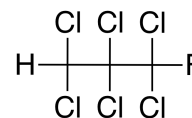


HCFC-221aa

Molecular Formula: CHCl₂CCl₂CCl₂F
 Name: 1,1,2,2,3,3-Hexachloro-1-fluoropropane
 CAS number: 422-28-6
 Molecular Weight: 268.76



Global Atmospheric Lifetime (years): 0.929
 Tropospheric Atmospheric Lifetime (years): 0.979
 Stratospheric Atmospheric Lifetime (years): 20
 Ozone Depletion Potential (ODP): 0.027

	<i>Well-mixed</i>	<i>Lifetime adjusted</i>
Radiative Efficiency (RE):	0.251	0.183
Global Warming Potential (GWP _H):		
GWP ₂₀	195	142
GWP ₁₀₀	53	38
Global Temperature Potentials (GTP _H):		
GTP ₂₀		46
GTP ₅₀		7
GTP ₁₀₀		5

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

Atmospheric Loss Processes *****

OH Reactivity

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

$k_{\text{SAR}}(298 \text{ K}) = 5.99 \times 10^{-14}$; $k_{\text{SAR}}(272 \text{ K}) \approx 3.82 \times 10^{-14}$ cm³ molecule⁻¹ s⁻¹

$\tau_{\text{Global}}^{\text{OH}} = 0.951$ years

$\tau_{\text{Trop}}^{\text{OH}} = 0.979$ years

$\tau_{\text{Strat}}^{\text{OH}} = 33.1$ years

Fractional Atmospheric Loss: 0.976

O(¹D) Reactivity

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

$k_{\text{Est}}(T) = 2.0 \times 10^{-10}$ cm³ molecule⁻¹ s⁻¹

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

Fractional Atmospheric Loss: 0.005

UV Photolysis

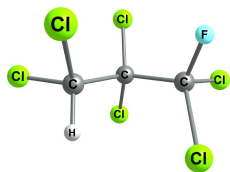
UV Spectrum: *No Recommendation*

$\tau_{\text{hv}} = 50$ years

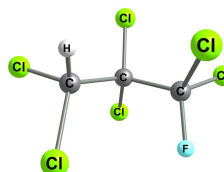
Fractional Atmospheric Loss: 0.019



Molecular Structure and Infrared Spectrum (4 conformers)



E = 0
Population = 0.48



$\Delta E = 0 \text{ kcal mol}^{-1}$
Population = 0.48

Optimized Coordinates (Angstroms)

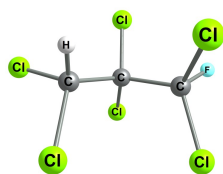
Atom	X	Y	Z
C	-1.314359388600	0.292159877300	0.549001211200
C	-0.080590862000	-0.366838172000	-0.149434979700
C	1.241381231400	0.500146916300	-0.029611073200
Cl	0.199509175400	-1.932340675700	0.677194163600
Cl	-0.398203716500	-0.623063812300	-1.885154511400
H	-1.093690392600	0.388042256000	1.608066862900
Cl	-1.680850768900	1.931124394700	-0.056683353200
Cl	-2.769882597100	-0.733584278400	0.416410864000
Cl	1.525142956900	0.989078960900	1.677986860200
Cl	2.671432034700	-0.383347292700	-0.633250937300
F	1.118532327400	1.606730825900	-0.759816107200

Atom	X	Y	Z
C	-1.326065422500	-0.404741036200	0.461678013000
C	-0.103017258800	0.430458768900	-0.039206231400
C	1.234035482200	-0.416183969000	-0.134679778100
Cl	-0.422018758200	1.112866095800	-1.655320054300
Cl	0.147534233200	1.739819297200	1.158867117700
H	-1.105630042900	-0.762200690700	1.463245836100
Cl	-2.799466806900	0.596424974900	0.584199902200
Cl	-1.662081209300	-1.842605614800	-0.541834880200
Cl	2.649135336800	0.615411773800	-0.485774796600
Cl	1.523409561400	-1.317104403200	1.395046722200
F	1.132314885000	-1.303471196700	-1.122199850800

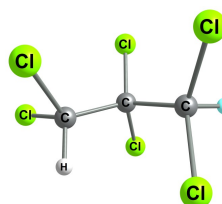
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
57.1880	0.0171
81.0986	0.00927
129.4447	0.0539
173.3692	0.0185
183.3989	0.0410
200.7717	0.00337
215.0046	0.0181
236.4910	0.0221
260.6945	0.0510
274.5351	0.0146
327.0938	0.381
344.3571	0.0567
380.9073	0.0250
395.7321	0.183
495.6697	0.634
580.7208	5.57
678.0972	16.7
752.6002	18.9
775.5754	23.0
840.4322	9.33
865.3557	9.31
979.3582	2.45
1027.8440	7.63
1159.2804	14.5
1229.0485	3.30
1279.2703	0.588
3168.7515	0.526

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
57.1856	0.0171
81.0978	0.00927
129.4445	0.0539
173.3677	0.0185
183.3985	0.0410
200.7713	0.00337
215.0024	0.0181
236.4903	0.0221
260.6937	0.0510
274.5346	0.0146
327.0935	0.381
344.3563	0.0567
380.9067	0.0250
395.7349	0.183
495.6714	0.634
580.7189	5.57
678.1002	16.7
752.5904	18.9
775.5800	23.0
840.4339	9.32
865.3571	9.31
979.3557	2.45
1027.8391	7.63
1159.2779	14.5
1229.0478	3.30
1279.2689	0.588
3168.7553	0.526



$E = 1.91 \text{ kcal mol}^{-1}$
Population = 0.019



$\Delta E = 1.91 \text{ kcal mol}^{-1}$
Population = 0.019

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.148073848200	-0.344581034200	0.682727495600
C	-0.185552018600	0.463533000700	-0.238852464000
C	1.362609521400	0.143471128000	-0.068841864900
Cl	-0.609796200300	0.285344522700	-1.958923826400
Cl	-0.367811474800	2.193922588700	0.241931774100
H	-0.876192274900	-0.140726443000	1.714474223100
Cl	-2.843934802000	0.179820359700	0.481164083600
Cl	-1.047319972800	-2.111360460100	0.459421005700
Cl	1.809714755200	0.135586463700	1.674468002200
Cl	1.890109341000	-1.388844700700	-0.811239974600
F	2.047749974100	1.117702574400	-0.668567454300

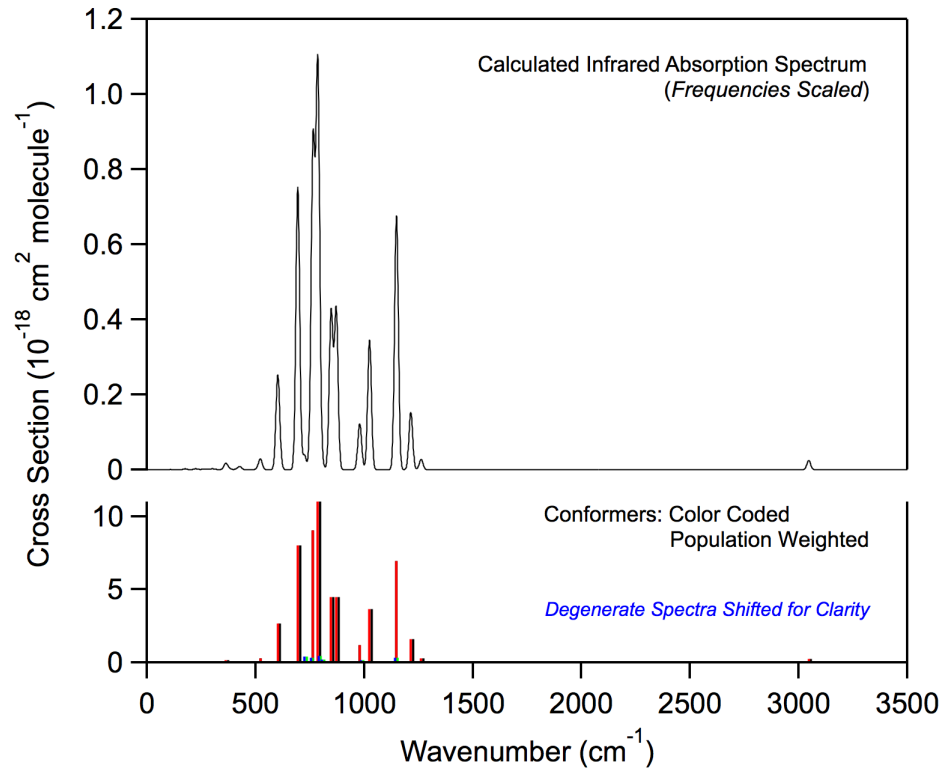
Atom	X	Y	Z
C	-1.136202553300	-0.227905506600	-0.707829912600
C	-0.135821046600	0.392200102800	0.313698571700
C	1.396317021000	0.036031570800	0.081627672400
Cl	-0.244920943100	2.181103557900	0.098023318700
Cl	-0.560336324300	-0.022736030400	1.992380763000
H	-0.859960241800	0.116029898600	-1.700489733600
Cl	-1.111167874100	-2.010885542900	-0.751303406300
Cl	-2.806919522300	0.331666695500	-0.412595504600
Cl	1.859980890800	-1.610845430900	0.581855235300
Cl	1.835517932000	0.269649145500	-1.648000765000
F	2.125465661600	0.879994539600	0.812571761000

Infrared Absorption Spectrum (unscaled frequencies)

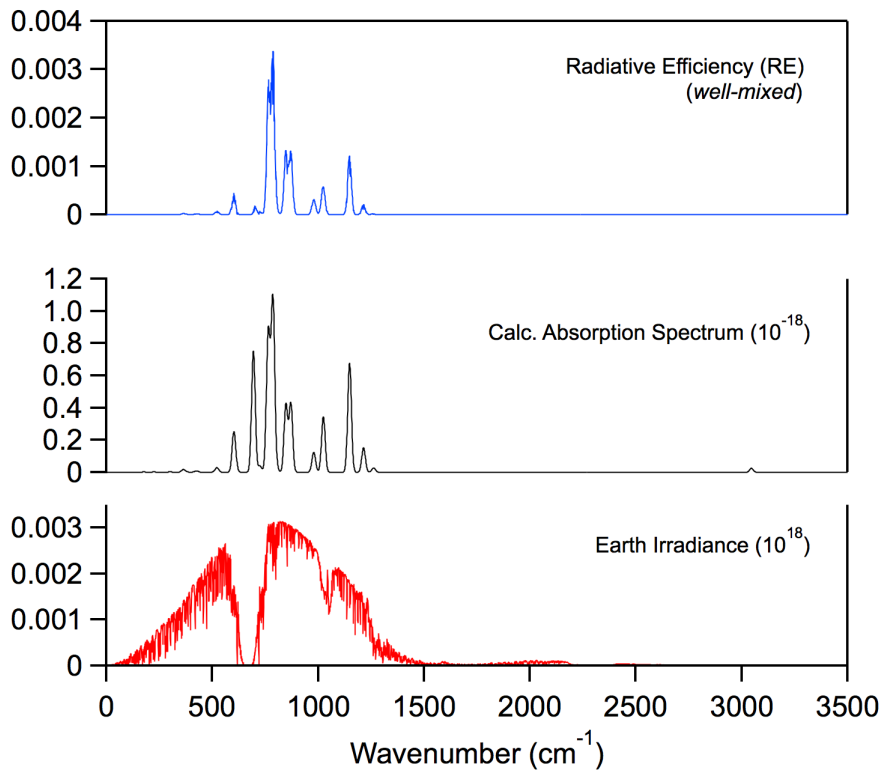
Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
50.2358	0.0224
78.9543	0.0168
135.8415	0.0186
166.2752	0.0192
177.5991	0.0623
206.0014	0.0237
219.5397	0.00852
228.1606	0.0155
278.3139	0.0336
288.8037	0.0428
294.8755	0.173
353.4377	0.0444
379.7765	0.245
394.0130	0.0483
480.2057	0.864
595.0128	3.48
710.5071	21.6
741.4135	16.4
779.6352	22.8
795.7185	10.8
861.8237	4.09
985.2838	8.01
1033.8524	1.24
1153.3720	16.1
1227.3094	2.30
1281.8344	0.664
3166.5759	0.620

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
50.2368	0.0224
78.9546	0.0168
135.8425	0.0186
166.2739	0.0192
177.5997	0.0623
206.0010	0.0237
219.5395	0.00852
228.1599	0.0155
278.3130	0.0336
288.8040	0.0428
294.8750	0.173
353.4366	0.0444
379.7776	0.245
394.0132	0.0483
480.2051	0.864
595.0161	3.48
710.5066	21.6
741.4145	16.4
779.6361	22.8
795.7191	10.8
861.8275	4.09
985.2783	8.01
1033.8475	1.23
1153.3777	16.1
1227.3056	2.30
1281.8306	0.664
3166.5879	0.620

Infrared Spectrum

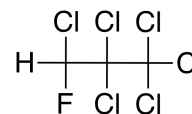


Radiative Efficiency



HCFC-221ab

Molecular Formula: CHClFCCl₂CCl₃
 Name: 1,1,1,2,2,3-Hexachloro-3-fluoropropane
 CAS number: 422-26-4
 Molecular Weight: 268.76



Global Atmospheric Lifetime (years): 2.67
 Tropospheric Atmospheric Lifetime (years): 2.96
 Stratospheric Atmospheric Lifetime (years): 27.3
 Ozone Depletion Potential (ODP): 0.069

	<i>Well-mixed</i>	<i>Lifetime adjusted</i>
Radiative Efficiency (RE):	0.207	0.181
Global Warming Potential (GWP _H):		
GWP ₂₀	462	404
GWP ₁₀₀	125	109
Global Temperature Potentials (GTP _H):		
GTP ₂₀		164
GTP ₅₀		20
GTP ₁₀₀		15

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

Atmospheric Loss Processes *****

OH Reactivity

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

$k_{SAR}(298\text{ K}) = 1.98 \times 10^{-14}$; $k_{SAR}(272\text{ K}) \approx 1.27 \times 10^{-14}$ cm³ molecule⁻¹ s⁻¹

$\tau_{Global}^{OH} = 2.86$ years

$\tau_{Trop}^{OH} = 2.96$ years

$\tau_{Strat}^{OH} = 89.6$ years

Fractional Atmospheric Loss: 0.932

O(¹D) Reactivity

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

$k_{Est}(T) = 2.0 \times 10^{-10}$ cm³ molecule⁻¹ s⁻¹

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

Fractional Atmospheric Loss: 0.014

UV Photolysis

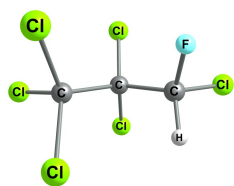
UV Spectrum: *No Recommendation*

$\tau_{hv} = 50$ years

Fractional Atmospheric Loss: 0.053



Molecular Structure and Infrared Spectrum (1 conformer)



E = 0

Population = 0.993

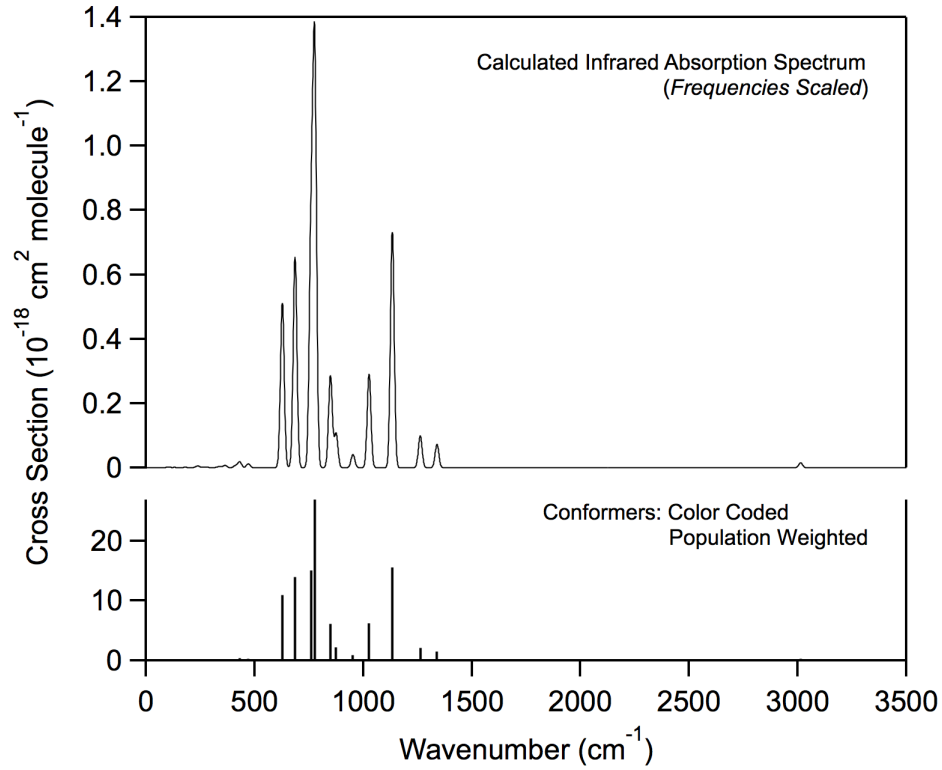
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.376146619200	-0.620563607200	0.600664515400
C	-0.354546393400	0.290028799000	-0.154988541600
C	1.156365346800	-0.131824145300	0.117560714400
Cl	-0.666352914700	0.226630365700	-1.908058662900
Cl	-0.588719260500	1.957088169500	0.457889361400
H	-1.191218759900	-0.555554473000	1.672592459200
Cl	-3.070121747500	-0.106311739400	0.338890287800
F	-1.255335369200	-1.896580582700	0.189660487300
Cl	2.274762613000	1.047507210800	-0.622257834200
Cl	1.453782360400	-0.173691500000	1.892094537300
Cl	1.530848744200	-1.743947497300	-0.549603324000

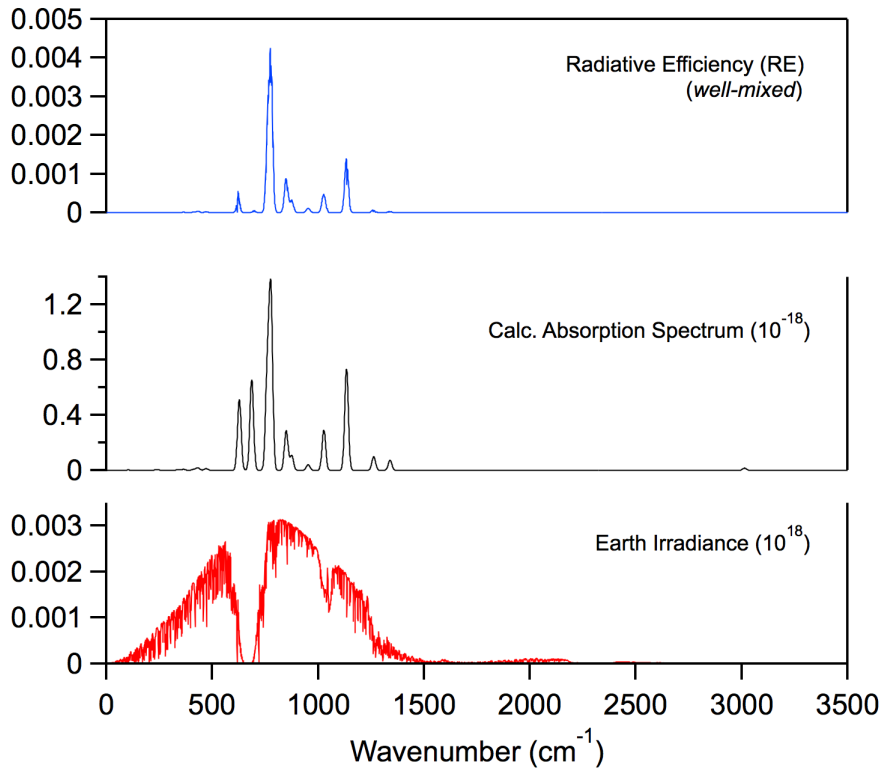
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
51.4796	0.0545
81.7610	0.0228
133.4146	0.0293
171.3195	0.00668
192.2541	0.0728
199.8495	0.0479
221.6944	0.0161
227.6455	0.00402
240.3498	0.0301
279.0748	0.0112
300.7887	0.0820
328.1626	0.153
379.1507	0.140
399.9146	0.393
441.5105	0.263
607.6943	11.0
669.6351	14.1
747.8084	15.2
765.4535	27.1
842.0516	6.14
869.7185	2.25
951.7936	0.888
1030.4472	6.25
1143.7302	15.7
1279.8815	2.12
1361.3815	1.56
3134.1416	0.336

Infrared Spectrum

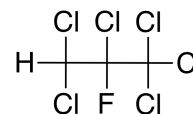


Radiative Efficiency



HCFC-221ba

Molecular Formula: CHCl₂CClFCCl₃
 Name: 1,1,1,2,3,3-Hexachloro-2-fluoropropane
 CAS number: 422-40-2
 Molecular Weight: 268.76



Global Atmospheric Lifetime (years): 1.11
 Tropospheric Atmospheric Lifetime (years): 1.17
 Stratospheric Atmospheric Lifetime (years): 20
 Ozone Depletion Potential (ODP): 0.032

	<i>Well-mixed</i>	<i>Lifetime adjusted</i>
Radiative Efficiency (RE):	0.229	0.174
Global Warming Potential (GWP _H):		
GWP ₂₀	212	161
GWP ₁₀₀	58	44
Global Temperature Potentials (GTP _H):		
GTP ₂₀		53
GTP ₅₀		8
GTP ₁₀₀		6

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

Atmospheric Loss Processes *****

OH Reactivity

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

$k_{\text{SAR}}(298 \text{ K}) = 5.01 \times 10^{-14}$; $k_{\text{SAR}}(272 \text{ K}) \approx 3.20 \times 10^{-14}$ cm³ molecule⁻¹ s⁻¹

$\tau_{\text{Global}}^{\text{OH}} = 1.14$ years

$\tau_{\text{Trop}}^{\text{OH}} = 1.17$ years

$\tau_{\text{Strat}}^{\text{OH}} = 38.9$ years

Fractional Atmospheric Loss: 0.972

O(¹D) Reactivity

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

$k_{\text{Est}}(T) = 2.0 \times 10^{-10}$ cm³ molecule⁻¹ s⁻¹

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

Fractional Atmospheric Loss: 0.006

UV Photolysis

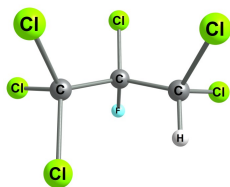
UV Spectrum: *No Recommendation*

$\tau_{\text{hv}} = 50$ years

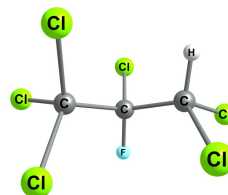
Fractional Atmospheric Loss: 0.022



Molecular Structure and Infrared Spectrum (2 conformers)



E = 0
Population = 0.962



$\Delta E = 1.96 \text{ kcal mol}^{-1}$
Population = 0.035

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.422286622900	-0.377537125400	-0.476966542200
C	0.223139668600	0.569744921300	-0.153405416900
C	-1.212945424300	-0.108773906200	-0.140405654000
Cl	0.491435940500	1.459703201700	1.368715357800
F	0.178634321600	1.454453684200	-1.174502856200
H	1.181842753700	-0.930115344400	-1.380628115400
Cl	2.868481459300	0.603361054800	-0.856036164200
Cl	1.792847065700	-1.567916910900	0.787376288800
Cl	-2.445885801200	1.186103138300	-0.120349001700
Cl	-1.408092196100	-1.043747327200	-1.667743725000
Cl	-1.483278410800	-1.183358386200	1.243662829000

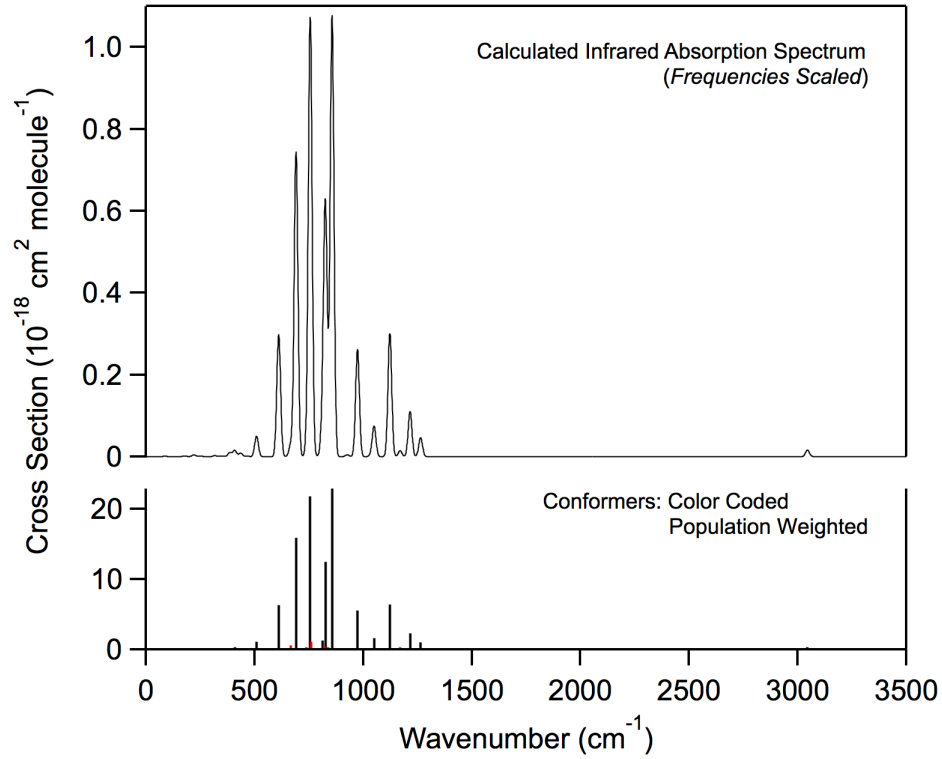
Atom	X	Y	Z
C	1.437757100100	-0.120666595200	0.490972548900
C	0.215562486900	0.357065559100	-0.360346849700
C	-1.209423533200	-0.233257330800	0.023098090900
Cl	0.165273093400	2.149241441900	-0.128883813900
F	0.416482055800	0.089653733800	-1.656584141500
H	1.337093934900	0.264047725900	1.500385721300
Cl	1.620256053100	-1.891113997200	0.624381866400
Cl	2.940793130700	0.561679003100	-0.200203001900
Cl	-2.499115824500	0.706579440000	-0.786539297100
Cl	-1.375894990100	-1.916626923400	-0.547848080600
Cl	-1.434948507100	-0.160043057100	1.794969957100

Infrared Absorption Spectrum (unscaled frequencies)

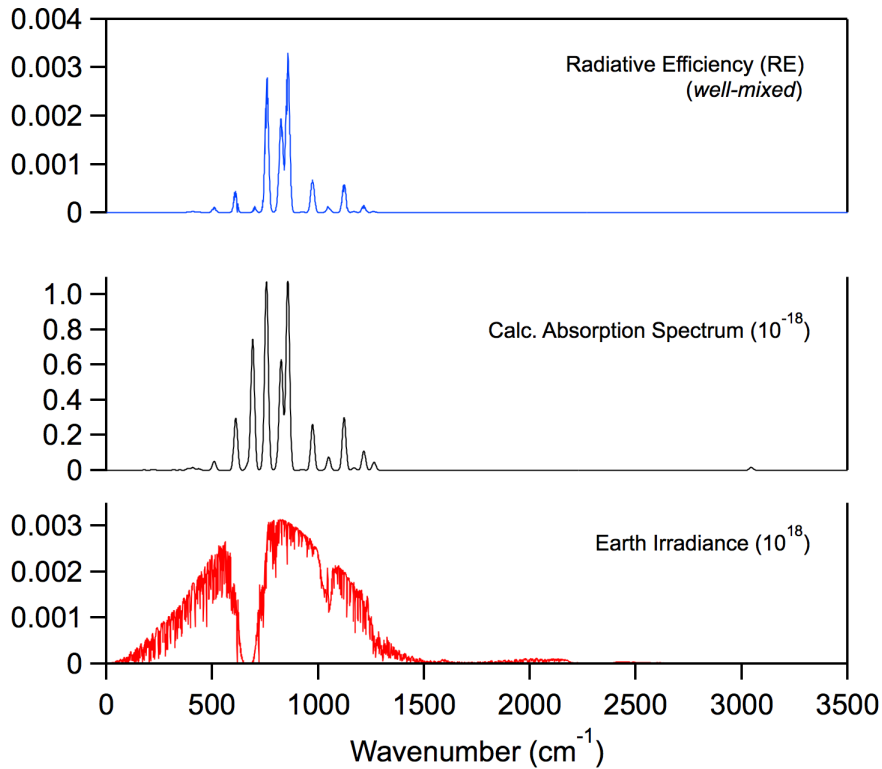
Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
35.1303	0.0295
81.9497	0.0139
131.2315	0.0482
168.4339	0.0105
176.0426	0.0814
192.5157	0.0168
210.0578	0.0198
232.8149	0.0131
277.2239	0.0478
288.7673	0.0139
311.0644	0.0445
351.1668	0.215
375.4271	0.335
404.2539	0.191
481.9321	1.11
589.8864	6.62
674.6206	16.5
743.3363	22.6
803.2131	1.29
817.3263	12.9
850.1147	23.8
973.9787	5.82
1054.6591	1.65
1131.6798	6.67
1230.3955	2.39
1281.6214	1.02
3166.7029	0.361

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
42.5731	0.0174
65.3502	0.0228
137.5449	0.0177
171.6010	0.0255
184.9352	0.0806
214.1958	0.0122
219.4292	0.0359
237.1647	0.00859
263.8896	0.0287
273.8627	0.0403
304.8470	0.0143
324.3596	0.146
369.1713	0.235
399.9611	0.0898
435.4678	1.02
649.2306	17.7
725.8971	8.65
747.2946	32.4
763.3744	1.27
812.2035	15.2
830.0394	9.09
923.5593	2.77
1035.6433	1.22
1181.6938	8.75
1223.6190	2.24
1299.7381	0.258
3181.2798	0.657

Infrared Spectrum

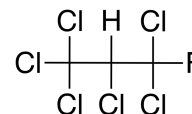


Radiative Efficiency



HCFC-221da

Molecular Formula: CCl₃CHClCCl₂F
 Name: 1,1,1,2,3,3-Hexachloro-3-fluoropropane
 CAS number: 431-79-8
 Molecular Weight: 268.76



Global Atmospheric Lifetime (years): 3.29
 Tropospheric Atmospheric Lifetime (years): 3.71
 Stratospheric Atmospheric Lifetime (years): 29.0
 Ozone Depletion Potential (ODP): 0.083

	<i>Well-mixed</i>	<i>Lifetime adjusted</i>
Radiative Efficiency (RE):	0.272	0.243
Global Warming Potential (GWP _H):		
GWP ₂₀	749	668
GWP ₁₀₀	203	181
Global Temperature Potentials (GTP _H):		
GTP ₂₀		297
GTP ₅₀		34
GTP ₁₀₀		25

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

Atmospheric Loss Processes *****

OH Reactivity

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

$$k_{\text{SAR}}(298 \text{ K}) = 1.58 \times 10^{-14}; k_{\text{SAR}}(272 \text{ K}) \approx 1.01 \times 10^{-14} \quad \text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$\tau_{\text{Global}}^{\text{OH}} = 3.59 \text{ years}$$

$$\tau_{\text{Trop}}^{\text{OH}} = 3.71 \text{ years}$$

$$\tau_{\text{Strat}}^{\text{OH}} = 110.0 \text{ years}$$

Fractional Atmospheric Loss: 0.916

O(¹D) Reactivity

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

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

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

Fractional Atmospheric Loss: 0.018

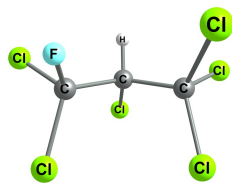
UV Photolysis

UV Spectrum: *No Recommendation*

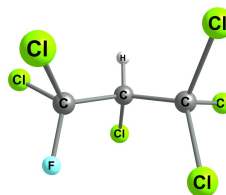
$$\tau_{\text{hv}} = 50 \text{ years}$$

Fractional Atmospheric Loss: 0.066

Molecular Structure and Infrared Spectrum (2 conformers)



E = 0
Population = 0.880



$\Delta E = 1.18 \text{ kcal mol}^{-1}$
Population = 0.120

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.297986304700	-0.129441091200	-0.070213273200
C	0.104367416600	0.429847375500	-0.485663334700
C	1.382643480600	-0.422380005700	-0.172832744700
H	0.068278609800	0.507580144100	-1.573323793700
Cl	0.335276622800	2.083211259100	0.146100003400
Cl	-2.546100089300	1.016719168000	-0.681296444100
Cl	-1.606062763400	-1.702080801400	-0.879302941000
Cl	-1.499390268500	-0.317961757600	1.686682904600
Cl	2.735826591600	0.240600753600	-1.166871277700
Cl	1.872208111900	-0.441074031100	1.540648557400
F	1.201391592700	-1.687140013400	-0.563261656400

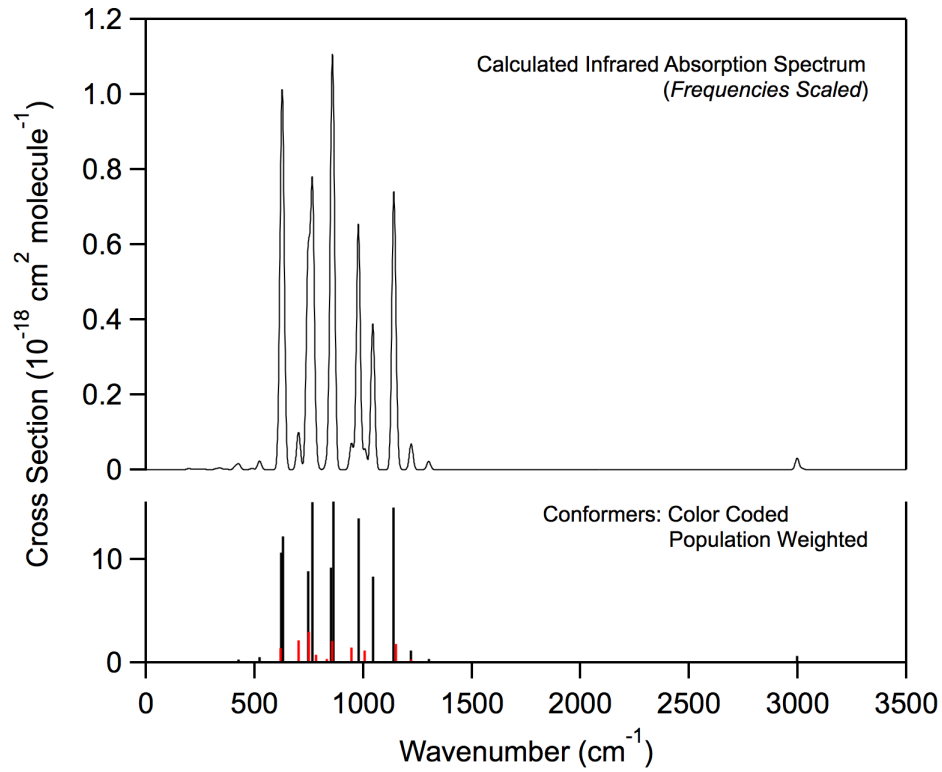
Atom	X	Y	Z
C	-1.253044573100	-0.156594573500	-0.076550409700
C	0.124182504200	0.495796321900	-0.449256754000
C	1.433610229000	-0.078651214000	0.198289555000
H	0.222082715500	0.416105348400	-1.530839687700
Cl	0.109985545400	2.245887784500	-0.044452255700
Cl	-2.593022404800	0.874629019900	-0.684870089100
Cl	-1.431176948500	-1.734352145900	-0.919106502200
Cl	-1.439785682600	-0.379825570800	1.681024782200
Cl	1.594878115300	-1.857501792700	0.123003892500
Cl	2.841113312100	0.629381259200	-0.683578448500
F	1.521166187600	0.278421563000	1.478877917400

Infrared Absorption Spectrum (unscaled frequencies)

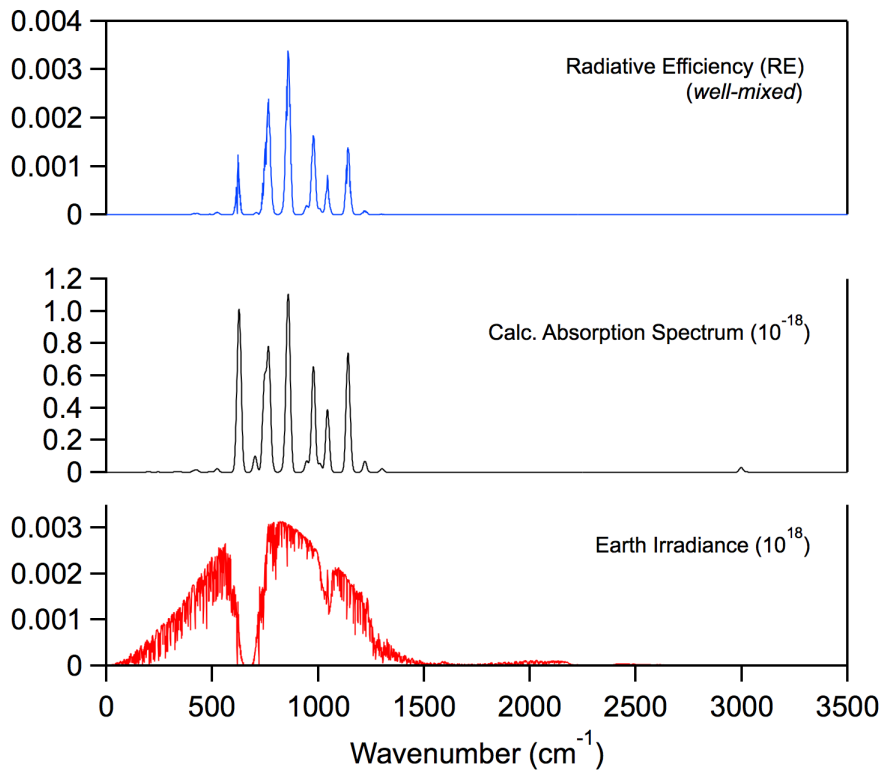
Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
17.1350	0.00120
80.3299	0.00340
151.4758	0.0651
167.5919	0.0151
179.3773	0.0136
195.1540	0.0226
204.9878	0.0358
225.1940	0.0216
282.9620	0.0271
288.5778	0.0394
304.1814	0.0978
377.7266	0.144
378.6138	0.0370
395.0065	0.303
496.4349	0.562
602.6999	12.1
610.8002	13.9
732.3431	10.1
754.2827	17.7
845.1505	10.4
855.2462	17.7
978.1897	15.8
1048.6030	9.42
1150.5382	17.0
1235.7622	1.32
1322.0837	0.395
3116.9720	0.748

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
37.3527	0.00226
69.3671	0.00653
145.1889	0.0506
167.8623	0.0325
184.7801	0.00495
205.5212	0.00110
231.2228	0.0214
235.4991	0.0501
264.1639	0.0228
292.0401	0.00392
316.7994	0.0932
334.3850	0.264
382.6702	0.165
395.2959	0.300
460.3029	0.621
598.2179	11.7
686.5260	17.8
735.8552	25.0
770.3369	6.56
823.9445	2.69
851.4699	17.6
944.8494	12.4
1010.3629	9.79
1162.5427	15.1
1235.7140	2.45
1318.9048	1.19
3141.7708	0.604

Infrared Spectrum

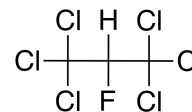


Radiative Efficiency



HCFC-221ea

Molecular Formula: CCl₃CHFCCl₃
 Name: 1,1,1,3,3,3-Hexachloro-2-fluoropropane
 CAS number: –
 Molecular Weight: 268.76



Global Atmospheric Lifetime (years): 3.51
 Tropospheric Atmospheric Lifetime (years): 3.99
 Stratospheric Atmospheric Lifetime (years): 29.5
 Ozone Depletion Potential (ODP): 0.088

	<i>Well-mixed</i>	<i>Lifetime adjusted</i>
Radiative Efficiency (RE):	0.245	0.219
Global Warming Potential (GWP _H):		
GWP ₂₀	717	644
GWP ₁₀₀	195	175
Global Temperature Potentials (GTP _H):		
GTP ₂₀		295
GTP ₅₀		33
GTP ₁₀₀		24

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

Atmospheric Loss Processes *****

OH Reactivity

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

$$k_{\text{SAR}}(298 \text{ K}) = 1.47 \times 10^{-14}; k_{\text{SAR}}(272 \text{ K}) \approx 0.938 \times 10^{-14} \quad \text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$\tau_{\text{Global}}^{\text{OH}} = 3.86 \text{ years}$$

$$\tau_{\text{Trop}}^{\text{OH}} = 3.99 \text{ years}$$

$$\tau_{\text{Strat}}^{\text{OH}} = 117.3 \text{ years}$$

Fractional Atmospheric Loss: 0.911

O(¹D) Reactivity

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

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

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

Fractional Atmospheric Loss: 0.019

UV Photolysis

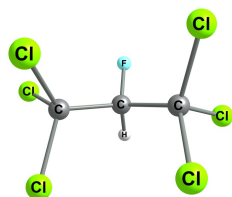
UV Spectrum: *No Recommendation*

$$\tau_{\text{hv}} = 50 \text{ years}$$

Fractional Atmospheric Loss: 0.070



Molecular Structure and Infrared Spectrum (1 conformer)



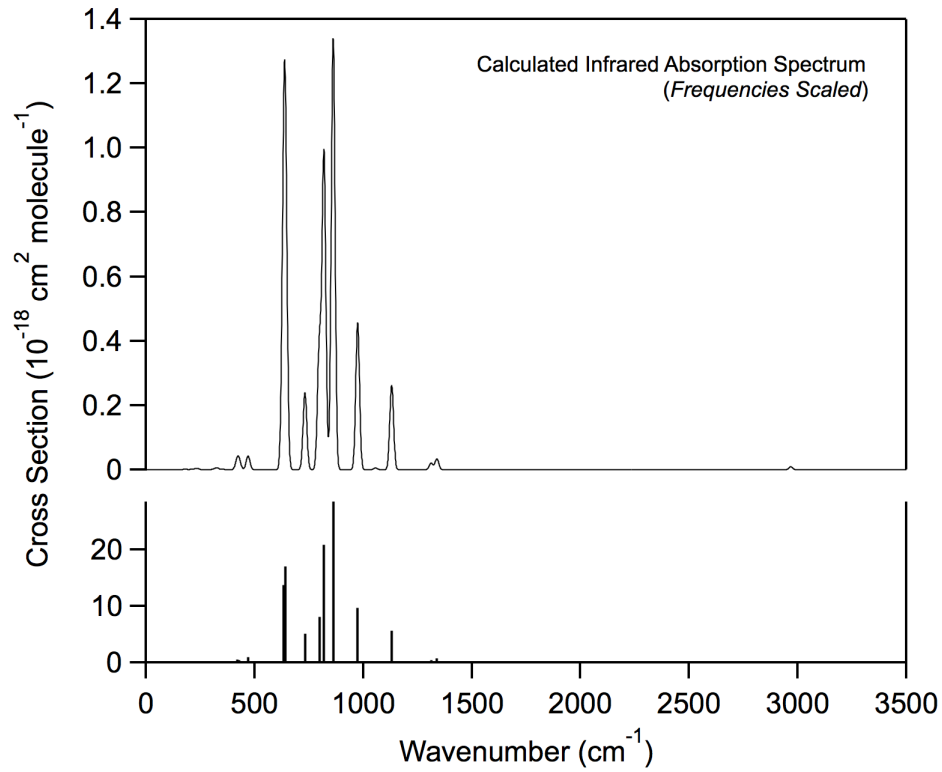
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.373371876800	0.014681235500	-0.061446672900
C	0.001186183900	-0.484070676000	-0.638421874200
C	-1.365062233600	0.030679591000	-0.061999873700
H	0.017368211300	-0.208325162800	-1.696962072300
F	-0.046383412700	-1.837131409400	-0.524780997700
Cl	2.628802693500	-1.109569364300	-0.691380002400
Cl	1.745610745700	1.645874663000	-0.702576948000
Cl	1.457838195100	0.029656141600	1.714192794700
Cl	-2.602806827900	-0.459416589000	-1.284241602100
Cl	-1.775020253000	-0.761798399500	1.481543827500
Cl	-1.433704179200	1.796672969800	0.131108421200

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
29.9659	0.00284
81.9693	0.00933
134.5064	0.0398
167.8948	0.0384
182.2570	0.0119
191.9434	0.0798
197.0462	0.00943
262.3640	0.00618
274.0724	0.0237
285.0477	0.0221
289.4582	0.112
316.8146	0.0295
387.6573	0.582
397.4803	0.476
440.6630	0.912
613.7855	13.8
622.8926	17.0
717.9036	5.11
787.8907	8.10
810.5000	20.9
855.3527	28.5
974.7484	9.74
1061.7573	0.114
1140.5923	5.59
1332.7304	0.429
1361.0968	0.715
3085.8319	0.194

Infrared Spectrum



Radiative Efficiency

