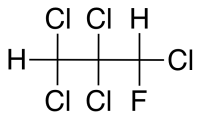
HCFC-231aa

Molecular Formula: $CHCl_2CCl_2CHClF$
Name: 1,1,2,2,3-Pentachloro-3-fluoropropane
CAS number: –
Molecular Weight: 234.31



Global Atmospheric Lifetime (years): 0.799
  Tropospheric Atmospheric Lifetime (years): 0.839
  Stratospheric Atmospheric Lifetime (years): 20
Ozone Depletion Potential (ODP): 0.022

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.183	0.128
Global Warming Potential (GWP_H):		
GWP_{20}	140	98
GWP_{100}	38	27
Global Temperature Potentials (GTP_H)		
GTP_{20}		31
GTP_{50}		5
GTP_{100}		4

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 6.99 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 4.46 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 0.815$ years
$\tau^{OH}_{Trop} = 0.839$ years
$\tau^{OH}_{Strat} = 28.8$ years

Fractional Atmospheric Loss: 0.980

O(^{1}D) Reactivity

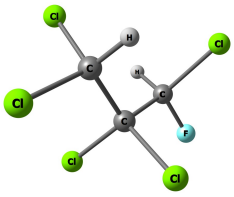
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 2.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)} = 185$ years
Fractional Atmospheric Loss: 0.004

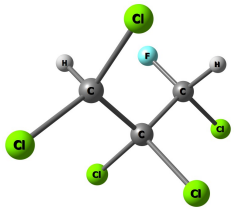
UV Photolysis

UV Spectrum: *No Recommendation*
$\tau_{hv} = 50$ years
Fractional Atmospheric Loss: 0.016

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.568



$\Delta E = 0.29$ kcal mol^{-1}
Population = 0.348

Optimized Coordinates (Angstroms)

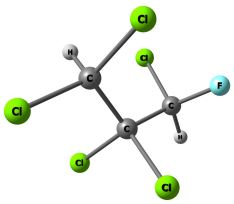
Atom	X	Y	Z
C	-0.934051291161	0.520659902431	0.493435275914
C	0.149719808976	-0.387652209208	-0.137705780674
C	1.428411970193	0.394935419053	-0.547230898210
Cl	-1.304692017138	1.921627877307	-0.567060288152
Cl	-2.425279517361	-0.362772608546	0.893608856795
H	-0.543129056852	0.929887490009	1.421074059432
Cl	-0.449150205227	-1.164478811430	-1.640200063281
Cl	0.596783039820	-1.642384262309	1.060037752113
H	1.190216114949	1.108628513256	-1.334988806332
Cl	2.102130492779	1.349226298489	0.823376957812
F	2.362838661023	-0.468783609053	-0.973824065417

Atom	X	Y	Z
C	-1.213252377925	0.244565436913	-0.540174658235
C	0.138872818100	-0.239416897318	0.059425386170
C	1.248262077033	0.796299669381	-0.275070135622
Cl	-2.557396835919	-0.869122568013	-0.204434064681
Cl	-1.627861193634	1.900245329192	0.021516844868
H	-1.099371537982	0.305986959180	-1.618952255363
Cl	0.528881294164	-1.801165717743	-0.730757139148
Cl	0.041492053253	-0.423379635825	1.828694802618
H	1.051412447502	1.726450661968	0.256464738109
Cl	2.881961520545	0.265856048320	0.200741046568
F	1.221729734862	1.021546713945	-1.611505565285

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
69.3211	0.0530
86.9040	0.0968
128.0919	0.0170
169.7778	0.0172
182.9198	0.275
204.3871	0.0231
227.5283	0.0124
276.5720	0.0849
284.7972	0.0998
348.9394	0.110
357.9324	0.285
415.8076	0.460
586.6040	4.46
622.1193	7.33
727.5516	14.6
750.2204	21.5
780.9040	10.7
837.6614	4.98
1025.2512	2.03
1056.5391	3.64
1160.7385	16.8
1229.1681	2.50
1268.4243	2.53
1278.8057	1.34
1365.3017	1.14
3138.7902	0.352
3163.9105	0.632

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
68.6558	0.0672
78.6562	0.106
122.8213	0.0362
170.9196	0.0385
193.1612	0.208
198.5411	0.00701
221.7948	0.0250
247.5381	0.0144
303.2851	0.173
339.9309	0.216
375.0023	0.165
434.5945	0.271
569.3803	6.84
629.9939	6.28
702.9239	15.4
748.0898	14.7
846.4699	9.07
858.0235	8.43
1009.5426	2.64
1046.5421	7.16
1115.9156	13.9
1231.3987	2.48
1272.2242	0.709
1286.8170	2.55
1355.6680	1.32
3139.1160	0.358
3165.3381	0.642



$\Delta E = 1.29$ kcal mol^{-1}
Population = 0.065

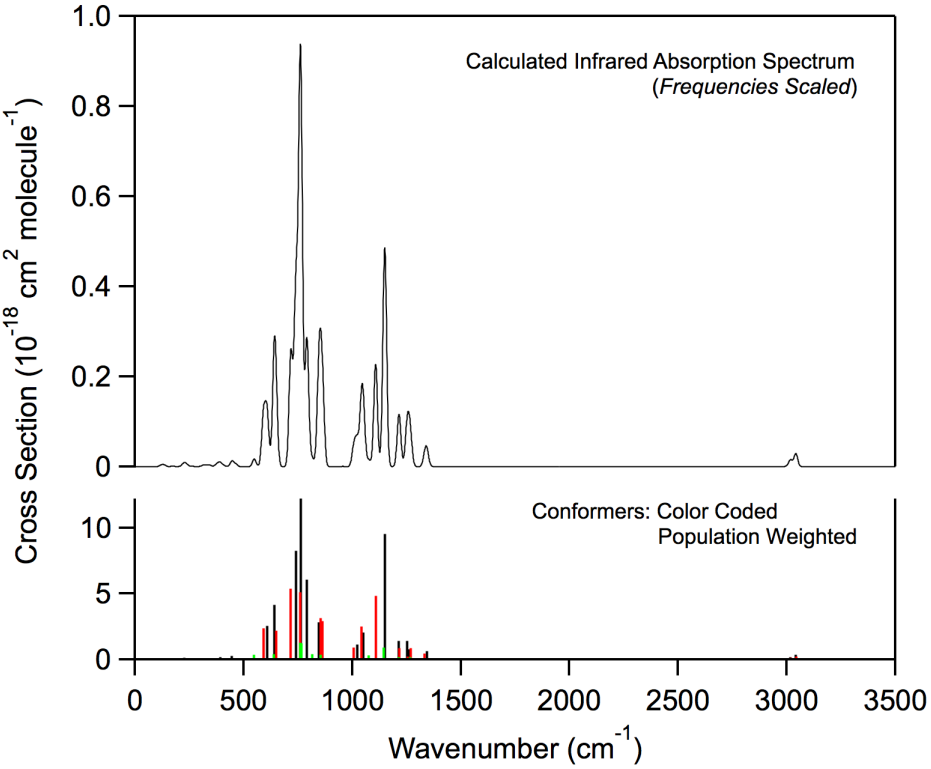
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-0.766258045827	0.361886926208	-0.706135296834
C	0.083048865174	-0.435177572621	0.315534202430
C	1.538000396215	0.089522120016	0.524121490982
Cl	-2.396657662965	-0.332067989280	-0.917335829826
Cl	-0.882124774315	2.092197048262	-0.278260292207
H	-0.272070642675	0.309196228960	-1.672558095551
Cl	0.254868008452	-2.118496285133	-0.302521941893
Cl	-0.682365196898	-0.467206295402	1.931510296404
H	2.103853210603	-0.673475754797	1.059750548880
Cl	2.388374018738	0.354831263660	-1.042265074946
F	1.552700823497	1.237227310125	1.220062992562

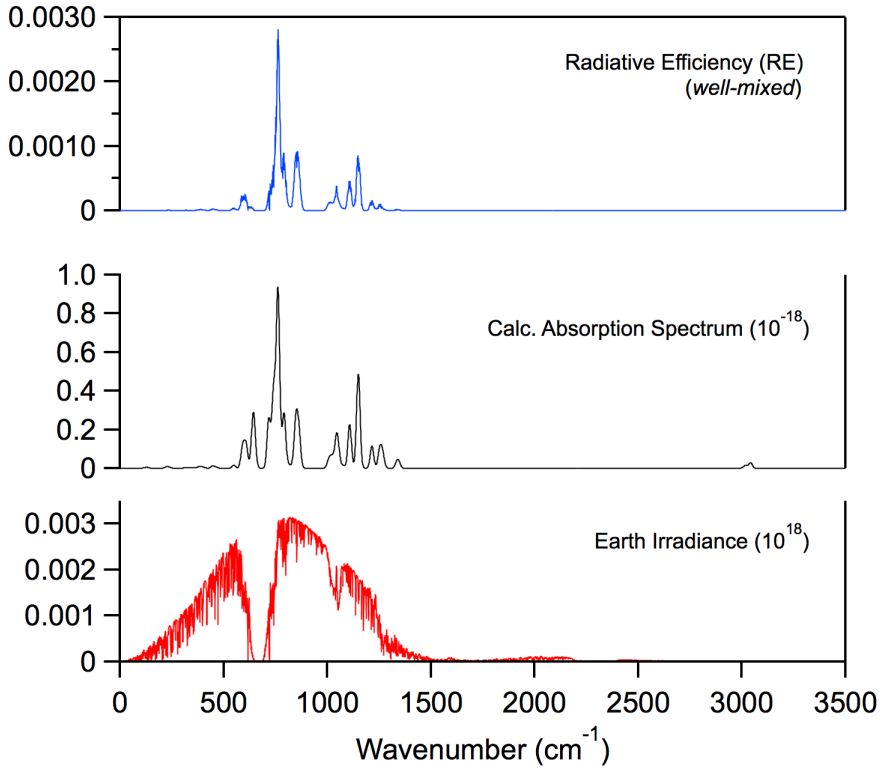
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
59.9612	0.0332
88.8172	0.0356
142.1090	0.0848
164.8350	0.0378
181.3817	0.0383
209.9222	0.0874
233.6712	0.00470
262.6640	0.106
312.2183	0.385
331.7354	0.125
365.6225	0.0955
431.7296	0.431
524.2662	5.59
620.7792	6.14
746.8958	19.7
754.3668	19.3
805.7401	6.19
847.3303	5.61
956.9540	0.230
1082.1357	5.02
1156.6302	14.3
1229.4484	3.14
1276.0285	1.61
1282.6762	2.73
1375.4416	0.913
3122.7178	0.414
3161.6642	0.583

Infrared Spectrum

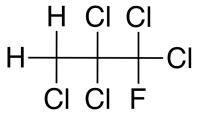


Radiative Efficiency



HCFC-231ab

Molecular Formula:	$CH_2ClCCl_2CCl_2F$
Name:	1,1,2,2,3-Pentachloro-1-fluoropropane
CAS number:	1538604-29-3
Molecular Weight:	234.31



Global Atmospheric Lifetime (years):	1.61
Tropospheric Atmospheric Lifetime (years):	1.73
Stratospheric Atmospheric Lifetime (years):	23.0
Ozone Depletion Potential (ODP):	0.042

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.221	0.180
Global Warming Potential (GWP_H):		
GWP_{20}	341	278
GWP_{100}	92	75
Global Temperature Potentials (GTP_H)		
GTP_{20}		97
GTP_{50}		13
GTP_{100}		10

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 3.40 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 2.17 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 1.67$ years

$\tau^{OH}_{Trop} = 1.73$ years

$\tau^{OH}_{Strat} = 55.2$ years

Fractional Atmospheric Loss: 0.959

$O(^1D)$ 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: 0.009

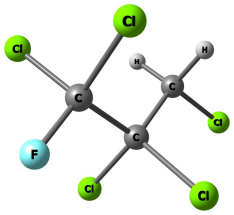
UV Photolysis

UV Spectrum: *No Recommendation*

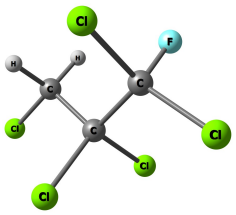
$\tau_{hv} = 50$ years

Fractional Atmospheric Loss: 0.032

Molecular Structure and Infrared Spectrum (7 conformers)



E = 0
Population = 0.230



$\Delta E = 0.10$ kcal mol^{-1}
Population = 0.196

Optimized Coordinates (Angstroms)

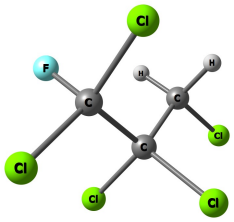
Atom	X	Y	Z
C	-1.034350216635	0.006795358813	1.127767114188
C	-0.341823912800	-0.000362736045	-0.240494393756
C	1.227018329826	0.001710212416	-0.100485945644
Cl	-2.818183051340	0.004760252275	1.025550994922
H	-0.739876080145	-0.882331063876	1.682795231095
H	-0.741335033072	0.902611668576	1.672718842906
Cl	-0.796392399819	1.452384323284	-1.191251765138
Cl	-0.794007913939	-1.464492469140	-1.174785074072
Cl	1.801867231494	1.464143909609	0.771314212044
Cl	1.804249549768	-1.449845652777	0.787764233580
F	1.778466496665	-0.004663807460	-1.309452450099

Atom	X	Y	Z
C	-1.317511596937	-0.787420125938	0.665355961665
C	-0.344308971810	0.163061003023	-0.055453152251
C	1.124856959274	-0.138629103470	0.427884190795
Cl	-3.034908626761	-0.479634776298	0.283621225115
H	-1.102629683303	-1.812839597703	0.372660828729
H	-1.190998656954	-0.669528096289	1.740663166562
Cl	-0.713042745356	1.859483338983	0.404049635139
Cl	-0.456813346878	-0.032121086132	-1.824705101174
Cl	1.579573300068	-1.845998607669	0.088818923638
Cl	2.333030108884	0.940767962856	-0.306412030646
F	1.155337259774	0.027891088637	1.758472352428

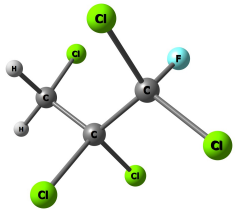
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
74.5129	0.00362
88.6301	0.191
130.1818	0.114
165.3896	0.0657
207.2491	0.0248
222.5383	0.00621
249.2892	0.191
275.0897	0.0102
299.1270	0.179
327.6388	0.0808
374.6216	0.125
385.9443	0.0367
476.4535	0.756
564.6286	1.92
709.2136	20.9
720.2167	18.2
797.3624	5.24
821.4385	22.2
969.0886	2.67
999.5893	5.40
1068.5207	2.63
1181.8776	15.5
1223.6359	1.25
1314.5315	1.04
1462.7954	0.697
3111.3035	0.789
3179.8539	0.0284

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
72.9992	0.00639
91.7330	0.242
126.0103	0.140
172.3698	0.0570
194.7043	0.00963
228.6856	0.0704
240.8856	0.0460
275.4616	0.0763
304.4738	0.193
330.8719	0.236
380.6754	0.0228
389.4914	0.0996
494.0917	0.565
547.7127	3.52
690.0614	17.6
737.9358	16.0
800.2795	15.7
862.0500	10.0
972.8484	6.94
1001.1329	7.26
1057.9038	4.51
1132.4273	12.9
1224.2613	2.17
1313.1168	1.10
1463.6346	0.626
3112.4777	0.579
3182.9846	0.0409



$\Delta E = 0.10$ kcal mol^{-1}
Population = 0.196



$\Delta E = 0.17$ kcal mol^{-1}
Population = 0.172

Optimized Coordinates (Angstroms)

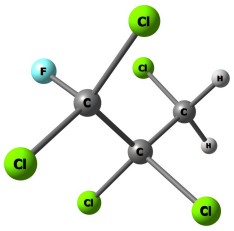
Atom	X	Y	Z
C	-1.315429471687	-0.804301783092	-0.643851064763
C	-0.343439318961	0.163162356713	0.055686319656
C	1.126079443887	-0.147106829281	-0.421104009903
Cl	-3.033199005887	-0.490521242380	-0.268730787667
H	-1.189208956187	-0.709966175004	-1.721514650598
H	-1.099110188219	-1.822726930119	-0.328659254303
Cl	-0.455467337056	0.006874001610	1.828827272462
Cl	-0.714544654957	1.848539560973	-0.441043857969
Cl	2.332866933065	0.949863508872	0.289030504638
Cl	1.583170396273	-1.845963840589	-0.044546477291
F	1.156169159728	-0.009922627703	-1.755044994262

Atom	X	Y	Z
C	-1.536891128170	-0.035404927623	-0.937072076710
C	-0.266957714960	0.535656535678	-0.278945571708
C	0.675196828435	-0.534463909904	0.386501802259
Cl	-2.656246865319	-0.894813960605	0.168851115722
H	-2.086768603099	0.799625610777	-1.366528887434
H	-1.251644860999	-0.734014898901	-1.720812803958
Cl	-0.712577064774	1.733440400566	0.975562690674
Cl	0.611623392918	1.357896117159	-1.615755580112
Cl	1.035180294243	-1.864572182828	-0.768176511456
Cl	2.210684169297	0.177761232582	0.958534323333
F	0.050856552428	-1.062972016903	1.438826499390

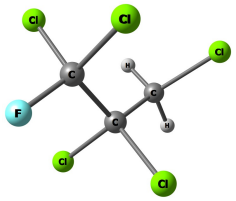
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
72.9997	0.00639
91.7343	0.242
126.0104	0.140
172.3697	0.0570
194.7040	0.00963
228.6855	0.0704
240.8853	0.0460
275.4618	0.0763
304.4741	0.193
330.8719	0.236
380.6753	0.0228
389.4916	0.0996
494.0917	0.565
547.7125	3.52
690.0615	17.6
737.9363	16.0
800.2803	15.7
862.0501	10.0
972.8478	6.94
1001.1332	7.26
1057.9038	4.51
1132.4277	12.9
1224.2594	2.17
1313.1152	1.10
1463.6326	0.626
3112.4780	0.579
3182.9849	0.0409

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
55.9927	0.0308
104.3078	0.0899
149.0130	0.0307
176.2712	0.0439
188.3038	0.0961
231.3987	0.00966
259.2484	0.0963
272.4735	0.170
308.8129	0.318
342.8952	0.339
380.9752	0.0253
392.3984	0.0997
471.3764	2.58
519.3066	2.80
684.4954	13.2
749.2469	13.3
818.7264	23.3
853.8178	14.2
908.6573	9.83
998.7981	0.0896
1084.9258	4.97
1156.4211	12.3
1243.2089	0.739
1311.2470	4.22
1457.5091	1.94
3117.8971	0.613
3185.7874	0.0406



$\Delta E = 0.17$ kcal mol^{-1}
Population = 0.172



$\Delta E = 1.54$ kcal mol^{-1}
Population = 0.017

Optimized Coordinates (Angstroms)

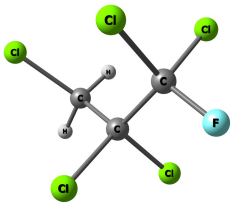
Atom	X	Y	Z
C	-1.544439213538	-0.008990832271	0.920559632222
C	-0.257547369151	0.543106155887	0.279414233972
C	0.673718288279	-0.540098002838	-0.380163959963
Cl	-2.665632566982	-0.844321696141	-0.201829481054
H	-1.280084103494	-0.715771533056	1.704299532689
H	-2.084845668281	0.833452719505	1.347553895110
Cl	0.619675237439	1.344405834915	1.629763672212
Cl	-0.668358617674	1.753753180990	-0.974626812958
Cl	2.227539094322	0.148219143364	-0.931585292579
Cl	0.997792622873	-1.881142893013	0.772499139271
F	0.052464296206	-1.053301077342	-1.441848558923

Atom	X	Y	Z
C	-1.078290535998	0.671409339185	-1.133916739677
C	-0.046338404982	0.720945795453	0.002994103269
C	0.777923579721	-0.586928595132	0.301746351498
Cl	-2.515731696163	-0.362857706728	-0.856202365376
H	-1.444734741549	1.684816815970	-1.283266688554
H	-0.590623762503	0.318587842517	-2.040788415429
Cl	-0.789039408496	1.285492222039	1.528813125047
Cl	1.153364005086	1.966923263396	-0.540140690056
Cl	-0.193815315075	-1.870962112655	1.068725110524
Cl	1.501494559198	-1.234716005167	-1.212969844084
F	1.770628720761	-0.278916858878	1.137656052838

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
55.9927	0.0308
104.3104	0.0899
149.0147	0.0307
176.2725	0.0439
188.3059	0.0961
231.3994	0.00966
259.2495	0.0962
272.4736	0.170
308.8147	0.318
342.8957	0.339
380.9754	0.0253
392.3987	0.0997
471.3764	2.58
519.3071	2.80
684.4961	13.2
749.2460	13.3
818.7278	23.3
853.8177	14.2
908.6591	9.83
998.7996	0.0896
1084.9271	4.97
1156.4231	12.3
1243.2069	0.739
1311.2447	4.22
1457.5094	1.94
3117.8975	0.613
3185.7879	0.0406

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
47.8698	0.0792
106.1025	0.0863
145.9169	0.0295
169.6357	0.0392
218.8978	0.0331
225.6828	0.279
245.8228	0.113
277.1102	0.268
292.8090	0.177
326.7492	0.0590
381.9743	0.0327
389.4432	0.0661
451.3404	1.11
576.0481	2.51
685.8795	11.9
740.6951	22.8
783.9582	16.1
840.9312	12.4
900.6795	7.56
1016.7268	1.03
1083.9800	4.10
1163.9705	13.4
1250.1842	0.802
1315.9223	2.47
1457.2097	2.07
3116.8421	0.582
3183.9966	0.0494



$\Delta E = 1.54$ kcal mol^{-1}
Population = 0.017

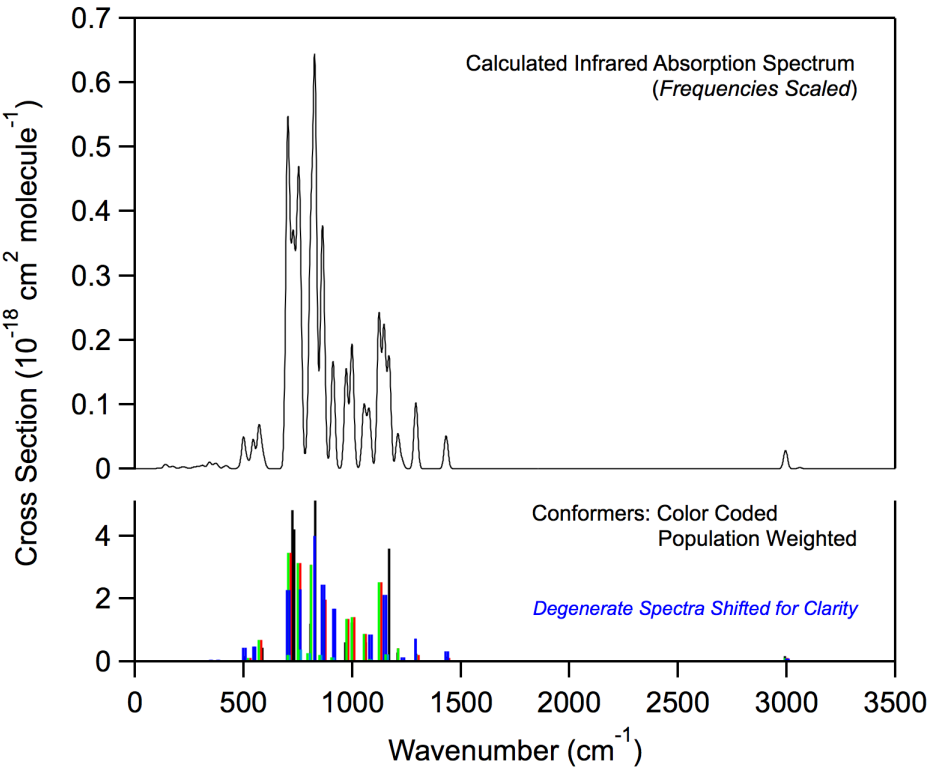
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.078973476292	0.683504302208	1.131669021004
C	-0.047303341529	0.723286455625	-0.005881274942
C	0.778734573062	-0.586312486698	-0.291901889658
Cl	-2.515012868104	-0.355463048330	0.864445290723
H	-0.590642277739	0.340318399884	2.041874495623
H	-1.446812412291	1.697819147107	1.271102170079
Cl	1.150753610982	1.976227566586	0.524720958511
Cl	-0.791076921423	1.271741328997	-1.537035525296
Cl	1.503494747229	-1.218135186364	1.228975866324
Cl	-0.191347050512	-1.879195082218	-1.046005390920
F	1.770851416617	-0.285160396795	-1.131003721448

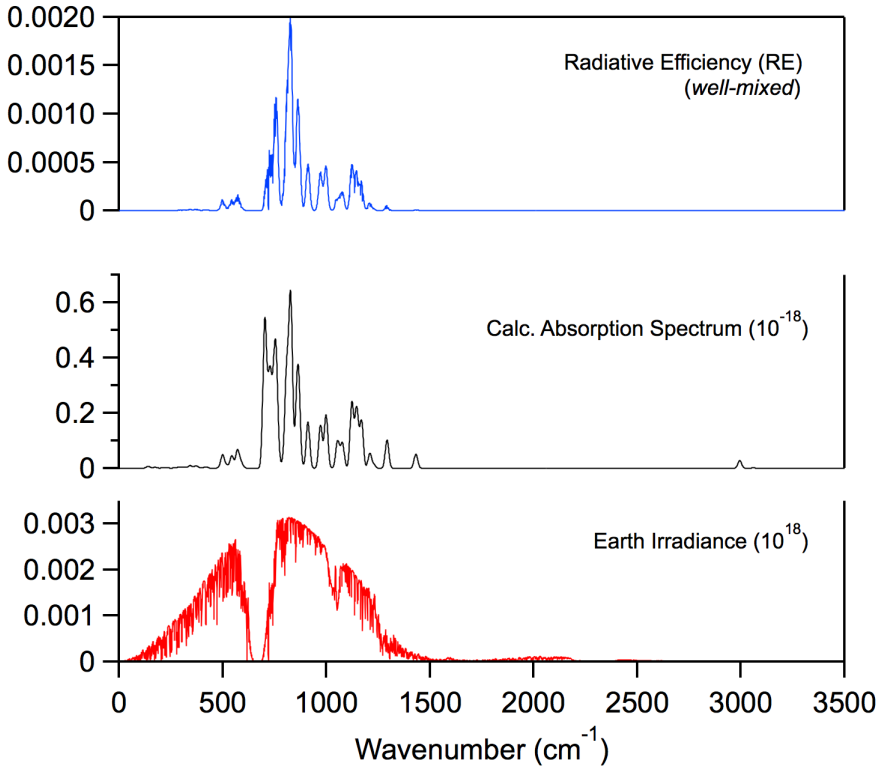
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
47.8707	0.0792
106.1029	0.0863
145.9167	0.0295
169.6360	0.0392
218.8976	0.0331
225.6829	0.279
245.8228	0.113
277.1104	0.268
292.8089	0.177
326.7494	0.0590
381.9746	0.0327
389.4436	0.0661
451.3405	1.11
576.0483	2.51
685.8810	11.9
740.6952	22.8
783.9585	16.1
840.9320	12.4
900.6796	7.56
1016.7271	1.03
1083.9795	4.10
1163.9698	13.4
1250.1834	0.802
1315.9217	2.47
1457.2085	2.07
3116.8422	0.582
3183.9966	0.0494

Infrared Spectrum

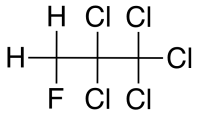


Radiative Efficiency



HCFC-231ac

Molecular Formula: $CH_2FCCl_2CCl_3$
Name: 1,1,1,2,2-Pentachloro-3-fluoropropane
CAS number: –
Molecular Weight: 234.31



Global Atmospheric Lifetime (years): 2.33
  Tropospheric Atmospheric Lifetime (years): 2.55
  Stratospheric Atmospheric Lifetime (years): 26.2
Ozone Depletion Potential (ODP): 0.058

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.181	0.156
Global Warming Potential (GWP_H):		
GWP_{20}	405	348
GWP_{100}	110	94
Global Temperature Potentials (GTP_H)		
GTP_{20}		135
GTP_{50}		17
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*

$k_{SAR}(298\ K) = 2.30 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 1.47 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 2.47$ years
$\tau^{OH}_{Trop} = 2.55$ years
$\tau^{OH}_{Strat} = 78.5$ years

Fractional Atmospheric Loss: 0.941

O(^{1}D) Reactivity

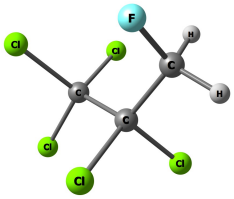
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 2.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)} = 185$ years
Fractional Atmospheric Loss: 0.012

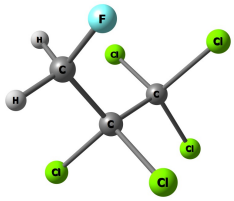
UV Photolysis

UV Spectrum: *No Recommendation*
$\tau_{hv} = 50$ years
Fractional Atmospheric Loss: 0.047

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.368



E = 0
Population = 0.368

Optimized Coordinates (Angstroms)

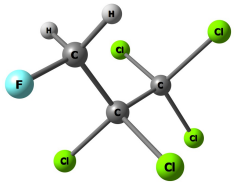
Atom	X	Y	Z
C	1.501044145564	0.653765470113	-1.177224937317
C	0.788785181185	-0.181273671372	-0.090278504984
C	-0.765184349518	0.062010943683	0.031321070586
H	0.995116873470	0.503937873002	-2.134756603450
F	1.515011441399	1.982276924977	-0.868128826399
H	2.529015485364	0.287151141154	-1.239521838682
Cl	1.567970280822	0.146090649782	1.487908237529
Cl	1.080412530254	-1.895117224218	-0.556805290760
Cl	-1.493380586502	-1.030399332707	1.242257367910
Cl	-1.103553443180	1.750550047417	0.503693423742
Cl	-1.548320558859	-0.242006821832	-1.559060098175

Atom	X	Y	Z
C	1.491933738865	0.686773544812	1.171268050565
C	0.793642431000	-0.165225214999	0.088427009696
C	-0.764857926518	0.048270695912	-0.031126800577
H	2.526753426482	0.339842000731	1.232900879136
F	1.480263360015	2.014261497789	0.857711474808
H	0.990624933083	0.530654270555	2.130222492326
Cl	1.118407922021	-1.871674932085	0.560136631567
Cl	1.563704747402	0.171463396870	-1.492273776110
Cl	-1.474446805423	-1.061768117630	-1.237068419295
Cl	-1.539290014144	-0.265110112610	1.561697593951
Cl	-1.135887812783	1.728519970653	-0.508510136068

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
60.4536	0.0774
123.4538	0.239
163.0202	0.00802
174.9234	0.0646
203.3774	0.162
221.5524	0.0412
237.8582	0.0257
269.6933	0.208
283.8119	0.381
311.7009	0.0858
346.1774	0.369
377.0190	0.0313
410.3051	0.301
526.3743	6.16
678.5597	12.6
757.3542	29.2
781.8261	12.6
855.5804	2.81
902.4211	1.17
1059.0641	1.63
1111.3915	0.412
1132.6002	13.9
1295.3845	0.894
1417.8417	0.954
1493.1237	1.28
3068.1786	1.29
3127.7471	0.997

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
60.4535	0.0774
123.4539	0.239
163.0200	0.00802
174.9235	0.0646
203.3775	0.162
221.5524	0.0412
237.8581	0.0257
269.6932	0.208
283.8118	0.381
311.7008	0.0858
346.1771	0.369
377.0188	0.0313
410.3049	0.301
526.3740	6.16
678.5594	12.6
757.3534	29.2
781.8256	12.6
855.5803	2.81
902.4203	1.17
1059.0634	1.63
1111.3907	0.412
1132.6003	13.9
1295.3841	0.894
1417.8413	0.954
1493.1237	1.28
3068.1795	1.29
3127.7480	0.997



$\Delta E = 0.20$ kcal mol^{-1}
Population = 0.264

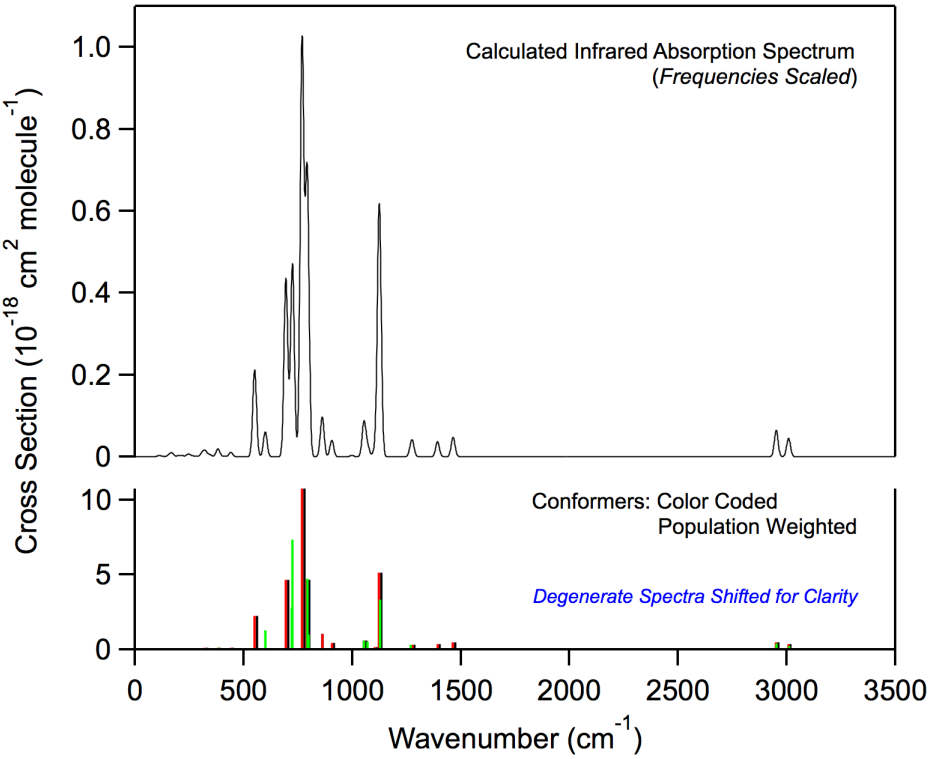
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.388191472821	0.005730190205	-1.361336314618
C	0.698820852543	-0.001189891342	0.019341041482
C	-0.871493953809	0.000318524067	-0.089909372472
H	1.095281229110	0.905825133656	-1.907570690550
F	2.740072504238	0.003985367931	-1.184369891806
H	1.094208648775	-0.888157003958	-1.917107087866
Cl	1.235972410131	1.452694665116	0.923961897128
Cl	1.234242485771	-1.465226723945	0.908484156528
Cl	-1.641759239828	-0.007756401542	1.514497037188
Cl	-1.417647648721	1.458495967688	-0.987243180778
Cl	-1.419362761030	-1.447583827877	-1.002697594236

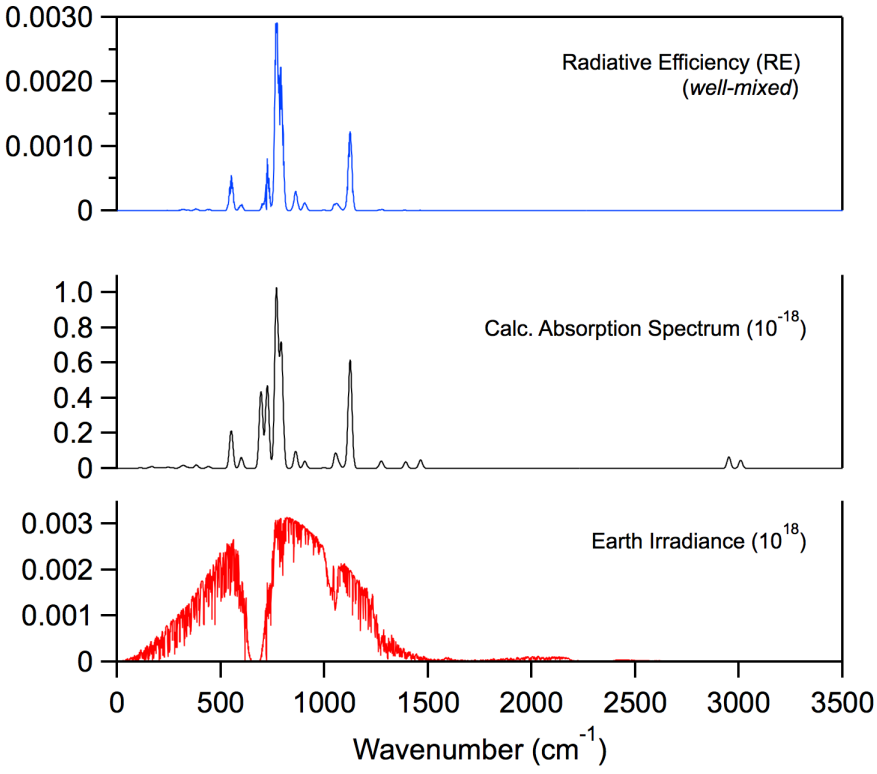
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
76.4397	0.0614
109.6562	0.345
154.1914	0.183
164.3835	0.0393
203.2056	0.0724
220.3380	0.0004
229.0646	0.0327
271.4123	0.0595
299.0049	0.209
300.1406	0.0768
346.0226	0.0613
350.3188	0.476
407.4570	0.0439
578.0795	4.91
708.4187	10.6
711.4143	27.8
782.1077	17.9
788.4061	3.75
1000.0102	0.271
1059.4882	2.29
1077.4946	1.95
1137.9402	12.6
1287.4533	1.16
1415.9447	0.296
1500.5478	0.373
3070.0812	1.59
3132.2430	0.943

Infrared Spectrum

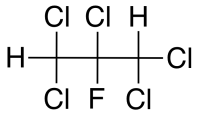


Radiative Efficiency



HCFC-231ba

Molecular Formula:	$CHCl_2CClFCHCl_2$
Name:	1,1,2,3,3-Pentachloro-2-fluoropropane
CAS number:	–
Molecular Weight:	234.31



Global Atmospheric Lifetime (years):	0.561
Tropospheric Atmospheric Lifetime (years):	0.586
Stratospheric Atmospheric Lifetime (years):	20
Ozone Depletion Potential (ODP):	0.015

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.181	0.114
Global Warming Potential (GWP_H):		
GWP_{20}	98	62
GWP_{100}	26	17
Global Temperature Potentials (GTP_H)		
GTP_{20}		19
GTP_{50}		3
GTP_{100}		2

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 1.0 \times 10^{-13}$; $k_{SAR}(272\ K) \approx 0.639 \times 10^{-13}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 0.570$ years

$\tau^{OH}_{Trop} = 0.586$ years

$\tau^{OH}_{Strat} = 20.8$ years

Fractional Atmospheric Loss: 0.986

$O(^1D)$ 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: 0.003

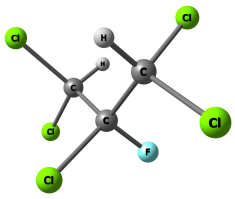
UV Photolysis

UV Spectrum: *No Recommendation*

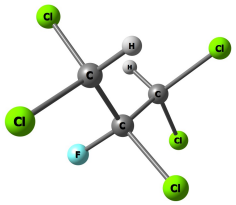
$\tau_{hv} = 50$ years

Fractional Atmospheric Loss: 0.011

Molecular Structure and Infrared Spectrum (2 conformers)



E = 0
Population = 0.50



E = 0
Population = 0.50

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.293446539647	0.286722013939	0.342957656643
C	0.017430622055	-0.367710245918	-0.250208833803
C	-1.217670171166	0.572084080202	-0.213253090420
Cl	2.710673965829	-0.768863649020	0.130905540570
Cl	1.599841812235	1.879379025237	-0.434494956779
H	1.164522083183	0.468947900870	1.405161197040
Cl	-0.310229029941	-1.881009878963	0.659609731592
F	0.239127444424	-0.670433651138	-1.544715647931
H	-0.986715846989	1.458513000473	-0.797502079171
Cl	-2.628364819772	-0.193485573896	-0.981295093753
Cl	-1.583862599506	1.122653978215	1.445617576012

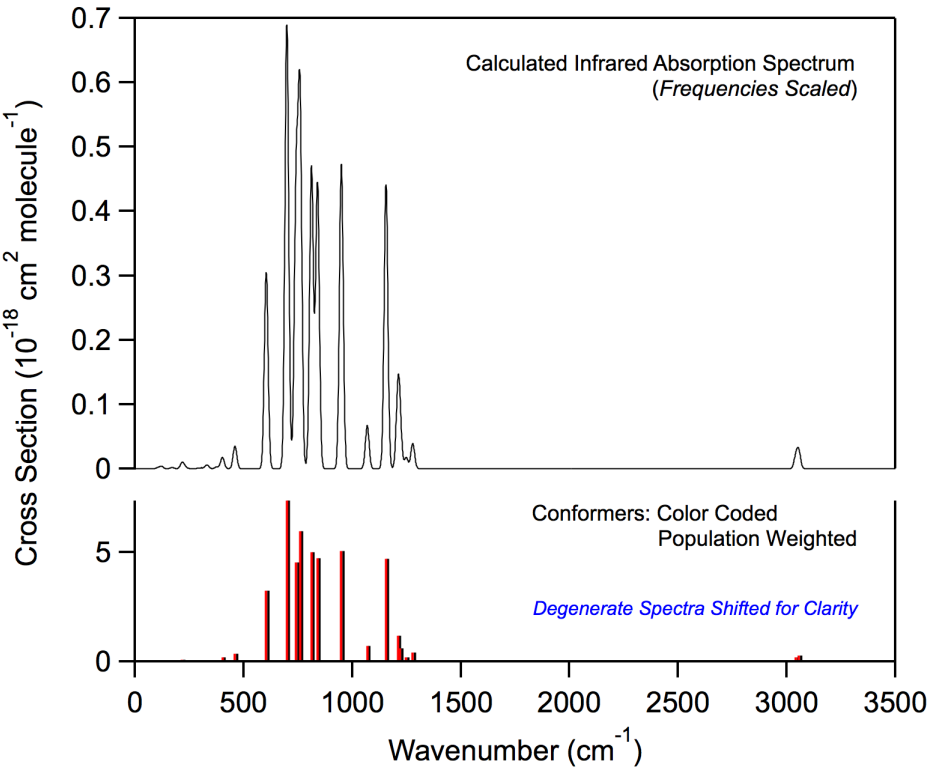
Atom	X	Y	Z
C	1.214976645865	0.576206204430	-0.199553674044
C	-0.023371762393	-0.358454856089	-0.253917540734
C	-1.294394285122	0.285047173591	0.361510650945
Cl	1.590856983562	1.084133041393	1.470715819268
Cl	2.619479234660	-0.174470424408	-0.993217266741
H	0.984166927808	1.477636876295	-0.760439297335
Cl	0.303625556634	-1.894973004148	0.616364599707
F	-0.252211947653	-0.628144069513	-1.554470837331
H	-1.159824422221	0.440356824845	1.427284583807
Cl	-1.599238506060	1.897533324326	-0.374577247581
Cl	-2.716079425080	-0.760431090722	0.130107210040

Infrared Absorption Spectrum (unscaled frequencies)

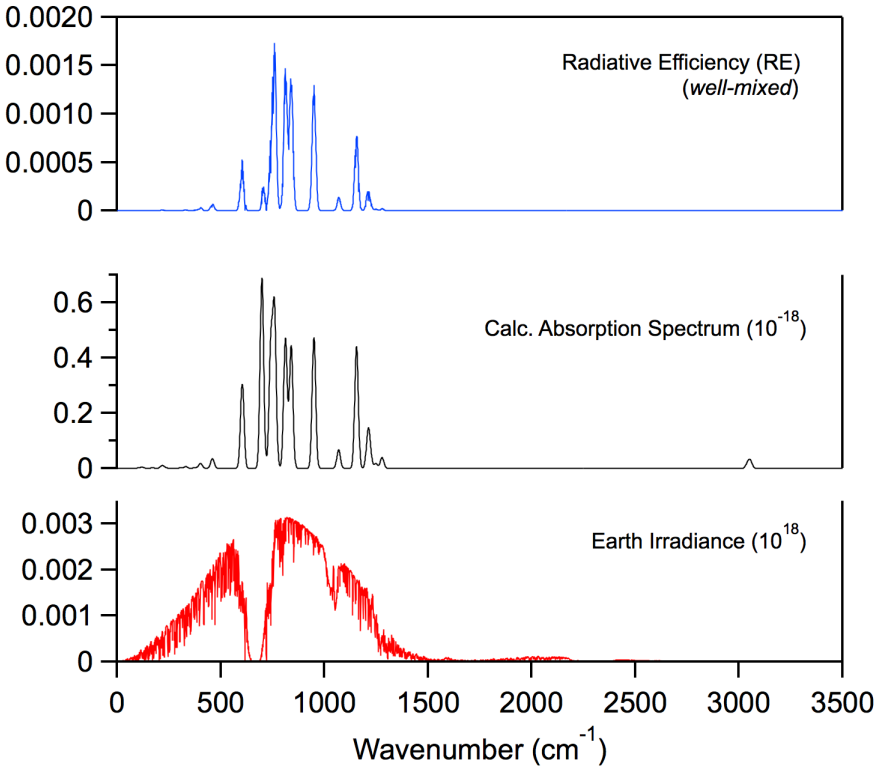
Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
54.7150	0.0325
71.9126	0.0800
123.8472	0.0390
172.7059	0.190
184.7215	0.0663
205.8868	0.00643
244.3748	0.00872
265.8590	0.0287
294.0057	0.128
341.5792	0.0602
369.3325	0.377
430.3263	0.746
582.7328	6.50
683.1235	14.7
728.5814	9.03
747.3163	11.9
803.2970	9.99
832.6731	9.44
948.8790	10.1
1075.1206	1.43
1166.5175	9.41
1224.8581	2.34
1234.5850	1.21
1265.0436	0.369
1296.9013	0.836
3164.3773	0.406
3178.8787	0.554

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
54.7149	0.0325
71.9125	0.0800
123.8472	0.0390
172.7058	0.190
184.7215	0.0663
205.8868	0.00643
244.3747	0.00872
265.8590	0.0287
294.0058	0.128
341.5792	0.0602
369.3326	0.377
430.3263	0.746
582.7328	6.50
683.1235	14.7
728.5814	9.03
747.3162	11.9
803.2971	9.99
832.6731	9.44
948.8790	10.1
1075.1204	1.43
1166.5175	9.41
1224.8584	2.34
1234.5853	1.21
1265.0440	0.369
1296.9016	0.836
3164.3770	0.406
3178.8784	0.554

Infrared Spectrum

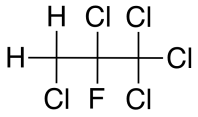


Radiative Efficiency



HCFC-231bb

Molecular Formula:	$CH_2ClCClFCCl_3$
Name:	1,1,1,2,3-Pentachloro-2-fluoropropane
CAS number:	421-94-3
Molecular Weight:	234.31



Global Atmospheric Lifetime (years):	2.54
Tropospheric Atmospheric Lifetime (years):	2.80
Stratospheric Atmospheric Lifetime (years):	26.9
Ozone Depletion Potential (ODP):	0.063

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.188	0.163
Global Warming Potential (GWP_H):		
GWP_{20}	458	397
GWP_{100}	124	108
Global Temperature Potentials (GTP_H)		
GTP_{20}		158
GTP_{50}		20
GTP_{100}		15

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 2.09 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 1.34 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 2.71$ years

$\tau^{OH}_{Trop} = 2.80$ years

$\tau^{OH}_{Strat} = 85.3$ years

Fractional Atmospheric Loss: 0.936

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: 0.014

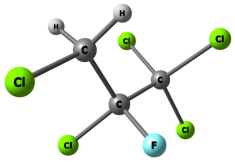
UV Photolysis

UV Spectrum: *No Recommendation*

$\tau_{hv} = 50$ years

Fractional Atmospheric Loss: 0.050

Molecular Structure and Infrared Spectrum (1 conformer)



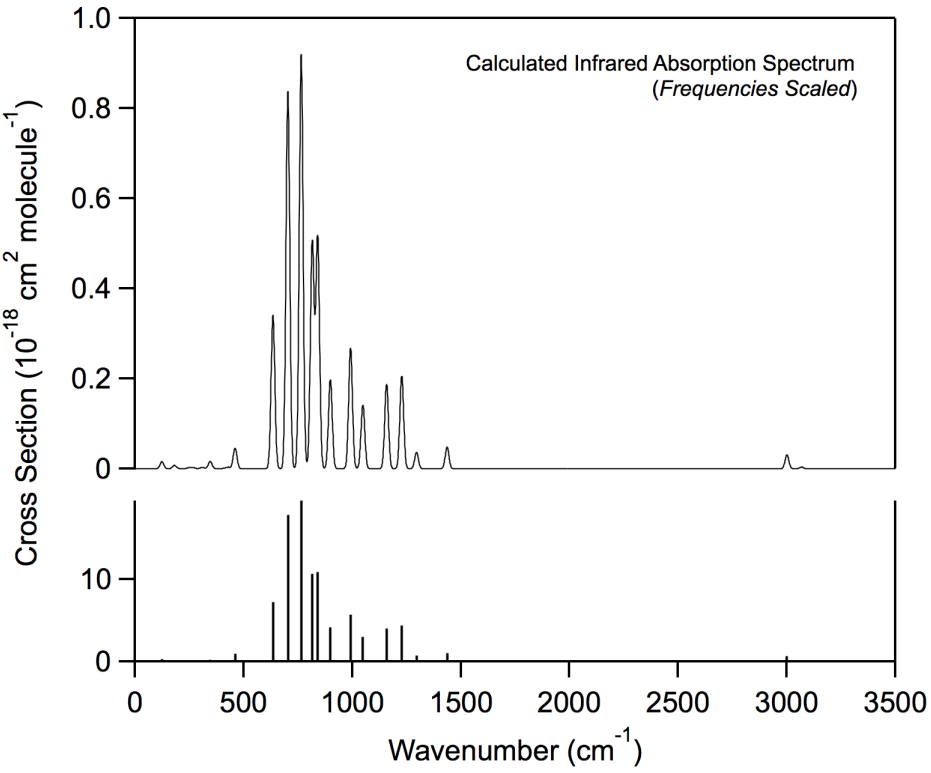
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.439060377619	0.809314759753	0.478644472410
C	0.489406962311	-0.136011314792	-0.270716775821
C	-1.029266438571	0.161444909053	0.040663379069
Cl	3.126706239334	0.625964554095	-0.085430371276
H	1.148639648253	1.840752962920	0.286987383871
H	1.413768272774	0.602837062429	1.545384782586
Cl	0.866088032884	-1.843044579888	0.152195129696
F	0.642561283390	0.014829682387	-1.600515837851
Cl	-2.076936689017	-0.955931636586	-0.865092799081
Cl	-1.353594455855	0.023828045428	1.791246146475
Cl	-1.401505233120	1.837800555202	-0.496496510077

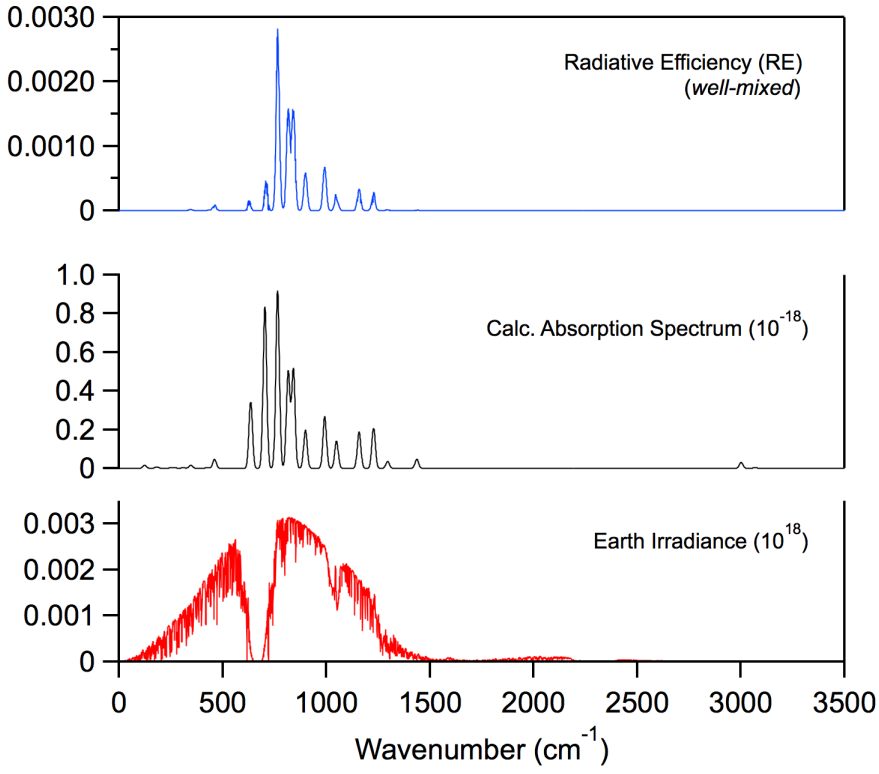
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
70.2500	0.00883
74.3847	0.321
135.1859	0.158
169.9173	0.0122
204.5170	0.0441
226.9933	0.0463
231.2661	0.00844
270.3779	0.0698
307.4863	0.105
310.3009	0.242
380.4991	0.0227
398.0207	0.0667
430.9206	0.975
615.6614	7.27
688.3597	17.8
753.1451	19.6
807.0805	10.7
833.6008	10.9
895.3612	4.20
993.8087	5.69
1053.8556	3.01
1169.4370	4.00
1243.4200	4.38
1315.3123	0.764
1464.3260	1.01
3120.9475	0.656
3192.6239	0.0766

Infrared Spectrum

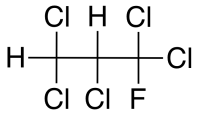


Radiative Efficiency



HCFC-231da

Molecular Formula:	$CHCl_2CHClCCl_2F$
Name:	1,1,2,3,3-Pentachloro-1-fluoropropane
CAS number:	1538604-31-7
Molecular Weight:	234.31



Global Atmospheric Lifetime (years):	0.535
Tropospheric Atmospheric Lifetime (years):	0.557
Stratospheric Atmospheric Lifetime (years):	20
Ozone Depletion Potential (ODP):	0.015

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.220	0.136
Global Warming Potential (GWP_H):		
GWP_{20}	113	70
GWP_{100}	31	19
Global Temperature Potentials (GTP_H)		
GTP_{20}		22
GTP_{50}		3
GTP_{100}		3

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 1.05 \times 10^{-13}$; $k_{SAR}(272\ K) \approx 0.672 \times 10^{-13}$ cm^3 $molecule^{-1}$ s^{-1}

τ^{OH}_{Global} = 0.542 years
τ^{OH}_{Trop} = 0.557 years
τ^{OH}_{Strat} = 20 years

Fractional Atmospheric Loss: 0.986

O(^{1}D) Reactivity

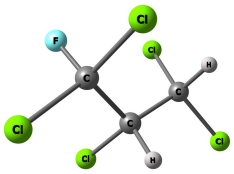
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 2.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)}$ = 185 years
Fractional Atmospheric Loss: 0.003

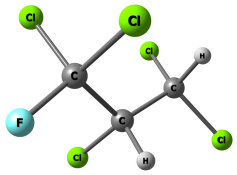
UV Photolysis

UV Spectrum: *No Recommendation*
τ_{hv} = 50 years
Fractional Atmospheric Loss: 0.011

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.815



$\Delta E = 1.19$ kcal mol^{-1}
Population = 0.109

Optimized Coordinates (Angstroms)

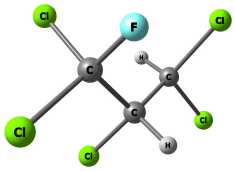
Atom	X	Y	Z
C	1.283876560104	-0.534139272085	-0.356727938473
C	0.085523824683	0.433297827854	-0.398874704872
C	-1.258929505019	-0.188296401119	0.063327380267
Cl	2.672255069401	0.191642958590	-1.230452532891
Cl	1.751800243027	-1.037080001574	1.288367064754
H	1.033361583573	-1.441366912153	-0.898611312892
H	-0.045333722772	0.734464596215	-1.438460876259
Cl	0.405565557023	1.920925365576	0.542287155500
Cl	-2.613733940697	0.933323433404	-0.286175533697
Cl	-1.561401096689	-1.728691309480	-0.835956300149
F	-1.259776572634	-0.460364285227	1.364359598713

Atom	X	Y	Z
C	1.153924317845	-0.607455547292	-0.362493009861
C	0.165699459377	0.567909939624	-0.448917472963
C	-1.341239099736	0.230040102830	-0.301849508580
Cl	2.696464780265	-0.134244909450	-1.155019131411
Cl	1.462423493343	-1.213488983728	1.283163204094
H	0.767590157161	-1.444764348317	-0.937592570497
H	0.247024252484	0.965049077093	-1.462778706049
Cl	0.592056333543	1.915453956311	0.644878825307
Cl	-1.781117279027	-1.011170309306	-1.545765265401
Cl	-1.845836620691	-0.333539888061	1.306738162848
F	-2.033584794564	1.337209910296	-0.592569527488

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
40.8233	0.0343
74.7083	0.0248
133.9367	0.164
174.0697	0.0321
179.7705	0.0370
200.9141	0.00359
250.9059	0.00915
263.3737	0.129
308.3238	0.394
324.9592	0.109
381.0101	0.258
456.4545	0.560
563.3632	5.74
660.7377	6.88
694.6234	17.0
761.0813	24.7
816.1272	1.24
853.6778	14.4
960.5322	7.26
1029.5279	9.82
1183.4321	12.4
1223.0862	0.463
1243.3936	7.47
1294.6278	1.95
1322.5008	1.71
3125.6713	0.567
3165.9095	0.217

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
34.6325	0.0378
77.9318	0.0361
137.7897	0.138
159.6725	0.0625
172.3316	0.00400
204.0008	0.0335
247.9290	0.0557
253.4835	0.216
309.0180	0.161
357.5308	0.0940
384.2491	0.166
475.4988	0.821
577.4360	4.31
623.1212	10.1
687.7040	6.63
761.8685	7.84
770.1355	22.2
851.5139	19.2
1027.9762	7.14
1050.6802	8.10
1145.6901	16.1
1222.4165	1.92
1238.2026	3.64
1296.2475	1.89
1322.6354	0.816
3105.6009	0.683
3158.1052	0.294



$\Delta E = 1.55$ kcal mol^{-1}
Population = 0.060

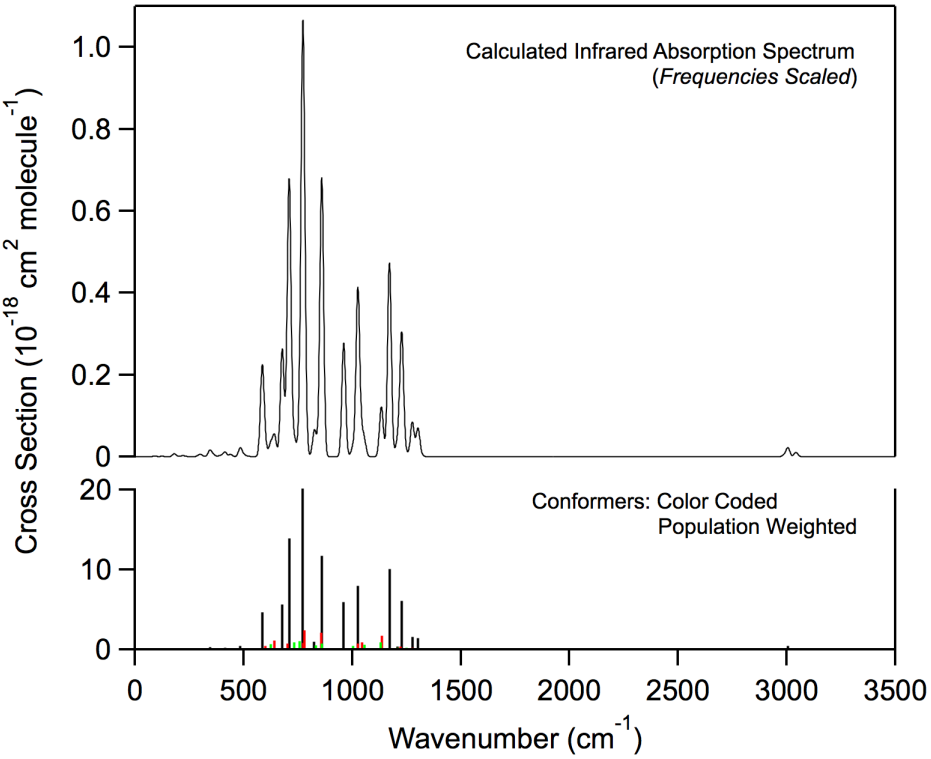
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.389610266777	-0.142471666188	0.306396151334
C	0.123717025189	0.396741839357	-0.397760477803
C	-1.174870756232	-0.430280019640	-0.165923861494
Cl	1.722827661260	-1.864257301748	-0.056675018455
Cl	2.814127844860	0.834843864623	-0.178140082694
H	1.294014299972	-0.056702694148	1.385390697115
H	0.285134795002	0.423408656454	-1.476755635517
Cl	-0.126778476042	2.084134065579	0.156792768485
Cl	-1.506930139687	-0.683631712437	1.577916438082
Cl	-2.581507670206	0.366364797036	-0.945385710474
F	-1.046220850893	-1.626889828889	-0.748933268581

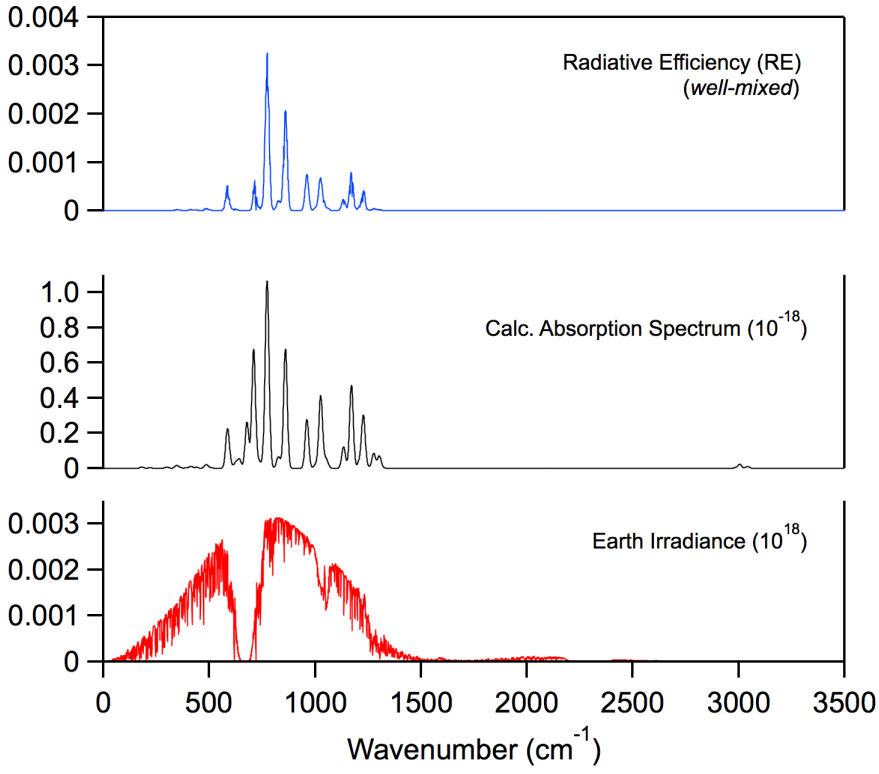
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
38.2477	0.0200
63.5897	0.0191
143.3913	0.0889
175.5582	0.0376
191.2742	0.0712
214.2850	0.0339
252.9486	0.0572
277.4636	0.0297
334.0707	0.133
358.7728	0.872
378.5498	0.288
408.7574	1.96
496.0735	0.365
604.2688	11.2
718.7911	15.6
745.0341	18.2
823.7948	8.48
852.5661	12.8
1004.9396	7.69
1062.2807	9.56
1140.9208	15.3
1202.4965	0.674
1222.6146	3.37
1265.0933	3.22
1341.4294	1.08
3116.9042	0.368
3164.4429	0.355

Infrared Spectrum

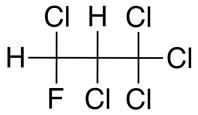


Radiative Efficiency



HCFC-231db

Molecular Formula:	$CHClFCHClCCl_3$
Name:	1,1,1,2,3-Pentachloro-3-fluoropropane
CAS number:	1943659-45-7
Molecular Weight:	234.31



Global Atmospheric Lifetime (years):	1.34
Tropospheric Atmospheric Lifetime (years):	1.43
Stratospheric Atmospheric Lifetime (years):	21.3
Ozone Depletion Potential (ODP):	0.036

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.183	0.144
Global Warming Potential (GWP_H):		
GWP_{20}	236	186
GWP_{100}	64	50
Global Temperature Potentials (GTP_H)		
GTP_{20}		63
GTP_{50}		9
GTP_{100}		7

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 4.09 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 2.61 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 1.39$ years

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

$\tau^{OH}_{Strat} = 46.6$ years

Fractional Atmospheric Loss: 0.966

$O(^1D)$ 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: 0.007

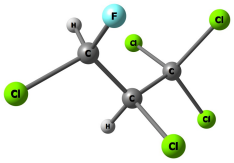
UV Photolysis

UV Spectrum: *No Recommendation*

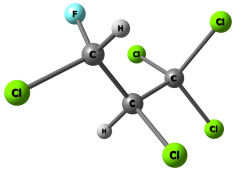
$\tau_{hv} = 50$ years

Fractional Atmospheric Loss: 0.027

Molecular Structure and Infrared Spectrum (2 conformers)



E = 0
Population = 0.862



$\Delta E = 1.17$ kcal mol^{-1}
Population = 0.120

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.441863031805	-0.744631276653	0.020575532322
C	0.387906302783	0.286932584835	-0.430833794235
C	-1.078028547723	-0.140190227384	-0.134499835853
Cl	2.997848538733	-0.436841143189	-0.834179446433
F	1.650322603275	-0.690481513257	1.348441735378
H	1.143712500387	-1.754720891068	-0.260189265793
H	0.457030433907	0.396516049431	-1.512822845660
Cl	0.755949800157	1.882248785262	0.286597790070
Cl	-2.208384133602	1.081278799737	-0.790427131967
Cl	-1.384495413545	-1.693836261244	-1.009290322668
Cl	-1.392091116176	-0.377191906471	1.601035584838

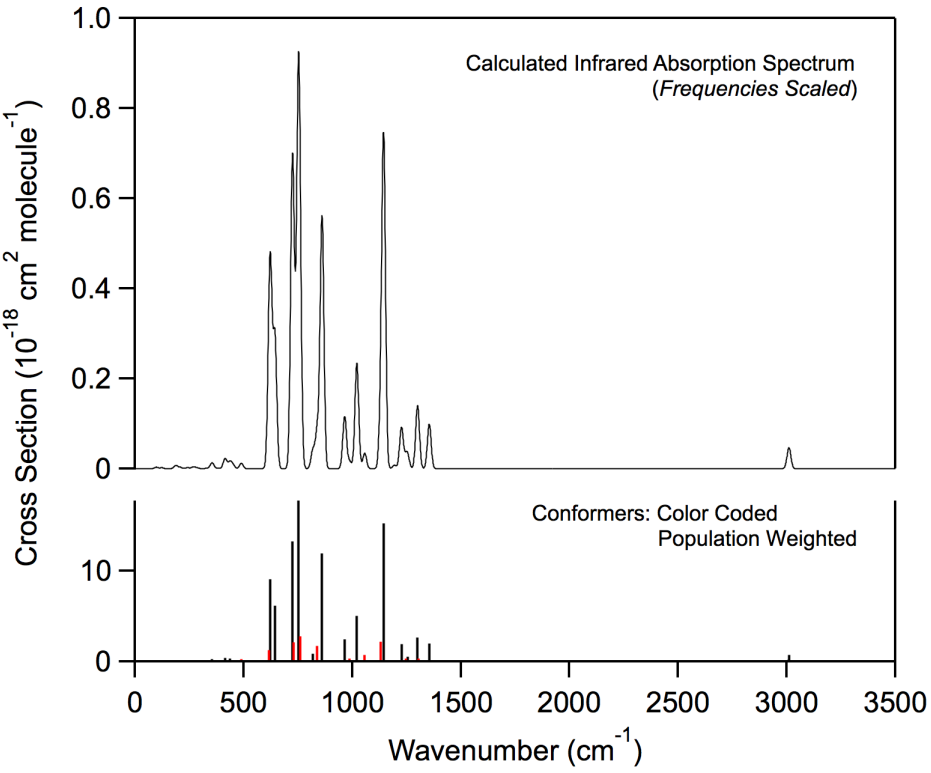
Atom	X	Y	Z
C	-1.489959244093	0.521355632868	0.362430343741
C	-0.404350708674	-0.279337446080	-0.397492420594
C	1.059485541247	0.141739031219	-0.074382476342
Cl	-3.089830543333	0.255427938199	-0.419266624686
H	-1.578949076956	0.172345353226	1.391110408097
F	-1.235646082826	1.845379090359	0.356378115460
H	-0.537088998482	-0.170897611082	-1.473806634065
Cl	-0.683816620165	-2.006806573777	0.001388591493
Cl	2.215336907487	-1.013490495579	-0.807218679470
Cl	1.382920796223	1.748784417233	-0.805043638354
Cl	1.336341029573	0.215435663415	1.693315014720

Infrared Absorption Spectrum (unscaled frequencies)

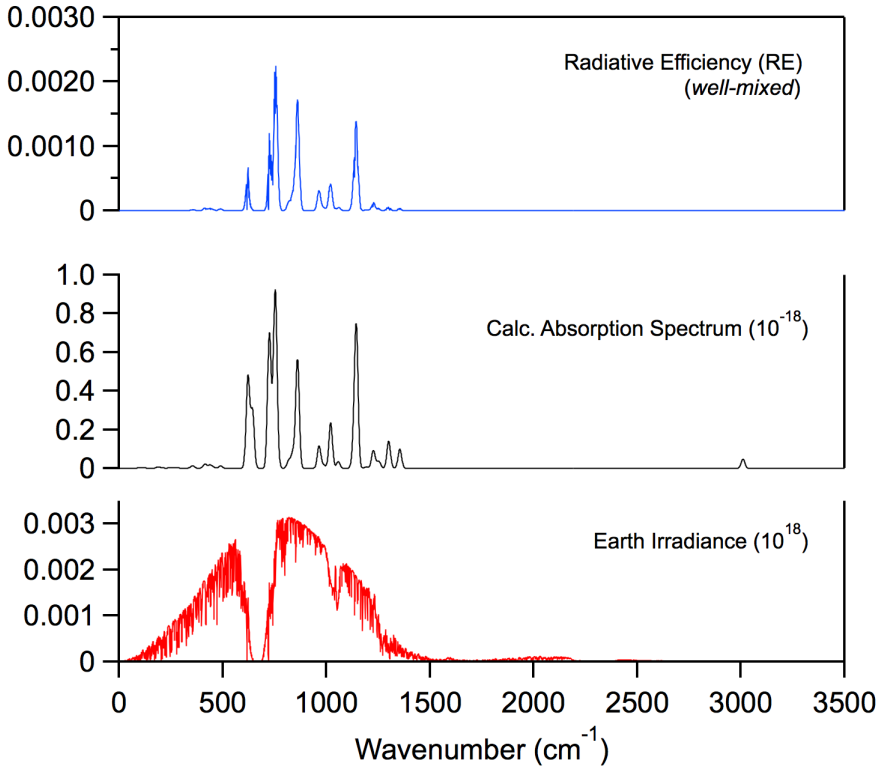
Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
46.6223	0.0746
73.5809	0.0509
142.1207	0.168
163.2939	0.0741
198.6409	0.0430
212.6027	0.00809
227.3289	0.0825
244.2468	0.0506
296.5964	0.00687
318.9426	0.325
381.4357	0.476
406.1862	0.364
602.3773	10.5
625.0685	7.16
710.1726	15.4
740.1300	20.5
809.8952	1.00
854.6848	13.8
964.9426	2.87
1024.2741	5.81
1155.1206	17.6
1242.0054	2.25
1271.9691	0.649
1319.9840	3.10
1377.0619	2.34
3127.3422	0.234
3131.8485	0.825

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
48.4996	0.0522
63.3833	0.0257
142.2009	0.0695
171.2014	0.0295
198.1313	0.0898
218.0632	0.0103
228.7135	0.0323
274.0364	0.0891
295.9913	0.112
349.6159	0.207
387.2459	0.609
420.9704	1.36
461.3133	2.16
596.2182	10.2
717.5312	17.7
748.3505	23.1
831.1225	14.0
839.9401	0.937
989.3790	2.83
1062.5660	6.09
1141.4307	18.4
1207.6372	1.38
1262.9892	2.76
1324.3916	2.94
1383.9731	1.07
3125.1406	0.739
3135.9833	0.334

Infrared Spectrum

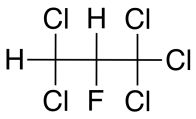


Radiative Efficiency



HCFC-231ea

Molecular Formula:	$CHCl_2CHFCCl_3$
Name:	1,1,1,3,3-Pentachloro-2-fluoropropane
CAS number:	–
Molecular Weight:	234.31



Global Atmospheric Lifetime (years):	0.762
Tropospheric Atmospheric Lifetime (years):	0.799
Stratospheric Atmospheric Lifetime (years):	20
Ozone Depletion Potential (ODP):	0.021

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.190	0.131
Global Warming Potential (GWP_H):		
GWP_{20}	139	96
GWP_{100}	38	26
Global Temperature Potentials (GTP_H)		
GTP_{20}		30
GTP_{50}		4
GTP_{100}		4

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 7.34 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 4.68 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 0.777$ years

$\tau^{OH}_{Trop} = 0.799$ years

$\tau^{OH}_{Strat} = 27.6$ years

Fractional Atmospheric Loss: 0.981

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: 0.004

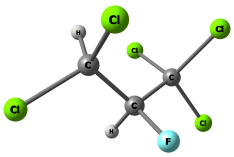
UV Photolysis

UV Spectrum: *No Recommendation*

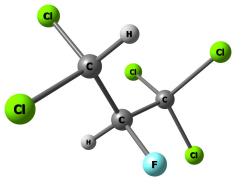
$\tau_{hv} = 50$ years

Fractional Atmospheric Loss: 0.015

Molecular Structure and Infrared Spectrum (2 conformers)



E = 0
Population = 0.805



$\Delta E = 0.85$ kcal mol^{-1}
Population = 0.193

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.448918592837	0.031176415140	0.467681228948
C	0.240648900856	-0.722788401833	-0.135861966740
C	-1.159162968200	-0.103550523793	0.145148579978
Cl	2.765252644428	-1.158133882610	0.778167441301
Cl	2.045373374858	1.342076993356	-0.579282456763
H	1.200289953129	0.466742104598	1.430546996230
H	0.211941287707	-1.714636280602	0.326372257611
F	0.395381135255	-0.859648510739	-1.476590291769
Cl	-2.383418362621	-1.208133492679	-0.558319933931
Cl	-1.397567514732	-0.031817616329	1.926096791015
Cl	-1.365064043519	1.514765195491	-0.559786645880

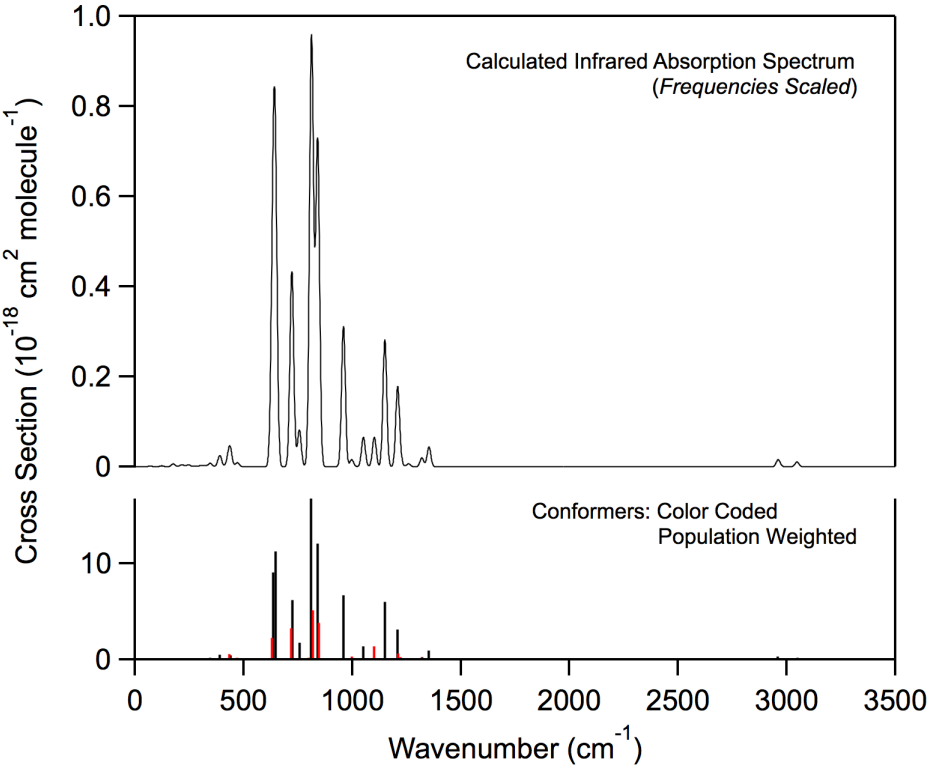
Atom	X	Y	Z
C	1.488350302569	0.065158983878	0.351529775144
C	0.251996738347	0.582311101818	-0.417325536307
C	-1.139265041127	-0.013438098192	-0.030132555426
Cl	1.848057241207	-1.658633428338	0.082969402183
Cl	2.899567894214	1.062516699572	-0.136468817913
H	1.357150166475	0.210798829525	1.420310269242
H	0.385847444781	0.436867786700	-1.493758497411
F	0.186471875841	1.918647839058	-0.135763730386
Cl	-2.396751189162	1.036345772349	-0.765317713518
Cl	-1.358529238037	-1.660864114774	-0.673432233029
Cl	-1.352393195108	-0.012666371597	1.749547637420

Infrared Absorption Spectrum (unscaled frequencies)

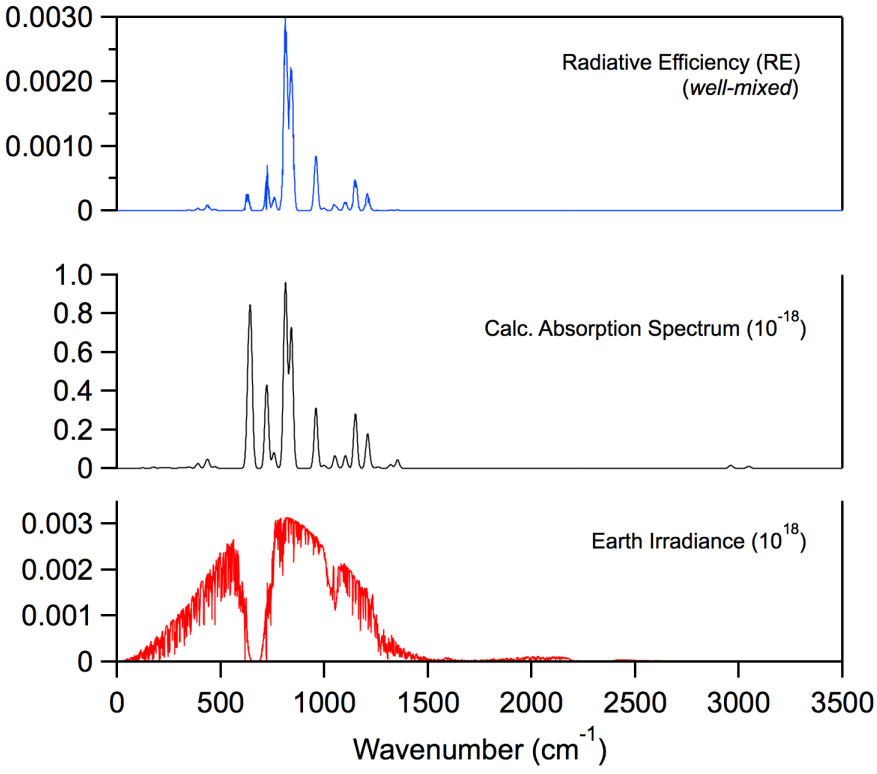
Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
17.4836	0.0304
73.0842	0.0487
129.0578	0.157
169.0293	0.0874
193.2119	0.0229
205.3882	0.0915
236.3979	0.0228
260.9175	0.0379
286.0790	0.0554
309.9746	0.198
356.6412	0.635
408.7144	0.537
617.3990	11.3
627.9581	14.0
708.9577	7.71
744.3417	2.15
801.9563	20.8
832.3044	15.0
959.1227	8.28
1056.2665	1.72
1160.8790	7.47
1222.8438	3.91
1276.0315	0.176
1341.4744	0.319
1376.0450	1.17
3076.9697	0.361
3171.1161	0.233

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
16.8915	0.0245
76.3253	0.0235
135.2892	0.0521
172.1921	0.0570
181.2818	0.141
210.7884	0.0229
265.2228	0.125
277.1095	0.0828
294.1335	0.0278
347.0382	0.158
391.2984	0.528
402.7386	3.05
442.2463	0.989
610.1803	11.7
704.8253	16.8
788.1773	1.10
810.3109	26.5
837.9277	19.6
999.4795	1.73
1072.2106	0.123
1109.5570	7.25
1224.8868	3.22
1238.7018	1.16
1340.7756	0.823
1360.8393	0.0123
3085.2657	0.336
3163.7745	0.263

Infrared Spectrum

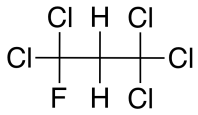


Radiative Efficiency



HCFC-231fa

Molecular Formula:	$CCl_2FCH_2CCl_3$
Name:	1,1,1,3,3-Pentachloro-3-fluoropropane
CAS number:	313696-58-1
Molecular Weight:	234.31



Global Atmospheric Lifetime (years):	6.26
Tropospheric Atmospheric Lifetime (years):	7.71
Stratospheric Atmospheric Lifetime (years):	33.2
Ozone Depletion Potential (ODP):	0.143

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.228	0.213
Global Warming Potential (GWP_H):		
GWP_{20}	1313	1226
GWP_{100}	371	346
Global Temperature Potentials (GTP_H)		
GTP_{20}		755
GTP_{50}		83
GTP_{100}		49

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 7.60 \times 10^{-15}$; $k_{SAR}(272\ K) \approx 4.85 \times 10^{-15}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 7.44$ years

$\tau^{OH}_{Trop} = 7.71$ years

$\tau^{OH}_{Strat} = 212.5$ 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

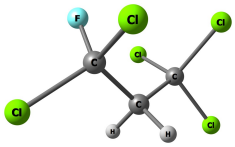
UV Photolysis

UV Spectrum: *No Recommendation*

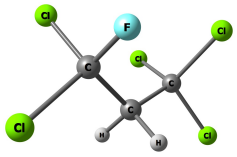
$\tau_{hv} = 50$ years

Fractional Atmospheric Loss: 0.125

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.364



$\Delta E = 0.09$ kcal mol^{-1}
Population = 0.314

Optimized Coordinates (Angstroms)

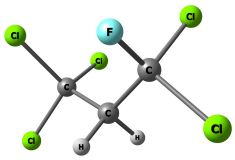
Atom	X	Y	Z
C	-1.418807363469	0.102565524614	0.125277429808
C	-0.137084345612	0.688930122500	-0.502978106699
C	1.226772330736	0.171366678435	-0.006634211112
Cl	-1.956617684826	-1.405370695944	-0.692551503086
F	-1.274396748412	-0.162235422033	1.425329439112
Cl	-2.736299752923	1.329544275391	-0.046442323951
H	-0.134768797901	1.763776231378	-0.314241784461
H	-0.193415279934	0.535297762605	-1.580809511081
Cl	2.471709785688	0.915367540830	-1.084005418934
Cl	1.553467018991	0.713414657638	1.672131964065
Cl	1.391502837662	-1.603725675414	-0.092699973662

Atom	X	Y	Z
C	-1.430676794744	-0.196956835573	0.197198130347
C	-0.137307394247	-0.679590736942	-0.480557286271
C	1.232783080513	-0.094431682965	-0.077846771359
Cl	-2.790435726617	-1.110520041987	-0.581228740219
F	-1.441124622646	-0.508069846664	1.497525665473
Cl	-1.761225279752	1.552839751573	0.043616813740
H	-0.242444374325	-0.549573804096	-1.558089349133
H	-0.093742634654	-1.751278705268	-0.271526412703
Cl	2.472693492008	-1.187788322487	-0.814606782487
Cl	1.500290664380	1.547014331167	-0.739423720570
Cl	1.485679590084	-0.068565106758	1.690834453181

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
23.6568	0.00611
92.6529	0.0896
131.9433	0.0966
180.4567	0.00603
197.8655	0.00460
219.6004	0.0561
271.1610	0.0356
287.0127	0.0238
306.0370	0.0666
348.8099	0.0544
384.2920	0.359
394.7431	0.335
454.0414	0.731
575.2491	8.12
638.9491	17.7
687.2565	25.2
729.6342	4.29
838.1121	15.5
941.8271	7.62
1024.3873	25.3
1061.6739	15.0
1193.3818	16.3
1288.0961	1.05
1361.1559	1.61
1450.9189	1.04
3097.0622	0.106
3155.0647	0.0792

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
16.9421	0.0005
116.0262	0.0906
129.1925	0.124
179.6473	0.00691
196.3793	0.00845
212.2959	0.0613
265.5789	0.0307
287.7860	0.0193
309.4843	0.0349
363.6957	0.0631
377.9534	0.331
396.4403	0.324
454.4599	0.885
575.8395	9.68
623.6692	16.6
705.6516	17.4
722.9689	7.28
848.1958	28.0
921.7741	1.39
1025.5117	17.8
1068.2392	17.4
1179.8841	18.6
1302.8436	1.08
1362.5752	1.17
1439.9188	0.778
3087.3477	0.0788
3151.5197	0.0840



$\Delta E = 0.09$ kcal mol^{-1}
Population = 0.314

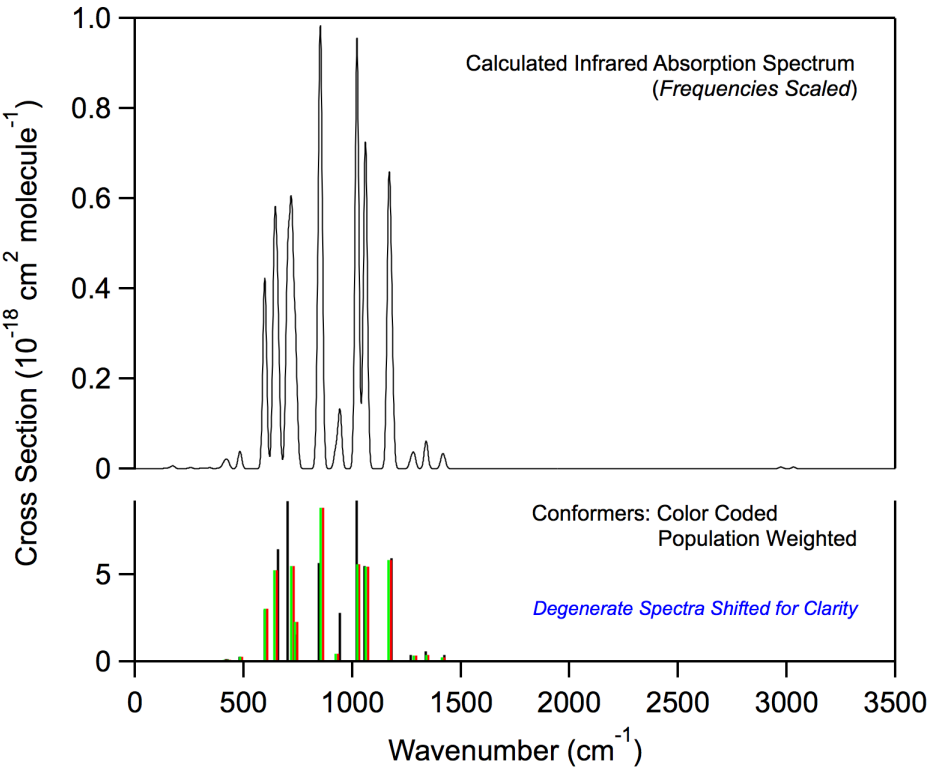
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.431292970601	0.189767006813	0.186784451980
C	-0.136803563105	0.680112391953	-0.483253255314
C	1.233135119257	0.094095225113	-0.081273519388
Cl	-1.758308113794	-1.559302699299	0.018103288725
F	-1.446083945038	0.490339110244	1.489546923426
Cl	-2.790381595132	1.107229063850	-0.588220051173
H	-0.095736624492	1.750148906032	-0.265440992005
H	-0.238567764504	0.558631346968	-1.562104485723
Cl	1.480913575361	0.054341422752	1.687874221623
Cl	1.505466108260	-1.541470228604	-0.755330093073
Cl	2.473261773789	1.195538454178	-0.805518489077

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
16.9442	0.0005
116.0244	0.0906
129.1919	0.124
179.6477	0.00691
196.3792	0.00845
212.2956	0.0613
265.5785	0.0307
287.7861	0.0193
309.4844	0.0349
363.6959	0.0631
377.9529	0.331
396.4402	0.324
454.4598	0.885
575.8396	9.68
623.6691	16.6
705.6517	17.4
722.9690	7.28
848.1958	28.0
921.7741	1.39
1025.5112	17.8
1068.2393	17.4
1179.8841	18.6
1302.8444	1.08
1362.5757	1.17
1439.9193	0.778
3087.3478	0.0788
3151.5196	0.0840

Infrared Spectrum



Radiative Efficiency