212
501.1104	1.07
555.8797	10.2
610.0287	4.19
755.7970	28.2
821.0032	18.8
854.7349	2.24
931.2757	6.89
1125.6262	1.39
1146.1079	5.80
1176.5862	29.7
1199.8461	13.4
1393.9140	2.65
1403.9274	5.74
3065.6556	3.16

Infrared Spectrum

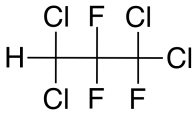


Radiative Efficiency



HCFC-223ca

Molecular Formula:	$CHCl_2CF_2CCl_2F$
Name:	1,1,3,3-Tetrachloro-1,2,2-trifluoropropane
CAS number:	422-52-6
Molecular Weight:	235.85



Global Atmospheric Lifetime (years):	1.38
Tropospheric Atmospheric Lifetime (years):	1.47
Stratospheric Atmospheric Lifetime (years):	21.6
Ozone Depletion Potential (ODP):	0.029

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.295	0.234
Global Warming Potential (GWP_H):		
GWP_{20}	388	308
GWP_{100}	105	83
Global Temperature Potentials (GTP_H)		
GTP_{20}		105
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*

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

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

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

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

Fractional Atmospheric Loss: 0.965

O(^{1}D) Reactivity

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

$k_{Est}(T) = 2.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 185$ years

Fractional Atmospheric Loss: 0.007

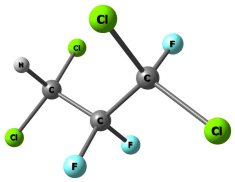
UV Photolysis

UV Spectrum: *No Recommendation*

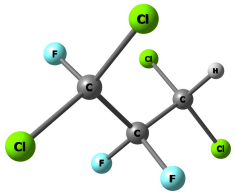
$\tau_{hv} = 50$ years

Fractional Atmospheric Loss: 0.028

Molecular Structure and Infrared Spectrum (2 conformers)



E = 0
Population = 0.500



E = 0
Population = 0.500

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.359468818486	-0.184942348620	0.408494227416
C	0.107623986487	0.559905019216	-0.123690683098
C	-1.232902692224	-0.257289791041	-0.107458029934
Cl	1.763697314298	-1.614250017433	-0.572300614694
Cl	2.727692901861	0.963064325298	0.459765460939
H	1.182348878421	-0.519453310092	1.426348299651
F	0.311350601109	0.957077299706	-1.387268617765
F	-0.077575431120	1.641527391537	0.653047734606
Cl	-1.542346146214	-0.916164093677	1.530077867210
Cl	-2.571171973878	0.818335393233	-0.597473133259
F	-1.163467257224	-1.264237868128	-0.975062511073

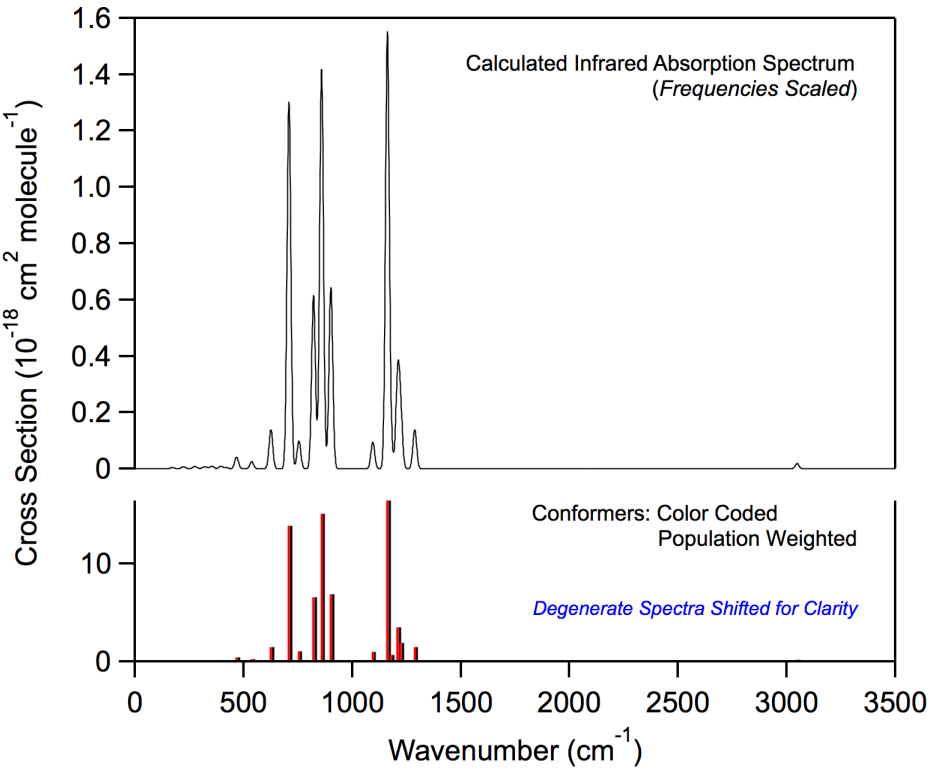
Atom	X	Y	Z
C	1.361112708764	0.203174723168	0.404893550057
C	0.111449005787	-0.574363321401	-0.083890349387
C	-1.231016733959	0.239175016289	-0.116071692096
Cl	2.732000211754	-0.936620266260	0.523725469753
Cl	1.762742370971	1.573996206759	-0.657096329645
H	1.182401885184	0.595882453269	1.401457170657
F	-0.071805723459	-1.609432738010	0.754307905440
F	0.317109269347	-1.043848209026	-1.322101028228
Cl	-2.566367680332	-0.866323204458	-0.543574636915
Cl	-1.543295845531	0.991414553814	1.480178743471
F	-1.163272468526	1.194135785856	-1.040714803107

Infrared Absorption Spectrum (unscaled frequencies)

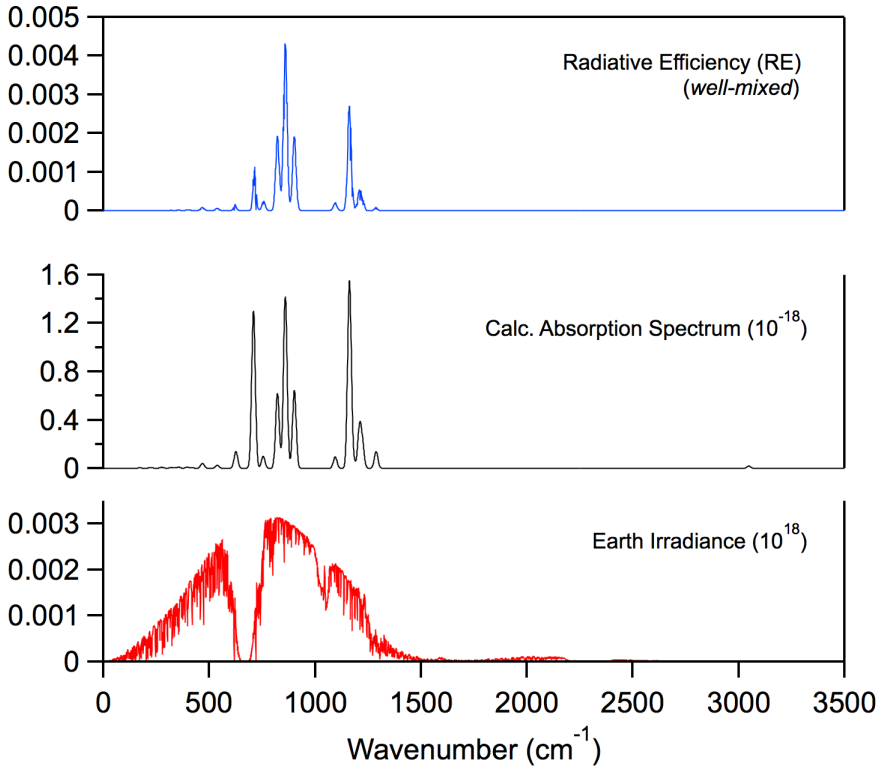
Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
31.4825	0.0217
75.2482	0.0203
125.2681	0.0902
177.9804	0.135
188.5579	0.0248
232.6175	0.139
242.3635	0.0484
280.7790	0.132
292.5799	0.0557
318.3335	0.197
361.7976	0.200
387.5456	0.0977
438.1400	0.879
512.2137	0.526
605.5912	2.96
693.5385	27.8
742.1287	2.10
813.2819	13.1
852.4881	30.2
897.9388	13.7
1102.1711	2.01
1173.2778	32.9
1191.5494	1.37
1223.8300	6.97
1238.5133	3.83
1306.6897	2.94
3170.3978	0.389

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
31.4812	0.0217
75.2472	0.0203
125.2681	0.0902
177.9797	0.135
188.5573	0.0248
232.6171	0.139
242.3619	0.0484
280.7787	0.132
292.5791	0.0557
318.3323	0.197
361.7972	0.200
387.5458	0.0977
438.1395	0.880
512.2137	0.526
605.5911	2.96
693.5382	27.8
742.1290	2.10
813.2814	13.1
852.4879	30.2
897.9369	13.7
1102.1682	2.01
1173.2775	32.9
1191.5471	1.37
1223.8310	6.97
1238.5132	3.83
1306.6905	2.94
3170.3979	0.389

Infrared Spectrum

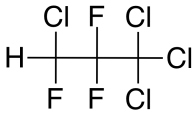


Radiative Efficiency



HCFC-223cb

Molecular Formula:	$CHClFCF_2CCl_3$
Name:	1,1,1,3-Tetrachloro-2,2,3-trifluoropropane
CAS number:	422-50-4
Molecular Weight:	235.85



Global Atmospheric Lifetime (years):	3.88
Tropospheric Atmospheric Lifetime (years):	4.45
Stratospheric Atmospheric Lifetime (years):	30.2
Ozone Depletion Potential (ODP):	0.073

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.263	0.238
Global Warming Potential (GWP_H):		
GWP_{20}	969	877
GWP_{100}	264	239
Global Temperature Potentials (GTP_H)		
GTP_{20}		422
GTP_{50}		46
GTP_{100}		33

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

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

OH Reactivity

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

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

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

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

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

Fractional Atmospheric Loss: 0.901

$O(^1D)$ Reactivity

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

$k_{Est}(T) = 2.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 185$ years

Fractional Atmospheric Loss: 0.021

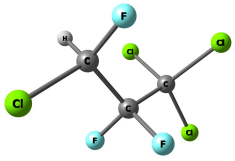
UV Photolysis

UV Spectrum: *No Recommendation*

$\tau_{hv} = 50$ years

Fractional Atmospheric Loss: 0.078

Molecular Structure and Infrared Spectrum (1 conformer)



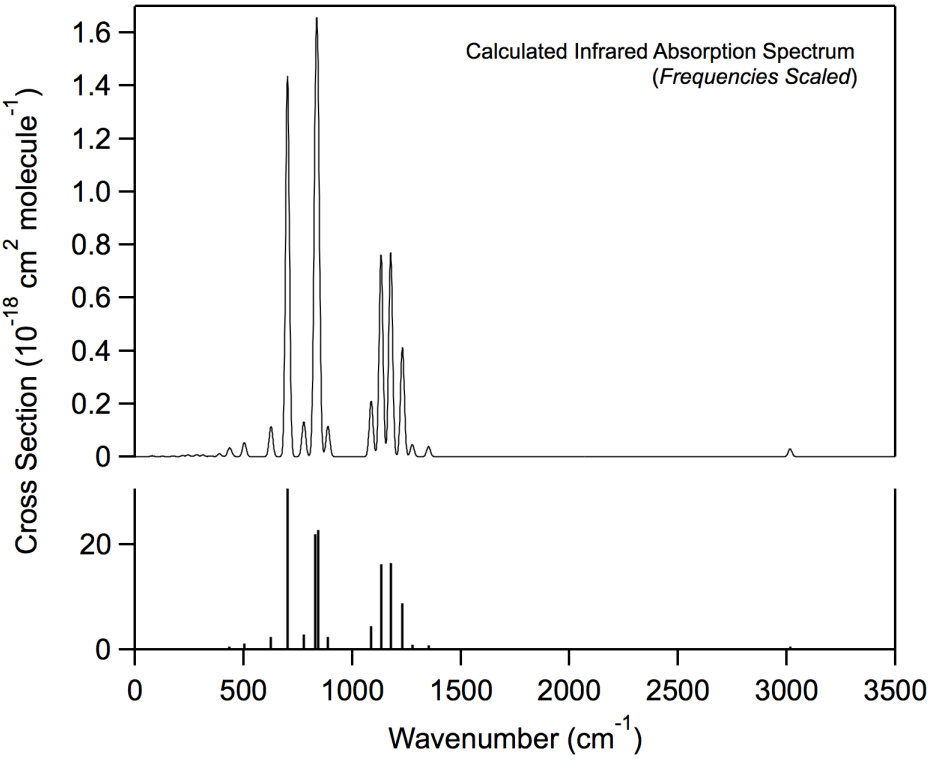
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.525843485180	0.431032696716	0.424307217653
C	0.413261706164	-0.451240529500	-0.198575168154
C	-1.063096360729	0.038565853838	0.048701242412
Cl	3.113418602529	-0.347183450584	0.139622952026
F	1.521719788356	1.652135788495	-0.141933209484
H	1.397653967077	0.513471465249	1.503103522754
F	0.518662894772	-1.677039349999	0.343144294114
F	0.599604291915	-0.538615079338	-1.522109515989
Cl	-2.165787362731	-1.203603142813	-0.608059263829
Cl	-1.336788161119	0.204535795151	1.811812809655
Cl	-1.372158851413	1.588109952785	-0.764999881158

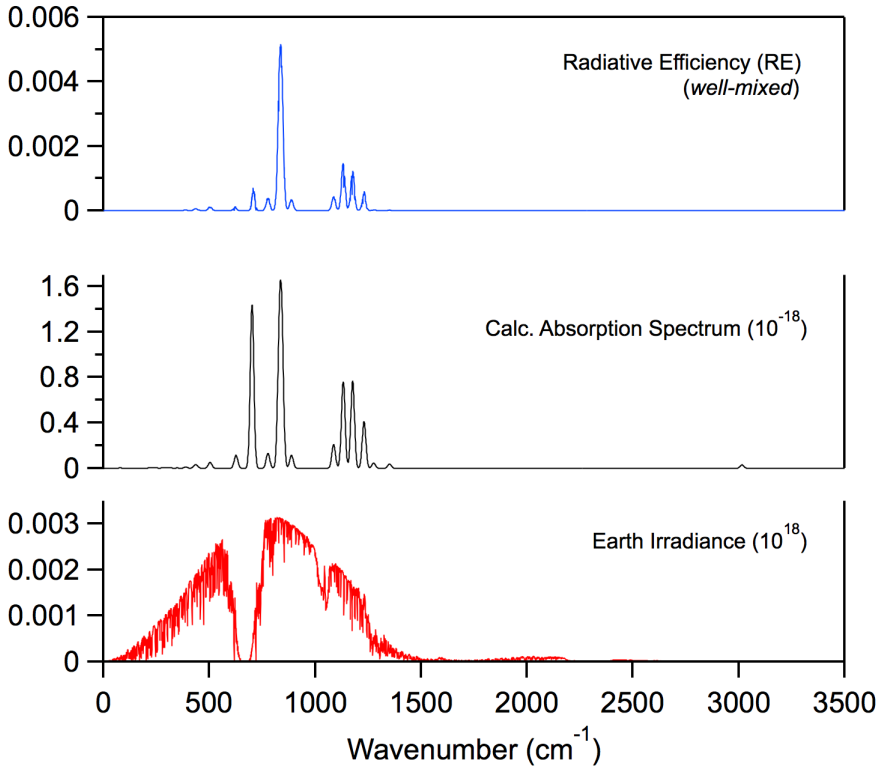
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
26.2603	0.0733
77.3086	0.0379
129.0812	0.0560
174.7479	0.0868
201.9072	0.133
215.9957	0.0104
243.2045	0.150
266.3954	0.0234
275.4448	0.115
312.1331	0.0696
354.8944	0.242
402.3487	0.588
412.7441	0.200
476.3008	1.13
606.0815	2.43
686.4113	30.6
765.9114	2.82
822.8910	21.9
835.2367	22.8
883.5102	2.45
1094.3619	4.46
1142.4323	16.2
1189.4144	16.4
1246.5297	8.78
1294.5567	0.980
1373.7291	0.821
3136.4497	0.632

Infrared Spectrum

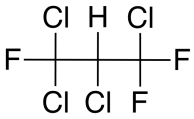


Radiative Efficiency



HCFC-223da

Molecular Formula:	$CCl_2FCHClCClF_2$
Name:	1,1,2,3-Tetrachloro-1,3,3-trifluoropropane
CAS number:	431-83-4
Molecular Weight:	235.85



Global Atmospheric Lifetime (years):	6.48
Tropospheric Atmospheric Lifetime (years):	7.86
Stratospheric Atmospheric Lifetime (years):	37.1
Ozone Depletion Potential (ODP):	0.111

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.334	0.313
Global Warming Potential (GWP_H):		
GWP_{20}	1975	1849
GWP_{100}	561	525
Global Temperature Potentials (GTP_H)		
GTP_{20}		1157
GTP_{50}		130
GTP_{100}		74

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 7.46 \times 10^{-15}$; $k_{SAR}(272\ K) \approx 4.76 \times 10^{-15}$ cm^3 $molecule^{-1}$ s^{-1}

τ^{OH}_{Global} = 7.58 years
τ^{OH}_{Trop} = 7.86 years
τ^{OH}_{Strat} = 216.1 years

Fractional Atmospheric Loss: 0.855

$O(^1D)$ Reactivity

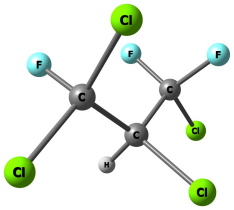
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 2.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)}$ = 185 years
Fractional Atmospheric Loss: 0.035

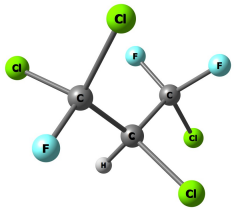
UV Photolysis

UV Spectrum: *No Recommendation*
τ_{hv} = 59 years
Fractional Atmospheric Loss: 0.110

Molecular Structure and Infrared Spectrum (6 conformers)



E = 0
Population = 0.338



$\Delta E = 0.1$ kcal mol^{-1}
Population = 0.285

Optimized Coordinates (Angstroms)

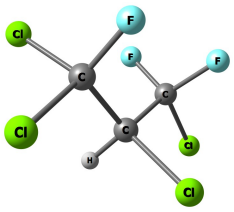
Atom	X	Y	Z
C	-1.205291359359	-0.319961179286	0.335107136252
C	0.162203642510	0.422070494904	0.362163733986
C	1.387857827836	-0.486347901550	0.063813662655
Cl	-2.511977481206	0.812297582442	0.823477694017
Cl	-1.589904604226	-1.043547947475	-1.249098555601
F	-1.169807547410	-1.297474683461	1.251282908352
H	0.274711089652	0.795423298108	1.380649452877
Cl	0.176512048061	1.818907023971	-0.738233161200
F	1.312869115270	-1.614380496316	0.773199839919
F	1.469147820415	-0.807552134553	-1.222332489480
Cl	2.906662448458	0.359629943216	0.541218778224

Atom	X	Y	Z
C	-1.304492439747	0.087910451936	0.310941485791
C	0.214306598928	0.304624501832	0.571731382377
C	1.188992447230	-0.525884079875	-0.304354609295
Cl	-1.764296569378	0.254643071668	-1.404715864147
Cl	-1.809929365631	-1.521666789009	0.934773526386
F	-1.978559018467	1.002705902389	1.016874153242
H	0.383950529909	0.036403700515	1.614146343190
Cl	0.609236832238	2.039592657624	0.403019357182
F	0.786052106295	-1.795448870485	-0.384449465130
F	1.279500829046	-0.043150218764	-1.538560084995
Cl	2.833058049577	-0.515088327831	0.434569775399

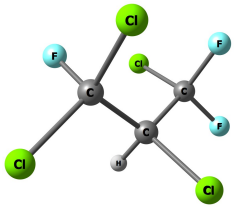
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
33.7884	0.000
73.6851	0.0104
144.7583	0.100
177.0522	0.0560
192.6190	0.0205
211.3282	0.0462
240.0329	0.0622
268.8421	0.0370
321.2534	0.0416
376.7010	0.0805
384.0559	0.0151
419.4530	0.0640
429.0923	0.383
494.7616	0.553
602.6425	3.50
614.0553	16.3
727.4020	24.7
850.6093	8.80
893.0339	6.25
947.0452	20.1
1050.9633	30.0
1126.5953	3.23
1175.0151	30.9
1222.9345	23.3
1257.0876	8.48
1329.5626	3.42
3123.5805	0.587

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
39.4453	0.001
73.6391	0.00511
146.9114	0.152
167.6290	0.0316
196.1626	0.00490
215.5705	0.0507
246.1456	0.0991
278.2648	0.111
326.2644	0.0868
346.2160	0.143
388.5812	0.0846
419.4156	0.0412
429.7521	0.171
476.8034	1.64
600.1170	5.52
641.7964	8.51
765.6725	28.2
834.4689	18.4
849.7514	8.40
939.3623	14.8
1052.4243	27.6
1147.1666	10.8
1173.9977	23.9
1230.2123	18.7
1257.7645	6.95
1329.4645	4.29
3132.6825	0.666



$\Delta E = 0.61$ kcal mol^{-1}
Population = 0.120



$\Delta E = 0.61$ kcal mol^{-1}
Population = 0.120

Optimized Coordinates (Angstroms)

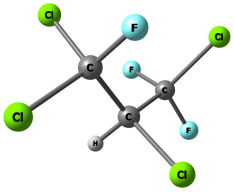
Atom	X	Y	Z
C	-1.236662670220	-0.133508312590	-0.137803966769
C	0.147055540025	0.347006007946	0.387867515711
C	1.349134704976	-0.476346164842	-0.162482008908
Cl	-1.641866455189	-1.758110315294	0.518026149238
Cl	-2.539849937303	0.989053891741	0.371637091221
F	-1.225838311679	-0.200536379806	-1.470677993019
H	0.144179631766	0.280844115155	1.474091818367
Cl	0.411454066792	2.058292919430	-0.064298093887
F	1.178350049650	-1.781958974032	0.049158158587
F	1.499881123128	-0.286828581062	-1.469317677989
Cl	2.868677258053	0.005721793354	0.677973007447

Atom	X	Y	Z
C	-0.997489017220	-0.528659979516	0.113082913313
C	0.097826507349	0.506119678837	0.494791476193
C	1.534838411017	0.219663532475	-0.022687423005
Cl	-2.498356180936	-0.153237450934	1.031110790241
Cl	-1.358967619079	-0.580377308498	-1.632575363987
F	-0.598052889019	-1.749131805548	0.492431572966
H	0.149674682861	0.518230148928	1.583845635327
Cl	-0.374740800858	2.147673257880	-0.031345241721
F	1.574121171963	0.065876839187	-1.342174699531
F	2.314950347914	1.252818928539	0.302434550527
Cl	2.249966386010	-1.239448841349	0.754473789676

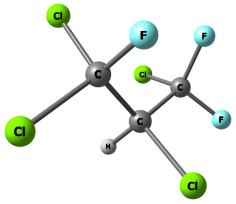
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
24.4442	0.00322
68.8029	0.00611
153.6767	0.0680
180.9816	0.0567
212.5119	0.0990
225.6709	0.0818
241.1688	0.133
255.2897	0.0274
321.0117	0.0246
339.8651	0.0631
377.4797	0.167
418.8636	0.136
428.2612	0.164
459.0082	0.788
603.0351	4.72
674.5391	24.8
778.6479	30.5
814.5665	1.76
880.9078	2.18
952.8991	18.4
967.2849	14.1
1166.0850	21.4
1173.9093	13.3
1217.9732	27.2
1260.1329	11.0
1323.8839	5.43
3151.3768	0.616

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
19.7246	0.00312
81.6586	0.00928
153.6480	0.0658
173.3547	0.0560
178.2275	0.0588
236.3931	0.0732
245.1413	0.128
273.7903	0.135
308.0070	0.0747
367.7574	0.189
381.5452	0.0570
397.9596	0.310
425.3268	0.178
498.1274	0.209
591.3990	5.34
653.7062	10.8
756.4580	26.3
821.8977	15.4
851.0669	13.4
955.3676	13.5
1054.5081	16.9
1142.5865	14.9
1175.5586	26.3
1218.4727	19.3
1250.6881	8.91
1333.8013	3.99
3126.7120	0.608



$\Delta E = 0.71$ kcal mol^{-1}
Population = 0.101



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

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.103030612015	-0.173632753087	-0.241533364371
C	0.073499626357	0.437129541628	0.564206138254
C	1.454968812530	-0.273411353796	0.479278170834
Cl	-1.292336872541	-1.927625244584	0.079672862615
Cl	-2.630688163637	0.649924813978	0.236433747507
F	-0.929158732747	-0.002458113591	-1.550694272890
H	-0.198958024251	0.413709950746	1.620367757912
Cl	0.273926873366	2.151333214475	0.095105950142
F	2.346019342393	0.471074927253	1.138501532975
F	1.390781799954	-1.453084204643	1.103994212623
Cl	2.052955950590	-0.533562778379	-1.185755735601

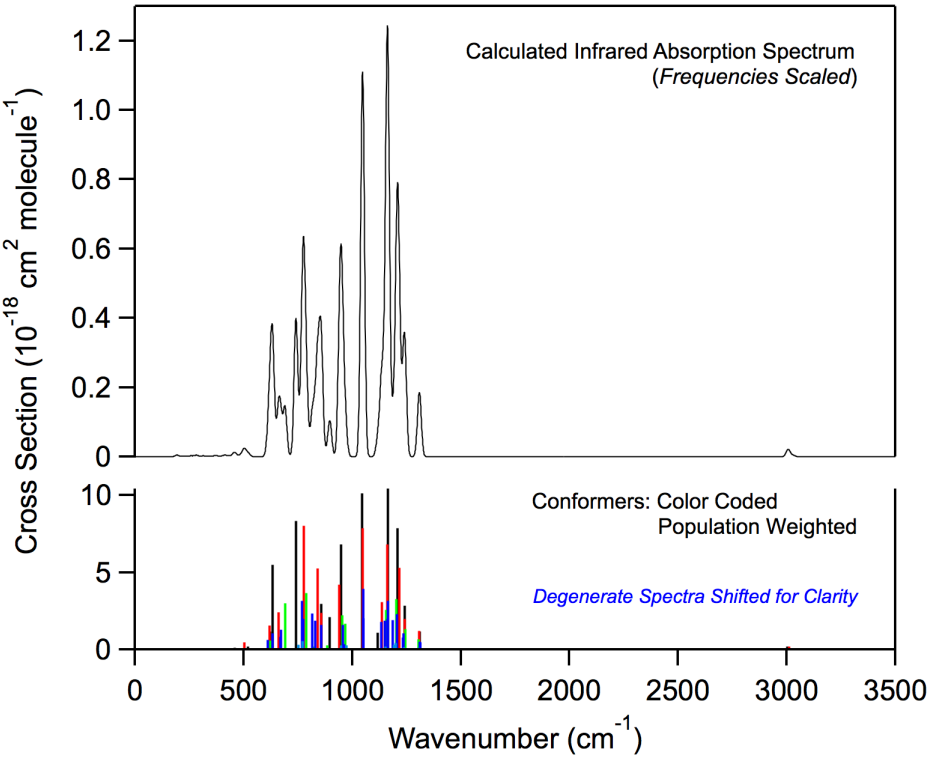
Atom	X	Y	Z
C	-1.071688811817	-0.235422107041	-0.271325730530
C	0.055170121709	0.519233130735	0.487444760529
C	1.504341664266	0.225247409825	-0.024597354162
Cl	-0.792327090368	-2.005377645852	-0.311711741340
Cl	-2.645150089701	0.061782121520	0.546946747053
F	-1.158282974573	0.200573578453	-1.527925398728
H	-0.000819009936	0.265198246150	1.543038808015
Cl	-0.266300367710	2.280174605057	0.343907422936
F	1.510600821710	-0.038395260487	-1.330086583739
F	2.299839133110	1.268919986609	0.191187526815
Cl	2.232866603310	-1.166878064968	0.862649543151

Infrared Absorption Spectrum (unscaled frequencies)

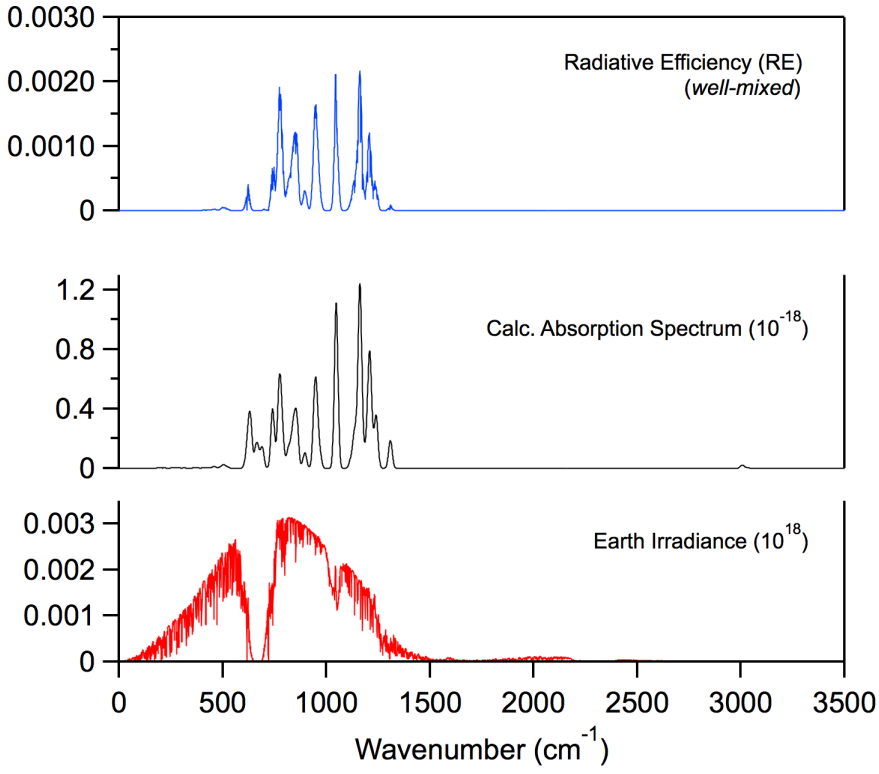
Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
39.3523	0.00116
75.8778	0.00691
148.6461	0.0723
180.4263	0.0360
203.5844	0.0642
222.5034	0.0662
237.6521	0.111
293.7180	0.0772
309.8476	0.0418
334.9043	0.115
382.6450	0.102
425.6285	0.00480
436.3119	0.372
466.0086	0.510
612.6895	10.3
652.4201	8.01
762.1764	19.5
806.8491	23.2
847.0946	0.630
961.8882	3.53
1054.7491	39.0
1161.0755	18.6
1173.0644	19.6
1197.8039	18.7
1247.9333	7.80
1330.1203	5.19
3121.0839	0.494

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
45.4066	0.00893
62.3353	0.00314
145.4786	0.0384
179.9231	0.0599
211.3614	0.128
222.2202	0.0621
246.5942	0.0339
296.2263	0.244
305.7078	0.0773
328.6972	0.0730
383.5944	0.0888
408.3404	0.486
424.1000	0.158
466.6769	0.281
589.1021	5.01
738.4875	18.3
760.3983	33.9
796.0243	4.14
850.6818	3.30
947.1885	17.5
972.5854	17.0
1165.0716	11.2
1204.0391	18.5
1212.8764	25.9
1253.9459	9.02
1326.2449	6.38
3160.3131	0.616

Infrared Spectrum

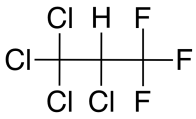


Radiative Efficiency



HCFC-223db

Molecular Formula:	$CCl_3CHClCF_3$
Name:	1,1,1,2-Tetrachloro-3,3,3-trifluoropropane
CAS number:	431-81-2
Molecular Weight:	235.85



Global Atmospheric Lifetime (years):	6.47
Tropospheric Atmospheric Lifetime (years):	8.02
Stratospheric Atmospheric Lifetime (years):	33.4
Ozone Depletion Potential (ODP):	0.117

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.245	0.229
Global Warming Potential (GWP_H):		
GWP_{20}	1443	1351
GWP_{100}	409	383
Global Temperature Potentials (GTP_H)		
GTP_{20}		844
GTP_{50}		94
GTP_{100}		54

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 7.31 \times 10^{-15}$; $k_{SAR}(272\ K) \approx 4.66 \times 10^{-15}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 7.74$ years

$\tau^{OH}_{Trop} = 8.02$ years

$\tau^{OH}_{Strat} = 220.2$ years

Fractional Atmospheric Loss: 0.836

O(^{1}D) Reactivity

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

$k_{Est}(T) = 2.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 185$ years

Fractional Atmospheric Loss: 0.035

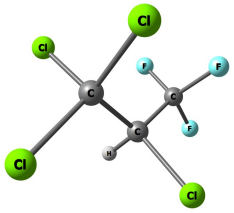
UV Photolysis

UV Spectrum: *No Recommendation*

$\tau_{hv} = 50$ years

Fractional Atmospheric Loss: 0.129

Molecular Structure and Infrared Spectrum (1 conformer)



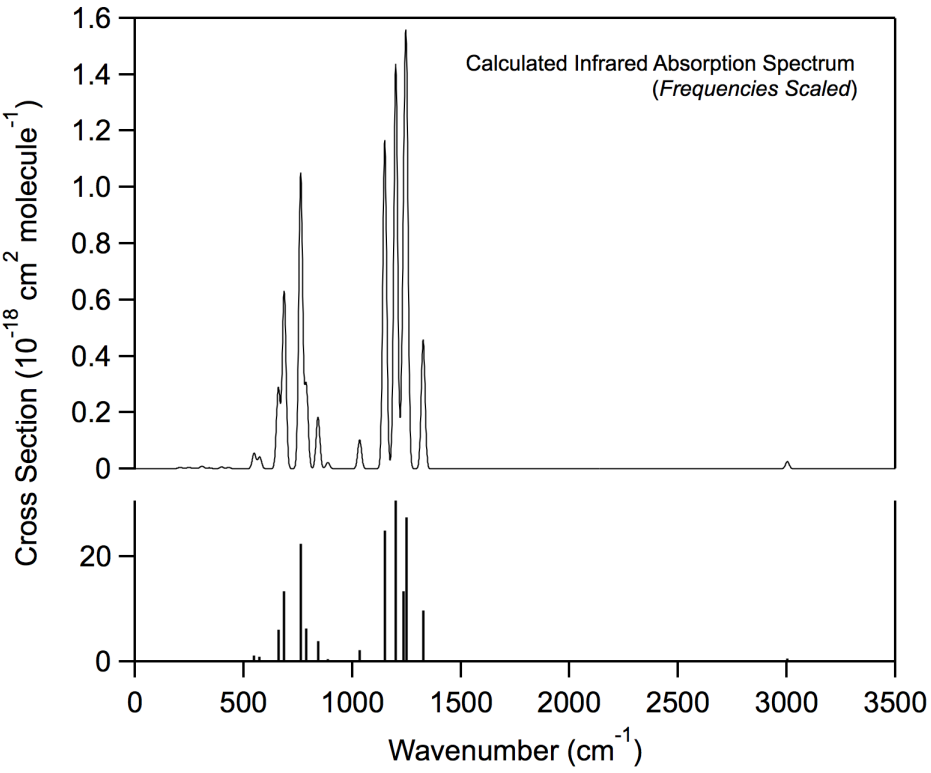
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	0.935989065147	-0.150503322734	-0.031342056377
C	-0.439000763613	0.363350372062	-0.544548017002
C	-1.711254047525	-0.404461835409	-0.091465864809
Cl	2.230755437110	0.891939397309	-0.713535431874
Cl	1.049658317329	-0.140846525854	1.746700117167
Cl	1.221619266076	-1.815929403858	-0.639271285035
H	-0.408477739472	0.304276326277	-1.633272371774
Cl	-0.685271981079	2.084453100863	-0.115638670892
F	-2.760578655367	0.118610262112	-0.732280438424
F	-1.650695000055	-1.696788638078	-0.414675326016
F	-1.929450898552	-0.310581732690	1.215496345037

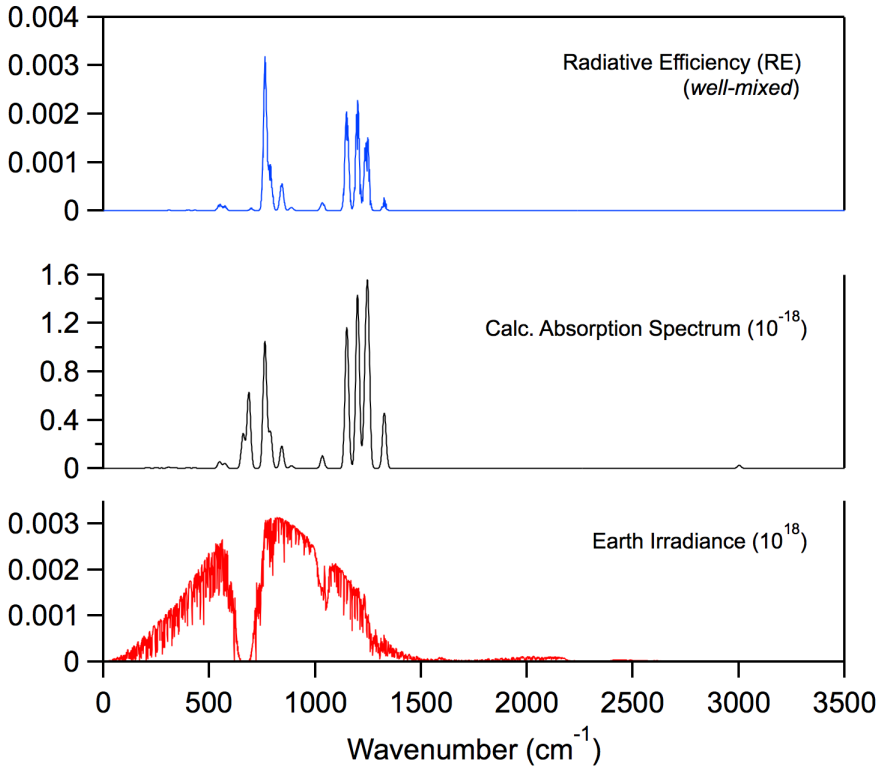
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
26.5401	0.00118
83.4618	0.00327
159.5709	0.0791
170.8140	0.0457
203.9030	0.0862
218.2075	0.0253
235.7896	0.0511
269.0468	0.194
293.0502	0.0370
308.9502	0.0585
365.7667	0.141
399.2690	0.102
523.8196	1.16
550.6932	0.887
641.7961	6.08
670.2399	13.4
750.7596	22.4
778.1041	6.28
835.0546	3.90
883.0622	0.471
1038.2359	2.19
1160.2799	24.9
1213.9695	30.6
1252.9638	13.4
1265.8642	27.4
1347.6962	9.75
3122.9123	0.534

Infrared Spectrum

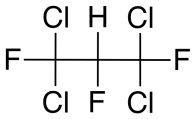


Radiative Efficiency



HCFC-223ea

Molecular Formula:	$CCl_2FCHFCCl_2F$
Name:	1,1,3,3-Tetrachloro-1,2,3-trifluoropropane
CAS number:	–
Molecular Weight:	235.85



Global Atmospheric Lifetime (years):	6.28
Tropospheric Atmospheric Lifetime (years):	7.74
Stratospheric Atmospheric Lifetime (years):	33.2
Ozone Depletion Potential (ODP):	0.114

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.302	0.282
Global Warming Potential (GWP_H):		
GWP_{20}	1732	1619
GWP_{100}	489	457
Global Temperature Potentials (GTP_H)		
GTP_{20}		997
GTP_{50}		110
GTP_{100}		64

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 7.58 \times 10^{-15}$; $k_{SAR}(272\ K) \approx 4.84 \times 10^{-15}$ cm^3 $molecule^{-1}$ s^{-1}

τ^{OH}_{Global} = 7.47 years
τ^{OH}_{Trop} = 7.74 years
τ^{OH}_{Strat} = 213.1.5 years

Fractional Atmospheric Loss: 0.841

O(^{1}D) Reactivity

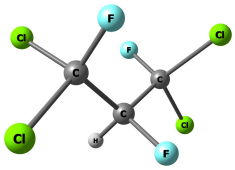
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 2.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)}$ = 185 years
Fractional Atmospheric Loss: 0.034

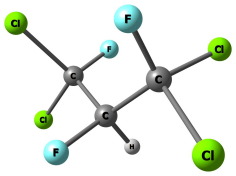
UV Photolysis

UV Spectrum: *No Recommendation*
τ_{hv} = 50 years
Fractional Atmospheric Loss: 0.125

Molecular Structure and Infrared Spectrum (6 conformers)



E = 0
Population = 0.424



E = 0
Population = 0.424

Optimized Coordinates (Angstroms)

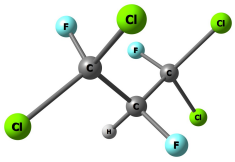
Atom	X	Y	Z
C	-1.328337501801	-0.054034834279	-0.134508337039
C	-0.010012716263	0.613419641928	0.346880001809
C	1.299561802957	-0.205749552937	0.166714878781
Cl	-1.745899825843	-1.462480299719	0.888070718341
Cl	-2.640483254976	1.168052182391	-0.013628424755
F	-1.245859726455	-0.449761864015	-1.404527208518
H	-0.120530599059	0.819775755815	1.415502567846
F	0.149226219286	1.775866256783	-0.338774290897
F	1.194729658879	-1.398561035346	0.756598481284
Cl	1.729046410515	-0.439119579523	-1.547705320050
Cl	2.615306532759	0.707271328902	0.990468933197

Atom	X	Y	Z
C	-1.300781408990	0.207958093608	-0.174707633797
C	0.008116960454	-0.614069143936	-0.346581451230
C	1.327300206168	0.058091091535	0.125825037680
Cl	-2.617846971189	-0.713685705822	-0.986665078118
Cl	-1.728552942318	0.461385987015	1.537291474339
F	-1.195746554612	1.393809710264	-0.778424842390
H	0.117516106294	-0.832860156259	-1.412842885708
F	-0.151210206109	-1.768395341819	0.352637508200
F	1.246231942366	0.468612406535	1.391230575457
Cl	2.638568168406	-1.166153586945	0.017972317385
Cl	1.744809699529	1.454285645822	-0.913442021820

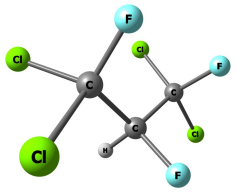
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
10.2549	0.00455
89.0761	0.0149
137.8939	0.0709
181.9919	0.0941
186.0671	0.0496
224.9824	0.158
240.0388	0.114
284.8456	0.129
291.8341	0.113
328.8594	0.0570
373.7471	0.0412
378.9291	0.0325
434.3784	0.950
465.3400	0.811
550.5125	0.580
628.1023	20.3
714.3672	29.8
841.5458	29.5
877.4131	11.3
945.6148	3.59
1075.5063	21.7
1147.8392	11.2
1175.7928	12.9
1204.9850	19.1
1338.0910	0.992
1362.5121	0.735
3090.3895	0.365

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
10.2592	0.00455
89.0735	0.0149
137.8935	0.0709
181.9912	0.0941
186.0679	0.0496
224.9831	0.158
240.0383	0.114
284.8466	0.129
291.8347	0.113
328.8584	0.0570
373.7463	0.0412
378.9287	0.0325
434.3782	0.950
465.3406	0.811
550.5127	0.580
628.1021	20.3
714.3657	29.8
841.5468	29.5
877.4117	11.3
945.6136	3.59
1075.5047	21.7
1147.8387	11.2
1175.7936	12.9
1204.9843	19.1
1338.0910	0.992
1362.5156	0.735
3090.3899	0.365



$\Delta E = 0.90$ kcal mol^{-1}
Population = 0.093



$\Delta E = 1.79$ kcal mol^{-1}
Population = 0.021

Optimized Coordinates (Angstroms)

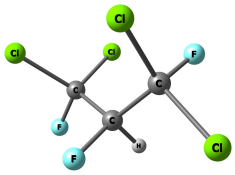
Atom	X	Y	Z
C	-1.322050614045	-0.025171051483	-0.303208330986
C	0.001403152191	-0.711981718723	0.148187050364
C	1.326969493055	-0.087318067432	-0.366267353409
Cl	-2.645170304076	-1.237433381941	-0.124368545176
Cl	-1.730315225642	1.415203092419	0.659683270337
F	-1.241434422930	0.313266199654	-1.593209317086
H	-0.016023199965	-1.720808759480	-0.279409177634
F	0.020462105796	-0.784079171079	1.498136224659
F	1.325388147265	-0.123385112960	-1.703668716400
Cl	1.613274962911	1.584089721091	0.171052151087
Cl	2.668747905440	-1.136812750066	0.216509744244

Atom	X	Y	Z
C	-1.315709709654	0.029661813839	0.157587964063
C	0.000674892352	-0.597733850305	-0.409806415530
C	1.314588832762	-0.090059673780	0.250779624054
Cl	-1.723233919323	1.537117618870	-0.725714015656
Cl	-2.666354066399	-1.129760547214	-0.042194040182
F	-1.194814484302	0.312917814386	1.457529421432
H	0.036856881163	-0.416615961335	-1.485349176561
F	-0.013676517504	-1.938117316404	-0.163190747160
F	1.332539555412	-0.453264634021	1.534496995050
Cl	2.689346117652	-0.903234481346	-0.579505083636
Cl	1.529994417842	1.676449217310	0.144751474127

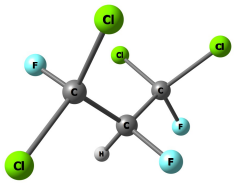
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
12.8468	0.00465
81.4626	0.0252
135.4137	0.128
185.4729	0.0289
189.0842	0.0520
204.7605	0.0727
218.5652	0.122
276.5091	0.0964
300.9137	0.0662
352.3783	0.0215
373.4091	0.00649
381.7579	0.0297
439.5650	0.590
506.9609	0.325
582.0340	0.118
633.1730	22.2
638.6783	21.2
758.5200	12.1
885.4128	28.2
1022.0404	20.6
1096.6582	6.82
1159.4097	5.30
1177.2022	38.9
1187.0173	1.61
1346.3100	0.0570
1362.2574	1.49
3067.5064	0.508

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
30.2849	0.00538
72.6348	0.00727
134.2381	0.0416
185.5550	0.0649
202.4294	0.0251
225.8841	0.307
241.6111	0.0342
298.9625	0.0584
314.4285	0.0891
334.1257	0.0922
360.9092	0.0388
378.9887	0.0237
428.8581	1.55
459.1220	0.647
472.9858	1.21
665.3464	31.0
808.6187	6.68
853.7148	30.0
862.1420	25.4
951.3816	7.52
982.0862	16.7
1129.3173	6.12
1174.3745	1.42
1202.5202	32.0
1334.3673	1.02
1362.6802	0.305
3118.3918	0.236



$\Delta E = 1.94$ kcal mol^{-1}
Population = 0.016



$\Delta E = 1.94$ kcal mol^{-1}
Population = 0.016

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.408454566684	-0.190689911121	0.324732453397
C	0.076172968303	-0.438479570078	0.720365348116
C	1.222261820874	-0.219744637930	-0.300349479809
Cl	-1.830843809458	1.532245489841	0.169864293957
Cl	-1.874802942438	-1.090507720032	-1.146713492767
F	-2.123653484962	-0.687766899099	1.350965249714
H	0.117786443909	-1.501069484589	0.989710780472
F	0.321587477749	0.321194757135	1.818431877348
F	1.055770949219	-1.030881285814	-1.348987484889
Cl	1.371768628455	1.455833962864	-0.879559350845
Cl	2.752299515034	-0.698758701176	0.523863805307

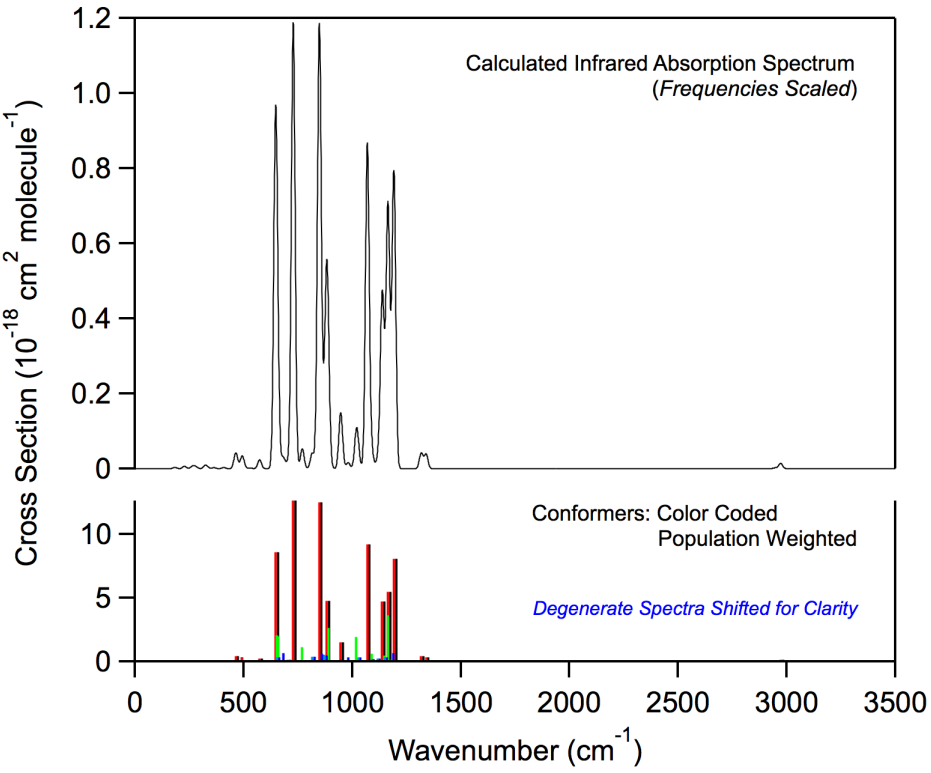
Atom	X	Y	Z
C	-1.225533019906	-0.229211422440	-0.294327438475
C	-0.080950541227	-0.429028407045	0.731941257509
C	1.405618921554	-0.205614060082	0.329149770023
Cl	-2.759346573247	-0.671237438685	0.543424019113
Cl	-1.360584432718	1.430550199012	-0.920707908554
F	-1.066641820418	-1.071137337365	-1.319616224332
H	-0.131779556268	-1.483156937205	1.031282767166
F	-0.319184628742	0.363568197664	1.808100451674
F	2.116883282802	-0.679688757355	1.368911639296
Cl	1.863381522025	-1.150826671633	-1.116302858066
Cl	1.843061846143	1.508459635135	0.125440524644

Infrared Absorption Spectrum (unscaled frequencies)

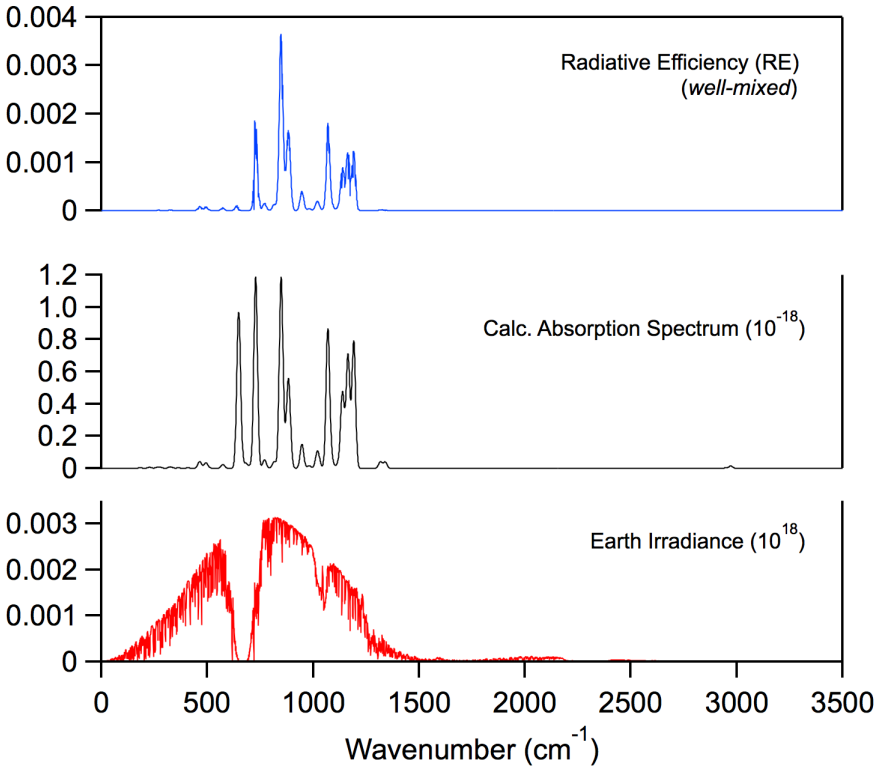
Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
10.6269	0.000
93.0344	0.0196
140.4872	0.0957
183.5983	0.114
188.6909	0.0173
191.4995	0.0885
249.8249	0.0963
282.9463	0.139
313.5270	0.197
324.6755	0.162
377.6213	0.00771
388.5906	0.0258
439.2363	0.734
478.4240	1.41
548.0743	0.668
634.7425	19.6
687.9387	9.81
806.7093	23.3
865.3448	29.2
1031.1000	19.9
1094.5860	13.0
1125.6121	13.6
1160.0460	21.2
1175.1062	5.54
1345.2146	0.335
1354.8050	2.03
3058.2150	0.469

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
10.6233	0.000
93.0347	0.0196
140.4877	0.0957
183.5977	0.114
188.6902	0.0173
191.4994	0.0885
249.8249	0.0963
282.9461	0.139
313.5268	0.197
324.6755	0.162
377.6209	0.00771
388.5907	0.0258
439.2364	0.734
478.4239	1.41
548.0747	0.668
634.7424	19.6
687.9389	9.81
806.7086	23.3
865.3448	29.2
1031.0998	19.9
1094.5865	13.0
1125.6124	13.6
1160.0460	21.2
1175.1073	5.54
1345.2154	0.335
1354.8051	2.03
3058.2154	0.469

Infrared Spectrum

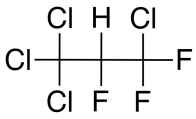


Radiative Efficiency



HCFC-223eb

Molecular Formula:	$CCl_3CHFCClF_2$
Name:	1,1,1,3-Tetrachloro-2,3,3-trifluoropropane
CAS number:	54002-59-4
Molecular Weight:	235.85



Global Atmospheric Lifetime (years):	6.46
Tropospheric Atmospheric Lifetime (years):	8.02
Stratospheric Atmospheric Lifetime (years):	33.4
Ozone Depletion Potential (ODP):	0.117

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.280	0.262
Global Warming Potential (GWP_H):		
GWP_{20}	1650	1545
GWP_{100}	468	438
Global Temperature Potentials (GTP_H)		
GTP_{20}		966
GTP_{50}		108
GTP_{100}		62

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 7.32 \times 10^{-15}$; $k_{SAR}(272\ K) \approx 4.67 \times 10^{-15}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 7.73$ years

$\tau^{OH}_{Trop} = 8.02$ years

$\tau^{OH}_{Strat} = 220.0$ years

Fractional Atmospheric Loss: 0.836

O(^{1}D) Reactivity

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

$k_{Est}(T) = 2.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 185$ years

Fractional Atmospheric Loss: 0.035

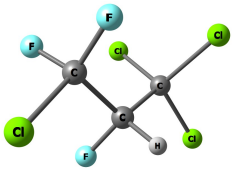
UV Photolysis

UV Spectrum: *No Recommendation*

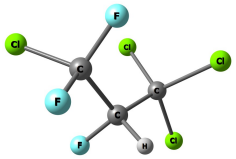
$\tau_{hv} = 50$ years

Fractional Atmospheric Loss: 0.129

Molecular Structure and Infrared Spectrum (2 conformers)



E = 0
Population = 0.932



$\Delta E = 1.82$ kcal mol^{-1}
Population = 0.043

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.130682348676	0.015360929575	-0.079294029065
C	0.293854457937	-0.508311703499	-0.423292699496
C	1.507673315545	0.294211351370	0.117247318494
Cl	-1.408805275495	1.604882701490	-0.845527220288
Cl	-2.289888869692	-1.167894705971	-0.779852740130
Cl	-1.403423405454	0.119064603978	1.677520975601
H	0.366179697698	-0.532367838656	-1.514669901326
F	0.412296593218	-1.765035695746	0.082243589213
F	1.472982822625	1.566175896228	-0.273550111789
F	1.569314963061	0.256187004299	1.443841706939
Cl	3.012739049234	-0.455061543069	-0.539125888152

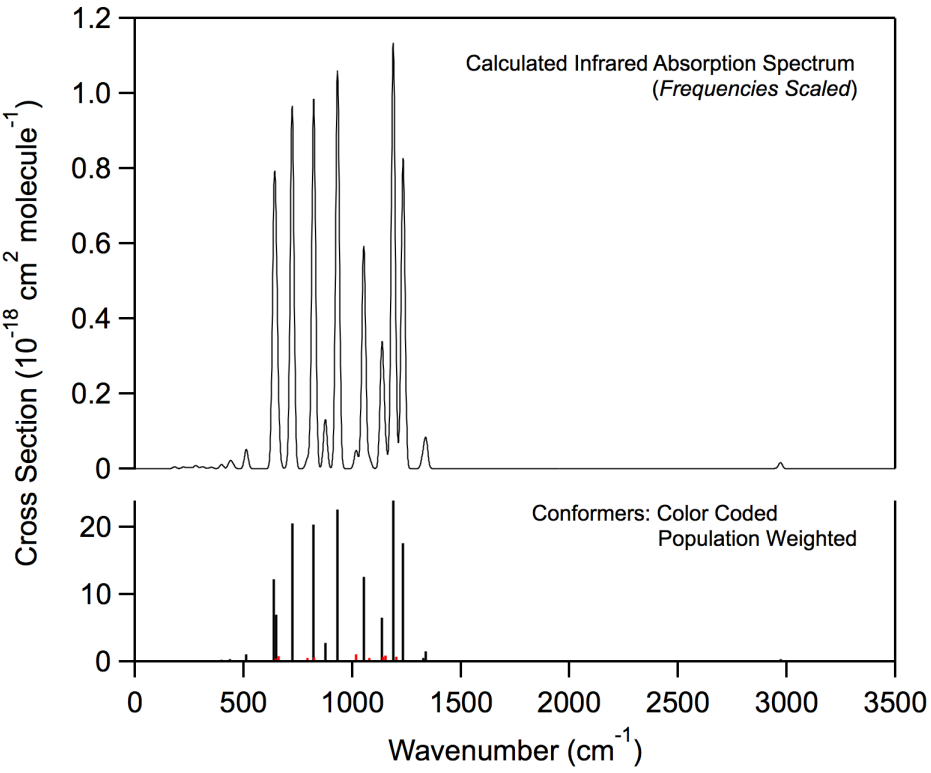
Atom	X	Y	Z
C	-1.067162141017	0.116498881739	-0.000211131306
C	0.178041893437	-0.130545821727	-0.896073420021
C	1.578465378202	0.288979394973	-0.348401141003
Cl	-2.468119935693	-0.640185116229	-0.831023304709
Cl	-0.901863154226	-0.594630747249	1.622617004532
Cl	-1.367847342802	1.877055044376	0.123523294940
H	0.025516972770	0.464719807131	-1.803267394842
F	0.243057454895	-1.444266147905	-1.228782841232
F	2.351200137557	0.531337197347	-1.417170973858
F	1.515567589909	1.406401750937	0.373311943802
Cl	2.373445146968	-0.986661243391	0.619619963697

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
16.4914	0.000
91.0591	0.00521
136.1074	0.111
177.8176	0.0921
194.2512	0.0361
212.2376	0.0594
239.7040	0.196
271.6644	0.107
292.0621	0.0208
315.0529	0.0899
365.3954	0.257
405.8156	0.408
419.7878	0.232
485.5848	1.12
620.8770	13.2
631.6646	7.48
709.0889	22.1
814.1784	21.9
870.8957	3.01
930.2806	24.2
1058.0673	13.6
1146.6341	7.00
1201.6454	25.7
1249.8933	18.9
1347.0953	0.569
1361.0771	1.66
3089.5636	0.374

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
27.4708	0.00830
72.7590	0.0170
139.4939	0.0673
172.7763	0.0720
195.5529	0.0274
216.3396	0.116
258.9408	0.193
272.0084	0.203
284.9861	0.0516
330.2374	0.177
359.3665	0.214
416.5996	0.0793
423.5994	0.0102
486.2282	1.15
627.4875	10.3
644.0146	18.0
688.5930	3.66
784.2031	13.2
815.4005	14.5
1021.0015	24.4
1086.3147	13.1
1153.7596	16.8
1164.1328	20.7
1215.7488	16.3
1343.2252	1.80
1366.8683	1.84
3069.4150	0.457

Infrared Spectrum



Radiative Efficiency