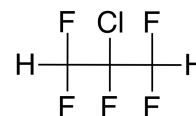


HCFC-235ba

Molecular Formula: CHF₂CClFCHF₂
 Name: 2-Chloro-1,1,2,3,3-pentafluoropropane
 CAS number: 144429-90-3
 Molecular Weight: 168.49



Global Atmospheric Lifetime (years): 8.80
 Tropospheric Atmospheric Lifetime (years): 9.50
 Stratospheric Atmospheric Lifetime (years): 120.7
 Ozone Depletion Potential (ODP): 0.018

	<i>Well-mixed</i>	<i>Lifetime adjusted</i>
Radiative Efficiency (RE):	0.237	0.225
Global Warming Potential (GWP _H):		
GWP ₂₀	2497	2371
GWP ₁₀₀	754	716
Global Temperature Potentials (GTP _H):		
GTP ₂₀		1698
GTP ₅₀		238
GTP ₁₀₀		102

* RE units: W m² ppb⁻¹
 * GWP and GTP: Relative to CO₂

Atmospheric Loss Processes *****

OH Reactivity

$k_{\text{Rec}}(T)$, *No recommendation*

$k_{\text{SAR}}(298 \text{ K}) = 6.18 \times 10^{-15}$; $k_{\text{SAR}}(272 \text{ K}) \approx 3.94 \times 10^{-15}$ cm³ molecule⁻¹ s⁻¹

$\tau_{\text{Global}}^{\text{OH}} = 9.16$ years

$\tau_{\text{Trop}}^{\text{OH}} = 9.50$ years

$\tau_{\text{Strat}}^{\text{OH}} = 256.3$ years

Fractional Atmospheric Loss: 0.961

O(¹D) Reactivity

$k_{\text{Rec}}(T)$, *No recommendation*

$k_{\text{Est}}(T) = 0.8 \times 10^{-10}$ cm³ molecule⁻¹ s⁻¹

$\tau_{\text{O}(\text{1D})} = 465$ years

Fractional Atmospheric Loss: 0.019

UV Photolysis

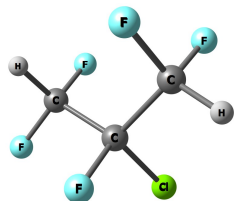
UV Spectrum: *No Recommendation*

$\tau_{\text{hv}} = 450$ years

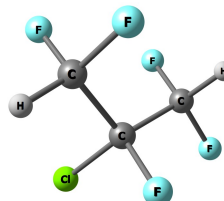
Fractional Atmospheric Loss: 0.020



Molecular Structure and Infrared Spectrum (8 conformers)



E = 0
Population = 0.208



E = 0
Population = 0.208

Optimized Coordinates (Angstroms)

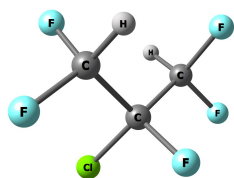
Atom	X	Y	Z
C	-1.467031469236	0.270179149498	0.069175415793
C	0.040837458546	0.255005559281	0.388317414028
C	0.722542485234	-1.088564067061	0.060615896299
F	-1.684669804377	0.168842686426	-1.249972816092
F	-2.024408792005	-0.804904437441	0.680471314269
H	-1.927126578989	1.185439472842	0.458591616125
F	0.154861410340	0.445182976995	1.726751954764
Cl	0.839316372463	1.598554636793	-0.473389924215
H	0.237034564664	-1.893711277910	0.623839904588
F	0.630388811650	-1.339584146655	-1.257397553608
F	2.019622541709	-1.022986552769	0.407685778049

Atom	X	Y	Z
C	-0.723071681020	-1.086812273211	0.091830244335
C	-0.040710223149	0.266231395112	0.376338058665
C	1.464807552707	0.273913533459	0.046025857180
F	-2.017706990599	-1.012762615145	0.446246635530
F	-0.640071657225	-1.375056306432	-1.219157582794
H	-0.232526433141	-1.875136008089	0.674163640842
F	-0.145357994488	0.494214519890	1.709622388140
Cl	-0.847033520051	1.583937719379	-0.517376465677
H	1.926543273665	1.200341553970	0.405977525301
F	2.027902069831	-0.782797406069	0.683554687142
F	1.673094603471	0.135391887135	-1.271249988664

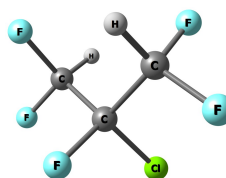
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
57.1543	0.222
93.4227	0.104
163.1140	0.167
180.6564	0.0236
205.4888	0.304
276.7971	0.677
316.1877	0.150
368.9063	0.169
405.6760	0.172
498.6965	2.53
555.3442	2.40
614.7273	1.35
651.9736	8.04
722.5337	9.45
1023.4615	12.8
1115.1657	6.63
1143.7606	2.69
1161.1562	9.80
1170.5091	32.4
1194.1807	23.5
1216.4335	15.0
1372.1594	4.96
1385.0621	1.15
1400.2822	4.72
1416.1111	4.39
3072.7648	3.01
3074.1936	3.53

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
57.1540	0.222
93.4224	0.104
163.1139	0.167
180.6564	0.0236
205.4887	0.304
276.7970	0.677
316.1878	0.150
368.9063	0.169
405.6761	0.172
498.6965	2.53
555.3442	2.40
614.7275	1.35
651.9735	8.04
722.5337	9.45
1023.4616	12.8
1115.1662	6.63
1143.7608	2.69
1161.1565	9.80
1170.5098	32.4
1194.1809	23.5
1216.4340	15.0
1372.1596	4.96
1385.0623	1.15
1400.2822	4.72
1416.1114	4.39
3072.7651	3.01
3074.1937	3.53



$\Delta E = 0.07 \text{ kcal mol}^{-1}$
Population = 0.184



$\Delta E = 0.07 \text{ kcal mol}^{-1}$
Population = 0.184

Optimized Coordinates (Angstroms)

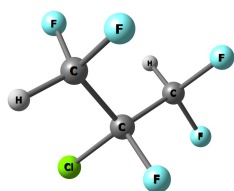
Atom	X	Y	Z
C	-1.305662641713	-0.345309868939	-0.462201430766
C	-0.028922528254	0.122245902643	0.262725143091
C	1.127855675303	-0.875708955073	0.070533433874
F	-1.571156507817	-1.610317997036	-0.048019011720
F	-2.333180378004	0.440897840445	-0.108674040755
H	-1.180273629966	-0.337712716459	-1.548631110219
F	-0.285536898034	0.198366825760	1.587339559167
Cl	0.428676683359	1.735657282822	-0.358286129166
H	0.876460346838	-1.828571234524	0.549617907660
F	1.321307864943	-1.073775749299	-1.252519549308
F	2.253863013346	-0.387290330340	0.611208228142

Atom	X	Y	Z
C	-1.128315501442	-0.873552066367	0.069070617139
C	0.030462192288	0.121637557376	0.263541557572
C	1.306180592929	-0.346678483804	-0.462692737716
F	-2.253282491767	-0.384226604938	0.611089725717
F	-1.322333260401	-1.068003256915	-1.254435591530
H	-0.878745634930	-1.828077600893	0.545792728897
F	0.287396386281	0.194020092479	1.588303397260
Cl	-0.424019248639	1.737461801003	-0.353473258676
H	1.180666623968	-0.336186386490	-1.549083926281
F	2.335299665780	0.436629032197	-0.107389642507
F	1.569221675935	-1.613215083649	-0.051628869875

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
70.3593	0.248
76.0770	0.225
149.3482	0.0366
190.5746	0.131
218.1148	0.787
259.3353	0.0705
313.1893	0.106
356.7546	0.357
391.1385	0.0330
490.4061	0.405
557.2585	2.95
587.1738	0.982
671.7187	11.9
820.6926	11.1
994.0288	16.0
1088.2122	7.50
1119.6419	10.6
1146.1630	19.4
1183.5684	12.9
1202.7036	18.9
1228.8481	18.2
1382.7034	2.48
1392.0345	4.23
1399.1475	1.00
1409.3815	6.30
3076.8110	2.78
3097.7746	2.74

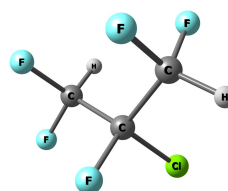
Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
70.3591	0.248
76.0771	0.225
149.3483	0.0366
190.5744	0.131
218.1147	0.787
259.3349	0.0705
313.1892	0.106
356.7546	0.357
391.1385	0.0330
490.4061	0.405
557.2585	2.95
587.1738	0.982
671.7185	11.9
820.6924	11.1
994.0285	16.0
1088.2117	7.50
1119.6427	10.6
1146.1636	19.4
1183.5685	12.9
1202.7034	18.9
1228.8481	18.2
1382.7034	2.48
1392.0345	4.23
1399.1475	1.00
1409.3814	6.30
3076.8109	2.78
3097.7741	2.74



$\Delta E = 0.62 \text{ kcal mol}^{-1}$
Population = 0.073

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-0.714036120065	-0.876783447020	-0.601840208939
C	-0.116126461896	0.199048338704	0.329411938031
C	1.404067501377	0.396728419890	0.154948485389
F	-0.119463386978	-2.055869410530	-0.326053408921
F	-2.029171504455	-0.995269206117	-0.348045860405
H	-0.557960713880	-0.621859596800	-1.654312056887
F	-0.347597308318	-0.145630627015	1.611612916182
Cl	-0.918797610615	1.767942117435	-0.024007752756
H	1.751437011577	1.262016535212	0.730139219489
F	2.047191354096	-0.707901296615	0.573372396810
F	1.672159239156	0.583017172858	-1.156621667992



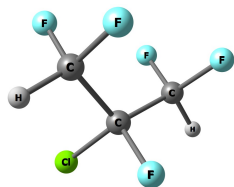
$\Delta E = 0.62 \text{ kcal mol}^{-1}$
Population = 0.073

Atom	X	Y	Z
C	-1.415720935875	0.354615250300	0.159331213075
C	0.109541787895	0.197993341585	0.331223753887
C	0.736049352701	-0.854878492535	-0.607439463355
F	-1.690215916647	0.541800535397	-1.150786322165
F	-2.027588502469	-0.770053038564	0.571195229862
H	-1.786318930834	1.206254921880	0.740365100730
F	0.351787968951	-0.148350480836	1.610983105141
Cl	0.868102158334	1.790746304029	-0.012781775646
H	0.571885069474	-0.597639759083	-1.658115927421
F	2.054223393398	-0.938515893442	-0.355539949903
F	0.174641555073	-2.051722688732	-0.338730964206

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
53.3879	0.158
88.7972	0.122
162.3382	0.0713
191.0967	0.0677
221.7504	0.632
268.8932	0.228
314.4802	0.108
338.5426	0.399
409.8868	0.416
470.6391	1.17
539.7833	3.84
582.2893	1.21
692.0436	6.21
839.7640	8.13
926.5278	24.9
1120.7876	2.37
1140.5571	13.6
1152.4393	17.8
1158.7433	11.3
1204.3411	16.4
1228.8828	27.5
1383.4936	2.36
1388.4348	1.29
1404.4598	5.04
1417.8659	4.03
3076.4819	3.29
3092.5353	2.92

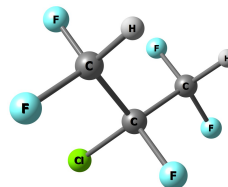
Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
53.3879	0.158
88.7967	0.122
162.3369	0.0713
191.0962	0.0677
221.7505	0.632
268.8931	0.228
314.4799	0.108
338.5428	0.399
409.8865	0.416
470.6395	1.17
539.7833	3.84
582.2892	1.21
692.0438	6.21
839.7642	8.13
926.5272	24.9
1120.7880	2.37
1140.5565	13.6
1152.4392	17.8
1158.7439	11.3
1204.3423	16.4
1228.8836	27.5
1383.4941	2.36
1388.4355	1.29
1404.4605	5.04
1417.8666	4.03
3076.4823	3.29
3092.5354	2.92



$\Delta E = 0.74 \text{ kcal mol}^{-1}$
Population = 0.060

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	0.326849302034	-1.316607298907	-0.021453699311
C	-0.312224868519	0.009870627247	0.444858471285
C	0.353040404347	1.308428583328	-0.061675389661
F	0.313654606188	-1.397128106108	-1.362694844677
F	1.604777797566	-1.358633895454	0.404245685370
H	-0.224991501592	-2.161929943809	0.407334452931
F	-0.250154518467	0.029969807745	1.797064541910
Cl	-2.033215289210	0.019253184741	-0.063466266514
H	-0.181712296497	2.177330912821	0.340824930206
F	1.631673592096	1.337991462600	0.362953731846
F	0.341071772054	1.348053665797	-1.404758613385



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

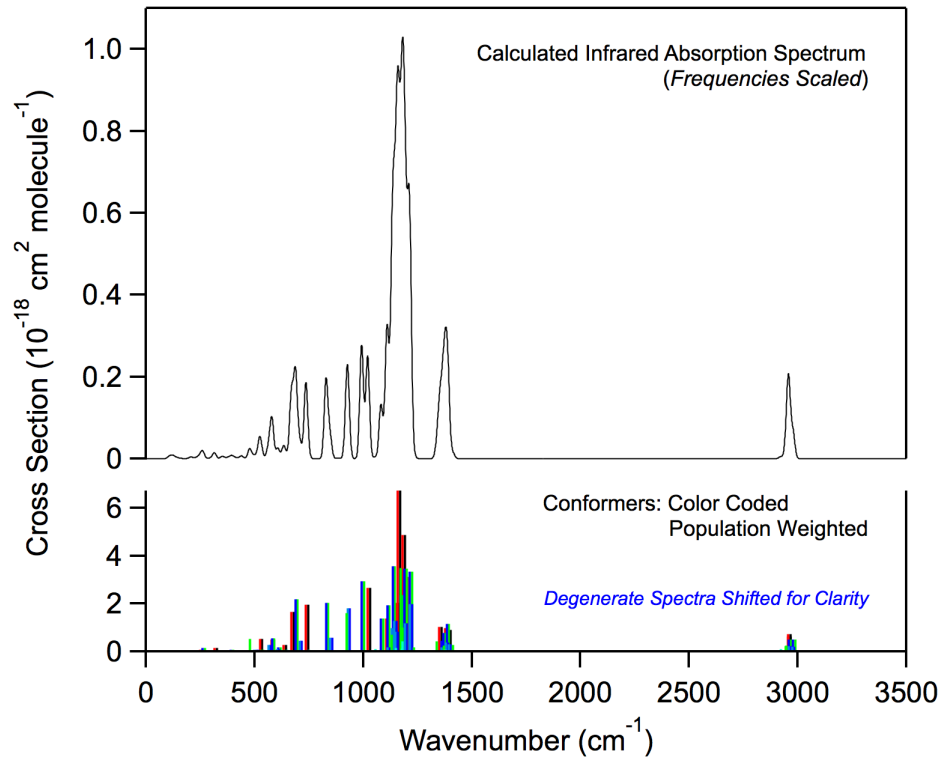
Atom	X	Y	Z
C	-1.285668758488	-0.573138159492	0.469170308053
C	-0.000076251672	0.267294838205	0.326539503122
C	1.286136724811	-0.572715173239	0.466033692683
F	-2.352576917047	0.241028460541	0.411563015970
F	-1.367722385902	-1.479761051120	-0.519099498080
H	-1.286683652370	-1.090338016340	1.439294088169
F	0.001037400432	1.149830947168	1.358738028727
Cl	-0.002109816483	1.146329863976	-1.222466857148
H	1.289687252668	-1.089916270651	1.436150859081
F	1.366079233648	-1.479309320445	-0.522435496561
F	2.352633170402	0.241802881398	0.405827355984

Infrared Absorption Spectrum (unscaled frequencies)

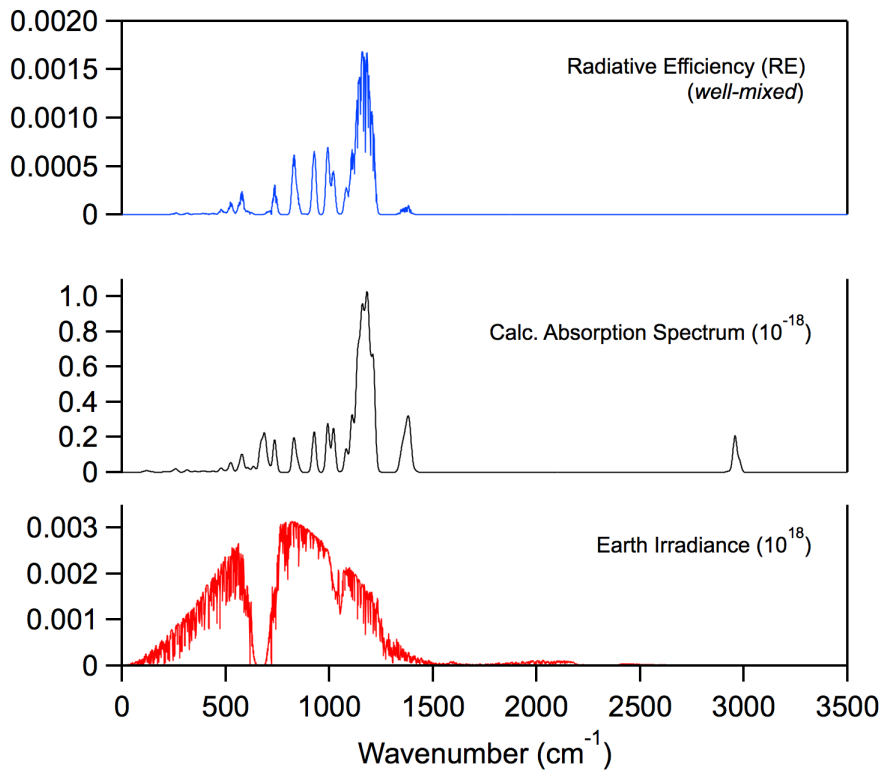
Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
31.2471	0.000
110.8590	0.367
176.3958	0.0151
179.0589	0.0137
206.1006	0.113
303.0512	0.0478
318.7362	0.168
379.7199	0.395
413.0409	0.317
448.5807	8.78
514.5006	1.07
583.6543	0.303
616.3454	1.32
878.7775	0.525
919.9141	26.8
1123.5940	0.253
1141.6752	11.7
1151.0944	0.0785
1183.8259	58.8
1193.5312	17.0
1248.8471	2.81
1359.1858	7.17
1385.8079	0.00317
1396.4151	4.22
1439.3425	4.71
3060.3137	3.74
3064.0134	4.09

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
50.1133	0.0889
85.7658	0.148
162.4308	0.119
185.1109	0.0957
212.8539	0.404
255.3949	0.222
338.1980	0.0993
364.8406	0.0404
370.9388	0.564
550.3077	0.166
556.9043	2.37
609.6556	5.70
632.4898	8.93
735.7151	7.84
1060.6393	9.36
1086.5493	5.24
1155.2532	3.38
1161.7609	16.1
1191.7630	12.5
1193.5421	43.2
1211.8328	3.57
1371.6782	2.92
1399.1382	7.07
1402.8040	7.52
1412.8976	2.59
3026.3582	0.194
3036.7616	10.4

Infrared Spectrum

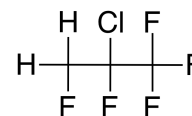


Radiative Efficiency



HCFC-235bb

Molecular Formula: CH₂FCClF₂
 Name: 2-Chloro-1,1,1,2,3-pentafluoropropane
 CAS number: 230956-35-1
 Molecular Weight: 168.49



Global Atmospheric Lifetime (years): 7.21
 Tropospheric Atmospheric Lifetime (years): 7.71
 Stratospheric Atmospheric Lifetime (years): 110.0
 Ozone Depletion Potential (ODP): 0.017

	<i>Well-mixed</i>	<i>Lifetime adjusted</i>
Radiative Efficiency (RE):	0.252	0.237
Global Warming Potential (GWP _H):		
GWP ₂₀	2273	2139
GWP ₁₀₀	656	618
Global Temperature Potentials (GTP _H):		
GTP ₂₀		1407
GTP ₅₀		167
GTP ₁₀₀		87

* RE units: W m² ppb⁻¹
 * GWP and GTP: Relative to CO₂

Atmospheric Loss Processes *****

OH Reactivity

$k_{\text{Rec}}(T)$, *No recommendation*

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

$$\tau_{\text{Global}}^{\text{OH}} = 7.44 \text{ years}$$

$$\tau_{\text{Trop}}^{\text{OH}} = 7.71 \text{ years}$$

$$\tau_{\text{Strat}}^{\text{OH}} = 212.5 \text{ years}$$

Fractional Atmospheric Loss: 0.968

O(¹D) Reactivity

$k_{\text{Rec}}(T)$, *No recommendation*

$$k_{\text{Est}}(T) = 0.8 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$\tau_{\text{O}(\text{1D})} = 465 \text{ years}$$

Fractional Atmospheric Loss: 0.016

UV Photolysis

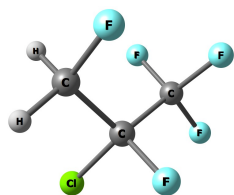
UV Spectrum: *No Recommendation*

$$\tau_{\text{hv}} = 450 \text{ years}$$

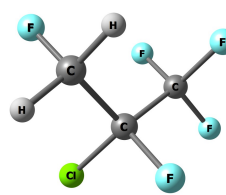
Fractional Atmospheric Loss: 0.016



Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.553



$\Delta E = 0.33 \text{ kcal mol}^{-1}$
Population = 0.315

Optimized Coordinates (Angstroms)

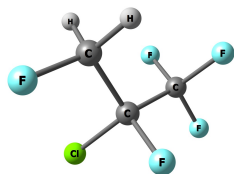
Atom	X	Y	Z
C	-0.349442678106	-1.586540296010	-0.540095629306
C	0.246879028311	-0.414445030611	0.237896701563
C	-0.422254024255	0.950523513369	-0.067252222384
H	0.179066406378	-2.497238059389	-0.241321777939
F	-1.679114368687	-1.704744460266	-0.235573286011
H	-0.226249844061	-1.417270428933	-1.613180781606
Cl	1.990989599133	-0.316374257896	-0.188753064116
F	0.120527051694	-0.626128573069	1.565252916236
F	0.220137897307	1.943037007083	0.539203015449
F	-0.422790702782	1.175333889513	-1.383514222181
F	-1.681004364933	0.940313696209	0.364149350295

Atom	X	Y	Z
C	1.130300454017	-1.142238412961	0.659638844499
C	0.343073317021	0.152903306563	0.450556446622
C	-1.055594267227	-0.067909132757	-0.177114663599
H	0.527243523307	-1.813414381882	1.280918772590
F	1.400020748518	-1.740336332237	-0.536581973866
H	2.061944312233	-0.892851586126	1.177200062498
Cl	1.265217126042	1.298590739581	-0.568848273722
F	0.140103384496	0.699526488581	1.674594783364
F	-1.742714603016	1.068232255753	-0.207749072011
F	-0.964122225034	-0.556379132868	-1.407826344938
F	-1.728006770357	-0.945871811647	0.579924418563

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
52.2026	0.0567
120.8448	0.519
181.5213	0.0879
190.1029	0.158
237.0654	0.703
310.6121	0.138
324.3486	0.202
331.2347	0.144
398.1072	0.137
450.9378	0.654
539.4800	1.55
581.7646	0.721
624.3217	6.02
770.5482	2.97
916.9023	18.6
955.1925	11.3
1097.9963	5.87
1129.5010	10.8
1203.6054	13.0
1232.7356	37.9
1246.4577	25.2
1269.6192	14.7
1342.7836	9.83
1422.6735	2.17
1490.2560	0.882
3061.4844	1.60
3123.3056	1.48

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
52.9979	0.0751
107.5608	0.332
168.5922	0.0101
201.3676	0.272
244.8330	0.795
301.5498	0.242
321.5787	0.308
364.0601	0.0131
392.5100	0.101
512.3519	0.809
520.5794	3.36
577.9984	1.28
628.5945	2.72
724.0453	8.24
840.0678	5.93
1082.4952	14.4
1111.2608	8.55
1139.5615	17.3
1170.0740	6.73
1219.5099	30.5
1254.2844	15.7
1262.9552	28.1
1329.9938	11.2
1424.5032	2.04
1499.9461	1.08
3050.3705	2.41
3109.1216	1.81



$\Delta E = 0.85 \text{ kcal mol}^{-1}$
Population = 0.132

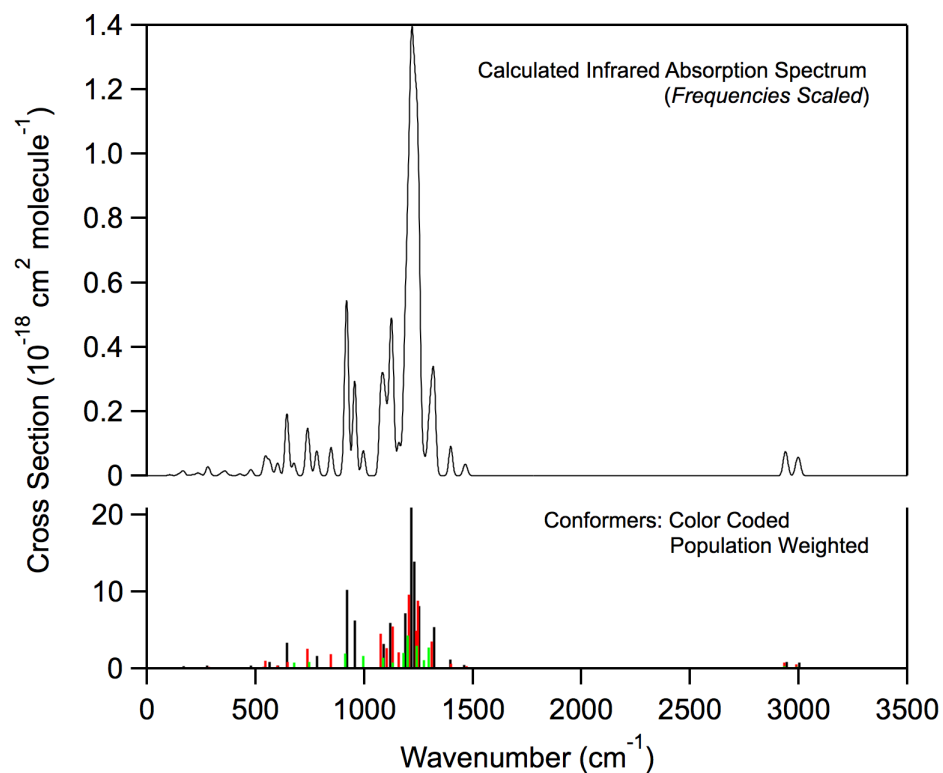
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.128911132542	-1.099172249940	-0.519794723121
C	0.313615977977	-0.046592876271	0.231291978050
C	-1.192399793539	-0.145753429348	-0.108377124525
H	0.977376627757	-0.982888796806	-1.596839733643
F	2.449374555055	-0.956425806237	-0.211590550044
H	0.783777509418	-2.088235302520	-0.198403790878
Cl	0.896617465475	1.601924749608	-0.162325695764
F	0.430164724573	-0.244286961063	1.564738897345
F	-1.903272608605	0.735264349583	0.579277682585
F	-1.39532870005	0.048472887015	-1.412361827224
F	-1.624331820649	-1.375172564021	0.202704887220

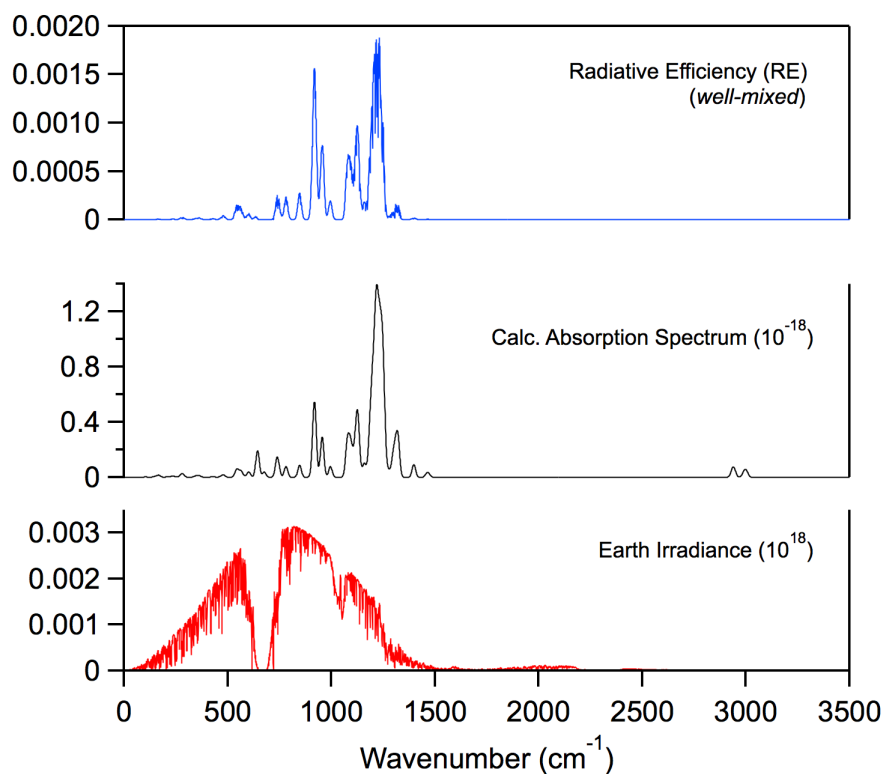
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
61.2144	0.0746
94.8043	0.534
159.8638	0.404
186.3540	0.202
241.0238	0.101
311.6846	0.224
320.0794	0.0496
351.4310	0.128
393.8734	0.0806
438.3304	0.726
550.3617	1.38
577.6586	0.328
659.3185	6.23
733.1410	6.35
908.6758	14.7
997.4034	12.6
1093.5514	10.5
1140.2710	5.70
1194.2204	15.6
1214.4585	32.6
1257.0663	22.3
1291.7592	8.33
1316.3875	20.5
1427.9832	0.939
1500.9401	0.429
3050.8364	2.18
3112.2711	1.65

Infrared Spectrum

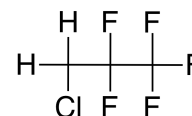


Radiative Efficiency



HCFC-235ca

Molecular Formula: CH₂ClCF₂CF₃
 Name: 3-Chloro-1,1,1,2,2-pentafluoropropane
 CAS number: 422-02-6
 Molecular Weight: 168.49



Global Atmospheric Lifetime (years): 9.82
 Tropospheric Atmospheric Lifetime (years): 10.6
 Stratospheric Atmospheric Lifetime (years): 126.5
 Ozone Depletion Potential (ODP): 0.018

	<i>Well-mixed</i>	<i>Lifetime adjusted</i>
Radiative Efficiency (RE):	0.225	0.215
Global Warming Potential (GWP _H):		
GWP ₂₀	2571	2451
GWP ₁₀₀	801	764
Global Temperature Potentials (GTP _H):		
GTP ₂₀		1830
GTP ₅₀		288
GTP ₁₀₀		110

* RE units: W m² ppb⁻¹
 * GWP and GTP: Relative to CO₂

Atmospheric Loss Processes *****

OH Reactivity

$k_{\text{Rec}}(T)$, *No recommendation*

$k_{\text{SAR}}(298 \text{ K}) = 5.51 \times 10^{-15}$; $k_{\text{SAR}}(272 \text{ K}) \approx 3.52 \times 10^{-15}$ cm³ molecule⁻¹ s⁻¹

$\tau_{\text{Global}}^{\text{OH}} = 10.3$ years

$\tau_{\text{Trop}}^{\text{OH}} = 10.6$ years

$\tau_{\text{Strat}}^{\text{OH}} = 284.1$ years

Fractional Atmospheric Loss: 0.957

O(¹D) Reactivity

$k_{\text{Rec}}(T)$, *No recommendation*

$k_{\text{Est}}(T) = 0.8 \times 10^{-10}$ cm³ molecule⁻¹ s⁻¹

$\tau_{\text{O}(\text{¹D})} = 465$ years

Fractional Atmospheric Loss: 0.021

UV Photolysis

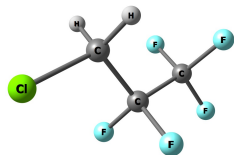
UV Spectrum: *No Recommendation*

$\tau_{\text{hv}} = 450$ years

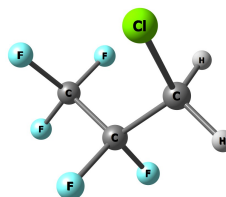
Fractional Atmospheric Loss: 0.022



Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.622



$\Delta E = 0.71 \text{ kcal mol}^{-1}$
Population = 0.189

Optimized Coordinates (Angstroms)

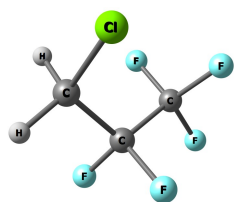
Atom	X	Y	Z
C	1.329234998005	0.092349337833	0.000000000000
C	-0.183125677394	0.274023851326	0.000000000000
C	-0.926759808599	-1.085851435364	0.000000000000
Cl	2.164278457716	1.672985654631	0.000000000000
H	1.629767851071	-0.455027097949	0.892551427837
H	1.629767851071	-0.455027097949	-0.892551427837
F	-0.589081688915	0.949383927822	-1.093117410224
F	-0.589081688915	0.949383927822	1.093117410224
F	-2.239170280763	-0.897804965926	0.000000000000
F	-0.589657506693	-1.790132051093	-1.084111051215
F	-0.589657506693	-1.790132051093	1.084111051215

Atom	X	Y	Z
C	1.189912953646	0.731137561017	0.646613606399
C	-0.148154841499	0.745198611298	-0.087424777102
C	-1.009851994614	-0.535631286552	0.046731631744
Cl	2.380910735724	-0.395802082771	-0.067604917682
H	1.601991608988	1.738855068385	0.590996147930
H	1.030473345326	0.451207266733	1.686744266972
F	0.012640524767	0.998413691179	-1.397884756850
F	-0.876001011440	1.753732497410	0.455345263001
F	-2.224778974138	-0.312097681150	-0.445479569630
F	-0.465033433539	-1.555482217317	-0.607144477179
F	-1.124223913220	-0.863426428233	1.338480582396

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
59.7350	0.0794
71.9872	0.523
133.5381	0.257
216.3175	0.223
228.1548	0.238
304.5661	0.0709
335.9247	0.160
361.5257	0.0114
437.1847	0.0442
520.8508	1.62
582.2095	0.436
587.5776	0.0800
707.9812	11.2
783.5122	3.71
799.9621	1.17
908.5091	0.629
1038.9602	17.3
1112.2099	12.4
1223.9964	28.3
1225.3257	39.1
1263.7041	7.28
1284.4441	19.8
1315.5924	8.73
1357.8615	12.7
1465.9159	0.986
3107.7564	0.986
3173.7273	0.00284

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
40.5144	0.0936
95.8387	0.226
163.8161	0.199
215.7172	0.297
230.4669	0.607
323.0988	0.267
334.0214	0.0562
364.5443	0.0578
438.5852	0.448
518.4226	1.81
586.4416	0.187
609.2637	2.25
632.0845	2.98
768.7026	2.28
810.3187	5.21
895.4485	0.515
1070.5073	16.1
1147.0135	20.5
1187.9367	13.2
1227.0827	49.0
1244.1727	31.1
1264.2761	12.4
1316.5693	0.665
1386.6909	4.05
1464.2043	2.31
3103.8951	1.02
3172.7244	0.00822



$\Delta E = 0.71 \text{ kcal mol}^{-1}$
Population = 0.189

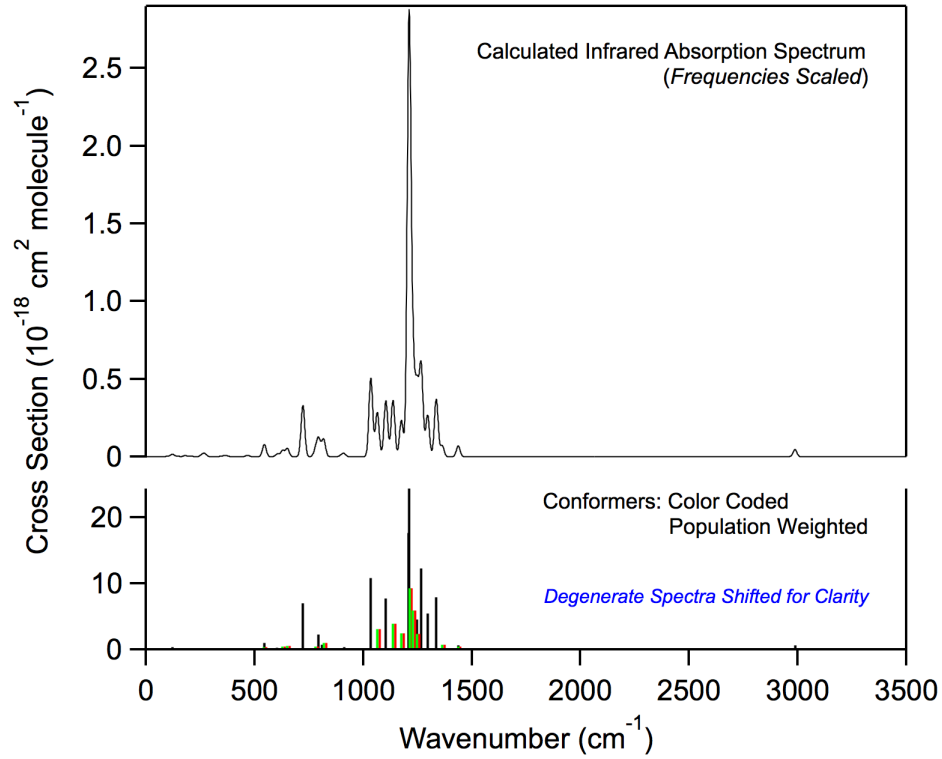
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.190062141059	0.730730982082	-0.646952292903
C	-0.147870885473	0.745149368349	0.087324787110
C	-1.009997528724	-0.535395339052	-0.046794677544
Cl	2.380829709068	-0.396650332267	0.066952948707
H	1.030349311520	0.450945303551	-1.687079943132
H	1.602469745110	1.738312923837	-0.591316865566
F	-0.875493826355	1.753962943268	-0.455224805446
F	0.013237133529	0.998194843858	1.397779145796
F	-2.224766179974	-0.311521607458	0.445652649004
F	-1.124702728837	-0.863036954385	-1.338553029671
F	-0.465385890922	-1.555478131784	0.606892083645

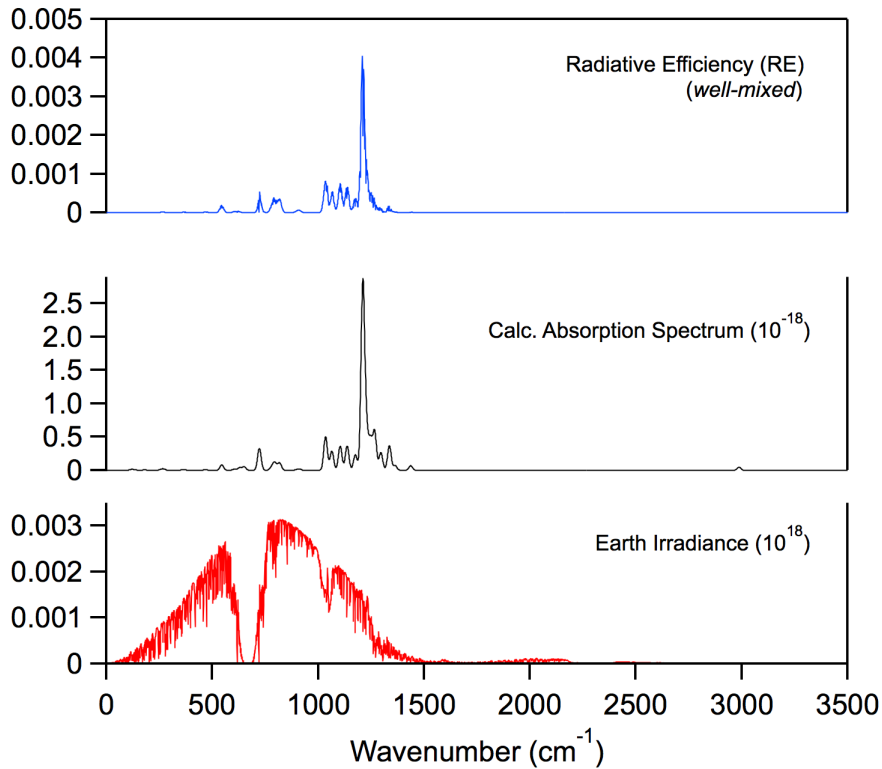
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
40.5144	0.0936
95.8387	0.226
163.8161	0.199
215.7172	0.297
230.4669	0.607
323.0987	0.267
334.0214	0.0562
364.5443	0.0578
438.5852	0.448
518.4226	1.81
586.4416	0.187
609.2637	2.25
632.0845	2.98
768.7026	2.28
810.3187	5.21
895.4485	0.515
1070.5073	16.1
1147.0134	20.5
1187.9367	13.2
1227.0827	49.0
1244.1727	31.1
1264.2761	12.4
1316.5693	0.665
1386.6909	4.05
1464.2043	2.31
3103.8951	1.02
3172.7244	0.00822

Infrared Spectrum

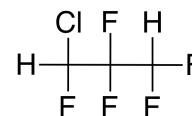


Radiative Efficiency



HCFC-235cb

Molecular Formula: CHClFCF₂CHF₂
 Name: 1-Chloro-1,2,2,3,3-pentafluoropropane
 CAS number: 679-99-2
 Molecular Weight: 168.49



Global Atmospheric Lifetime (years): 4.45
 Tropospheric Atmospheric Lifetime (years): 4.70
 Stratospheric Atmospheric Lifetime (years): 85.2
 Ozone Depletion Potential (ODP): 0.014

	<i>Well-mixed</i>	<i>Lifetime adjusted</i>
Radiative Efficiency (RE):	0.256	0.234
Global Warming Potential (GWP _H):		
GWP ₂₀	1505	1376
GWP ₁₀₀	412	377
Global Temperature Potentials (GTP _H):		
GTP ₂₀		711
GTP ₅₀		76
GTP ₁₀₀		53

* RE units: W m² ppb⁻¹
 * GWP and GTP: Relative to CO₂

Atmospheric Loss Processes *****

OH Reactivity

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

$$k_{SAR}(298\text{ K}) = 1.25 \times 10^{-14}; k_{SAR}(272\text{ K}) \approx 0.797 \times 10^{-14} \quad \text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$\tau_{Global}^{OH} = 4.54 \text{ years}$$

$$\tau_{Trop}^{OH} = 4.70 \text{ years}$$

$$\tau_{Strat}^{OH} = 135.9 \text{ years}$$

Fractional Atmospheric Loss: 0.980

O(¹D) Reactivity

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

$$k_{Est}(T) = 0.8 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$\tau_{O(^1D)} = 465 \text{ years}$$

Fractional Atmospheric Loss: 0.010

UV Photolysis

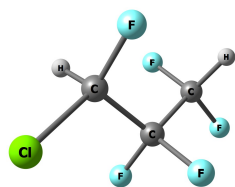
UV Spectrum: *No Recommendation*

$$\tau_{hv} = 450 \text{ years}$$

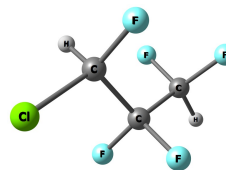
Fractional Atmospheric Loss: 0.010



Molecular Structure and Infrared Spectrum (7 conformers)



E = 0
Population = 0.380



$\Delta E = 0.05 \text{ kcal mol}^{-1}$
Population = 0.347

Optimized Coordinates (Angstroms)

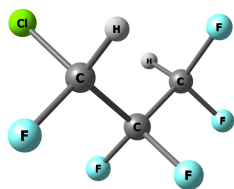
Atom	X	Y	Z
C	0.897633604395	-0.608531550423	-0.221546543308
C	-0.263934907125	0.349809094719	0.082246177989
C	-1.608519982713	-0.398874416244	0.191064527669
Cl	2.456567264291	0.255697693954	-0.195636129648
F	0.890742979752	-1.584327036663	0.721259503288
H	0.777984461449	-1.049613577961	-1.211580205862
F	-0.345984693726	1.260644276495	-0.904549137636
F	-0.056229111878	0.985611996390	1.250781698529
H	-1.627529847240	-1.055712194936	1.066258838442
F	-2.596816579362	0.506060040944	0.277213756956
F	-1.782548187844	-1.133746326276	-0.932606486418

Atom	X	Y	Z
C	0.710824458624	-0.431298103659	-0.507104602633
C	-0.229987443697	0.493450735586	0.283110849895
C	-1.726268100612	0.182817417153	0.071615585494
Cl	2.415057474854	0.031387497672	-0.223456782361
F	0.507408701107	-1.704188653283	-0.108210069976
H	0.520058957487	-0.338524342693	-1.577004713144
F	-0.033553419603	1.764912610530	-0.130351123623
F	0.026955415774	0.419303797824	1.600183981843
H	-2.335372057727	0.972664441324	0.527989561875
F	-1.970336935522	0.138678617891	-1.258847101718
F	-2.040784050684	-1.004735018344	0.612563414347

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
60.0278	0.179
68.4819	0.220
133.1199	0.100
213.7609	0.674
230.9041	0.209
252.4278	0.149
299.3319	0.306
373.6415	0.102
409.7465	0.233
478.7682	0.214
561.1655	3.77
601.6429	1.63
763.8728	19.7
798.5596	11.4
858.4540	1.79
1083.7320	11.0
1113.7874	19.8
1142.0300	14.4
1173.8848	15.4
1236.9972	22.5
1273.0039	14.1
1300.1721	0.850
1369.4581	1.35
1395.2892	1.80
1417.3490	3.66
3089.8435	3.29
3126.7282	0.833

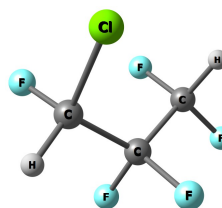
Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
45.6497	0.126
83.8398	0.160
148.8052	0.0773
207.5693	0.431
223.3543	0.237
234.2080	0.133
341.9675	0.0710
368.1124	0.205
433.4366	0.340
505.2629	1.10
562.0174	1.42
579.0416	14.2
662.3575	4.63
796.3344	3.34
866.9533	5.47
1128.2092	4.25
1134.0506	25.1
1152.8695	2.39
1186.4608	48.3
1210.1495	1.94
1249.1115	16.3
1307.8836	2.24
1373.6466	1.29
1387.0804	1.61
1418.7523	5.98
3063.8107	4.40
3122.9086	0.824



$\Delta E = 0.92 \text{ kcal mol}^{-1}$
Population = 0.080

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.029115628415	0.221015593665	0.570222626292
C	-0.312089211475	0.480774596506	-0.137157297676
C	-1.289529752227	-0.708424618719	-0.103029851742
Cl	1.888973321394	-1.162458238816	-0.186364088956
F	1.781700073679	1.331848896129	0.467530612536
H	0.866871742153	-0.032216955134	1.618396289178
F	-0.098714432179	0.822885662216	-1.421213000219
F	-0.886562783448	1.528050135086	0.494063846841
H	-0.959641815345	-1.523780987803	-0.753539939697
F	-1.375009172099	-1.152181508667	1.173796106133
F	-2.498930598869	-0.274389574462	-0.495311302688



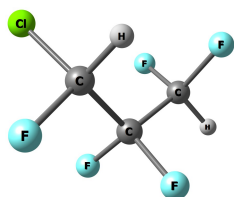
$\Delta E = 1.08 \text{ kcal mol}^{-1}$
Population = 0.061

Atom	X	Y	Z
C	1.083632237050	-0.140557561492	-0.639284001159
C	-0.353492882998	0.380569436837	-0.456416142384
C	-1.113148033435	-0.113452263020	0.789827070796
Cl	2.106973738180	0.287208837324	0.773623274867
F	1.070867312480	-1.474047103799	-0.808312807592
H	1.525393782819	0.346498164813	-1.512085894462
F	-1.042336543060	0.014967015767	-1.557882601109
F	-0.306296761090	1.729141173339	-0.410196128584
H	-0.642484438336	0.238544759393	1.713038516088
F	-2.371421127382	0.361297431659	0.715897301638
F	-1.151603284229	-1.459782890822	0.781687411901

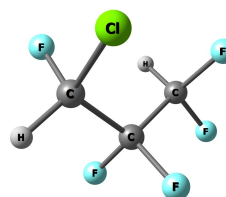
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
54.7124	0.183
76.1182	0.219
137.4236	0.0518
201.5438	0.669
241.9273	0.182
275.7086	0.133
302.3576	0.197
377.1819	0.406
403.5036	0.347
443.1433	0.881
561.6436	1.41
591.7498	2.14
776.2054	10.8
786.3509	8.37
874.8547	13.2
1076.3418	20.9
1131.9208	19.8
1140.6029	11.5
1175.2784	17.1
1230.8022	17.0
1262.8332	17.0
1292.6103	1.53
1379.1690	2.61
1395.8369	0.703
1422.6469	2.18
3095.0218	3.01
3126.7078	0.797

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
39.4665	0.177
86.7733	0.0931
152.8047	0.182
190.0574	0.154
240.0696	0.357
275.3624	0.506
320.3381	0.248
364.0209	0.363
416.0247	0.318
476.4947	0.744
531.2330	4.50
638.0034	1.58
668.6450	4.11
786.5294	9.35
866.5623	15.3
1132.2240	3.52
1151.2371	7.55
1161.2443	11.6
1186.8560	42.4
1189.1393	33.5
1232.9999	3.53
1303.9920	0.119
1371.3240	3.69
1404.6003	2.24
1429.3200	1.25
3089.4004	3.29
3100.3684	1.33



$\Delta E = 1.19 \text{ kcal mol}^{-1}$
Population = 0.051



$\Delta E = 1.29 \text{ kcal mol}^{-1}$
Population = 0.043

Optimized Coordinates (Angstroms)

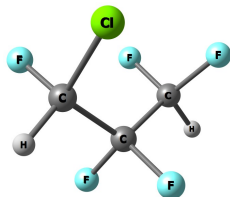
Atom	X	Y	Z
C	0.890780377082	0.307006073632	0.578204222447
C	-0.348190377557	0.627336709375	-0.279296468743
C	-1.551260955717	-0.319867419142	-0.113341711434
Cl	1.662489419027	-1.226028406520	0.080047647797
F	1.766369200015	1.322695246817	0.429765329387
H	0.607210966265	0.206912745656	1.626422421344
F	-0.023463114414	0.692423909502	-1.580856231631
F	-0.777069589465	1.854394273874	0.112636767089
H	-2.441537841174	0.143841596499	-0.555587083257
F	-1.318533244609	-1.503107884541	-0.701686939621
F	-1.758683839451	-0.519532845153	1.209555046623

Atom	X	Y	Z
C	1.067883943779	0.699573975261	0.030470110991
C	-0.425282796994	0.484130175217	0.340996023985
C	-1.178954719431	-0.451767584169	-0.624834435347
Cl	2.075036034712	-0.718608331258	0.420145842338
F	1.177596701557	0.997609002518	-1.288084274386
H	1.435674914865	1.536232074511	0.628655964210
F	-1.006120854674	1.706399406917	0.234619526463
F	-0.570249637679	0.055079146335	1.604157978332
H	-1.080680858138	-0.108718928936	-1.659834726666
F	-0.699910331142	-1.704488929235	-0.511947964447
F	-2.477538396856	-0.449502007162	-0.267683045473

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
41.2978	0.148
88.9653	0.117
147.8097	0.124
203.2762	0.468
217.6603	0.116
286.8506	0.608
323.6970	0.236
362.1956	0.159
402.1837	0.988
496.0499	0.253
547.9508	2.09
603.8977	4.37
701.6744	8.11
792.2325	6.84
851.9294	10.3
1123.9158	7.76
1139.1078	21.6
1144.8710	14.3
1168.8878	34.4
1226.5321	4.99
1248.2809	17.8
1293.6487	0.683
1386.6003	0.484
1391.7855	4.18
1420.2862	2.16
3063.6616	4.63
3124.8016	0.806

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
38.5724	0.178
81.4031	0.0789
153.1258	0.0858
187.2103	0.187
234.4530	0.496
275.1858	0.673
311.2442	0.129
366.6433	0.134
426.9534	0.536
486.6653	0.447
538.0376	4.67
621.7699	1.20
666.4791	3.58
822.4169	17.8
858.9832	6.14
1113.3332	15.4
1139.4706	16.9
1156.1719	6.65
1166.9821	40.0
1204.0583	3.79
1245.9190	15.2
1301.0491	5.19
1373.0347	3.16
1403.7210	1.33
1429.7088	1.41
3085.2715	3.33
3103.9661	1.30



$\Delta E = 1.53 \text{ kcal mol}^{-1}$
 Population = 0.029

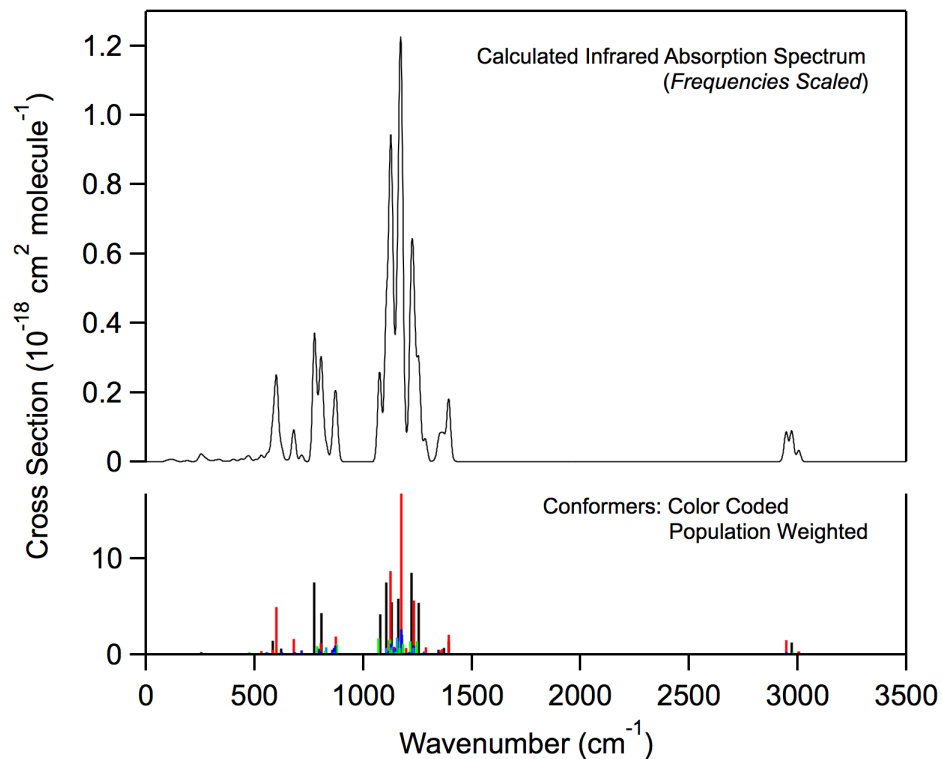
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	0.859799191792	0.801024641211	-0.141157524889
C	-0.500021281446	0.476718125519	0.506975604385
C	-1.317589128286	-0.716686064234	-0.025756038821
Cl	2.055119116011	-0.508942260232	0.086619065639
F	0.685080011658	1.045571102086	-1.454209624795
H	1.262821887595	1.689649634505	0.351888505133
F	-1.272214239307	1.579011693273	0.334516534135
F	-0.314684390722	0.297897992490	1.830205360893
H	-2.307109609213	-0.700704980385	0.449872884444
F	-1.458834723423	-0.613897116076	-1.360200913425
F	-0.700879834660	-1.875376768157	0.264423147300

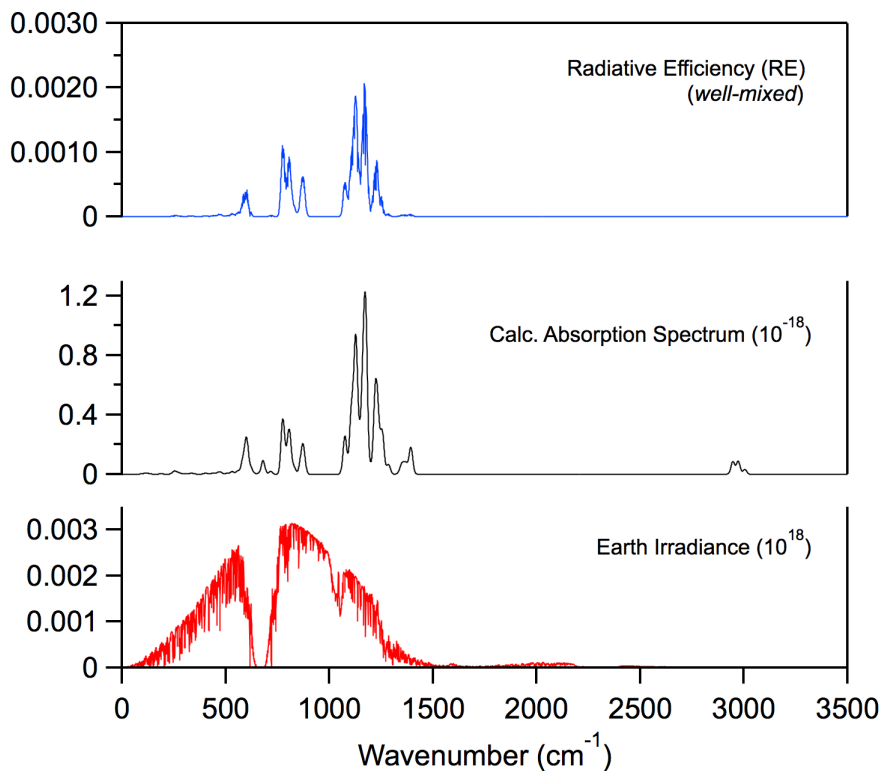
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
16.7851	0.00731
104.3554	0.324
158.2317	0.0546
191.9391	0.0459
211.5220	0.0988
300.4133	0.282
358.9849	0.0423
362.7526	0.0392
433.8827	2.02
447.3446	7.82
534.2112	0.842
569.3422	0.776
656.9868	0.908
814.9056	12.8
868.2024	3.83
1133.1913	8.46
1138.8302	17.9
1164.8376	9.25
1177.4231	25.1
1196.4550	38.5
1274.1241	0.379
1298.2338	4.60
1353.4669	3.72
1392.5775	2.77
1444.2529	1.34
3050.3791	5.16
3092.1799	1.67

Infrared Spectrum

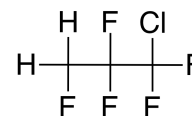


Radiative Efficiency



HCFC-235cc

Molecular Formula: CH₂FCF₂CClF₂
 Name: 1-Chloro-1,1,2,2,3-pentafluoropropane
 CAS number: 677-55-4
 Molecular Weight: 168.49



Global Atmospheric Lifetime (years): 14.2
 Tropospheric Atmospheric Lifetime (years): 15.7
 Stratospheric Atmospheric Lifetime (years): 145.8
 Ozone Depletion Potential (ODP): 0.021

	<i>Well-mixed</i>	<i>Lifetime adjusted</i>
Radiative Efficiency (RE):	0.292	0.282
Global Warming Potential (GWP _H):		
GWP ₂₀	4188	4040
GWP ₁₀₀	1501	1448
Global Temperature Potentials (GTP _H):		
GTP ₂₀		3384
GTP ₅₀		838
GTP ₁₀₀		231

* RE units: W m² ppb⁻¹
 * GWP and GTP: Relative to CO₂

Atmospheric Loss Processes *****

OH Reactivity

$k_{\text{Rec}}(T)$, *No recommendation*

$k_{\text{SAR}}(298 \text{ K}) = 3.72 \times 10^{-15}$; $k_{\text{SAR}}(272 \text{ K}) \approx 2.38 \times 10^{-15}$ cm³ molecule⁻¹ s⁻¹

$\tau_{\text{Global}}^{\text{OH}} = 15.2$ years

$\tau_{\text{Trop}}^{\text{OH}} = 15.7$ years

$\tau_{\text{Strat}}^{\text{OH}} = 404.3$ years

Fractional Atmospheric Loss: 0.938

O(¹D) Reactivity

$k_{\text{Rec}}(T)$, *No recommendation*

$k_{\text{Est}}(T) = 0.8 \times 10^{-10}$ cm³ molecule⁻¹ s⁻¹

$\tau_{\text{O}(\text{1D})} = 465$ years

Fractional Atmospheric Loss: 0.031

UV Photolysis

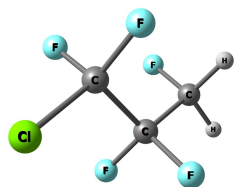
UV Spectrum: *No Recommendation*

$\tau_{\text{hv}} = 450$ years

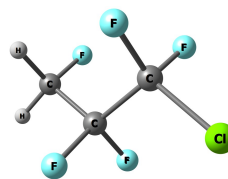
Fractional Atmospheric Loss: 0.031



Molecular Structure and Infrared Spectrum (9 conformers)



E = 0
Population = 0.289



E = 0
Population = 0.289

Optimized Coordinates (Angstroms)

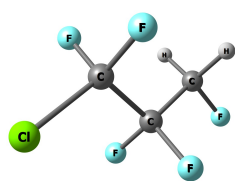
Atom	X	Y	Z
C	-1.944045588628	0.156697147022	0.420734303623
C	-0.546623435444	0.614170046294	0.000040677064
C	0.544755353021	-0.478444163292	0.147245541827
H	-2.615282665367	1.014964539732	0.305309043718
F	-2.362672676344	-0.873450072818	-0.373458452057
H	-1.922551135221	-0.160017205619	1.467564679318
F	-0.211652621250	1.655987719697	0.792092065527
F	-0.557078696998	1.024925841214	-1.280508005799
Cl	2.169935441502	0.177108646458	-0.209442990454
F	0.523805509696	-0.938391553340	1.404038221898
F	0.287958515032	-1.488288945350	-0.679130084667

Atom	X	Y	Z
C	-1.942070853243	0.153426863209	-0.428096624448
C	-0.546317366902	0.612874066107	-0.004028283625
C	0.546374107005	-0.479169757249	-0.145616657733
H	-1.917090323384	-0.165419729645	-1.474202088467
F	-2.362338849976	-0.875419617045	0.366915361465
H	-2.614338363819	1.011395481478	-0.316511205599
F	-0.561054947791	1.026247509591	1.275635264238
F	-0.209722762567	1.653330845970	-0.797179892556
Cl	2.169924536404	0.178407472075	0.214748074344
F	0.287820902535	-1.487523137046	0.682031215879
F	0.529674921737	-0.941707997445	-1.401522163498

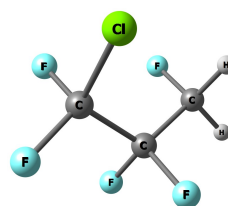
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
41.7241	0.0883
108.5618	0.491
170.4385	0.273
209.4089	0.440
218.7785	0.0771
305.5637	0.852
329.4103	0.0424
355.7617	0.0249
416.8444	0.139
423.7828	0.0163
523.8281	2.35
593.9874	4.77
601.7280	9.66
691.8500	0.617
899.0002	11.8
1005.1424	24.0
1120.4454	3.68
1146.1858	30.7
1185.4322	7.77
1207.8731	39.8
1238.7552	4.72
1258.0288	10.3
1337.7807	2.61
1428.2326	1.03
1495.8673	0.813
3052.2477	2.49
3113.9477	2.02

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
41.7242	0.0883
108.5617	0.491
170.4386	0.273
209.4088	0.440
218.7785	0.0771
305.5634	0.852
329.4103	0.0424
355.7619	0.0249
416.8444	0.139
423.7828	0.0163
523.8281	2.35
593.9873	4.77
601.7283	9.66
691.8500	0.617
899.0002	11.8
1005.1425	24.0
1120.4452	3.68
1146.1853	30.7
1185.4316	7.77
1207.8729	39.8
1238.7555	4.72
1258.0292	10.3
1337.7813	2.61
1428.2325	1.03
1495.8673	0.813
3052.2478	2.49
3113.9478	2.02



$\Delta E = 0.56 \text{ kcal mol}^{-1}$
Population = 0.112



$\Delta E = 0.81 \text{ kcal mol}^{-1}$
Population = 0.073

Optimized Coordinates (Angstroms)

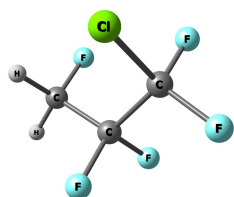
Atom	X	Y	Z
C	-1.784033082551	-0.687256497185	-0.001690377111
C	-0.595656816716	0.276253698384	-0.000353519562
C	0.758677513309	-0.476522844591	-0.000574193776
H	-1.743706997529	-1.314775198990	0.893815811242
F	-2.931069444348	0.053810516939	-0.001369570501
H	-1.743091518266	-1.313046084025	-0.898377535033
F	-0.643523549009	1.061505129828	1.092753194242
F	-0.642736963437	1.063566613849	-1.092010885063
Cl	2.140554667373	0.647204030169	0.000940328340
F	0.820757534302	-1.259761401206	1.082506050053
F	0.821512656872	-1.257766963171	-1.085051302831

Atom	X	Y	Z
C	-1.539734276092	-0.745703736555	0.641361700596
C	-0.669449500805	0.463339001598	0.313567611964
C	0.676185793344	0.177047173514	-0.409389876335
H	-2.444234774070	-0.366377402116	1.130374946042
F	-1.872880979868	-1.406953580705	-0.507569852093
H	-1.006179751742	-1.416464482228	1.320331886922
F	-0.393360476762	1.106105975846	1.468170139290
F	-1.348912193480	1.307640981224	-0.493166379155
Cl	1.740397479177	-0.874813061123	0.585798917798
F	0.448500959663	-0.413342323332	-1.578291024459
F	1.299204720636	1.332993453876	-0.627292070572

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
55.4271	0.246
83.2874	0.600
140.6594	0.442
214.7579	0.173
231.0342	0.0740
306.7319	0.503
319.2593	0.0712
359.9216	0.0836
368.7420	0.00251
426.9373	0.0349
529.4145	0.0000
548.5452	2.76
656.4696	1.51
787.1840	17.2
874.0154	27.7
984.2594	5.33
1112.2697	28.0
1134.7545	9.17
1187.3663	27.5
1201.8320	7.75
1232.2445	16.5
1297.4734	1.37
1311.1079	10.3
1435.9058	0.739
1503.0920	0.194
3058.4632	2.13
3116.6553	1.99

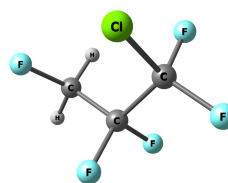
Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
39.7955	0.112
109.5955	0.390
181.1661	0.134
192.0288	0.204
245.8909	0.719
313.1230	0.392
321.1211	0.231
358.2627	0.166
416.5039	0.236
422.8430	0.189
466.6129	1.41
592.8244	4.44
643.6732	2.74
692.5320	3.29
934.8069	32.3
957.8310	10.8
1124.4997	6.73
1147.8242	19.4
1184.8872	21.9
1215.1807	39.1
1239.7958	6.56
1259.6775	1.84
1335.1515	8.13
1432.8715	0.690
1496.8742	1.29
3052.5185	2.39
3116.2881	2.13



$\Delta E = 0.81 \text{ kcal mol}^{-1}$
Population = 0.073

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.537107478150	-0.747955974885	-0.643600030890
C	-0.667161468105	0.461561282738	-0.316664426923
C	0.675713642611	0.176724455207	0.411979056664
H	-1.001610826617	-1.421288239911	-1.318483742624
F	-1.874780544638	-1.405226994994	0.506292524053
H	-2.439607303972	-0.369615345618	-1.137053519202
F	-1.348897464940	1.308942224744	0.484907079109
F	-0.386552191008	1.100377312808	-1.472369295658
Cl	1.742721913671	-0.879083698680	-0.576008830495
F	1.298745149306	1.332957504642	0.628320079975
F	0.443496571843	-0.409701526050	1.581983105990



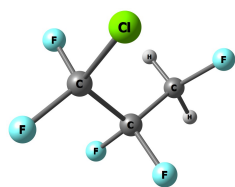
$\Delta E = 1.00 \text{ kcal mol}^{-1}$
Population = 0.053

Atom	X	Y	Z
C	-1.688873396943	-0.539086519228	0.541420353645
C	-0.768792590482	0.429042534698	-0.198666526066
C	0.735028774373	0.380610389389	0.188139527556
H	-2.716614071048	-0.261981859658	0.281479578232
F	-1.445982572769	-1.827353729097	0.159532100098
H	-1.538828100012	-0.430440779801	1.619754234617
F	-1.187633985534	1.681729877968	0.112397036625
F	-0.872895816583	0.262375543627	-1.527813730258
Cl	1.525251676809	-1.138151803791	-0.314738366971
F	1.360768473559	1.406731798445	-0.384873473220
F	0.835398608630	0.510438547448	1.516855265741

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
39.7973	0.112
109.5955	0.390
181.1663	0.134
192.0278	0.204
245.8913	0.719
313.1228	0.392
321.1213	0.231
358.2626	0.166
416.5045	0.236
422.8431	0.189
466.6130	1.41
592.8246	4.44
643.6732	2.74
692.5322	3.29
934.8071	32.3
957.8312	10.8
1124.5006	6.73
1147.8242	19.4
1184.8872	21.9
1215.1810	39.1
1239.7964	6.56
1259.6775	1.84
1335.1509	8.13
1432.8722	0.690
1496.8745	1.29
3052.5176	2.39
3116.2873	2.13

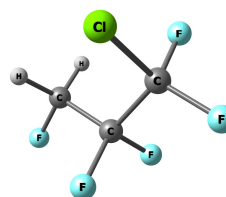
Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
39.9218	0.164
107.8220	0.464
172.5017	0.173
195.8741	0.0302
245.0910	1.02
310.6352	0.246
320.4769	0.286
345.7525	0.205
415.3391	0.468
427.4298	0.123
499.8232	0.264
590.9257	4.93
620.5116	2.45
707.0325	4.18
929.8996	19.5
972.7051	20.2
1134.0887	10.7
1135.8592	19.1
1167.5541	21.3
1199.6751	31.8
1242.7204	4.08
1269.4789	12.1
1338.4542	5.30
1432.8742	0.0916
1497.2698	0.804
3051.5198	2.54
3111.9813	2.07



$\Delta E = 1.00 \text{ kcal mol}^{-1}$
Population = 0.053

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.693655202982	-0.508043012078	-0.553331795301
C	-0.761322715046	0.442124894567	0.194659658603
C	0.743557172474	0.369279396862	-0.184125815538
H	-1.535899213433	-0.398789990163	-1.630503119009
F	-1.474773762082	-1.801372522361	-0.174049362416
H	-2.717944905847	-0.214269387926	-0.298116930993
F	-0.875514882035	0.273348956649	1.522712250266
F	-1.157121994133	1.702659501196	-0.114873997726
Cl	1.505118636502	-1.164163242186	0.318421379287
F	0.853394891860	0.501294046555	-1.511876496734
F	1.383478974721	1.382928358885	0.395387229562



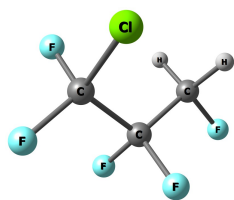
$\Delta E = 1.38 \text{ kcal mol}^{-1}$
Population = 0.028

Atom	X	Y	Z
C	-1.419220021788	-0.797936805991	0.601599864790
C	-0.636927397459	0.238211554770	-0.201039889323
C	0.866029381362	0.336609313974	0.175145117315
H	-1.314568745821	-0.583782246985	1.669772061518
F	-2.732593928486	-0.706028232695	0.233704551267
H	-1.041352982825	-1.800725439240	0.383132726982
F	-1.158192974620	1.465697300590	0.022518487919
F	-0.727798746499	-0.017256837094	-1.519614649211
Cl	1.744777697896	-1.181803699118	-0.202430236019
F	1.424224078394	1.338088346979	-0.494562169902
F	0.972163639846	0.583692744810	1.484855134665

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
39.9221	0.164
107.8191	0.464
172.4987	0.173
195.8724	0.0302
245.0896	1.02
310.6354	0.246
320.4759	0.286
345.7521	0.205
415.3391	0.468
427.4301	0.123
499.8226	0.264
590.9256	4.93
620.5114	2.45
707.0316	4.18
929.8990	19.5
972.7043	20.2
1134.0878	10.7
1135.8612	19.1
1167.5518	21.3
1199.6747	31.8
1242.7195	4.08
1269.4771	12.1
1338.4517	5.30
1432.8738	0.0916
1497.2688	0.804
3051.5205	2.54
3111.9816	2.07

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
55.6253	0.349
82.2573	0.434
152.7503	0.357
189.9251	0.144
263.2733	0.215
306.1080	0.417
323.2595	0.0810
332.1339	0.164
403.1635	0.0687
425.2639	0.223
474.2958	0.751
565.2493	1.63
647.4751	2.40
778.8951	8.53
928.1669	36.3
980.4819	8.13
1067.7426	26.4
1131.4675	8.54
1193.9614	7.04
1203.2289	33.1
1253.3371	2.86
1297.2281	18.2
1308.0309	7.09
1438.5273	0.470
1501.2299	0.295
3060.5238	2.14
3119.3364	1.83



$\Delta E = 1.38 \text{ kcal mol}^{-1}$
 Population = 0.028

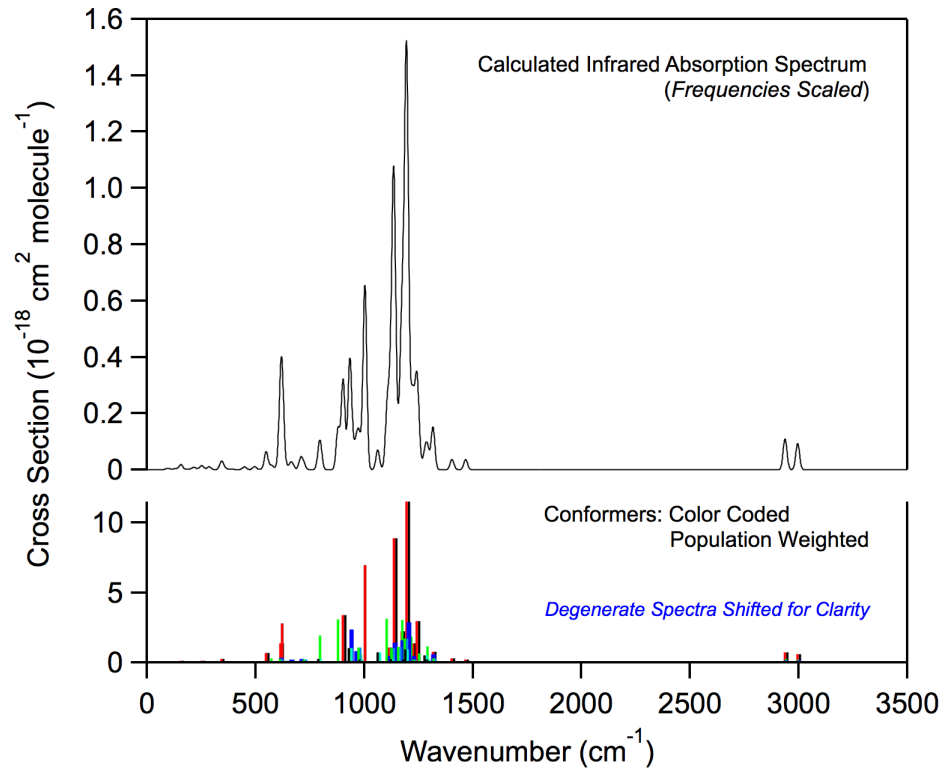
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.419071142463	-0.794292183455	-0.605304068612
C	-0.636231781188	0.239646261525	0.199649393242
C	0.867026723929	0.337287230786	-0.175526953716
H	-1.042283634722	-1.797837492178	-0.388452708209
F	-2.732559642266	-0.701795698950	-0.237966032043
H	-1.313624615922	-0.578296390062	-1.673027219560
F	-0.728077263541	-0.018130726534	1.517707339345
F	-1.156198476332	1.468034999177	-0.021964812797
Cl	1.744113055989	-1.182649428083	0.199775321205
F	0.974122138079	0.586646194281	-1.484727668518
F	1.425808638438	1.337014233493	0.496305409662

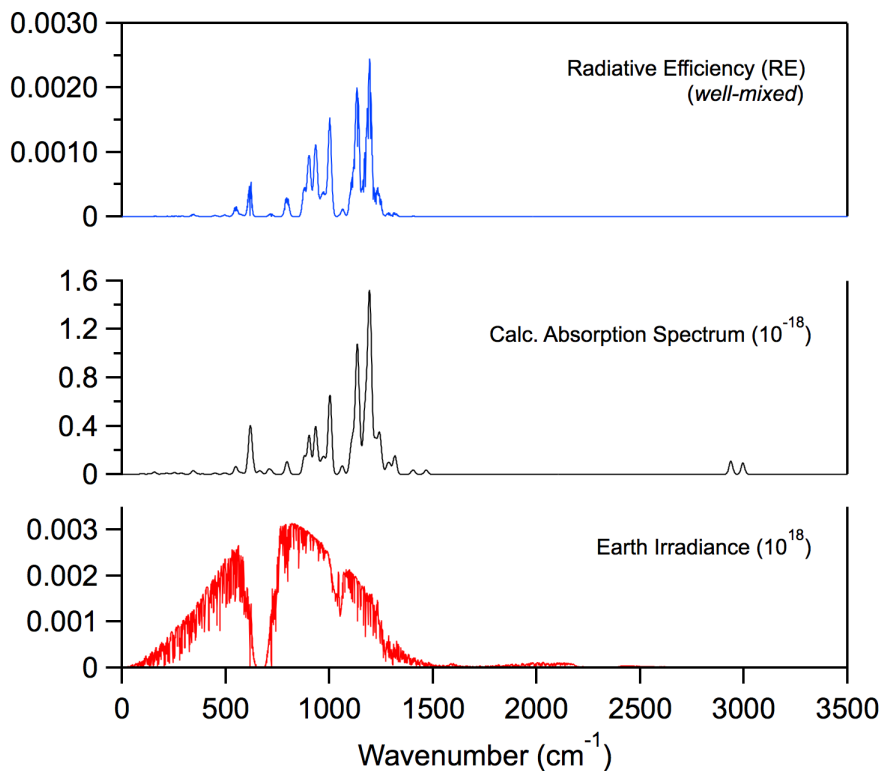
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
55.6260	0.349
82.2571	0.434
152.7505	0.357
189.9253	0.144
263.2734	0.215
306.1080	0.417
323.2595	0.0810
332.1338	0.164
403.1635	0.0687
425.2639	0.223
474.2956	0.751
565.2492	1.63
647.4749	2.40
778.8950	8.53
928.1669	36.3
980.4816	8.13
1067.7423	26.4
1131.4673	8.54
1193.9615	7.04
1203.2279	33.1
1253.3368	2.86
1297.2273	18.2
1308.0306	7.09
1438.5268	0.470
1501.2296	0.295
3060.5236	2.14
3119.3362	1.83

Infrared Spectrum

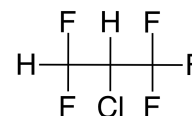


Radiative Efficiency



HCFC-235da

Molecular Formula: CHF₂CHClCF₃
 Name: 2-Chloro-1,1,1,3,3-pentafluoropropane
 CAS number: 28103-66-4
 Molecular Weight: 168.49



Global Atmospheric Lifetime (years): 7.55
 Tropospheric Atmospheric Lifetime (years): 8.09
 Stratospheric Atmospheric Lifetime (years): 112.5
 Ozone Depletion Potential (ODP): 0.017

	<i>Well-mixed</i>	<i>Lifetime adjusted</i>
Radiative Efficiency (RE):	0.241	0.227
Global Warming Potential (GWP _H):		
GWP ₂₀	2256	2128
GWP ₁₀₀	657	620
Global Temperature Potentials (GTP _H):		
GTP ₂₀		1429
GTP ₅₀		175
GTP ₁₀₀		88

* RE units: W m² ppb⁻¹
 * GWP and GTP: Relative to CO₂

Atmospheric Loss Processes *****

OH Reactivity

$k_{\text{Rec}}(T)$, *No recommendation*

$k_{\text{SAR}}(298 \text{ K}) = 7.25 \times 10^{-15}$; $k_{\text{SAR}}(272 \text{ K}) \approx 4.63 \times 10^{-15}$ cm³ molecule⁻¹ s⁻¹

$\tau_{\text{Global}}^{\text{OH}} = 7.80$ years

$\tau_{\text{Trop}}^{\text{OH}} = 8.09$ years

$\tau_{\text{Strat}}^{\text{OH}} = 221.8$ years

Fractional Atmospheric Loss: 0.967

O(¹D) Reactivity

$k_{\text{Rec}}(T)$, *No recommendation*

$k_{\text{Est}}(T) = 0.8 \times 10^{-10}$ cm³ molecule⁻¹ s⁻¹

$\tau_{\text{O}(\text{1D})} = 465$ years

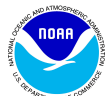
Fractional Atmospheric Loss: 0.016

UV Photolysis

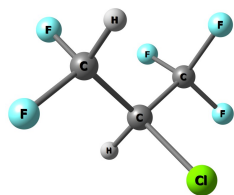
UV Spectrum: *No Recommendation*

$\tau_{\text{hv}} = 450$ years

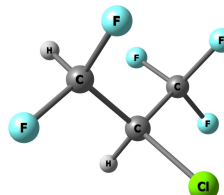
Fractional Atmospheric Loss: 0.017



Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.472



$\Delta E = 0.16 \text{ kcal mol}^{-1}$
Population = 0.361

Optimized Coordinates (Angstroms)

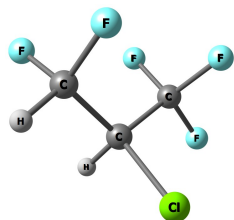
Atom	X	Y	Z
C	1.342464686384	-0.511199066152	0.308360701160
C	0.205886656933	0.224288097618	-0.415886017447
C	-1.181156550498	-0.310336909430	-0.031226146301
F	1.264421617799	-1.831341444187	0.024216341396
F	2.523737069918	-0.054518470244	-0.152742650681
H	1.297536371934	-0.370959458137	1.393434369192
H	0.335459408537	0.106359102853	-1.492734129007
Cl	0.313250625410	1.969206278008	-0.032082069514
F	-2.149157168546	0.446478661424	-0.544233437739
F	-1.337699973902	-1.551340284693	-0.500317580999
F	-1.331958743969	-0.344176507060	1.297810619940

Atom	X	Y	Z
C	1.198141588505	-0.876195943378	-0.251132628674
C	0.156445306083	0.212967636593	-0.528716483723
C	-1.248423245491	-0.209428745505	-0.084234416658
F	2.382613360327	-0.499678551666	-0.776351963295
F	1.355053550941	-1.060540228655	1.074000351809
H	0.891839586974	-1.825262024552	-0.708295780527
H	0.119776013646	0.382545395125	-1.606175287604
Cl	0.617501487635	1.753764204746	0.246481746584
F	-2.158821870425	0.684951372729	-0.465124953670
F	-1.549053097998	-1.382193674567	-0.674487318432
F	-1.340622680199	-0.374486440869	1.230589734190

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
48.1842	0.0648
75.7004	0.0918
168.0432	0.140
195.9082	0.106
226.3820	0.652
315.0559	0.0685
337.4586	0.125
395.9576	0.0554
446.5800	2.99
542.6028	1.19
566.5201	0.482
576.1990	0.783
699.7531	4.41
843.1103	5.48
892.7798	5.79
1076.1292	1.99
1121.8801	12.9
1131.8936	24.4
1171.4928	25.2
1231.7995	26.5
1246.2285	9.86
1266.4576	27.8
1335.9213	13.4
1397.0239	4.58
1418.1460	9.04
3081.3580	3.22
3123.4461	0.556

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
52.4289	0.106
82.4504	0.106
165.1135	0.369
185.8024	0.0327
205.5216	0.282
303.4979	0.0136
333.6410	0.130
359.4302	0.0444
518.0167	1.29
540.2652	0.858
573.1049	0.709
681.2257	7.07
700.1164	4.27
810.9521	1.91
897.6517	3.42
985.5394	2.97
1117.9493	17.6
1154.5542	25.3
1181.8911	18.1
1220.8900	25.8
1273.4914	3.45
1292.2598	29.3
1342.1256	14.5
1395.5916	11.3
1413.6198	5.38
3057.8060	3.60
3115.7775	0.724



$\Delta E = 0.62 \text{ kcal mol}^{-1}$
Population = 0.167

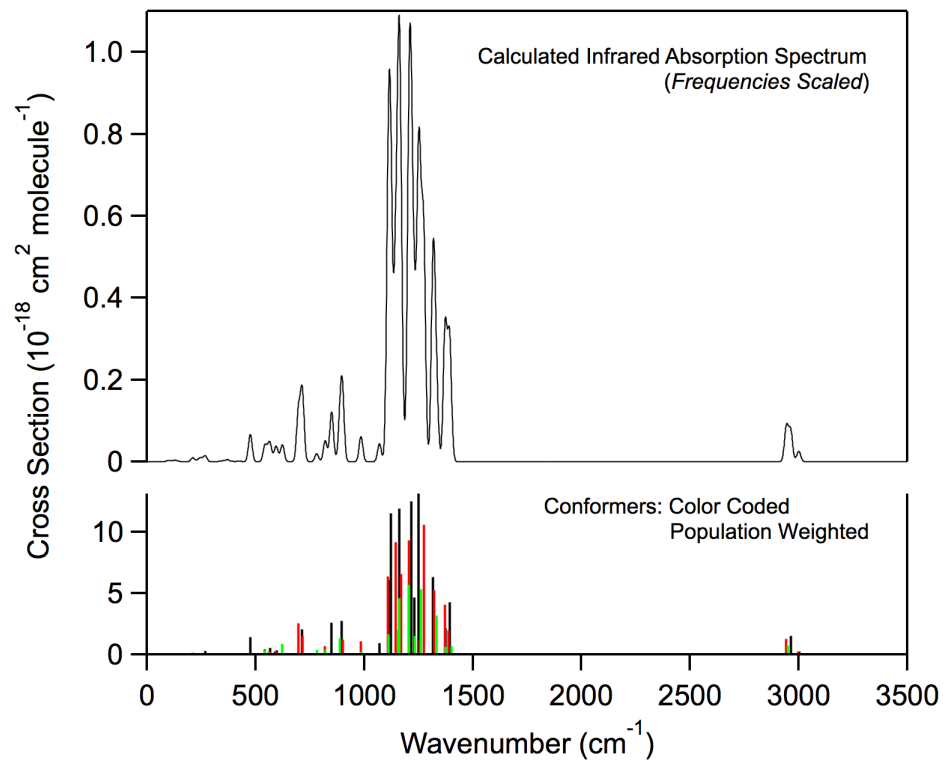
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.544198786196	0.072590687873	-0.269389679688
C	0.070063628952	0.342150876429	-0.604832974718
C	-0.922248826591	-0.617354286771	0.072288939963
F	1.730803657961	0.004925084898	1.062990462332
F	1.910217854277	-1.111436272364	-0.812357362909
H	2.180951227587	0.864981022979	-0.679311272856
H	-0.058502904354	0.239986177583	-1.683200868577
Cl	-0.329086429854	2.033872776895	-0.172475489197
F	-2.158752203155	-0.388060415441	-0.379212212082
F	-0.602120662927	-1.880703047486	-0.229418388709
F	-0.930915128093	-0.490121604593	1.395176846442

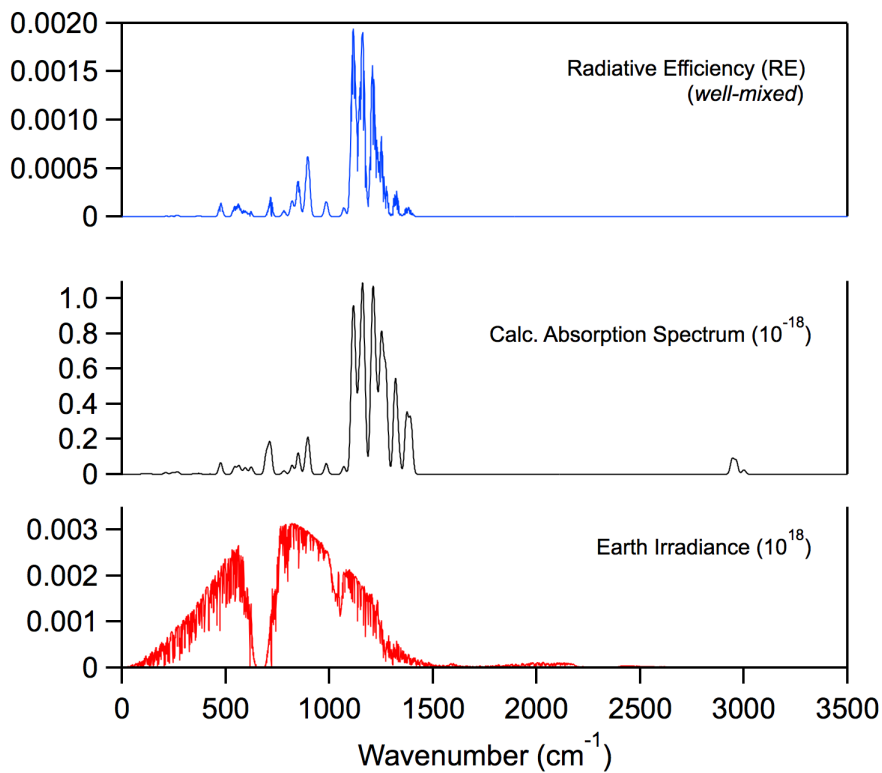
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
39.0856	0.0627
95.5991	0.124
172.1167	0.0559
198.5185	0.241
205.9463	0.191
299.5226	0.133
323.8185	0.0561
386.3674	0.0923
517.5644	2.21
533.8055	1.32
562.7379	0.252
603.1053	5.30
770.3753	2.50
813.6090	2.51
882.3768	8.08
988.5540	1.43
1119.6863	10.0
1167.2905	12.0
1172.0474	27.7
1219.4873	33.9
1249.8629	9.09
1278.7193	32.1
1354.8688	19.1
1397.8959	3.97
1426.1947	4.28
3065.8845	4.39
3121.4388	0.377

Infrared Spectrum

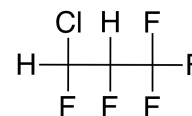


Radiative Efficiency



HCFC-235ea

Molecular Formula: CHClFCHFCF₃
 Name: 3-Chloro-1,1,1,2,3-pentafluoropropane
 CAS number: 134251-06-2
 Molecular Weight: 168.49



Global Atmospheric Lifetime (years): 7.36
 Tropospheric Atmospheric Lifetime (years): 7.88
 Stratospheric Atmospheric Lifetime (years): 111.1
 Ozone Depletion Potential (ODP): 0.017

	<i>Well-mixed</i>	<i>Lifetime adjusted</i>
Radiative Efficiency (RE):	0.241	0.227
Global Warming Potential (GWP _H):		
GWP ₂₀	2216	2088
GWP ₁₀₀	643	605
Global Temperature Potentials (GTP _H):		
GTP ₂₀		1386
GTP ₅₀		167
GTP ₁₀₀		86

* RE units: W m² ppb⁻¹
 * GWP and GTP: Relative to CO₂

Atmospheric Loss Processes *****

OH Reactivity

$k_{\text{Rec}}(T)$, *No recommendation*

$$k_{\text{SAR}}(298 \text{ K}) = 7.44 \times 10^{-15}; k_{\text{SAR}}(272 \text{ K}) \approx 4.75 \times 10^{-15} \quad \text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$\tau_{\text{Global}}^{\text{OH}} = 7.61 \text{ years}$$

$$\tau_{\text{Trop}}^{\text{OH}} = 7.88 \text{ years}$$

$$\tau_{\text{Strat}}^{\text{OH}} = 216.7 \text{ years}$$

Fractional Atmospheric Loss: 0.968

O(¹D) Reactivity

$k_{\text{Rec}}(T)$, *No recommendation*

$$k_{\text{Est}}(T) = 0.8 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$\tau_{\text{O}(\text{1D})} = 465 \text{ years}$$

Fractional Atmospheric Loss: 0.016

UV Photolysis

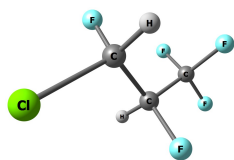
UV Spectrum: *No Recommendation*

$$\tau_{\text{hv}} = 450 \text{ years}$$

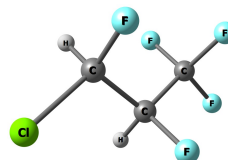
Fractional Atmospheric Loss: 0.016



Molecular Structure and Infrared Spectrum (6 conformers)



E = 0
Population = 0.504



$\Delta E = 0.53 \text{ kcal mol}^{-1}$
Population = 0.205

Optimized Coordinates (Angstroms)

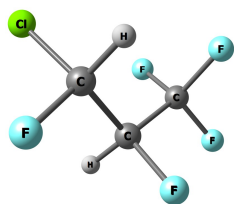
Atom	X	Y	Z
C	-1.022233100910	-0.364800532085	-0.359689900234
C	0.055336926004	0.431369296707	0.381085147410
C	1.473262430223	-0.056767953916	0.038536365446
F	-0.935696001152	-1.667221137634	-0.009323911862
Cl	-2.645416545499	0.266637109220	0.072721503021
H	-0.921418120977	-0.261766064643	-1.441464384602
H	-0.090235354122	0.345591893327	1.462914106189
F	-0.027329688326	1.738555719442	-0.003517903982
F	2.374971848799	0.781802178127	0.548088852728
F	1.691725436015	-1.270989878612	0.545027342978
F	1.654373169944	-0.111497629932	-1.286601217093

Atom	X	Y	Z
C	1.007038829809	-0.522899560226	-0.248889350899
C	-0.063966552114	0.565722664204	-0.204663769022
C	-1.483356007205	-0.021427857290	-0.152401631316
Cl	2.632681258118	0.231993289499	-0.395070690420
F	0.960640366161	-1.265953398938	0.876954400785
H	0.877494528822	-1.164989432128	-1.122188295521
H	0.007913779308	1.176030714102	-1.111354479847
F	0.103323214807	1.347016484435	0.898672615685
F	-2.384947858338	0.956213326335	-0.255804663979
F	-1.654709253530	-0.861552447785	-1.186695974462
F	-1.712713305838	-0.684797782209	0.975263838995

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
41.9735	0.0748
74.7415	0.0466
144.8578	0.171
224.7483	0.160
227.1776	0.662
279.8149	0.622
338.3842	0.0490
407.8933	0.212
430.3810	2.76
504.4952	0.0559
551.3838	0.486
581.0207	1.33
688.2600	13.3
793.9893	13.7
875.8285	1.51
1097.6421	1.63
1132.1662	5.42
1146.2680	12.4
1177.5802	27.5
1234.3181	43.2
1262.7155	14.7
1284.7973	19.4
1329.4206	2.60
1384.9410	10.9
1398.5485	1.76
3080.8883	0.856
3117.5449	1.33

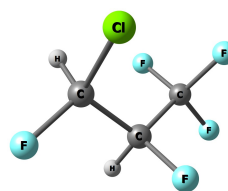
Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
43.7883	0.0978
79.4647	0.0789
144.7510	0.397
214.0462	0.345
227.7151	0.0939
268.1304	0.0436
300.3956	0.143
397.4353	0.295
407.0278	0.337
528.1769	0.495
569.7760	0.886
675.4403	14.3
768.8941	5.38
795.1179	12.0
868.4194	2.84
940.2151	1.10
1106.2215	11.4
1181.6296	3.52
1190.9143	37.8
1214.3037	32.3
1277.4589	1.15
1305.0083	33.7
1364.9836	3.90
1377.9043	7.27
1400.5419	4.59
3074.9811	1.07
3110.3175	1.40



$\Delta E = 0.76 \text{ kcal mol}^{-1}$
Population = 0.139

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.160176551018	0.456101546009	0.342797453044
C	-0.147828348819	0.646580185424	-0.430628043717
C	-1.284397919876	-0.298573917782	-0.009415011201
Cl	1.913823573508	-1.131287240612	-0.019661135547
F	2.005169780688	1.441514906395	-0.030109460680
H	0.998058521007	0.500603500082	1.420958869083
H	0.029882524655	0.536729709049	-1.505276336539
F	-0.574601489156	1.921148406777	-0.161176754951
F	-2.438572217094	0.146048438073	-0.505717334275
F	-1.084511360859	-1.536208773620	-0.461885896609
F	-1.394403615070	-0.348414759794	1.324341651393



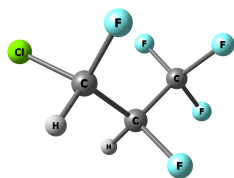
$\Delta E = 1.16 \text{ kcal mol}^{-1}$
Population = 0.071

Atom	X	Y	Z
C	-1.136025443509	0.263131379131	0.636621347475
C	0.149832083510	0.823145939889	0.025487944673
C	1.361090964107	-0.110348496357	0.140308865799
F	-2.024951039799	1.280353535059	0.745598899080
Cl	-1.858144296847	-1.033537582896	-0.365029212580
H	-0.944350028659	-0.161834062983	1.623591701352
H	0.393721598328	1.733297696363	0.588841207101
F	-0.029065287788	1.141561162308	-1.285707870962
F	2.464850564346	0.536275413373	-0.239626973240
F	1.513661059159	-0.483097259782	1.422038306216
F	1.241817827152	-1.202218724105	-0.606423214915

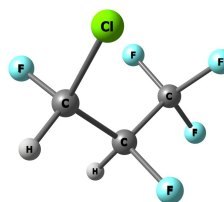
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
37.4500	0.0450
85.7472	0.0680
144.8213	0.0832
226.1400	0.860
237.4781	0.434
307.4652	0.170
336.0132	0.0883
419.1342	0.662
427.9649	1.64
455.0896	1.49
554.9585	0.529
580.0556	0.0694
708.3691	5.76
806.4360	15.5
881.1862	4.60
1080.8943	8.08
1111.3556	7.35
1136.1597	25.1
1183.4025	15.8
1236.8683	41.5
1252.8572	12.4
1285.3429	15.6
1332.7110	4.56
1380.6685	3.10
1407.8622	5.63
3083.3929	0.556
3119.2671	1.30

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
37.3311	0.0487
83.7113	0.0845
150.3823	0.417
201.0861	0.226
229.3424	0.163
279.1125	0.170
321.1168	0.204
403.4389	0.278
420.6474	0.539
520.1433	1.49
575.3135	0.0294
659.5062	10.4
717.4177	5.86
776.8129	4.41
886.0940	3.26
993.3671	4.01
1099.0726	18.9
1173.0760	33.0
1188.6424	7.85
1216.6902	37.0
1286.2696	5.08
1310.7102	20.5
1342.3327	4.92
1379.6601	3.57
1413.9706	5.22
3049.3413	1.36
3111.1498	1.25



$\Delta E = 1.26 \text{ kcal mol}^{-1}$
Population = 0.060



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

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.173821583239	0.692046673276	0.170611600957
C	0.238844253516	0.502316588728	0.730496811884
C	1.175334742383	-0.388879493605	-0.102812395973
F	-1.144086396761	0.923868322674	-1.158179340246
Cl	-2.210171365015	-0.737123259635	0.513085775670
H	-1.638820945279	1.542551286788	0.674724571789
H	0.176206147483	0.086363307804	1.740341066058
F	0.823397987144	1.743603575392	0.783297137255
F	2.333440586719	-0.529191905911	0.552276727449
F	0.650065849827	-1.601523514656	-0.285481770581
F	1.436255723222	0.149796419145	-1.290336184263

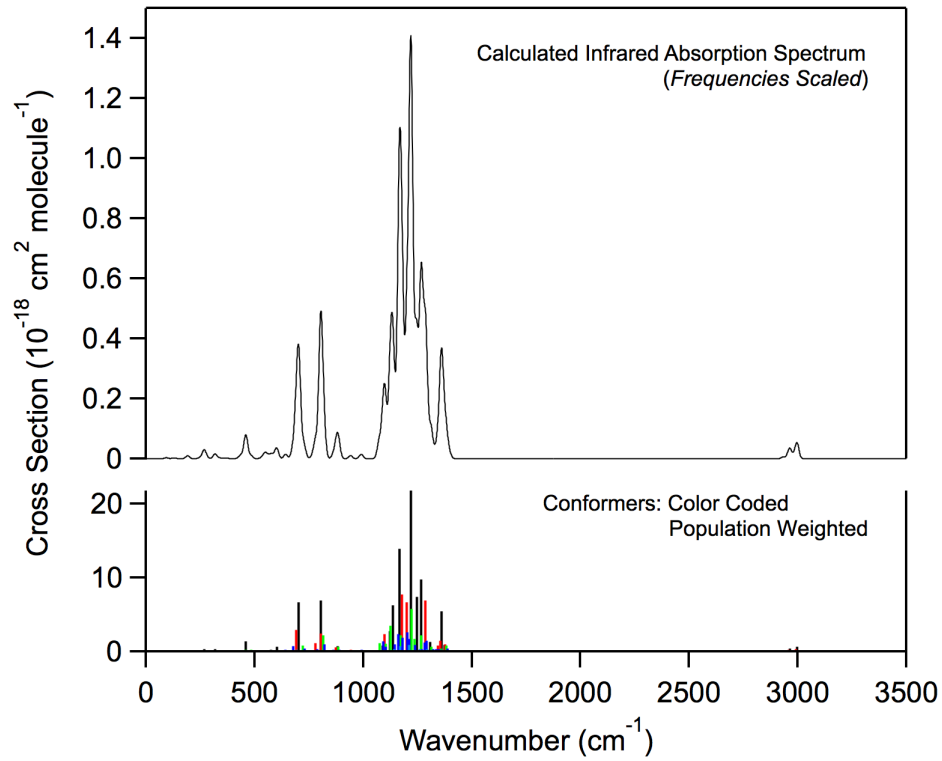
Atom	X	Y	Z
C	1.196302184140	-0.248788183431	-0.731903488403
C	-0.245282485503	0.246646127790	-0.889847740320
C	-1.236774971204	-0.120747258646	0.226083890346
Cl	1.983100622079	0.310008920767	0.778804545167
F	1.211418369362	-1.599468711458	-0.785454771125
H	1.797044170864	0.159284774192	-1.548331922815
H	-0.632042911106	-0.199835971693	-1.815046687444
F	-0.230513705029	1.606095008744	-1.012315409096
F	-2.476385084486	0.174773199834	-0.184884985444
F	-1.183718395599	-1.429028331647	0.486425341330
F	-1.007181793518	0.552688425547	1.348283227802

Infrared Absorption Spectrum (unscaled frequencies)

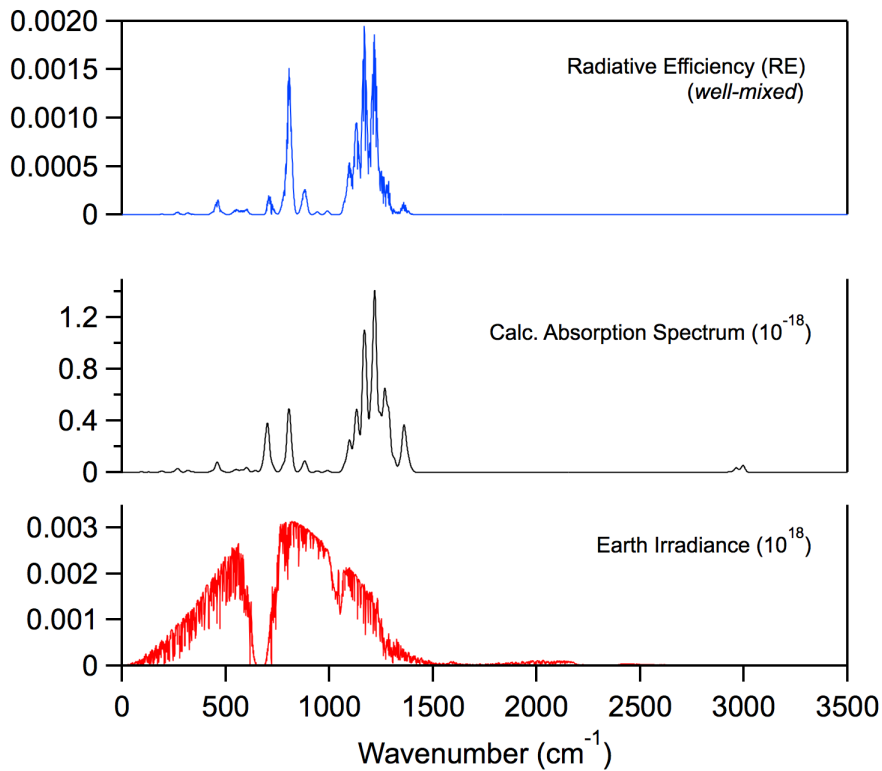
Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
34.8334	0.0522
91.1064	0.0758
157.3218	0.0634
204.1317	0.460
238.2700	0.446
288.2012	0.108
312.5246	0.120
389.9896	0.176
444.3283	0.754
521.8954	2.46
534.7450	1.74
622.2781	3.96
754.3251	3.18
812.6853	16.0
855.6608	4.26
983.6512	0.821
1111.8863	10.8
1156.3743	16.7
1192.5322	31.5
1224.2042	28.1
1253.8325	14.9
1300.9759	20.9
1357.1958	5.76
1368.2350	5.23
1425.2366	2.95
3088.8816	1.10
3098.8934	1.26

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
27.6887	0.0358
97.0885	0.0618
157.6536	0.103
190.5877	0.118
237.0068	0.333
270.9064	0.567
340.5684	0.0214
397.1697	0.139
504.8938	0.868
513.0738	2.23
533.0272	2.98
626.6928	3.75
676.9418	10.5
759.2248	0.429
873.7518	0.649
1071.4459	9.15
1126.0910	5.44
1152.0603	15.8
1183.0690	32.3
1225.3767	40.3
1278.0609	14.7
1313.1018	13.7
1335.7509	8.48
1374.8553	2.19
1423.5354	2.92
3048.7817	1.65
3094.2259	1.85

Infrared Spectrum

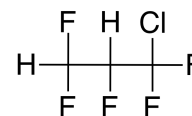


Radiative Efficiency



HCFC-235eb

Molecular Formula: CHF₂CHFCClF₂
 Name: 1-Chloro-1,1,2,3,3-pentafluoropropane
 CAS number: 162102-07-0
 Molecular Weight: 168.49



Global Atmospheric Lifetime (years): 3.18
 Tropospheric Atmospheric Lifetime (years): 3.33
 Stratospheric Atmospheric Lifetime (years): 69.4
 Ozone Depletion Potential (ODP): 0.012

	<i>Well-mixed</i>	<i>Lifetime adjusted</i>
Radiative Efficiency (RE):	0.308	0.274
Global Warming Potential (GWP _H):		
GWP ₂₀	1307	1163
GWP ₁₀₀	355	315
Global Temperature Potentials (GTP _H):		
GTP ₂₀		509
GTP ₅₀		59
GTP ₁₀₀		44

* RE units: W m² ppb⁻¹
 * GWP and GTP: Relative to CO₂

Atmospheric Loss Processes *****

OH Reactivity

$k_{\text{Rec}}(T)$, *No recommendation*

$$k_{\text{SAR}}(298 \text{ K}) = 1.76 \times 10^{-14}; k_{\text{SAR}}(272 \text{ K}) \approx 1.12 \times 10^{-14} \quad \text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$\tau_{\text{Global}}^{\text{OH}} = 3.23 \text{ years}$$

$$\tau_{\text{Trop}}^{\text{OH}} = 3.33 \text{ years}$$

$$\tau_{\text{Strat}}^{\text{OH}} = 99.8 \text{ years}$$

Fractional Atmospheric Loss: 0.986

O(¹D) Reactivity

$k_{\text{Rec}}(T)$, *No recommendation*

$$k_{\text{Est}}(T) = 0.8 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$\tau_{\text{O}(\text{1D})} = 465 \text{ years}$$

Fractional Atmospheric Loss: 0.007

UV Photolysis

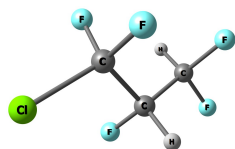
UV Spectrum: *No Recommendation*

$$\tau_{\text{hv}} = 450 \text{ years}$$

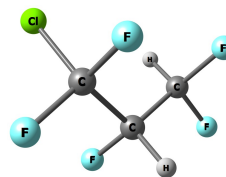
Fractional Atmospheric Loss: 0.007



Molecular Structure and Infrared Spectrum (9 conformers)



E = 0
Population = 0.366



$\Delta E = 0.21 \text{ kcal mol}^{-1}$
Population = 0.257

Optimized Coordinates (Angstroms)

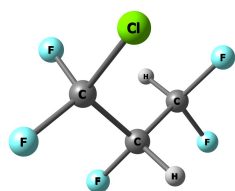
Atom	X	Y	Z
C	1.723767263909	-0.046050347966	0.230285965456
C	0.394750618359	0.494028660011	-0.315943574512
C	-0.806053579389	-0.356843119237	0.125242035458
F	1.913347190828	-1.312315696696	-0.199148927205
F	2.717297603218	0.725926448548	-0.257339566277
H	1.753811611183	-0.020370044670	1.325048933747
H	0.431646319655	0.513251623550	-1.409963533545
F	0.244709281927	1.759327387946	0.173789896218
Cl	-2.352794440071	0.449522805179	-0.298389779608
F	-0.764603530257	-1.547251396702	-0.474644943167
F	-0.776318339364	-0.551502319963	1.450551493435

Atom	X	Y	Z
C	1.529183840904	-0.195635558201	0.368454343530
C	0.469390742246	0.527996248198	-0.466262576870
C	-0.932938947746	-0.096786132183	-0.426470107737
F	1.629615629868	-1.478368826721	-0.041118538133
F	2.711725459864	0.419342466723	0.148571314411
H	1.305990872800	-0.167459307032	1.440237128664
H	0.788473830201	0.527267312112	-1.516515186707
F	0.378054519859	1.811516219940	-0.012587995467
Cl	-1.586318134113	-0.192453182318	1.248648420104
F	-1.761331500331	0.656140528122	-1.153618167593
F	-0.907628313553	-1.321554768641	-0.951957634202

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
42.8743	0.0808
80.1361	0.124
145.5928	0.157
215.1915	0.133
229.2836	0.635
298.1109	0.554
329.4185	0.0463
390.9263	0.680
414.6939	0.191
468.8856	5.86
514.3391	0.316
576.5327	1.93
642.4267	0.769
806.2368	21.4
963.0639	24.2
1109.7496	9.36
1139.8037	5.61
1140.8117	0.310
1159.0282	29.9
1193.2420	42.4
1240.2601	14.9
1304.2214	1.64
1357.0505	1.30
1401.3840	3.23
1426.7700	7.14
3074.0717	1.42
3088.1900	3.61

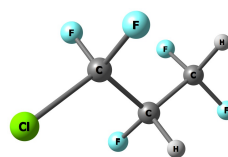
Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
39.0855	0.0803
88.7892	0.115
152.2834	0.200
190.3812	0.138
243.9480	0.491
308.9828	0.153
338.1366	0.447
395.7021	0.393
410.6006	0.114
460.5704	4.86
544.2258	0.365
575.2536	2.47
657.0801	0.692
689.3428	15.3
1053.6586	28.1
1106.6001	7.72
1141.6246	12.0
1147.0440	15.6
1155.1744	20.9
1211.5738	33.8
1215.3586	12.7
1307.8347	0.967
1354.6697	5.30
1401.7394	2.63
1430.9299	4.44
3053.6620	0.648
3083.6040	4.19



$\Delta E = 0.85 \text{ kcal mol}^{-1}$
Population = 0.088

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.534929907958	-0.291080313817	0.334705951270
C	0.492566392639	0.518101876967	-0.445836922448
C	-0.950479191888	0.350218257822	0.060038031085
F	1.313524933333	-1.613797507811	0.189198668413
F	2.746831512691	-0.002239388636	-0.185369485028
H	1.530842042580	-0.033019757426	1.399545309351
H	0.540429756416	0.261596346363	-1.508520538014
F	0.814521263054	1.839090150914	-0.270918880876
Cl	-1.647068447191	-1.234886052350	-0.408399147899
F	-0.988897607806	0.463924256861	1.394810592528
F	-1.710597561787	1.315165131114	-0.458363578382



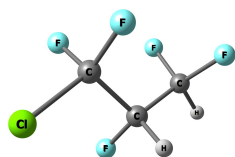
$\Delta E = 0.90 \text{ kcal mol}^{-1}$
Population = 0.080

Atom	X	Y	Z
C	1.690888934146	-0.252832572285	-0.358299895536
C	0.375502721146	0.536760142052	-0.315322025115
C	-0.835943161369	-0.376947024148	-0.086635264064
F	2.680308096197	0.600649673387	-0.705163163542
F	1.969752537500	-0.754191075424	0.860910194521
H	1.649710100321	-1.070229950763	-1.087746228478
H	0.243446133118	1.043473120294	-1.277328869044
F	0.439385783620	1.451742084707	0.690261556110
Cl	-2.363619073777	0.565099141788	-0.103993039766
F	-0.876753403320	-1.285033903584	-1.076124344349
F	-0.747238667583	-1.023452636024	1.072668079264

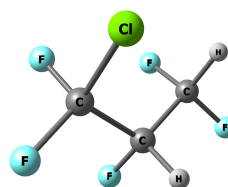
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
36.2471	0.0926
83.5928	0.0918
152.6563	0.0665
204.0127	0.336
251.4240	0.946
312.8004	0.277
317.2215	0.148
367.7900	1.14
420.1175	0.170
477.6690	1.82
514.2448	2.47
576.1023	1.97
618.7569	0.799
852.1683	16.1
960.9443	30.3
1097.7987	5.63
1118.7835	8.86
1138.5481	19.8
1157.2442	23.7
1196.7233	25.2
1239.8233	19.2
1304.7321	1.38
1357.9498	3.55
1401.2990	1.95
1430.2384	5.02
3073.5754	2.30
3092.6422	2.36

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
40.6482	0.110
81.9268	0.121
141.8959	0.350
218.3399	0.423
238.7832	0.207
255.8379	0.0714
314.6533	0.246
347.1517	0.138
419.7779	0.0755
465.8562	0.703
544.0456	3.99
627.4930	1.27
772.0306	21.5
837.1721	10.8
887.8420	3.38
988.3275	24.0
1140.4528	16.0
1146.6390	14.0
1166.6883	16.1
1199.1531	22.1
1266.3451	22.6
1327.4469	3.10
1377.3466	2.11
1415.9770	5.33
1420.4544	4.72
3063.6906	3.29
3076.7264	2.61



$\Delta E = 0.94 \text{ kcal mol}^{-1}$
Population = 0.074



$\Delta E = 1.22 \text{ kcal mol}^{-1}$
Population = 0.047

Optimized Coordinates (Angstroms)

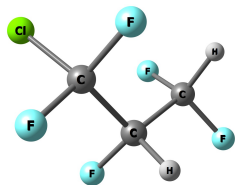
Atom	X	Y	Z
C	1.789355943135	0.208179596612	-0.366088097979
C	0.310183841782	0.530063784563	-0.628200496879
C	-0.675082454477	-0.313899802066	0.197762726053
F	2.057959523895	0.177879499133	0.954448086665
F	2.087915974926	-0.998004738453	-0.896474269144
H	2.416229552760	0.977319226748	-0.835743180720
H	0.106374306713	0.358811936348	-1.689939160343
F	0.110287699032	1.846609034668	-0.321554193301
Cl	-2.369995185258	0.050861064008	-0.301458742407
F	-0.440146394331	-1.611856572173	-0.009287981633
F	-0.560066808178	-0.057555029388	1.497246309687

Atom	X	Y	Z
C	1.421335075629	-0.651359120386	-0.075353480134
C	0.433795092375	0.410257233568	-0.570469604865
C	-0.962982567418	0.330038071551	0.061472688843
F	2.573341644733	-0.491798821923	-0.766341091720
F	1.680919754092	-0.459281427594	1.233432804989
H	1.051438737311	-1.671002344987	-0.227055519734
H	0.321874344179	0.315586894995	-1.655743898491
F	0.939082298569	1.643097475314	-0.264352364173
Cl	-1.763544738106	-1.227624986494	-0.391707727022
F	-0.909677591199	0.416527204832	1.386953004999
F	-1.712087050164	1.334241821123	-0.394208812692

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
34.0703	0.0757
95.7671	0.128
154.6368	0.0517
205.9442	0.246
225.2868	0.335
261.7334	0.114
329.5698	0.0682
401.9881	0.126
417.0850	0.146
474.9181	1.97
535.5909	8.77
617.8430	6.63
637.2142	3.70
846.6400	4.03
947.5567	23.8
992.1446	4.54
1135.6404	4.70
1147.0513	14.5
1190.5877	19.1
1197.4447	41.9
1260.2840	18.3
1333.4810	0.871
1357.8069	9.21
1405.4513	3.50
1430.8475	4.45
3048.6928	5.51
3082.3308	1.29

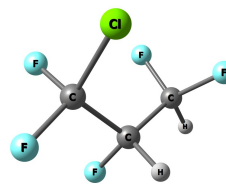
Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
41.0388	0.162
89.2383	0.0930
148.6316	0.253
207.1811	0.446
251.3616	0.0750
288.0045	0.0308
313.0296	0.499
350.7641	0.373
402.5147	0.269
419.5051	0.993
548.2540	2.37
627.3708	1.63
781.1876	9.12
844.6982	14.7
920.7364	11.9
965.3492	26.8
1111.0549	21.0
1133.1754	3.45
1192.0056	12.6
1198.8715	27.4
1268.4187	26.5
1333.1568	2.72
1374.0726	0.802
1414.9721	4.77
1421.3452	4.65
3073.9696	1.35
3081.1751	3.82



$\Delta E = 1.34 \text{ kcal mol}^{-1}$
Population = 0.038

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.529176192724	-0.154633774484	-0.527884057672
C	0.468673376408	0.745242708152	0.114229325406
C	-0.976802032072	0.390300382904	-0.263073041418
F	2.735273475930	0.433475808968	-0.348664450269
F	1.555253095452	-1.357500308128	0.076698885178
H	1.351658230862	-0.288289907052	-1.601266809803
H	0.630492671215	1.767535685169	-0.252632280564
F	0.602239901427	0.720591534129	1.467526631562
Cl	-1.524510990902	-1.175865924798	0.398301346654
F	-1.794264383770	1.347199867689	0.184292445896
F	-1.067972537273	0.357788927452	-1.603866994969



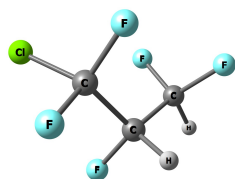
$\Delta E = 1.58 \text{ kcal mol}^{-1}$
Population = 0.025

Atom	X	Y	Z
C	1.651627587669	-0.267527247865	-0.278884216185
C	0.427809104784	0.547315281747	-0.718830589904
C	-0.854992271968	0.379219002751	0.112150751112
F	1.774582045156	-0.286687179942	1.063452998459
F	1.546872970467	-1.539656378409	-0.719828538292
H	2.550925006997	0.191044226162	-0.710021686295
H	0.195672351133	0.297880340007	-1.759163762778
F	0.772623144549	1.873611715916	-0.630371849173
Cl	-1.431516918075	-1.321952544741	0.095359203140
F	-0.671123704725	0.769339891895	1.370318578649
F	-1.807223315986	1.151822892481	-0.423768888733

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
38.5217	0.139
83.4561	0.133
155.4280	0.353
189.0197	0.228
243.7533	0.0977
277.3419	0.380
315.9613	0.261
350.6575	0.274
423.2307	0.0216
482.9251	0.261
558.8056	2.45
646.3197	1.25
685.7010	16.4
791.0758	8.55
923.3417	0.844
1063.3806	23.2
1124.3393	38.2
1144.4925	6.02
1187.2532	23.8
1200.1405	22.2
1219.6759	6.78
1327.4263	4.32
1378.4066	1.11
1418.4393	3.99
1423.8590	4.92
3045.9960	1.19
3068.5181	4.67

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
36.1212	0.0977
99.1293	0.159
150.6999	0.0281
217.5488	0.328
239.8635	0.615
281.6222	0.0510
312.0840	0.289
388.7369	0.374
415.1399	0.254
449.7823	1.31
539.4349	4.71
593.8608	1.18
719.4822	5.90
835.7017	8.10
937.8183	24.9
1005.7036	9.76
1113.9637	2.83
1145.6976	36.0
1168.0150	7.94
1195.4640	24.2
1255.5232	23.6
1332.1145	0.482
1364.7284	8.94
1408.1900	1.78
1431.1211	3.22
3050.5520	5.68
3082.3913	1.07



$\Delta E = 1.61 \text{ kcal mol}^{-1}$
Population = 0.024

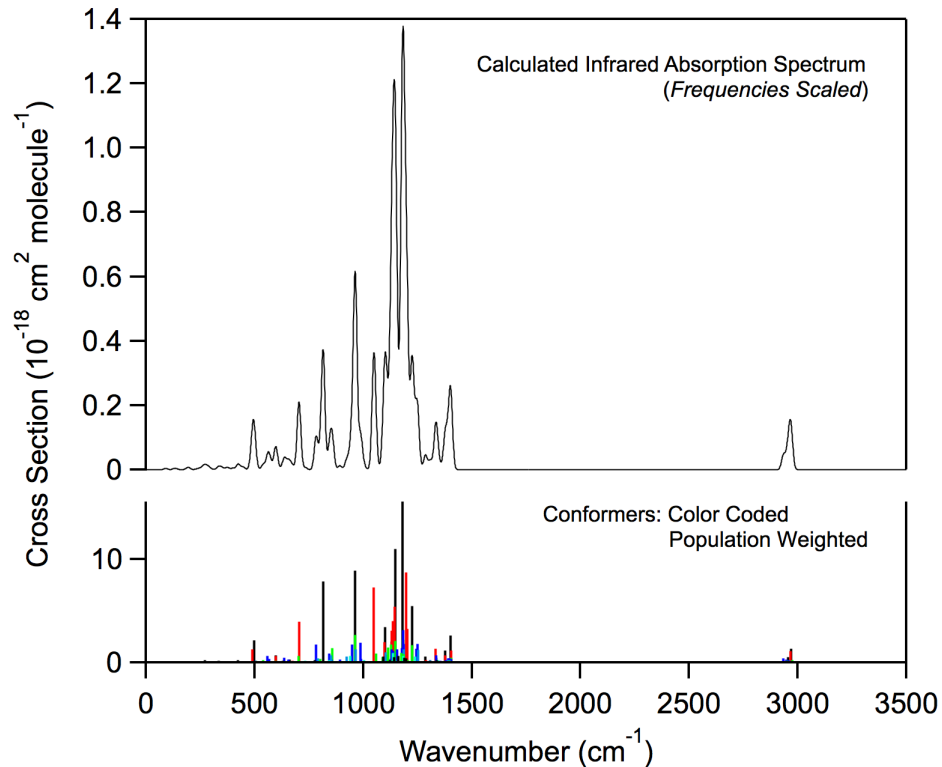
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.719597178679	0.164643253950	0.064727265410
C	0.397430869885	0.859259118830	0.411675890560
C	-0.865266718295	0.289716003148	-0.261593600447
F	1.629702504707	-1.175087462278	0.173445628888
F	2.060382095938	0.470709625240	-1.207034734329
H	2.502672714121	0.521124734043	0.746633579920
H	0.474700381183	1.901621969400	0.077621577400
F	0.233987404669	0.832203313978	1.766991871255
Cl	-1.403516422706	-1.262391566886	0.445024553361
F	-1.859521537073	1.176074124923	-0.117718892846
F	-0.639178471109	0.129259885650	-1.568618139172

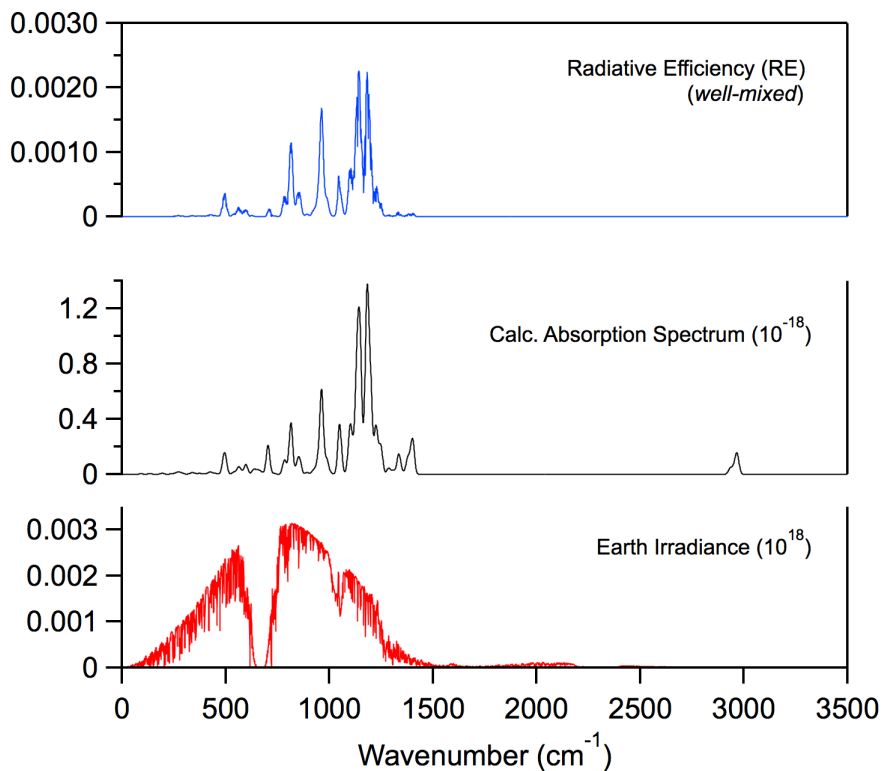
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength ($10^{-18} \text{ cm}^2 \text{ molecule}^{-1} \text{ cm}^{-1}$)
35.8371	0.0943
94.7919	0.129
159.7023	0.118
193.3195	0.120
227.2404	0.372
278.4917	0.365
336.0335	0.230
396.6751	0.337
422.1170	0.0972
475.9953	2.36
554.1523	3.72
610.5114	7.00
658.7093	3.18
767.3294	8.88
928.8370	3.00
1100.4991	24.7
1133.2556	8.74
1151.6517	21.7
1172.9341	27.2
1203.4786	19.5
1211.5989	17.0
1336.0756	0.707
1360.6961	8.94
1409.0965	3.46
1432.6321	1.10
3046.9253	5.01
3055.4687	2.35

Infrared Spectrum

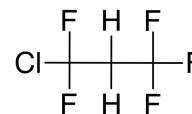


Radiative Efficiency



HCFC-235fa

Molecular Formula: $\text{CClF}_2\text{CH}_2\text{CF}_3$
 Name: 1-Chloro-1,1,3,3,3-pentafluoropropane
 CAS number: 460-92-4
 Molecular Weight: 168.49



Global Atmospheric Lifetime (years): 61.7
 Tropospheric Atmospheric Lifetime (years): 88.6
 Stratospheric Atmospheric Lifetime (years): 203.8
 Ozone Depletion Potential (ODP): 0.051

	<i>Well-mixed</i>	<i>Lifetime adjusted</i>
Radiative Efficiency (RE):	0.301	0.297
Global Warming Potential (GWP_H):		
GWP_{20}	6881	6787
GWP_{100}	5401	5327
Global Temperature Potentials (GTP_H):		
GTP_{20}		6941
GTP_{50}		5741
GTP_{100}		3434

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

Atmospheric Loss Processes *****

OH Reactivity

$k_{\text{Rec}}(T)$, *No recommendation*

$k_{\text{SAR}}(298 \text{ K}) = 6.62 \times 10^{-16}$; $k_{\text{SAR}}(272 \text{ K}) \approx 4.23 \times 10^{-16}$ $\text{cm}^3 \text{molecule}^{-1} \text{s}^{-1}$

$\tau_{\text{Global}}^{\text{OH}} = 84.6$ years

$\tau_{\text{Trop}}^{\text{OH}} = 88.6$ years

$\tau_{\text{Strat}}^{\text{OH}} = 1916.2$ years

Fractional Atmospheric Loss: 0.730

O(¹D) Reactivity

$k_{\text{Rec}}(T)$, *No recommendation*

$k_{\text{Est}}(T) = 0.8 \times 10^{-10} \text{ cm}^3 \text{molecule}^{-1} \text{s}^{-1}$

$\tau_{\text{O}(\text{1D})} = 465$ years

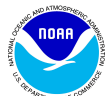
Fractional Atmospheric Loss: 0.133

UV Photolysis

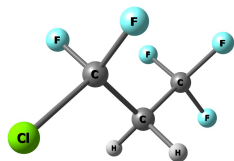
UV Spectrum: *No Recommendation*

$\tau_{\text{hv}} = 450$ years

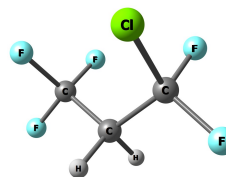
Fractional Atmospheric Loss: 0.137



Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.674



$\Delta E = 0.84 \text{ kcal mol}^{-1}$
Population = 0.163

Optimized Coordinates (Angstroms)

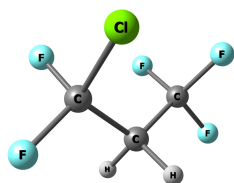
Atom	X	Y	Z
C	-0.070396085792	-0.973746662081	0.000000000000
C	0.760139450809	0.303279293474	0.000000000000
C	-0.070845105662	1.583379740163	0.000000000000
Cl	1.023483948488	-2.417962652916	0.000000000000
F	-0.852510038767	-1.050576158943	1.080004850536
F	-0.852510038767	-1.050576158943	-1.080004850536
H	1.395785368227	0.309492010692	-0.886515289866
H	1.395785368227	0.309492010692	0.886515289866
F	0.753622835805	2.640810226146	0.000000000000
F	-0.852029851178	1.674831175851	-1.080797350144
F	-0.852029851178	1.674831175851	1.080797350144

Atom	X	Y	Z
C	-1.076949980246	0.456320822951	0.052907413856
C	0.276561157888	0.641673508264	0.730204907540
C	1.477608063290	0.004088134995	0.043884617342
Cl	-1.670608137632	-1.244856783623	0.101417769269
F	-1.977302590636	1.216877746678	0.693307719184
F	-1.043912909543	0.850612656922	-1.223046993773
H	0.216661055782	0.260874089791	1.750576491767
H	0.459735700746	1.719185019806	0.771176043079
F	2.584121765855	0.320503926734	0.734449534086
F	1.398444645422	-1.328066458502	-0.003546984451
F	1.635461229075	0.451867335985	-1.205382517899

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
27.2415	0.00465
116.5145	0.367
147.5656	0.234
235.8771	0.0361
286.6539	0.00116
307.3808	0.0808
368.5969	0.183
413.2251	0.344
422.7251	0.00510
523.7117	0.868
538.7303	0.207
594.8958	1.01
637.6082	12.5
819.2310	11.8
849.7505	2.60
928.9751	5.24
949.9649	29.7
1073.5060	0.0
1193.4503	24.4
1227.7906	9.37
1253.4660	58.1
1290.8397	50.5
1326.2593	2.61
1389.0795	23.6
1453.2232	0.985
3102.3757	0.0157
3159.5803	0.00658

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
24.6122	0.00086
116.5404	0.204
157.6435	0.215
243.7767	0.145
289.7449	0.0134
319.3732	0.0664
380.9353	0.104
398.1511	0.169
428.2147	0.406
522.9251	1.17
538.7495	0.352
603.0868	2.70
682.8359	10.1
698.4425	6.23
866.4329	2.23
919.2080	7.69
998.0847	6.11
1119.2727	25.4
1169.3478	40.1
1214.4480	22.9
1240.7284	37.1
1290.1981	34.4
1319.9629	5.67
1400.7369	20.2
1456.0571	1.04
3083.6325	0.0666
3148.7031	0.0367



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

$$\text{Population} = 0.163$$

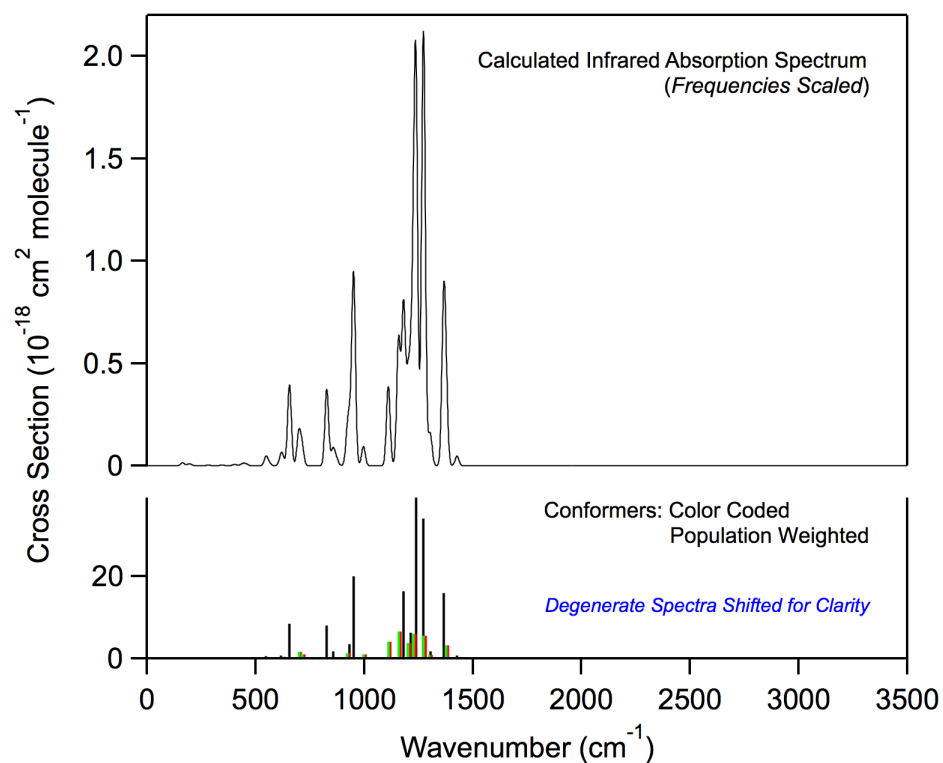
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.077068564070	-0.455853385884	0.052930505005
C	0.276394693562	-0.641357928578	0.730282128496
C	1.477651444953	-0.004541854144	0.043614959376
Cl	-1.670115007820	1.245560796249	0.100618513203
F	-1.044208244907	-0.850785999240	-1.222830274282
F	-1.977676316128	-1.215771435570	0.693730383482
H	0.459183697200	-1.718914785698	0.771779172473
H	0.216659371658	-0.260034357771	1.750467607438
F	2.584070519760	-0.321014595264	0.734305406183
F	1.635309528316	-0.452992991493	-1.205435745504
F	1.398964877477	1.327617537392	-0.004470655869

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
24.6121	0.0009
116.5403	0.204
157.6435	0.215
243.7767	0.145
289.7449	0.0134
319.3732	0.0664
380.9353	0.104
398.1511	0.169
428.2147	0.406
522.9251	1.17
538.7495	0.352
603.0868	2.70
682.8359	10.1
698.4425	6.23
866.4329	2.23
919.2080	7.69
998.0847	6.11
1119.2727	25.4
1169.3478	40.1
1214.4480	22.9
1240.7284	37.1
1290.1981	34.4
1319.9629	5.67
1400.7370	20.2
1456.0571	1.04
3083.6325	0.0666
3148.7031	0.0367

Infrared Spectrum



Radiative Efficiency

