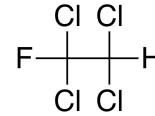


HCFC-121

Molecular Formula: CHCl₂CCl₂F
 Name: 1,1,2,2-Tetrachloro-1-fluoroethane
 CAS number: 354-14-3
 Molecular Weight: 185.84



Global Atmospheric Lifetime (years): 1.11
 Tropospheric Atmospheric Lifetime (years): 1.17
 Stratospheric Atmospheric Lifetime (years): 20
 Ozone Depletion Potential (ODP): 0.030

	<i>Well-mixed</i>	<i>Lifetime adjusted</i>
Radiative Efficiency (RE):	0.241	0.183
Global Warming Potential (GWP _H):		
GWP ₂₀	322	244
GWP ₁₀₀	87	66
Global Temperature Potentials (GTP _H):		
GTP ₂₀		80
GTP ₅₀		11
GTP ₁₀₀		9

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

Atmospheric Loss Processes *****

OH Reactivity

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

$$k_{\text{SAR}}(298 \text{ K}) = 5.01 \times 10^{-14}; k_{\text{SAR}}(272 \text{ K}) \approx 3.2 \times 10^{-14} \quad \text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

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

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

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

Fractional Atmospheric Loss: 0.972

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: 0.006

UV Photolysis

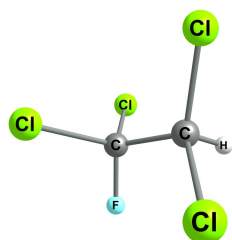
UV Spectrum: No Recommendation

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

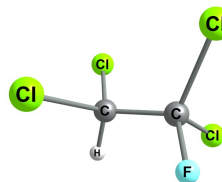
Fractional Atmospheric Loss: 0.022



Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.339



E = 0
Population = 0.339

Optimized Coordinates (Angstroms)

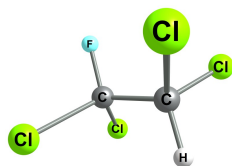
Atom	X	Y	Z
C	-0.631422869500	-0.379483134900	-0.213440560200
C	0.716498025000	0.313547838800	-0.543870693600
H	0.677025742900	0.616632173500	-1.588557041300
Cl	0.996565561900	1.769308524700	0.431638886300
Cl	2.060390810600	-0.850870551900	-0.387971000200
Cl	-1.978671507900	0.728241683300	-0.642510634800
Cl	-0.760576934500	-0.882808892400	1.488270121300
F	-0.734172828500	-1.462336641200	-0.992916077400

Atom	X	Y	Z
C	-0.630632473400	0.370150190400	-0.242726425700
C	0.715758587000	-0.342934832200	-0.534508128100
H	0.668910206100	-0.717682093800	-1.555369955400
Cl	2.059132511200	0.830708816200	-0.469861936100
Cl	1.005197955300	-1.727334251700	0.537355588800
Cl	-0.747710693300	0.990132558100	1.420963831000
Cl	-1.979493701200	-0.765789520600	-0.583740836300
F	-0.740724391700	1.396303133700	-1.094559138100

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
71.9737	0.0198
163.8017	0.0731
168.9619	0.0608
232.8956	0.0289
256.6603	0.0322
330.2977	0.0988
375.0120	0.105
385.1734	0.0480
490.8811	0.651
589.2189	6.90
739.1269	22.4
813.1034	19.7
833.6447	19.5
1040.7713	10.2
1141.8898	16.4
1225.8295	1.65
1274.3541	1.98
3142.0624	0.574

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
71.9713	0.0198
163.7996	0.0730
168.9593	0.0608
232.8971	0.0289
256.6609	0.0322
330.2987	0.0987
375.0136	0.105
385.1797	0.0478
490.8876	0.650
589.1931	6.90
739.1290	22.4
813.1225	19.7
833.6698	19.5
1040.7443	10.2
1141.8673	16.4
1225.8356	1.65
1274.3529	1.98
3142.0532	0.574



$\Delta E = 0.03 \text{ kcal mol}^{-1}$
Population = 0.322

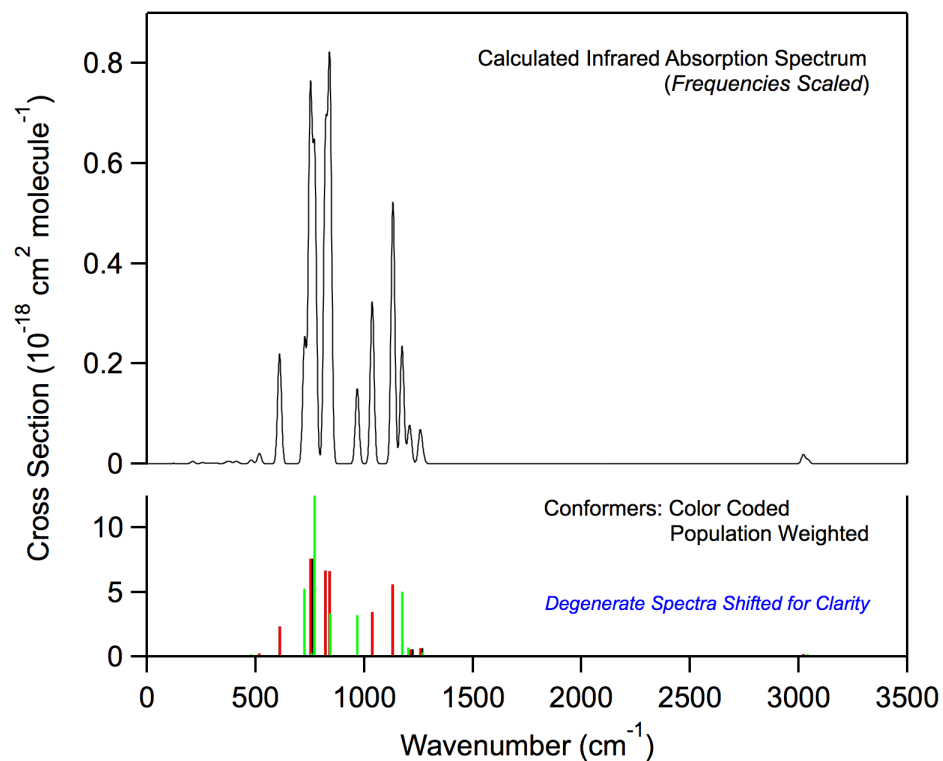
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-0.640260503100	0.013007129100	0.220185100100
C	0.738732253000	0.015148771700	-0.487800794700
H	0.592483637900	0.005662910900	-1.564512867500
Cl	1.658445766300	1.486045482400	-0.066668477900
Cl	1.675081812800	-1.438217632500	-0.043167241600
Cl	-1.563578734000	-1.451932760700	-0.249876100400
Cl	-1.580139659900	1.459558434100	-0.273244089900
F	-0.488667573200	0.024451664800	1.540975471900

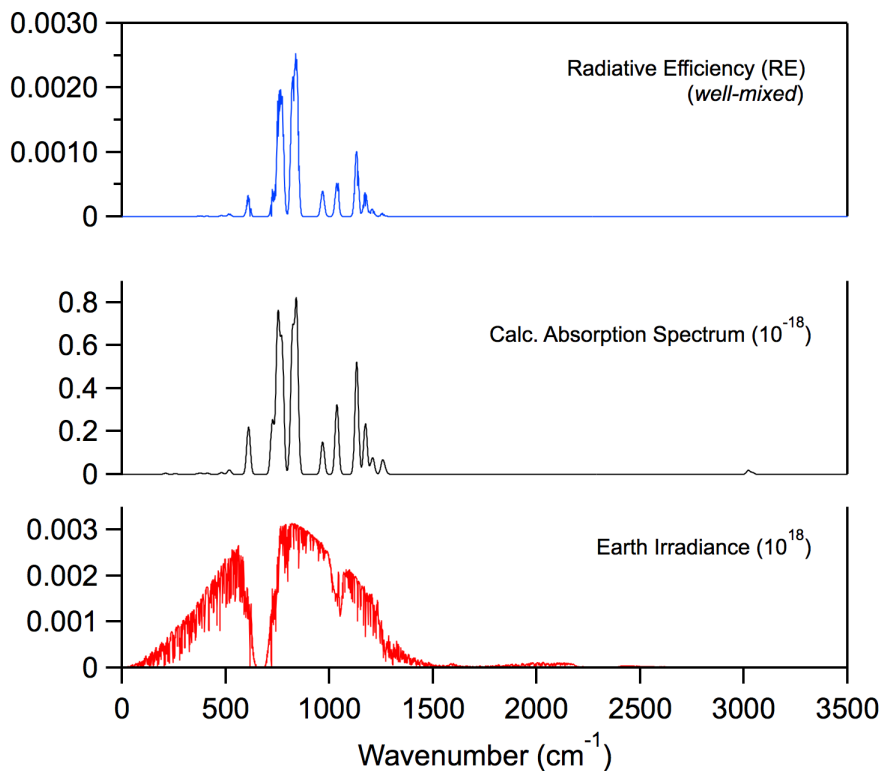
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength ($10^{-18} \text{ cm}^2 \text{ molecule}^{-1} \text{ cm}^{-1}$)
61.1598	0.0
160.9069	0.0501
213.1452	0.146
223.2854	0.00159
271.8216	0.0468
287.3978	0.0372
346.8698	0.278
382.9185	0.0523
451.0502	0.511
711.3754	16.4
746.4541	0.856
760.4949	38.8
836.1844	10.4
967.8414	9.95
1186.4357	15.5
1217.7949	2.15
1287.6008	0.967
3164.4264	0.539

Infrared Spectrum

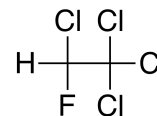


Radiative Efficiency



HCFC-121a

Molecular Formula: CHClFCCl₃
 Name: 1,1,1,2-Tetrachloro-2-fluoroethane
 CAS number: 354-11-0
 Molecular Weight: 185.84



Global Atmospheric Lifetime (years): 2.67
 Tropospheric Atmospheric Lifetime (years): 2.96
 Stratospheric Atmospheric Lifetime (years): 27.3
 Ozone Depletion Potential (ODP): 0.066

	<i>Well-mixed</i>	<i>Lifetime adjusted</i>
Radiative Efficiency (RE):	0.206	0.180
Global Warming Potential (GWP _H):		
GWP ₂₀	667	582
GWP ₁₀₀	181	158
Global Temperature Potentials (GTP _H):		
GTP ₂₀		237
GTP ₅₀		29
GTP ₁₀₀		22

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

Atmospheric Loss Processes *****

OH Reactivity

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

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

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

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

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

Fractional Atmospheric Loss: 0.933

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: 0.014

UV Photolysis

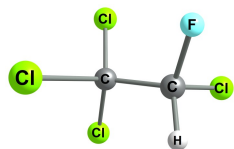
UV Spectrum: No Recommendation

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

Fractional Atmospheric Loss: 0.053



Molecular Structure and Infrared Spectrum (1 conformer)



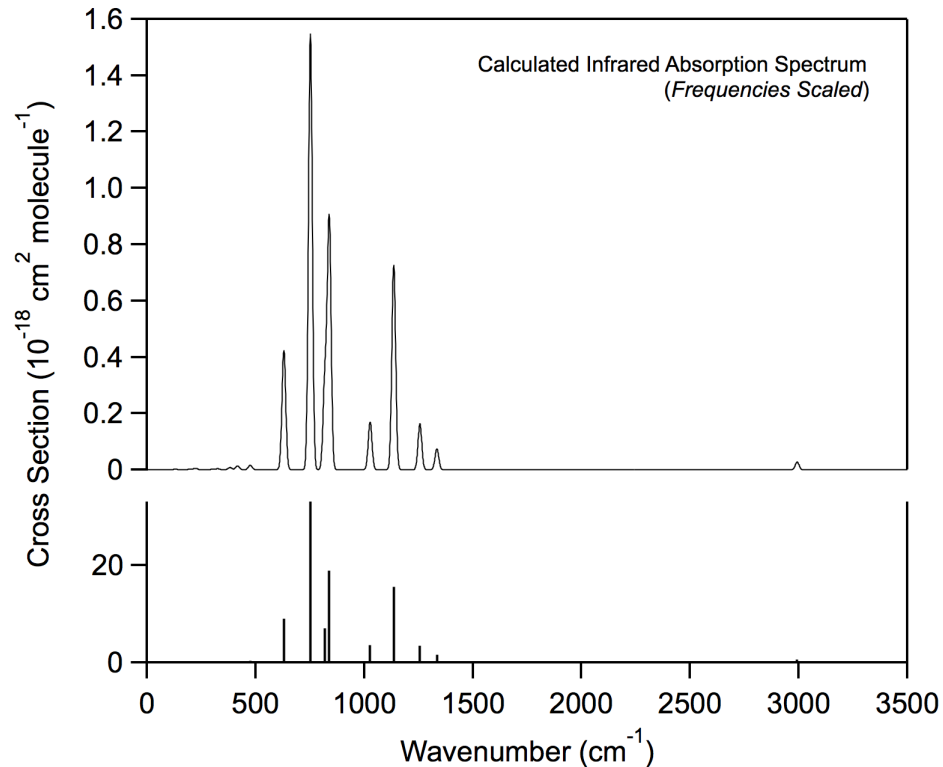
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-0.468787709700	0.093713654100	0.003708364000
C	0.777161808400	-0.548887521300	-0.665046903100
H	0.693566104900	-0.431528871300	-1.747210611300
Cl	2.304680815400	0.232510570800	-0.162284450500
F	0.823419801200	-1.852237087500	-0.339061635000
Cl	-0.584809122100	1.808133265200	-0.470584067300
Cl	-0.402787704400	-0.071955504600	1.771861978000
Cl	-1.899724993700	-0.789649505300	-0.629118674700

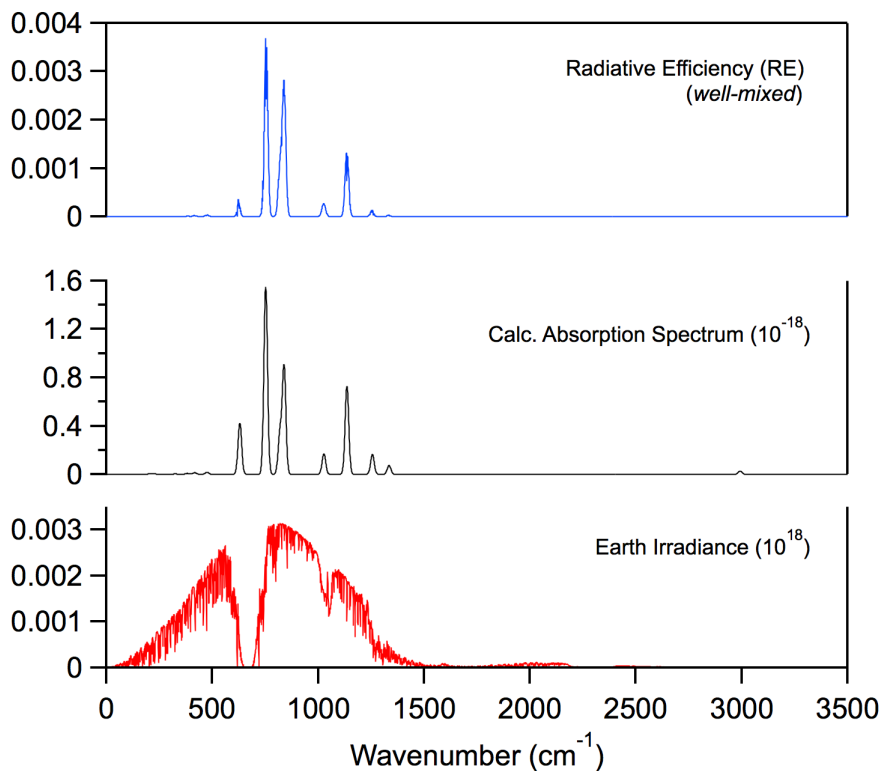
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
82.1680	0.0370
155.2977	0.0636
180.0417	0.102
231.8635	0.00404
262.8083	0.0392
288.0676	0.0751
347.8363	0.161
384.4855	0.287
446.2334	0.341
610.2462	9.03
739.6330	33.0
810.6596	6.99
831.5004	18.9
1030.5371	3.61
1145.8335	15.5
1273.3029	3.48
1356.1489	1.58
3112.1252	0.581

Infrared Spectrum

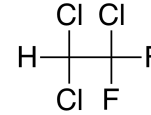


Radiative Efficiency



HCFC-122

Molecular Formula: CHCl₂CClF₂
 Name: 1,2,2-Trichloro-1,1-difluoroethane
 CAS number: 354-21-2
 Molecular Weight: 169.39



Global Atmospheric Lifetime (years): 1.39
 Tropospheric Atmospheric Lifetime (years): 1.47
 Stratospheric Atmospheric Lifetime (years): 24.5
 Ozone Depletion Potential (ODP): 0.030

	<i>Well-mixed</i>	<i>Lifetime adjusted</i>	
Radiative Efficiency (RE):	0.265	0.211	0.17 #
Global Warming Potential (GWP _H):			
GWP ₂₀	490	389	218 #
GWP ₁₀₀	133	105	59 #
Global Temperature Potentials (GTP _H):			
GTP ₂₀		133	70 #
GTP ₅₀		18	10 #
GTP ₁₀₀		15	8 #

* RE units: W m² ppb⁻¹

* GWP and GTP: Relative to CO₂

Value taken from WMO (2014)

Atmospheric Loss Processes *****

OH Reactivity

$$k_{\text{Rec}}(T) = 7.7 \times 10^{-13} \exp(-810/T); k_{\text{Rec}}(272 \text{ K}) = 3.92 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

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

$$\tau_{\text{Global}}^{\text{OH}} = 1.43 \text{ years}$$

$$\tau_{\text{Trop}}^{\text{OH}} = 1.47 \text{ years}$$

$$\tau_{\text{Strat}}^{\text{OH}} = 47.8 \text{ years}$$

Fractional Atmospheric Loss: 0.973

O(¹D) Reactivity

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

$$k_{\text{Est}}(T) = 1.9 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$\tau_{\text{O}(\text{1D})} = 195 \text{ years}$$

Fractional Atmospheric Loss: 0.007

UV Photolysis

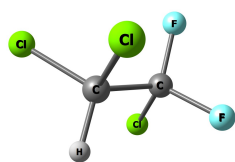
UV Spectrum: No Recommendation

$$\tau_{\text{hv}} = 68 \text{ years}$$

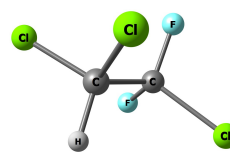
Fractional Atmospheric Loss: 0.020



Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.419



E = 0
Population = 0.419

Optimized Coordinates (Angstroms)

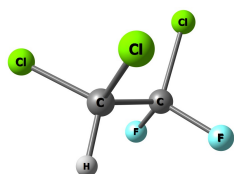
Atom	X	Y	Z
C	0.645669241920	-0.520529660882	0.133900675818
C	-0.590350130346	0.161980172557	-0.494911977520
F	0.567082433402	-0.544685077247	1.457911919806
F	0.726912040648	-1.774743877334	-0.313317340328
Cl	2.148971765688	0.339530355755	-0.354984820013
H	-0.456324970910	0.222239278222	-1.572002555062
Cl	-2.035101413833	-0.844110950882	-0.185356360333
Cl	-0.804915966569	1.810690759812	0.132972457632

Atom	X	Y	Z
C	0.646359251702	0.520217162383	0.134515357582
C	-0.590261654534	-0.160958613838	-0.494561228579
F	0.728220633327	1.774801653557	-0.311549811760
F	0.568189536972	0.543176665879	1.458572574549
Cl	2.148995305477	-0.340287384580	-0.355635138017
H	-0.456600043236	-0.220287285384	-1.571748626174
Cl	-0.805628877856	-1.810128516413	0.131840818216
Cl	-2.034313151851	0.845710318395	-0.183621945818

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
64.1413	0.00536
163.3573	0.0962
210.6579	0.147
241.8285	0.0899
299.8229	0.0491
340.4480	0.150
417.6964	0.317
425.7446	0.185
593.4702	2.29
741.0789	19.4
761.2593	12.0
819.9487	11.7
962.5047	25.4
1167.1937	23.1
1223.3952	2.56
1234.2848	18.3
1304.1067	4.28
3158.6807	0.498

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
64.1413	0.00536
163.3573	0.0962
210.6579	0.147
241.8285	0.0899
299.8229	0.0491
340.4480	0.150
417.6964	0.317
425.7446	0.185
593.4702	2.29
741.0789	19.4
761.2593	12.0
819.9488	11.7
962.5047	25.4
1167.1937	23.1
1223.3953	2.56
1234.2848	18.3
1304.1067	4.28
3158.6807	0.498



$\Delta E = 0.56 \text{ kcal mol}^{-1}$
 Population = 0.162

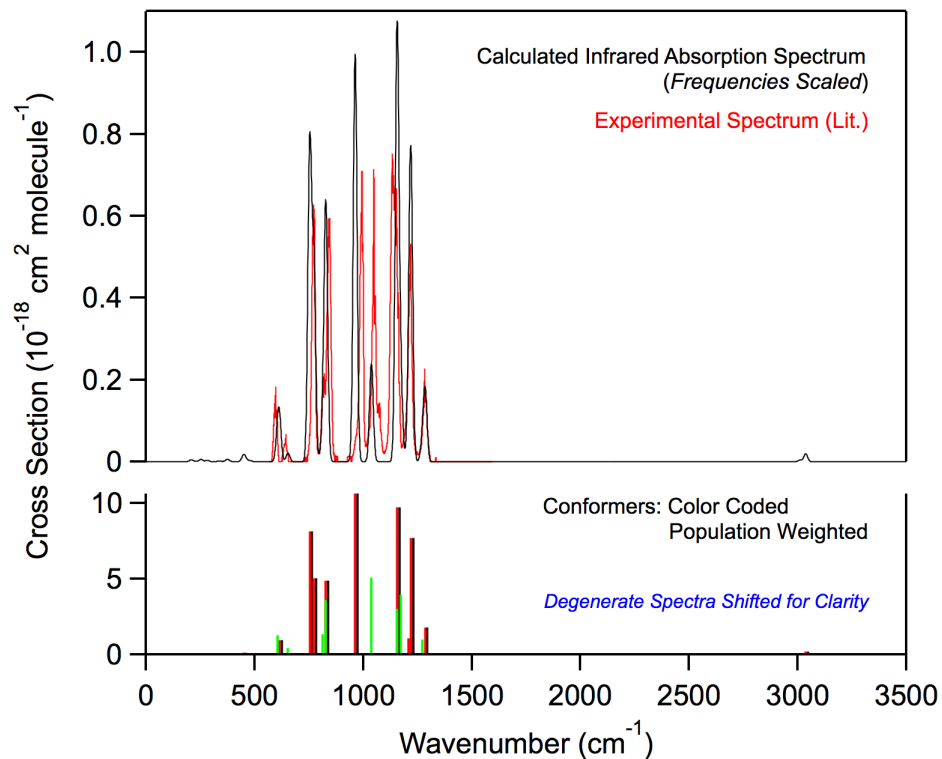
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	0.836528858399	0.018524486156	0.428303698157
C	-0.705881848622	0.002747222822	0.542469168092
F	1.291344937731	1.118261646920	1.034944013540
F	1.317039314114	-1.041660199167	1.083597153571
Cl	1.439220602304	-0.012137139281	-1.251119305912
H	-0.938996049847	0.023937427958	1.606583007971
Cl	-1.423199746593	1.455776246177	-0.186968098749
Cl	-1.388057067486	-1.498283691586	-0.120448636671

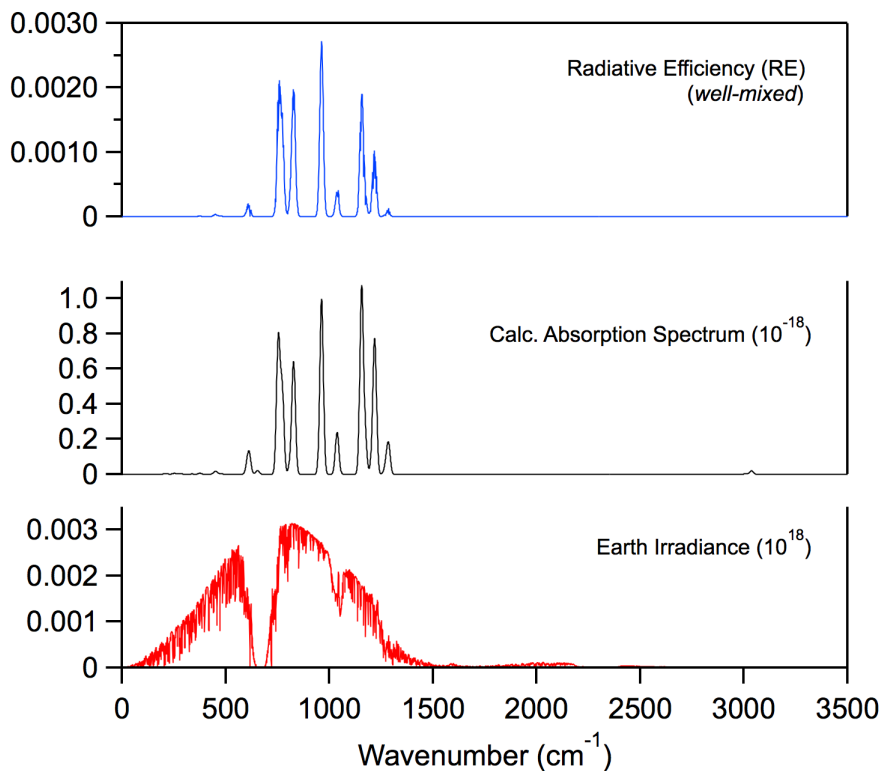
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
70.9140	0.0282
164.0640	0.0713
181.3428	0.143
248.4810	0.00752
312.7252	0.0243
372.6104	0.0586
421.4051	0.0332
449.4583	0.409
584.8132	7.88
635.2155	2.73
803.9394	8.28
819.1311	22.1
1041.7742	31.3
1165.9494	18.6
1185.2054	24.3
1229.3910	0.318
1290.2028	6.22
3130.2345	0.496

Infrared Spectrum

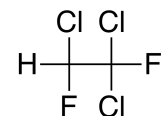


Radiative Efficiency



HCFC-122a

Molecular Formula: CHClFCCl₂F
 Name: 1,1,2-Trichloro-1,2-difluoroethane
 CAS number: 354-15-4
 Molecular Weight: 169.39



Global Atmospheric Lifetime (years): 3.20
 Tropospheric Atmospheric Lifetime (years): 3.54
 Stratospheric Atmospheric Lifetime (years): 34.1
 Ozone Depletion Potential (ODP): 0.060

	<i>Well-mixed</i>	<i>Lifetime adjusted</i>	
Radiative Efficiency (RE):	0.261	0.232	0.21 #
Global Warming Potential (GWP _H):			
GWP ₂₀	1110	988	945 #
GWP ₁₀₀	301	268	258 #
Global Temperature Potentials (GTP _H):			
GTP ₂₀		434	426 #
GTP ₅₀		50	48 #
GTP ₁₀₀		37	36 #

* RE units: W m² ppb⁻¹
 * GWP and GTP: Relative to CO₂
 # Value taken from WMO (2014)

Atmospheric Loss Processes *****

OH Reactivity

$$\begin{aligned}
 k_{\text{Rec}}(T) &= 9.0 \times 10^{-13} \exp(-1200/T); k_{\text{Rec}}(272 \text{ K}) = 1.09 \times 10^{-14} && \text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \\
 k_{\text{SAR}}(298 \text{ K}) &= 1.66 \times 10^{-14}; k_{\text{SAR}}(272 \text{ K}) \approx 1.06 \times 10^{-14} && \text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \\
 \tau_{\text{Global}}^{\text{OH}} &= 3.42 \text{ years} \\
 \tau_{\text{Trop}}^{\text{OH}} &= 3.54 \text{ years} \\
 \tau_{\text{Strat}}^{\text{OH}} &= 105.3 \text{ years}
 \end{aligned}$$

Fractional Atmospheric Loss: 0.937

O(¹D) Reactivity

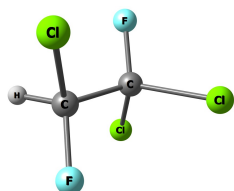
$$\begin{aligned}
 k_{\text{Rec}}(T) &, \text{ No recommendation} \\
 k_{\text{Est}}(T) &= 1.9 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \\
 \tau_{\text{O}(\text{1D})} &= 195 \text{ years} \\
 \text{Fractional Atmospheric Loss} &: 0.016
 \end{aligned}$$

UV Photolysis

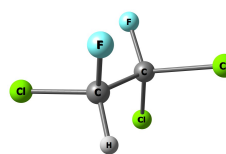
UV Spectrum: No Recommendation
 $\tau_{\text{hv}} = 68 \text{ years}$
 Fractional Atmospheric Loss: 0.047



Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.646



$\Delta E = 0.57 \text{ kcal mol}^{-1}$
Population = 0.248

Optimized Coordinates (Angstroms)

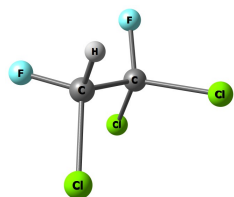
Atom	X	Y	Z
C	-0.697886875148	-0.819680782745	0.049568157503
C	0.478845222620	0.111054518097	-0.326377771089
H	-0.640128503726	-1.720936191065	-0.564871985765
F	-0.629381868043	-1.135400912419	1.351406855652
Cl	-2.267102939202	-0.040358159204	-0.311345069575
F	0.368783671600	0.455500783873	-1.610578764520
Cl	0.520055388010	1.573486610019	0.685170489614
Cl	1.999669903889	-0.826017866555	-0.119602911818

Atom	X	Y	Z
C	-0.718511083389	-0.577935295715	-0.504302806157
C	0.481806420737	0.080503625610	0.218507815416
H	-0.617201366638	-0.465622605854	-1.584184437012
F	-0.758494524398	-1.880095438650	-0.164566208729
Cl	-2.255377930648	0.195214476286	-0.011245785296
F	0.313186881438	0.025163689752	1.537420553564
Cl	1.964921577976	-0.837490166223	-0.209230117909
Cl	0.659857024922	1.782427714793	-0.292206013878

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
76.2738	0.0756
161.5694	0.140
192.3450	0.119
243.8237	0.0398
285.4229	0.0348
370.0764	0.0453
385.1042	0.0570
425.4632	0.392
556.7201	0.0619
614.9955	11.7
760.5845	39.9
842.0664	13.5
1061.9889	6.08
1164.9709	28.1
1175.7829	10.2
1278.5555	2.97
1360.4030	2.01
3105.6170	0.801

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
69.0679	0.0133
158.3331	0.0798
219.5983	0.170
243.1161	0.0857
305.5775	0.129
329.2016	0.143
385.3227	0.109
419.6910	0.683
464.9068	0.741
740.2165	31.5
790.8611	6.98
846.6372	28.9
975.4239	10.5
1128.1126	14.7
1209.9931	19.4
1278.2410	1.66
1365.7616	0.742
3126.9178	0.650



$$\Delta E = 1.07 \text{ kcal mol}^{-1}$$

$$\text{Population} = 0.107$$

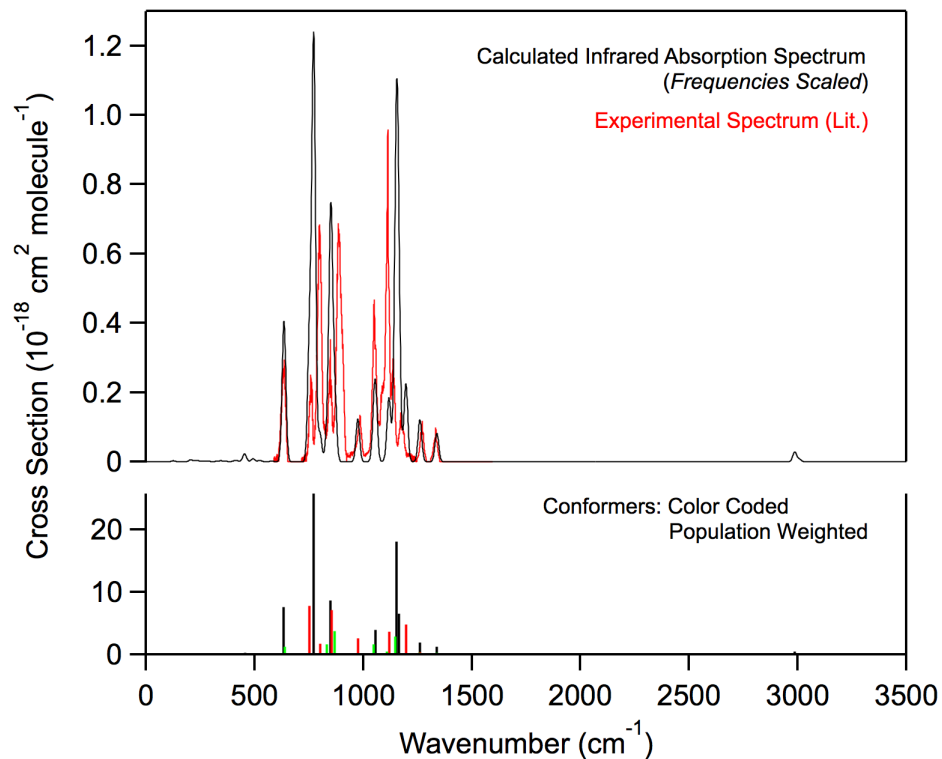
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-0.875091423655	-0.077778287509	-0.713292973228
C	0.607544418478	-0.143417047839	-0.269241748685
H	-0.927241189771	0.487787304332	-1.646862570346
F	-1.298599402623	-1.339723633567	-0.916757832319
Cl	-1.929165650026	0.732677483116	0.470267564302
F	1.264206873897	-0.780416992814	-1.251228964574
Cl	1.285256028987	1.502193894362	-0.117581336658
Cl	0.811522344714	-1.068080720080	1.237488861507

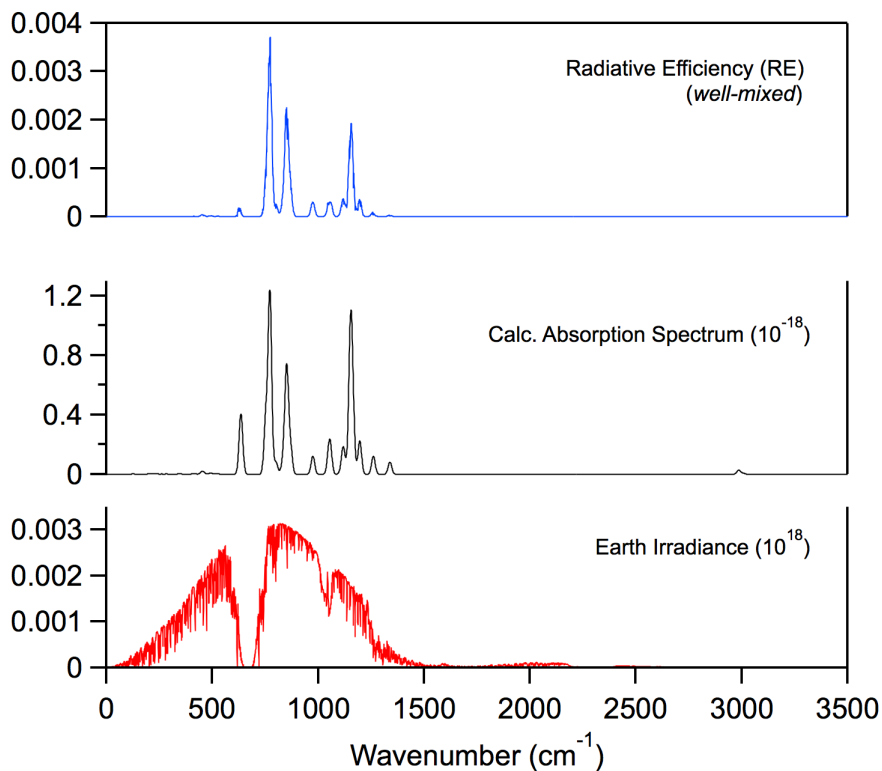
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
77.9438	0.0535
161.2556	0.0630
181.5276	0.149
255.4203	0.0172
309.4237	0.248
373.3228	0.0607
384.8345	0.0204
424.8007	0.633
497.6406	0.825
620.5019	11.9
825.3935	15.6
863.6232	35.5
1053.3648	15.4
1118.6131	4.49
1157.6077	27.5
1275.0159	2.53
1359.2487	2.80
3100.8512	0.885

Infrared Spectrum

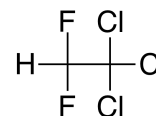


Radiative Efficiency



HCFC-122b

Molecular Formula: CHF₂CCl₃
 Name: 1,1,1-Trichloro-2,2-difluoroethane
 CAS number: 354-12-1
 Molecular Weight: 169.39



Global Atmospheric Lifetime (years): 9.31
 Tropospheric Atmospheric Lifetime (years): 12.6
 Stratospheric Atmospheric Lifetime (years): 35.5
 Ozone Depletion Potential (ODP): 0.170

	<i>Well-mixed</i>	<i>Lifetime adjusted</i>
Radiative Efficiency (RE):	0.224	0.213
Global Warming Potential (GWP _H):		
GWP ₂₀	2444	2326
GWP ₁₀₀	749	713
Global Temperature Potentials (GTP _H):		
GTP ₂₀		1702
GTP ₅₀		253
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*

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

$$\tau_{\text{Global}}^{\text{OH}} = 12.2 \text{ years}$$

$$\tau_{\text{Trop}}^{\text{OH}} = 12.6 \text{ years}$$

$$\tau_{\text{Strat}}^{\text{OH}} = 331.1 \text{ years}$$

Fractional Atmospheric Loss: 0.766

O(¹D) Reactivity

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

$$k_{\text{Est}}(T) = 1.9 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$\tau_{\text{O}(\text{1D})} = 195 \text{ years}$$

Fractional Atmospheric Loss: 0.048

UV Photolysis

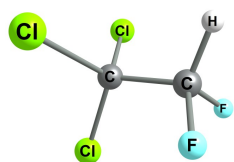
UV Spectrum: *No Recommendation*

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

Fractional Atmospheric Loss: 0.186



Molecular Structure and Infrared Spectrum (1 conformer)



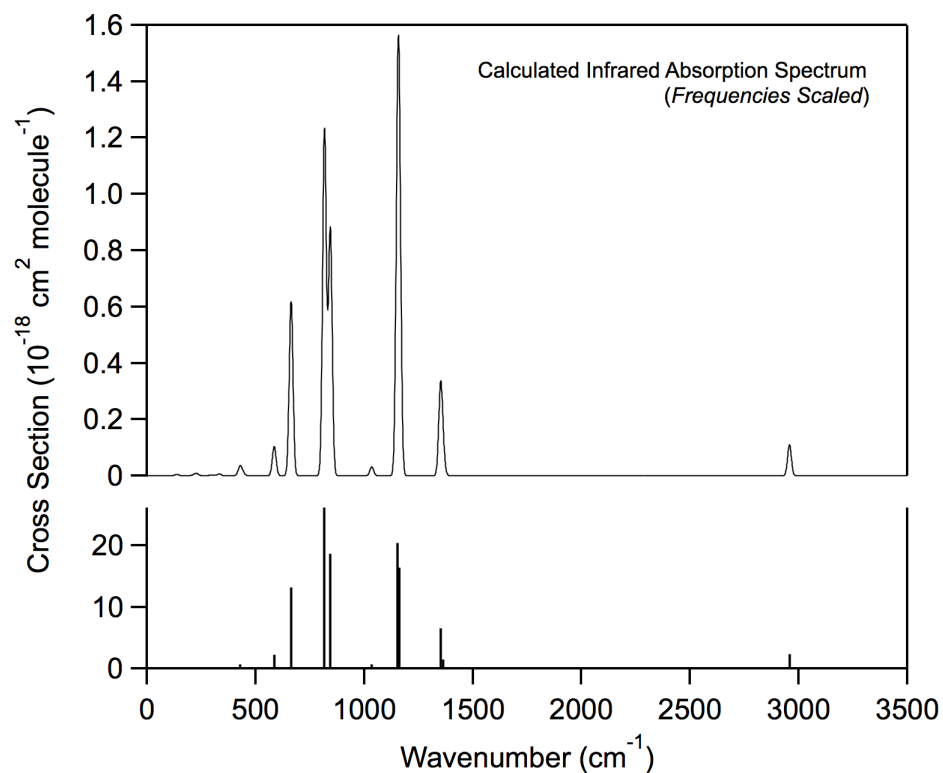
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	0.250259863200	-0.000550423800	0.005269067800
C	-1.105248784000	-0.001436550200	-0.752975442100
H	-0.921734021500	0.007287216300	-1.833329963700
F	-1.803268414600	-1.097275985200	-0.415934037200
F	-1.813559184700	1.082746524300	-0.400070119000
Cl	1.162157058800	-1.455214407100	-0.488308005200
Cl	-0.039677904800	-0.014650457100	1.759720975900
Cl	1.148335387700	1.469681082700	-0.467086476500

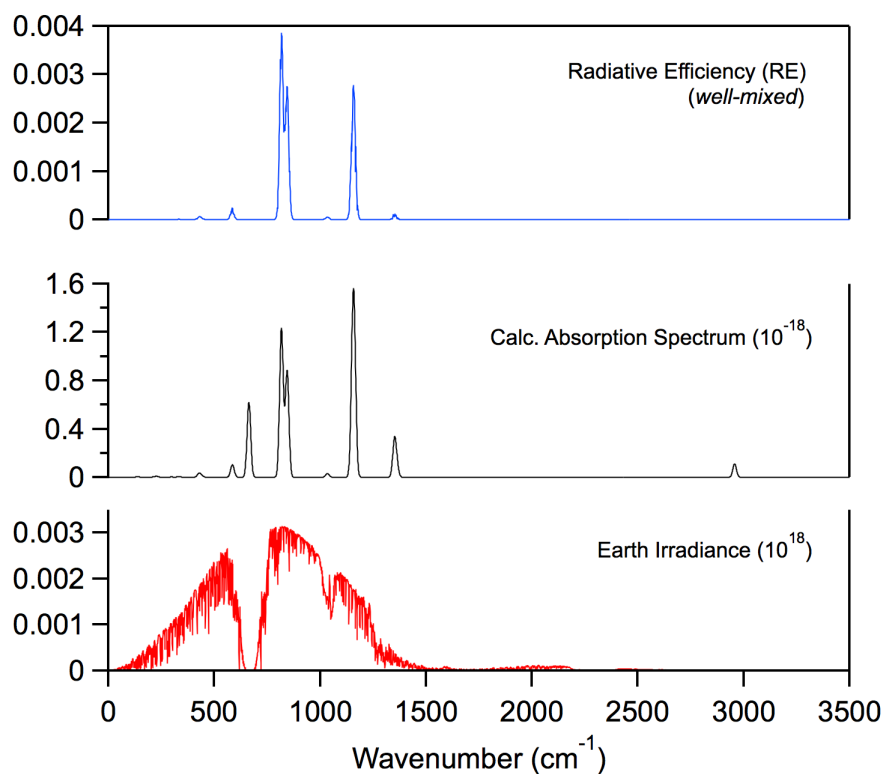
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
88.9543	0.102
171.0578	0.0652
185.6028	0.158
257.3850	0.0393
260.4029	0.0269
295.1618	0.137
396.5233	0.688
410.5108	0.210
563.2903	2.22
645.5946	13.2
808.2162	26.2
836.7400	18.7
1038.5986	0.667
1165.1416	20.4
1173.2797	16.4
1373.9652	6.56
1386.3275	1.51
3074.7609	2.36

Infrared Spectrum

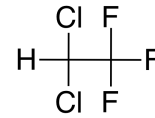


Radiative Efficiency



HCFC-123

Molecular Formula: CHCl₂CF₃
 Name: 2,2-Dichloro-1,1,1-trifluoroethane
 CAS number: 306-83-2
 Molecular Weight: 152.93



Global Atmospheric Lifetime (years):	1.81		1.3 [#]
Tropospheric Atmospheric Lifetime (years):	1.92		1.35 [#]
Stratospheric Atmospheric Lifetime (years):	30.8		36 [#]
Ozone Depletion Potential (ODP):	0.026		
	<i>Well-mixed</i>	<i>Lifetime adjusted</i>	
Radiative Efficiency (RE):	0.218	0.181	0.15 [#]
Global Warming Potential (GWP _H):			
GWP ₂₀	579	480	292 [#]
GWP ₁₀₀	157	130	79 [#]
Global Temperature Potentials (GTP _H):			
GTP ₂₀		173	98 [#]
GTP ₅₀		23	14 [#]
GTP ₁₀₀		18	11 [#]

* RE units: W m² ppb⁻¹

* GWP and GTP: Relative to CO₂

Value taken from WMO (2014)

Atmospheric Loss Processes *****

OH Reactivity

$$k_{\text{Rec}}(T) = 7.4 \times 10^{-13} \exp(-900/T); k_{\text{Rec}}(272 \text{ K}) = 2.70 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$k_{\text{SAR}}(298 \text{ K}) = 3.05 \times 10^{-14}; k_{\text{SAR}}(272 \text{ K}) \approx 1.95 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$\tau_{\text{Global}}^{\text{OH}} = 1.86 \text{ years}$$

$$\tau_{\text{Trop}}^{\text{OH}} = 1.92 \text{ years}$$

$$\tau_{\text{Strat}}^{\text{OH}} = 60.7 \text{ years}$$

Fractional Atmospheric Loss: 0.971

O(¹D) Reactivity

$$k_{\text{Rec}}(T) = 0.79 \times 2.0 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$k_{\text{Est}}(T) = 1.3 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$\tau_{\text{O}(\text{1D})} = 285 \text{ years}$$

Fractional Atmospheric Loss: 0.006

UV Photolysis

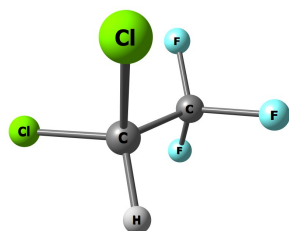
UV Spectrum: *Recommendation Available*

$$\tau_{\text{hv}} = 80 \text{ years}$$

Fractional Atmospheric Loss: 0.023



Molecular Structure and Infrared Spectrum (1 conformer)



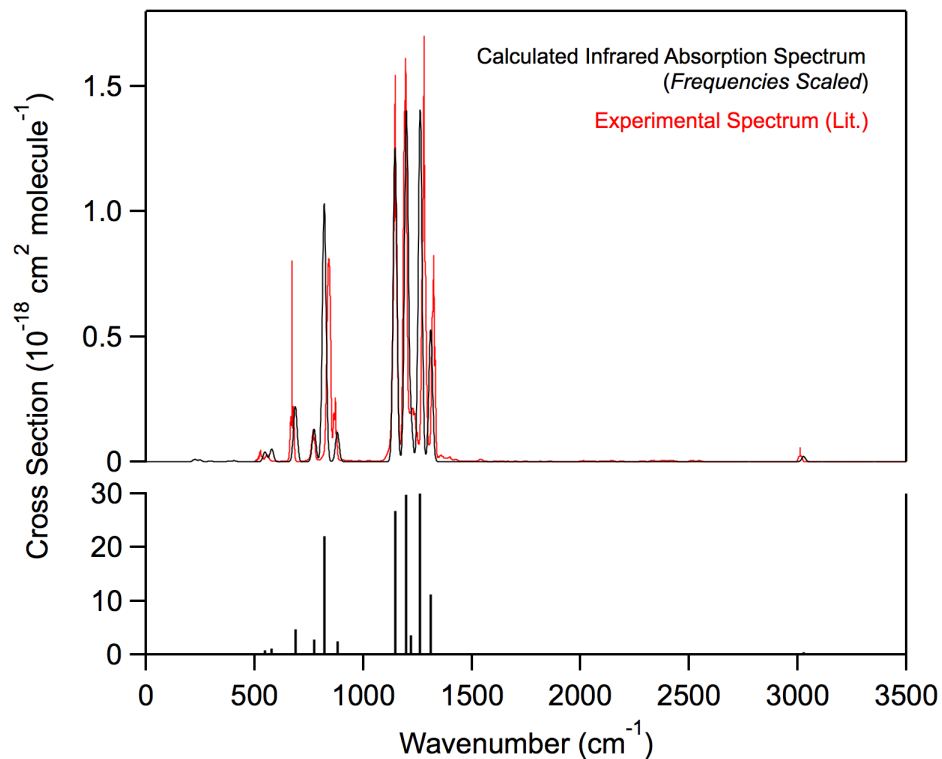
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.028638418108	-0.000933799283	0.001544699350
C	0.426159812304	-0.000077086525	-0.506804685085
F	-1.658609417744	-1.085017447843	-0.456193362423
F	-1.095617875109	0.005227099655	1.326493856701
F	-1.663478764577	1.075889484632	-0.466487619511
H	0.415388123164	-0.005282600329	-1.594636051275
Cl	1.260278443613	1.481248737626	0.022047502573
Cl	1.266934096456	-1.472524387932	0.036115659670

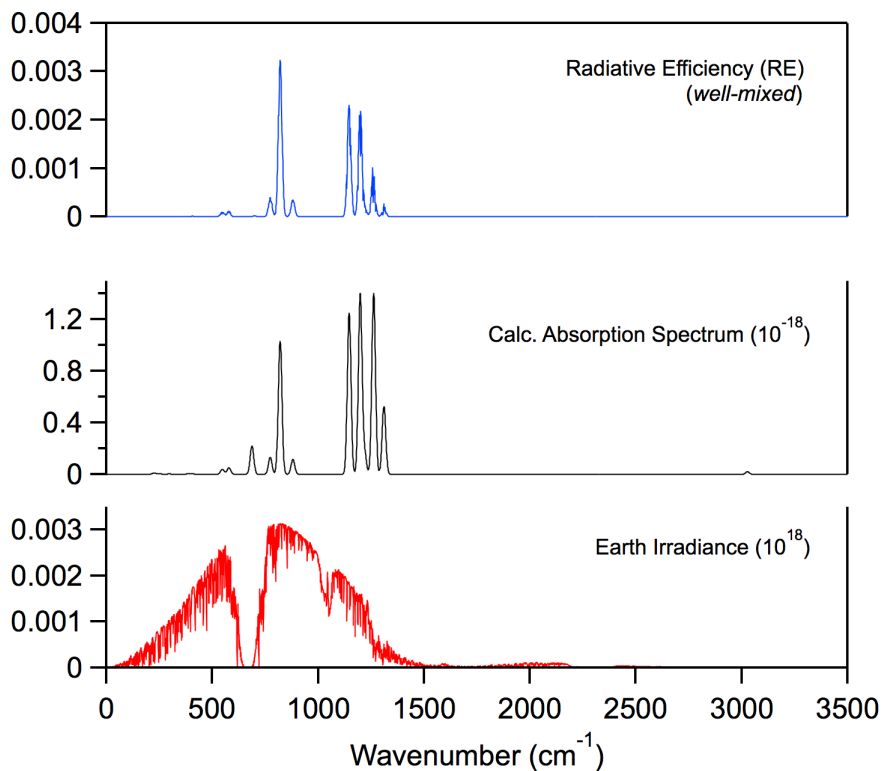
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
64.8170	0.00586
181.3170	0.196
206.5030	0.140
256.6169	0.0741
349.6218	0.0693
373.2482	0.0830
522.9445	0.840
555.7256	1.08
670.9326	4.69
762.2678	2.79
811.8741	22.0
875.7109	2.50
1157.0036	26.7
1212.2252	29.7
1233.8037	3.55
1279.5914	29.9
1330.9805	11.2
3148.7563	0.447

Infrared Spectrum

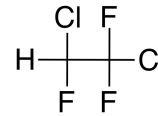


Radiative Efficiency



HCFC-123a

Molecular Formula: CHClFCClF₂
 Name: 1,2-Dichloro-1,1,2-trifluoroethane
 CAS number: 354-23-4
 Molecular Weight: 152.93



Global Atmospheric Lifetime (years): 4.16 4.0 #
 Tropospheric Atmospheric Lifetime (years): 4.45 4.3 #
 Stratospheric Atmospheric Lifetime (years): 63.8 ~65 #
 Ozone Depletion Potential (ODP): 0.038

	<i>Well-mixed</i>	<i>Lifetime adjusted</i>	
Radiative Efficiency (RE):	0.282	0.256	0.23 #
Global Warming Potential (GWP _H):			
GWP ₂₀	1712	1558	1350 #
GWP ₁₀₀	468	425	370 #
Global Temperature Potentials (GTP _H):			
GTP ₂₀		778	659 #
GTP ₅₀		84	72 #
GTP ₁₀₀		60	51 #

* RE units: W m² ppb⁻¹

* GWP and GTP: Relative to CO₂

Value taken from WMO (2014)

Atmospheric Loss Processes *****

OH Reactivity

$$k_{\text{Rec}}(T) = 8.6 \times 10^{-13} \exp(-1250/T); k_{\text{Rec}}(272 \text{ K}) = 8.68 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

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

$$\tau_{\text{Global}}^{\text{OH}} = 4.30 \text{ years}$$

$$\tau_{\text{Trop}}^{\text{OH}} = 4.45 \text{ years}$$

$$\tau_{\text{Strat}}^{\text{OH}} = 129.5 \text{ years}$$

Fractional Atmospheric Loss: 0.967

O(¹D) Reactivity

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

$$k_{\text{Est}}(T) = 1.3 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$\tau_{\text{O}(\text{1D})} = 285 \text{ years}$$

Fractional Atmospheric Loss: 0.015

UV Photolysis

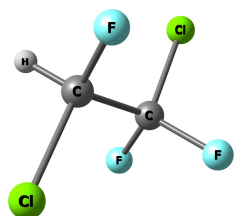
UV Spectrum: No Recommendation

$$\tau_{\text{hv}} = 225 \text{ years}$$

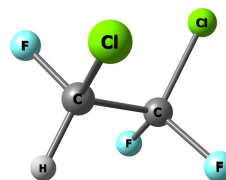
Fractional Atmospheric Loss: 0.018



Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.679



$\Delta E = 0.69 \text{ kcal mol}^{-1}$
Population = 0.210

Optimized Coordinates (Angstroms)

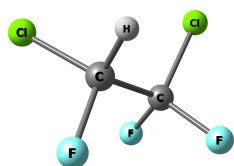
Atom	X	Y	Z
C	-0.602518312591	0.545851356957	-0.418553289521
C	0.504789053718	-0.394912848743	0.096220829218
H	-0.504306492464	0.687773041159	-1.495808406761
Cl	-2.205340145604	-0.194181210115	-0.114671730337
F	-0.515917336962	1.721746194425	0.225803503032
F	0.432697315430	-1.565963076844	-0.532887845370
Cl	2.109766518246	0.345897238990	-0.246097869530
F	0.392125400228	-0.593971695829	1.403754809269

Atom	X	Y	Z
C	-0.733185981304	0.724770501640	-0.062792181017
C	0.684954061119	0.201572101179	-0.374557423299
H	-0.972394364039	1.504126787885	-0.791826921540
Cl	-1.962152146600	-0.554955751001	-0.227972890619
F	-0.748375319159	1.236214895527	1.179794509725
F	1.512019998036	1.25424885232	-0.355023614450
Cl	1.253258222980	-0.999288202686	0.816514691502
F	0.710595528968	-0.327140187777	-1.596650170302

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
67.0791	0.0348
165.5038	0.184
233.9893	0.322
258.6746	0.0509
337.8067	0.102
386.2472	0.203
420.9408	0.126
476.6764	0.673
627.8601	1.96
762.3347	42.4
798.6172	2.29
967.1761	20.3
1145.6046	14.0
1198.6286	31.7
1260.8691	18.4
1288.8368	2.82
1375.3058	0.600
3120.5460	0.901

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
72.2873	0.0784
168.4233	0.161
197.1877	0.176
306.2097	0.0713
331.2348	0.0413
419.3674	0.0612
423.6036	0.215
495.6731	0.400
620.5712	13.8
654.3275	2.68
830.7976	17.3
1060.0576	30.9
1149.2391	13.8
1183.6412	30.0
1209.2877	21.3
1286.9348	1.03
1370.0652	4.44
3091.2788	1.32



$$\Delta E = 1.07 \text{ kcal mol}^{-1}$$

$$\text{Population} = 0.111$$

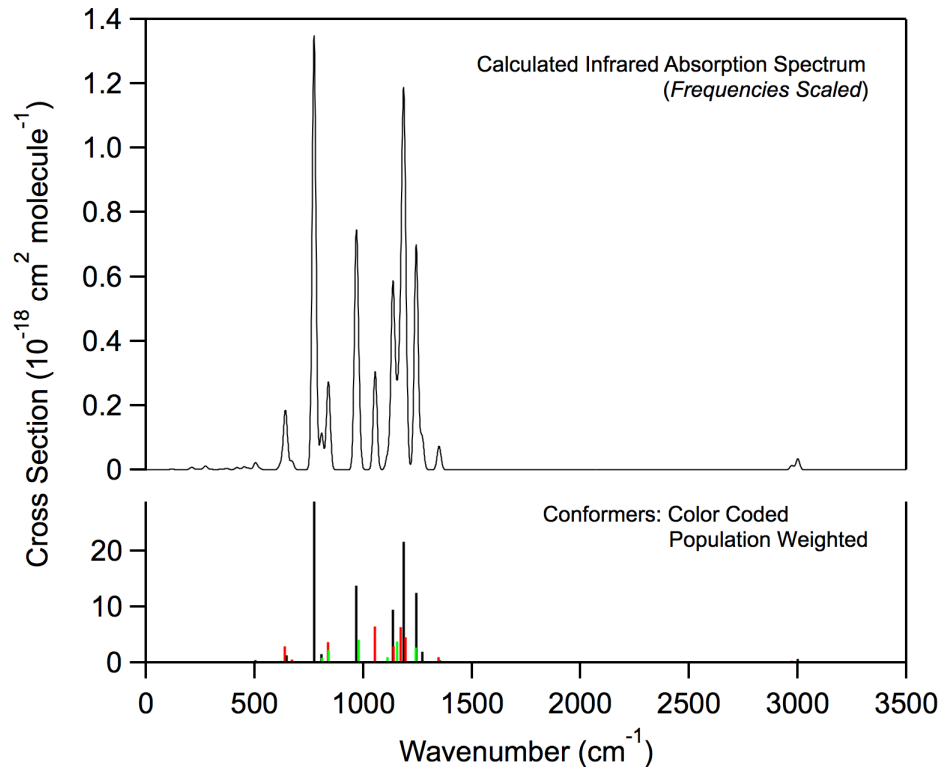
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-0.752263282789	0.339799746038	-0.547584225071
C	0.641970760073	0.367991491940	0.117359177721
H	-0.653128536832	0.161990222415	-1.619550279596
Cl	-1.778341450650	-0.948114770610	0.135223508929
F	-1.323051481436	1.541977160315	-0.324640589126
F	0.540841758273	0.479495904575	1.436414534638
Cl	1.584370277236	-1.099535324409	-0.295614386615
F	1.292216956126	1.438707569735	-0.348920740880

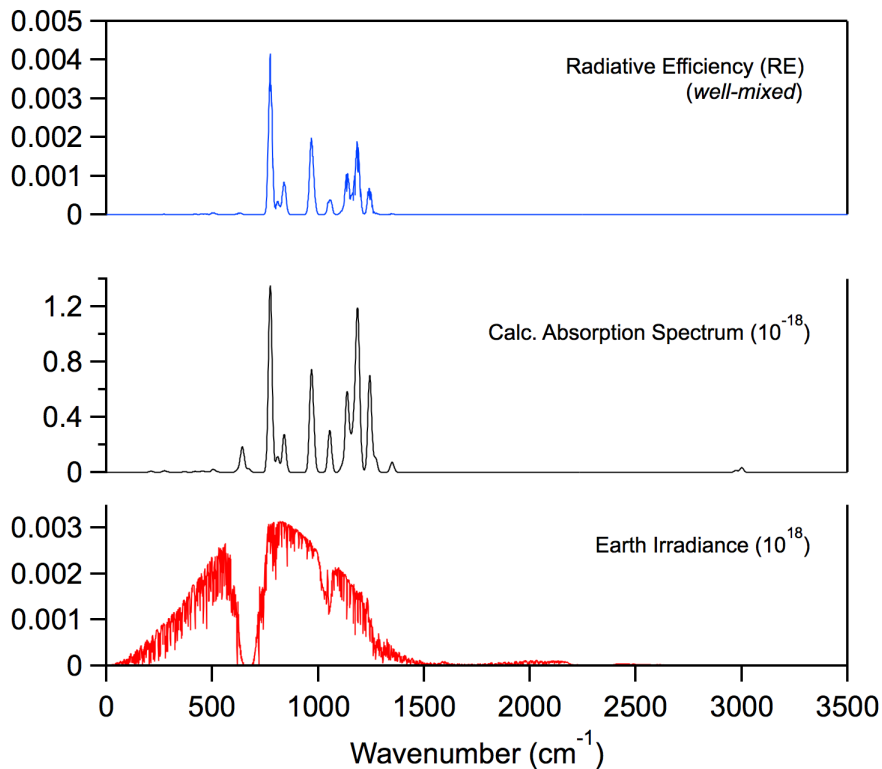
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength ($10^{-18} \text{ cm}^2 \text{ molecule}^{-1} \text{ cm}^{-1}$)
69.1038	0.0287
162.1250	0.0881
224.1692	0.310
307.8145	0.171
322.7747	0.183
400.8428	0.182
420.4199	0.423
443.5979	0.873
599.3654	3.23
799.8383	7.69
834.1091	20.4
978.3657	37.2
1121.0267	8.56
1167.0076	33.8
1256.4270	24.0
1289.3843	0.473
1372.0549	2.47
3118.8273	0.936

Infrared Spectrum

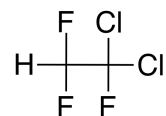


Radiative Efficiency



HCFC-123b

Molecular Formula: CHF₂CCl₂F
 Name: 1,1-Dichloro-1,2,2-trifluoroethane
 CAS number: 812-04-4
 Molecular Weight: 152.93



Global Atmospheric Lifetime (years): 11.8 ~6 #
 Tropospheric Atmospheric Lifetime (years): 15.1 ~7 #
 Stratospheric Atmospheric Lifetime (years): 53.8 ~50 #
 Ozone Depletion Potential (ODP): 0.124

	<i>Well-mixed</i>	<i>Lifetime adjusted</i>
Radiative Efficiency (RE):	0.250	0.240
Global Warming Potential (GWP _H):		
GWP ₂₀	3537	3394
GWP ₁₀₀	1173	1125
Global Temperature Potentials (GTP _H):		
GTP ₂₀		2694
GTP ₅₀		528
GTP ₁₀₀		167

* RE units: W m² ppb⁻¹
 * GWP and GTP: Relative to CO₂
 # Value taken from WMO (2014)

Atmospheric Loss Processes *****

OH Reactivity

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

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

$$\tau_{\text{Global}}^{\text{OH}} = 14.5 \text{ years}$$

$$\tau_{\text{Trop}}^{\text{OH}} = 15.1 \text{ years}$$

$$\tau_{\text{Strat}}^{\text{OH}} = 389.0 \text{ years}$$

Fractional Atmospheric Loss: 0.811

O(¹D) Reactivity

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

$$k_{\text{Est}}(T) = 1.3 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$\tau_{\text{O}(\text{1D})} = 285 \text{ years}$$

Fractional Atmospheric Loss: 0.041

UV Photolysis

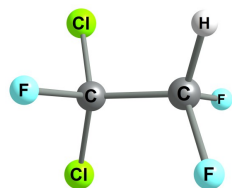
UV Spectrum: *No Recommendation*

$$\tau_{\text{hv}} = 80 \text{ years}$$

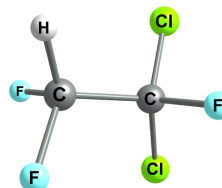
Fractional Atmospheric Loss: 0.147



Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.409



E = 0
Population = 0.409

Optimized Coordinates (Angstroms)

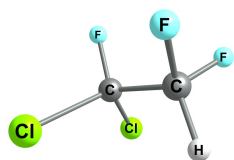
Atom	X	Y	Z
C	-0.258490226700	0.103098792900	-0.330156824300
C	0.995447157400	-0.785799053400	-0.157113184100
H	0.890158917200	-1.685462965400	-0.775827988200
F	2.070943048400	-0.085866488700	-0.557980343400
F	1.147323206800	-1.126917595000	1.129482570200
Cl	-1.708565359800	-0.833690468200	0.138782754600
F	-0.354199230300	0.427071264300	-1.624831308300
Cl	-0.120496512900	1.590144513500	0.638459323500

Atom	X	Y	Z
C	-0.257887624400	0.108283921300	0.330203939900
C	0.994614389900	-0.785038614200	0.169998618100
H	0.888419592800	-1.674957634800	0.802495806300
F	1.145120179500	-1.146061382100	-1.111320488500
F	2.071416431800	-0.080655649300	0.559387033900
Cl	-0.118293062000	1.580105999000	-0.661163967300
F	-0.352251935700	0.452208501800	1.619827685900
Cl	-1.709676972000	-0.833383141700	-0.123393628300

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
80.4277	0.141
182.3096	0.139
190.2250	0.185
267.8998	0.0903
316.3812	0.156
379.4360	0.0818
420.0768	0.431
509.2931	0.744
593.7904	2.67
652.3733	15.8
864.3673	36.0
1065.5227	5.92
1143.6764	10.9
1182.6390	38.1
1195.3732	8.54
1383.9905	6.90
1388.2346	2.01
3064.0283	3.14

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
80.4261	0.141
182.3085	0.139
190.2279	0.185
267.8999	0.0903
316.3804	0.156
379.4380	0.0818
420.0769	0.431
509.2933	0.744
593.7892	2.67
652.3750	15.8
864.3757	36.0
1065.5181	5.92
1143.6709	10.9
1182.6278	38.1
1195.3656	8.55
1383.9841	6.90
1388.2312	2.01
3064.0405	3.14



$\Delta E = 0.48 \text{ kcal mol}^{-1}$
 Population = 0.181

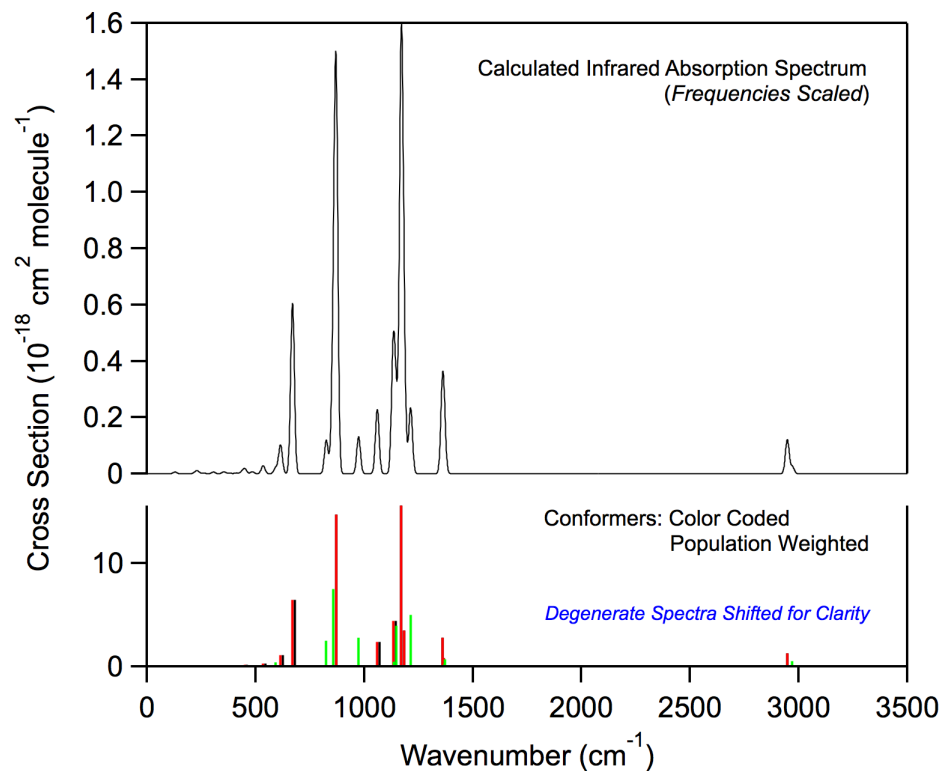
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-0.233893241600	-0.001040708300	0.213049072900
C	1.138597629500	-0.011160656800	-0.503899685900
H	1.014253406900	-0.012745245800	-1.591357152300
F	1.827377062800	1.076113404000	-0.115749178800
F	1.813796906700	-1.105225160400	-0.111034825600
Cl	-1.134286639100	1.472245979700	-0.250705548400
F	-0.038003411500	0.000638499600	1.531539475900
Cl	-1.152587713700	-1.465060112100	-0.244212157900

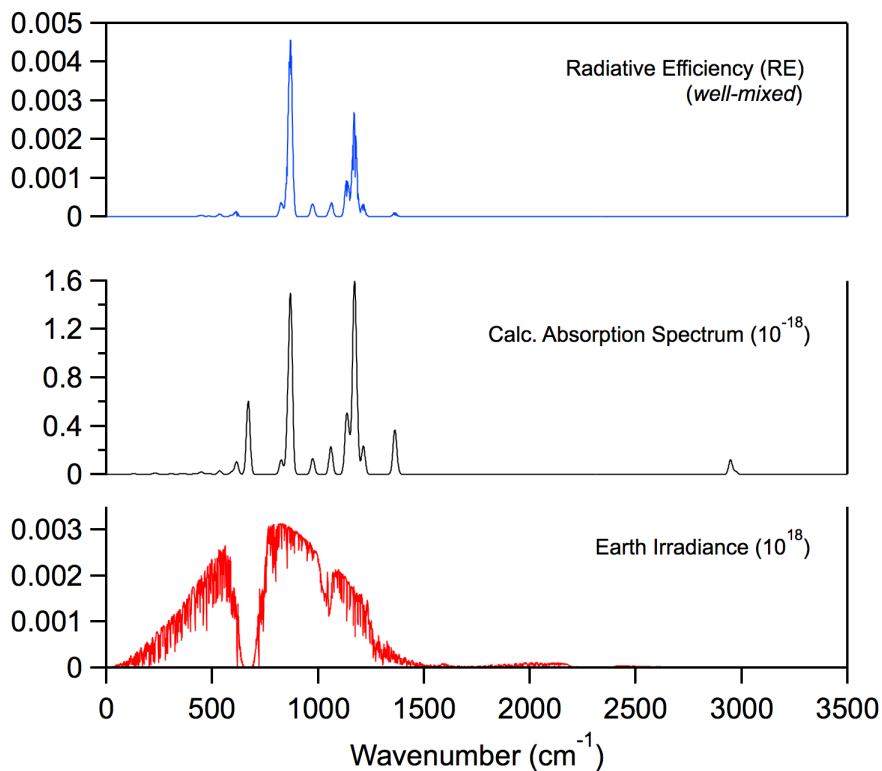
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength ($10^{-18} \text{ cm}^2 \text{ molecule}^{-1} \text{ cm}^{-1}$)
74.6693	0.0591
172.1816	0.118
222.5544	0.170
267.0000	0.283
329.6611	0.134
345.5223	0.254
407.0843	0.788
455.9967	0.820
570.4347	2.42
817.0996	14.0
850.4490	41.5
974.4834	15.5
1147.0082	2.65
1157.5951	22.0
1228.0973	27.6
1391.5330	1.49
1394.6280	3.94
3088.8085	2.90

Infrared Spectrum

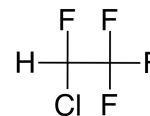


Radiative Efficiency



HCFC-124

Molecular Formula: CHClF₂
 Name: 2-Chloro-1,1,1,2-tetrafluoroethane
 CAS number: 2837-89-0
 Molecular Weight: 136.48



Global Atmospheric Lifetime (years): 5.47 5.9 #
 Tropospheric Atmospheric Lifetime (years): 5.80 6.3 #
 Stratospheric Atmospheric Lifetime (years): 98.0 111 #
 Ozone Depletion Potential (ODP): 0.018

	<i>Well-mixed</i>	<i>Lifetime adjusted</i>	
Radiative Efficiency (RE):	0.228	0.211	0.20 #
Global Warming Potential (GWP _H):			
GWP ₂₀	2006	1860	1870 #
GWP ₁₀₀	558	517	527 #
Global Temperature Potentials (GTP _H):			
GTP ₂₀		1070	1120 #
GTP ₅₀		114	121 #
GTP ₁₀₀		73	74 #

* RE units: W m² ppb⁻¹

* GWP and GTP: Relative to CO₂

Value taken from WMO (2014)

Atmospheric Loss Processes *****

OH Reactivity

$$k_{\text{Rec}}(T) = 7.1 \times 10^{-13} \exp(-1300/T); k_{\text{Rec}}(272 \text{ K}) = 5.96 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

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

$$\tau_{\text{Global}}^{\text{OH}} = 5.60 \text{ years}$$

$$\tau_{\text{Trop}}^{\text{OH}} = 5.80 \text{ years}$$

$$\tau_{\text{Strat}}^{\text{OH}} = 164.3 \text{ years}$$

Fractional Atmospheric Loss: 0.978

O(¹D) Reactivity

$$k_{\text{Rec}}(T) = 0.69 \times 0.86 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

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

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

Fractional Atmospheric Loss: 0.010

UV Photolysis

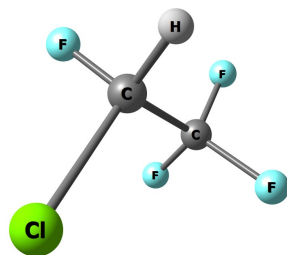
UV Spectrum: *Recommendation Available*

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

Fractional Atmospheric Loss: 0.012



Molecular Structure and Infrared Spectrum (1 conformer)



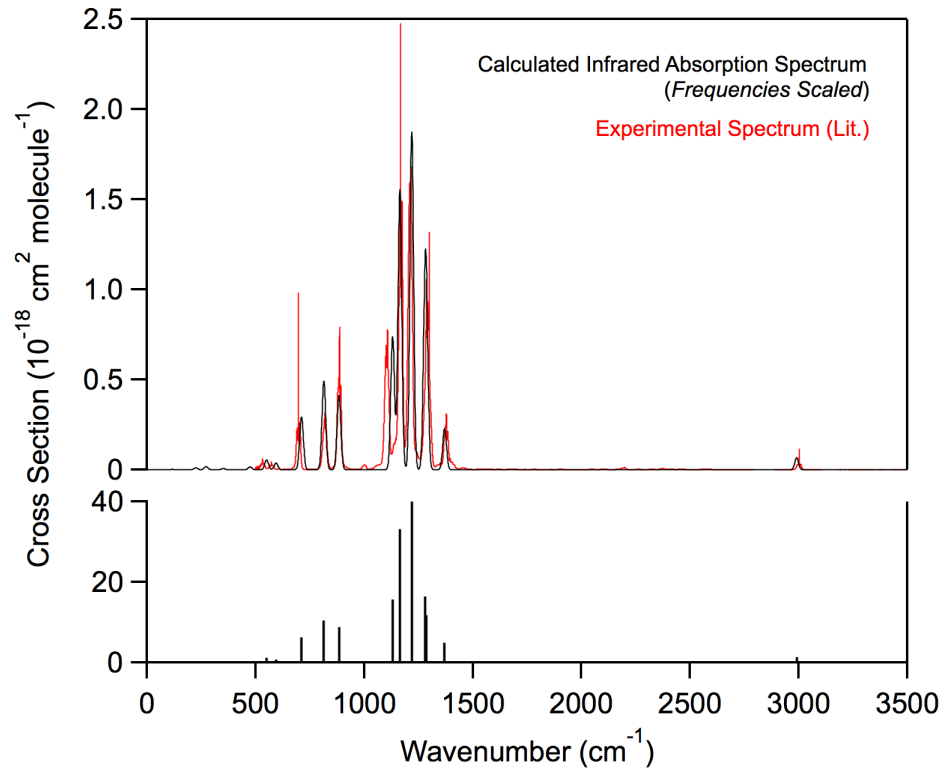
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	0.861839191713	-0.175211162303	0.000719303619
C	-0.441950284001	0.489867007826	0.474324624630
F	0.982461397225	-1.390303778354	0.532964407537
F	0.910699557254	-0.270972745389	-1.322335114956
F	1.891907188206	0.571483316920	0.411912932663
H	-0.456601898183	0.540227118248	1.565023669844
F	-0.498190362064	1.728571916346	-0.051453792178
Cl	-1.858194790150	-0.465429673293	-0.043958031159

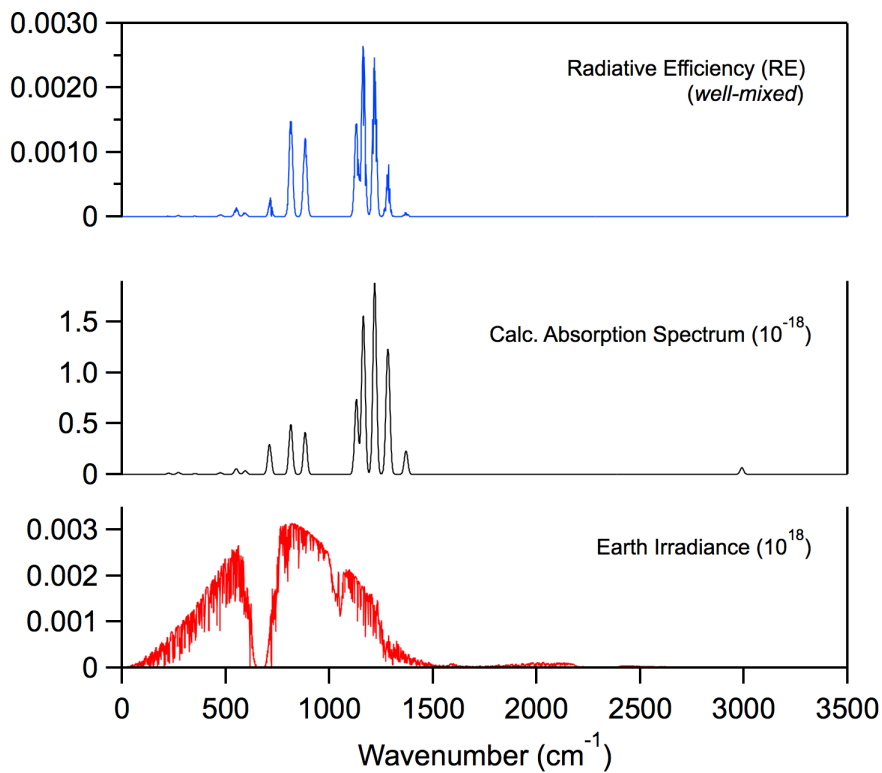
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
66.3815	0.0401
181.0721	0.220
231.4478	0.365
315.6989	0.137
371.1323	0.0118
445.2154	0.324
526.3697	1.17
572.2718	0.767
696.2492	6.24
805.1695	10.5
878.7622	8.78
1140.4091	15.7
1175.7992	33.1
1233.7632	40.0
1298.3789	16.5
1305.5965	11.8
1393.7719	4.88
3109.5782	1.40

Infrared Spectrum

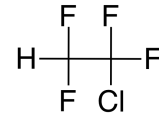


Radiative Efficiency



HCFC-124a

Molecular Formula: CHF₂CClF₂
 Name: 1-Chloro-1,1,2,2-tetrafluoroethane
 CAS number: 354-25-6
 Molecular Weight: 136.48



Global Atmospheric Lifetime (years): 17.0 ~9.2[#]
 Tropospheric Atmospheric Lifetime (years): 19.0 ~10[#]
 Stratospheric Atmospheric Lifetime (years): 161.2 ~120[#]
 Ozone Depletion Potential (ODP): 0.026

	<i>Well-mixed</i>	<i>Lifetime adjusted</i>
Radiative Efficiency (RE):	0.249	0.241
Global Warming Potential (GWP _H):		
GWP ₂₀	4827	4677
GWP ₁₀₀	1884	1826
Global Temperature Potentials (GTP _H):		
GTP ₂₀		4088
GTP ₅₀		1258
GTP ₁₀₀		327

* RE units: W m² ppb⁻¹

* GWP and GTP: Relative to CO₂

Value taken from WMO (2014)

Atmospheric Loss Processes *****

OH Reactivity

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

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

$$\tau_{\text{Global}}^{\text{OH}} = 18.3 \text{ years}$$

$$\tau_{\text{Trop}}^{\text{OH}} = 19.0 \text{ years}$$

$$\tau_{\text{Strat}}^{\text{OH}} = 478.6 \text{ years}$$

Fractional Atmospheric Loss: 0.930

O(¹D) Reactivity

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

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

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

Fractional Atmospheric Loss: 0.032

UV Photolysis

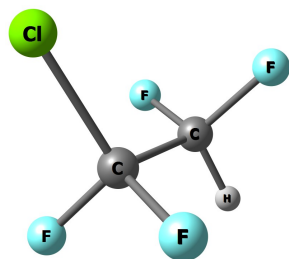
UV Spectrum: *No Recommendation*

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

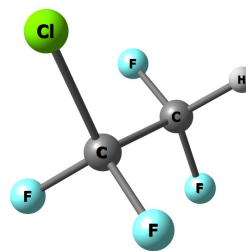
Fractional Atmospheric Loss: 0.038



Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.488



$\Delta E = 0.38 \text{ kcal mol}^{-1}$
Population = 0.256

Optimized Coordinates (Angstroms)

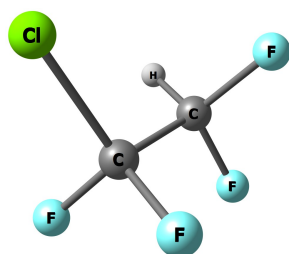
Atom	X	Y	Z
C	1.158040169121	-0.271267406322	0.017656324496
C	-0.372593733749	-0.452813328626	0.013597200740
F	1.534148720748	0.370778753679	-1.099219240806
F	1.519122722499	0.448484935076	1.091280116498
H	1.635096044697	-1.259662186453	0.055991272055
F	-0.714024137775	-1.188351920998	-1.046966668346
F	-0.728878665631	-1.111530414407	1.118830487714
Cl	-1.226135119910	1.113678568051	-0.047820492352

Atom	Z	Z	Z
C	0.977968645916	-0.364311854643	-0.456768904409
C	-0.251462057034	0.398587405832	0.078591648741
F	2.061010016831	0.403247299388	-0.227425048025
F	1.112041806966	-1.518930133385	0.213733471325
H	0.878849086170	-0.558228188838	-1.530348168152
F	-0.109879420176	0.643206060051	1.377427412434
F	-0.355985272311	1.559408825723	-0.570485222985
Cl	-1.743191806362	-0.560285414128	-0.190965188928

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
74.3707	0.167
185.8285	0.251
206.8491	0.246
333.8619	0.0511
359.4439	0.0172
420.2178	0.0460
517.0856	0.0001
562.6304	2.17
650.4395	19.0
683.6674	1.61
1075.7589	21.0
1163.7742	34.5
1173.1639	4.51
1210.2731	51.8
1227.4293	1.90
1389.4432	2.34
1405.4624	5.58
3051.6088	4.36

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
70.8907	0.0899
179.7901	0.167
240.5401	0.473
315.6756	0.246
344.5434	0.284
422.8034	0.197
450.8528	0.670
561.0247	2.57
643.2399	1.90
835.7053	17.2
975.3703	38.6
1142.7607	7.94
1170.7851	11.4
1200.4600	41.4
1275.8640	24.2
1393.1568	1.96
1412.4933	2.67
3079.5334	3.65



$\Delta E = 0.38 \text{ kcal mol}^{-1}$
Population = 0.256

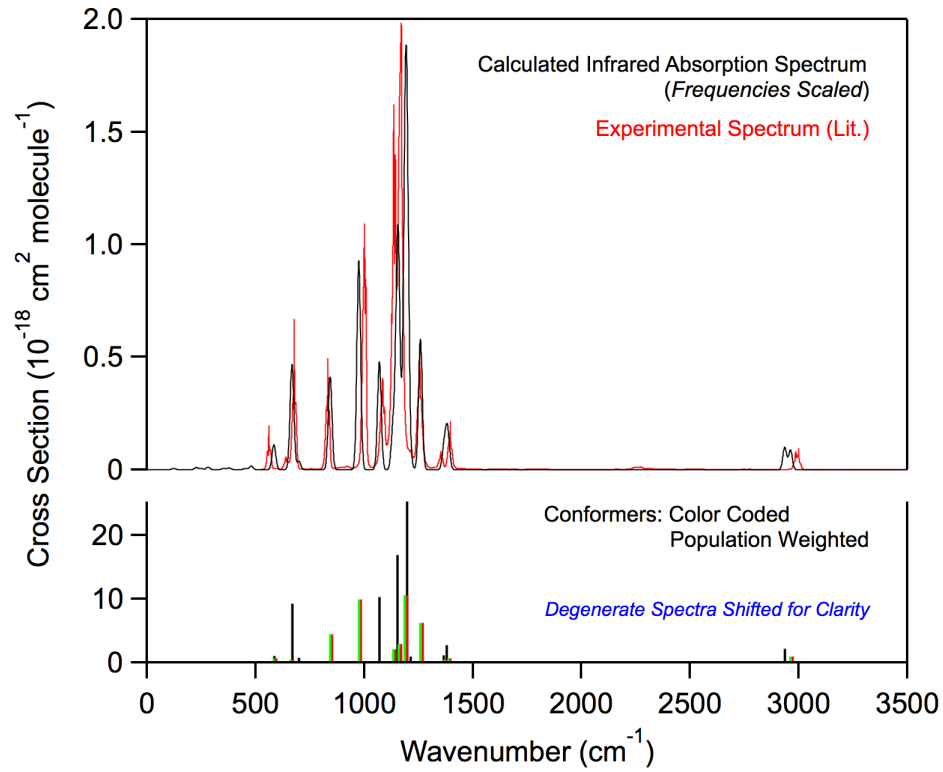
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	0.980090726459	0.364252889796	-0.454750425000
C	-0.250255800910	-0.403325318747	0.071745227106
F	1.111006594405	1.514517896193	0.223809725038
F	2.063149684050	-0.403806360676	-0.227170452675
H	0.884088062477	0.565200847407	-1.527319355233
F	-0.351683465193	-1.559906334432	-0.585343334580
F	-0.112433379237	-0.656434437805	1.369357986140
Cl	-1.742058422052	0.555932818264	-0.196031370798

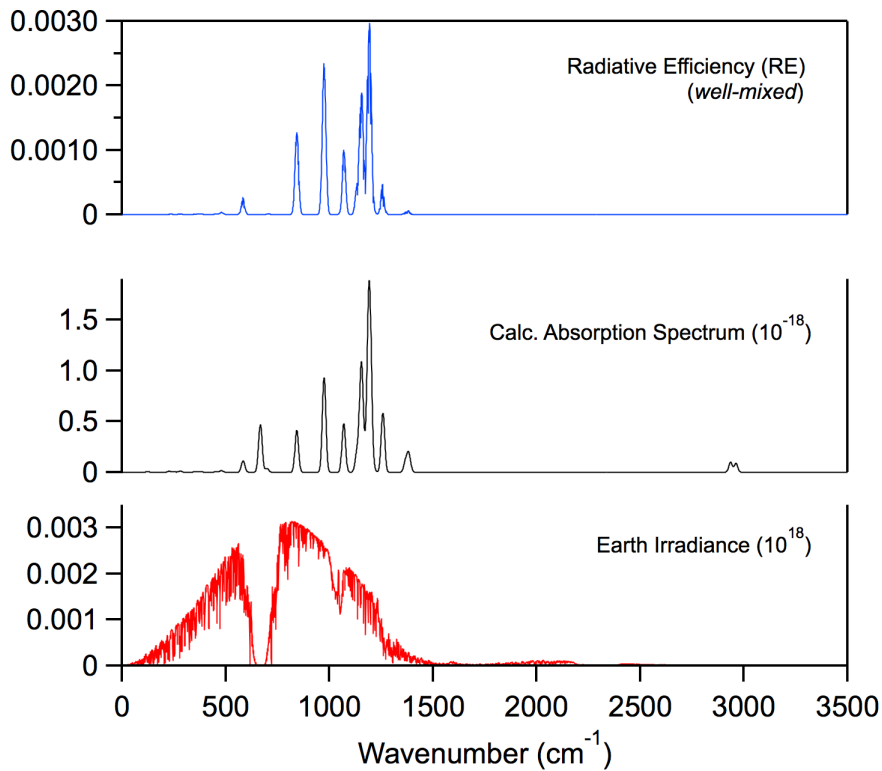
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength ($10^{-18} \text{ cm}^2 \text{ molecule}^{-1} \text{ cm}^{-1}$)
70.8912	0.0899
179.7902	0.167
240.5402	0.473
315.6755	0.246
344.5436	0.284
422.8034	0.197
450.8526	0.670
561.0248	2.57
643.2400	1.90
835.7051	17.2
975.3705	38.6
1142.7608	7.94
1170.7853	11.4
1200.4597	41.4
1275.8642	24.2
1393.1567	1.96
1412.4932	2.67
3079.5333	3.65

Infrared Spectrum

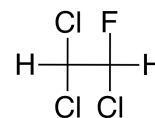


Radiative Efficiency



HCFC-131

Molecular Formula: CHCl₂CHClF
 Name: 1,2,2-Trichloro-1-fluoroethane
 CAS number: 359-28-4
 Molecular Weight: 151.39



Global Atmospheric Lifetime (years): 0.752
 Tropospheric Atmospheric Lifetime (years): 0.786
 Stratospheric Atmospheric Lifetime (years): 20
 Ozone Depletion Potential (ODP): 0.019

	<i>Well-mixed</i>	<i>Lifetime adjusted</i>
Radiative Efficiency (RE):	0.146	0.101
Global Warming Potential (GWP _H):		
GWP ₂₀	164	113
GWP ₁₀₀	44	31
Global Temperature Potentials (GTP _H):		
GTP ₂₀		36
GTP ₅₀		5
GTP ₁₀₀		4

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

Atmospheric Loss Processes *****

OH Reactivity

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

$$k_{\text{SAR}}(298 \text{ K}) = 7.46 \times 10^{-14}; k_{\text{SAR}}(272 \text{ K}) \approx 4.76 \times 10^{-14} \quad \text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$\tau_{\text{Global}}^{\text{OH}} = 0.764 \text{ years}$$

$$\tau_{\text{Trop}}^{\text{OH}} = 0.786 \text{ years}$$

$$\tau_{\text{Strat}}^{\text{OH}} = 27.1 \text{ years}$$

Fractional Atmospheric Loss: 0.985

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: 0.004

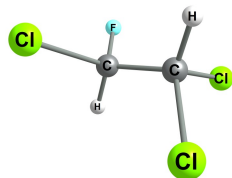
UV Photolysis

UV Spectrum: *No Recommendation*

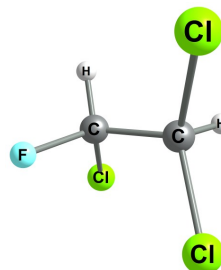
$$\tau_{\text{hv}} = 68 \text{ years}$$

Fractional Atmospheric Loss: 0.011

Molecular Structure and Infrared Spectrum (3 conformers)



$E = 0$
Population = 0.495



$\Delta E = 0.10 \text{ kcal mol}^{-1}$
Population = 0.420

Optimized Coordinates (Angstroms)

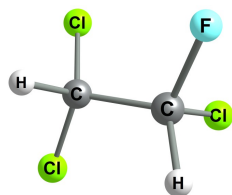
Atom	X	Y	Z
C	0.654530435800	0.595967006700	0.357073628500
C	-0.509489662200	-0.079676124500	-0.380688921300
H	-0.345474639200	-0.066801367600	-1.455957392300
Cl	-0.678518365100	-1.777689506100	0.135232823000
Cl	-2.013509709200	0.838465877500	-0.055807013100
H	0.562238469700	0.483608124600	1.438644974500
F	0.691617991800	1.901891996200	0.024221920400
Cl	2.213257478300	-0.157575006700	-0.131592019800

Atom	X	Y	Z
C	0.639472036700	-0.777807993000	0.057255667500
C	-0.496559027300	0.076126988200	-0.513489326800
H	-0.364944718300	0.212441732700	-1.583807586800
Cl	-2.039551470900	-0.816185099300	-0.280982692500
Cl	-0.563717648000	1.685745102000	0.241132083400
H	0.589629998300	-1.785290192800	-0.361589221300
F	0.573291046700	-0.836060606900	1.396518047900
Cl	2.232399782800	-0.101643930900	-0.443245971400

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
66.2679	0.0568
162.8470	0.0852
239.8841	0.0264
311.2165	0.927
331.1416	0.647
372.7919	1.40
442.1141	0.507
727.6749	24.8
783.3966	5.22
795.1294	13.6
1052.1640	2.00
1131.5264	17.9
1209.5063	3.57
1221.3110	2.90
1302.1340	1.55
1378.8721	0.773
3116.4550	0.678
3152.9552	0.365

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
74.0958	0.120
168.1862	0.284
208.1535	0.0904
247.7443	0.0829
318.2563	0.282
391.6573	0.266
615.8764	7.37
725.8054	21.0
743.3108	10.9
799.3765	5.70
964.3023	5.29
1161.7215	16.1
1219.4738	4.12
1273.1760	1.37
1277.2140	1.18
1380.4362	2.80
3103.0811	0.892
3158.1313	0.357



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

$$\text{Population} = 0.085$$

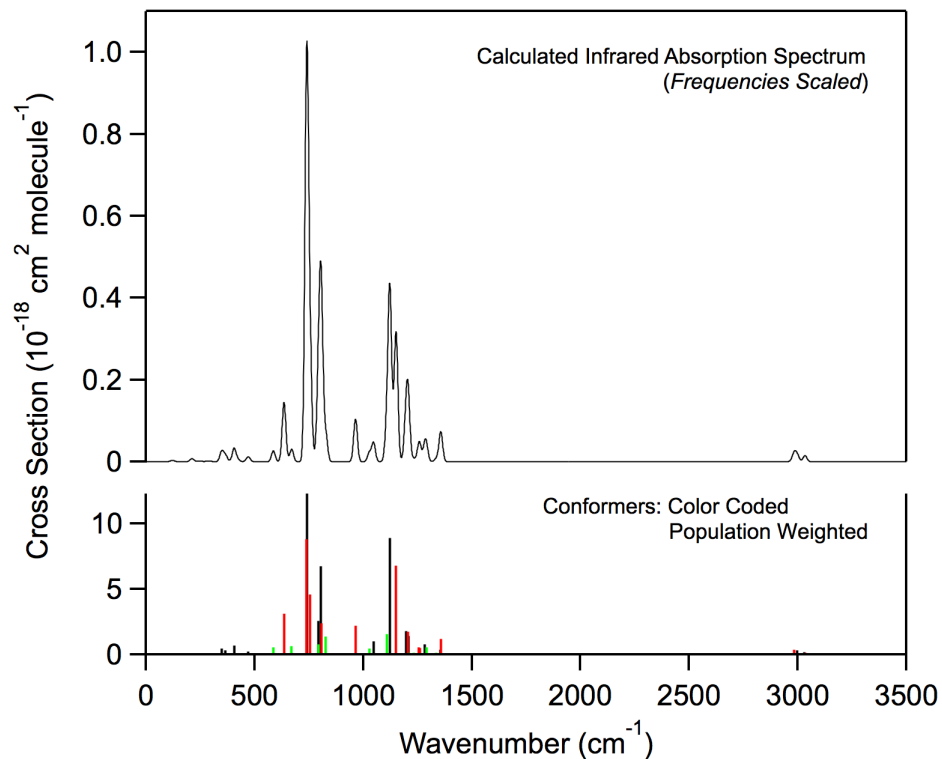
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	0.855723715600	0.124361379100	-0.719759361600
C	-0.634461280200	-0.201345161300	-0.559362684200
H	-0.989481675400	-0.597191282400	-1.510257020600
Cl	-0.922177840000	-1.466709702500	0.658916745300
Cl	-1.568307123000	1.284734734600	-0.234142170800
H	0.974497644000	0.915930320900	-1.463791584200
F	1.485960692900	-0.994295536300	-1.142728735800
Cl	1.625887866200	0.712261247900	0.782025811900

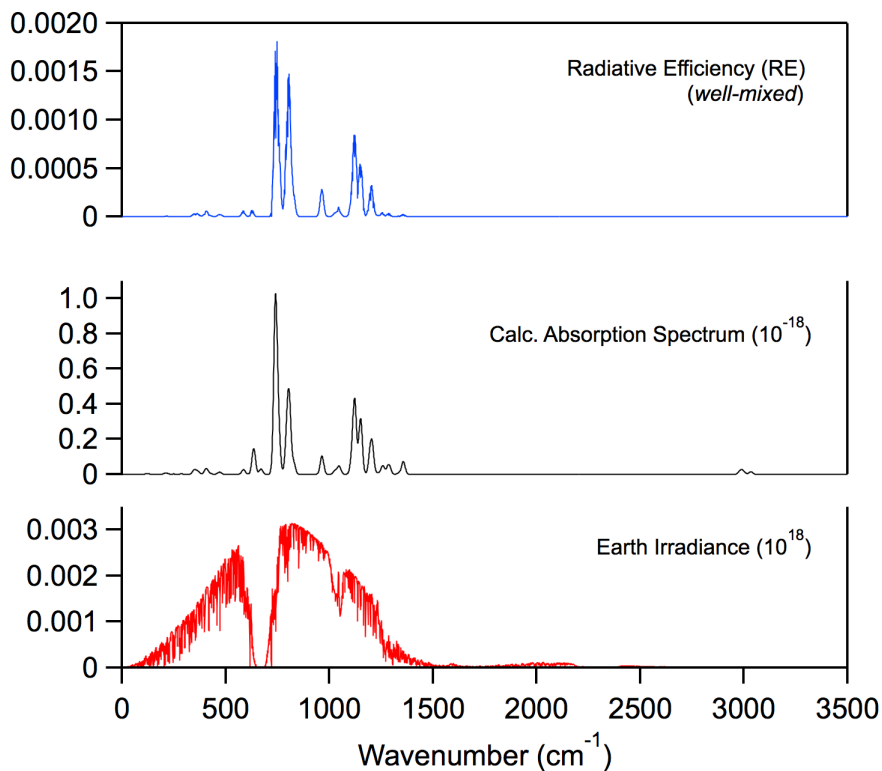
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
78.4623	0.0769
164.8281	0.0581
186.2055	0.194
264.3022	0.118
354.9836	0.246
431.5517	0.301
563.6581	6.67
652.9808	7.52
784.0983	9.23
819.4852	16.4
1031.4134	5.36
1116.2934	18.2
1226.1525	1.87
1247.8432	1.84
1310.4865	6.57
1358.2361	1.83
3095.5350	1.10
3127.9608	0.416

Infrared Spectrum

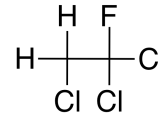


Radiative Efficiency



HCFC-131a

Molecular Formula: CH₂ClCCl₂F
 Name: 1,1,2-Trichloro-1-fluoroethane
 CAS number: 811-95-0
 Molecular Weight: 151.39



Global Atmospheric Lifetime (years): 2.57
 Tropospheric Atmospheric Lifetime (years): 2.80
 Stratospheric Atmospheric Lifetime (years): 31.4
 Ozone Depletion Potential (ODP): 0.056

	<i>Well-mixed</i>	<i>Lifetime adjusted</i>
Radiative Efficiency (RE):	0.195	0.169
Global Warming Potential (GWP _H):		
GWP ₂₀	744	647
GWP ₁₀₀	202	175
Global Temperature Potentials (GTP _H):		
GTP ₂₀		259
GTP ₅₀		32
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*

$k_{\text{SAR}}(298 \text{ K}) = 2.09 \times 10^{-14}$; $k_{\text{SAR}}(272 \text{ K}) \approx 1.34 \times 10^{-14}$ cm³ molecule⁻¹ s⁻¹

$\tau_{\text{Global}}^{\text{OH}} = 2.71$ years

$\tau_{\text{Trop}}^{\text{OH}} = 2.80$ years

$\tau_{\text{Strat}}^{\text{OH}} = 85.3$ years

Fractional Atmospheric Loss: 0.948

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: 0.014

UV Photolysis

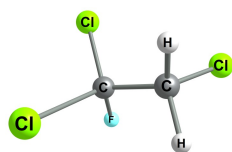
UV Spectrum: *No Recommendation*

$\tau_{\text{hv}} = 68$ years

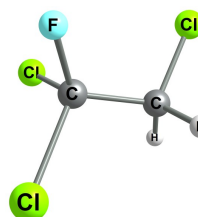
Fractional Atmospheric Loss: 0.038



Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.474



E = 0
Population = 0.474

Optimized Coordinates (Angstroms)

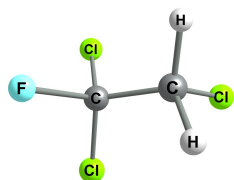
Atom	X	Y	Z
C	0.395656217200	-0.073378647000	0.201136319300
C	-0.696319075400	-0.845049590800	-0.535872607500
H	-0.582662268900	-0.713318327500	-1.609720861200
H	-0.607515538100	-1.898548927100	-0.270683208000
Cl	-2.336240725800	-0.303475628800	-0.062970373000
Cl	1.978127417800	-0.816469989500	-0.258779605200
F	0.252625524900	-0.185437119100	1.522618717000
Cl	0.408425448400	1.664356229800	-0.226876381300

Atom	X	Y	Z
C	0.395752409400	0.072802369400	0.201858952100
C	-0.694079071900	0.853531506800	-0.528733502600
H	-0.599812428900	1.905146511700	-0.257991802500
H	-0.583175582300	0.727134926500	-1.603508890800
Cl	-2.335554489500	0.317016888800	-0.055507494400
Cl	0.399593692300	-1.662637759800	-0.235614751300
F	0.255874502700	0.178319234300	1.524200284600
Cl	1.980753968200	0.811034322400	-0.257228795100

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
102.7542	0.332
160.2560	0.176
241.3438	0.0694
287.4555	0.191
344.4979	0.240
385.9482	0.225
437.9541	0.731
617.0557	7.92
744.5041	25.8
807.1344	15.5
915.4791	5.48
1019.1879	14.0
1175.5453	9.16
1248.1369	9.79
1302.7871	1.51
1455.2005	1.08
3107.9333	0.821
3182.6481	0.0311

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
102.7466	0.332
160.2547	0.176
241.3437	0.0695
287.4524	0.191
344.4929	0.240
385.9417	0.226
437.9477	0.730
617.0446	7.92
744.5125	25.8
807.1242	15.5
915.4894	5.48
1019.2024	14.0
1175.5814	9.16
1248.1683	9.79
1302.8020	1.51
1455.2041	1.08
3107.9118	0.821
3182.6412	0.0311



$$\Delta E = 1.31 \text{ kcal mol}^{-1}$$

$$\text{Population} = 0.052$$

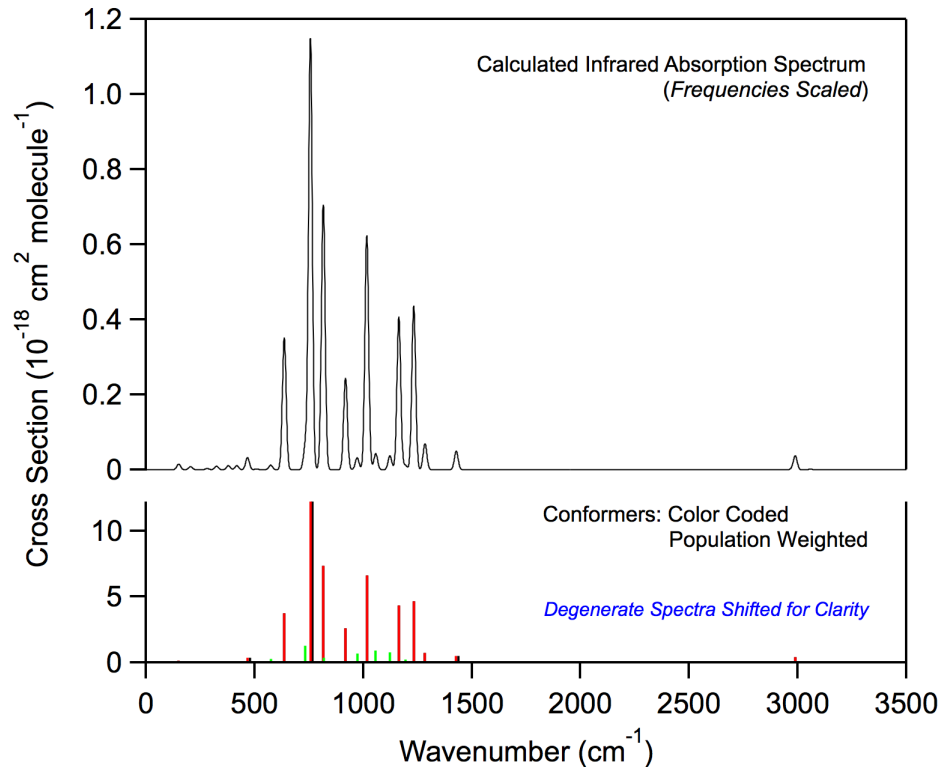
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	0.539328381300	0.000783984000	-0.368946381000
C	-0.855974358500	-0.010815619000	-0.997344994600
H	-0.949444813300	0.879979241500	-1.619218170000
H	-0.937985377700	-0.907990809800	-1.611617573200
Cl	-2.192620200500	-0.014381112900	0.179126455500
Cl	0.822957145100	1.474798133700	0.607556052700
F	1.418203358400	0.002098901600	-1.387761169900
Cl	0.841778865300	-1.461151719200	0.620007780400

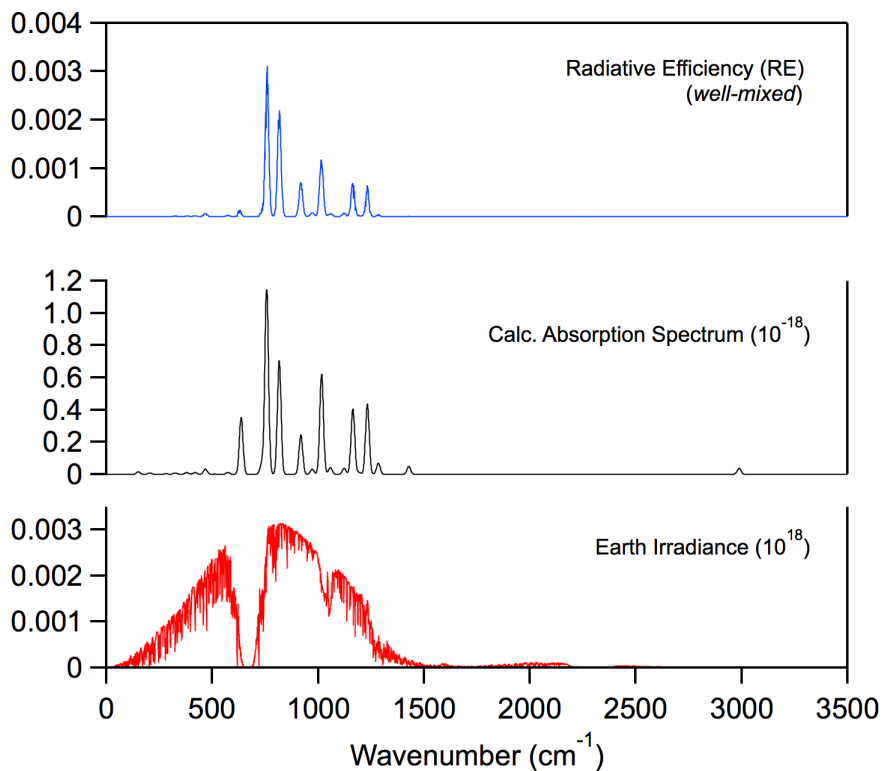
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength ($10^{-18} \text{ cm}^2 \text{ molecule}^{-1} \text{ cm}^{-1}$)
95.5869	0.196
156.0280	0.0822
261.4177	0.0217
284.9881	0.291
367.5611	0.119
389.1271	0.180
483.1238	0.780
550.8061	4.97
719.3561	25.0
810.3023	7.15
972.3685	13.2
1062.9081	17.6
1132.0527	15.3
1206.8040	4.86
1306.7850	0.880
1459.5406	0.705
3093.6860	1.04
3162.0803	0.0115

Infrared Spectrum

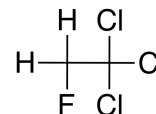


Radiative Efficiency



HCFC-131b

Molecular Formula: CH₂FCCl₃
 Name: 1,1,1-Trichloro-2-fluoroethane
 CAS number: 2366-36-1
 Molecular Weight: 151.39



Global Atmospheric Lifetime (years): 2.33
 Tropospheric Atmospheric Lifetime (years): 2.55
 Stratospheric Atmospheric Lifetime (years): 26.2
 Ozone Depletion Potential (ODP): 0.054

	<i>Well-mixed</i>	<i>Lifetime adjusted</i>
Radiative Efficiency (RE):	0.153	0.132
Global Warming Potential (GWP _H):		
GWP ₂₀	530	456
GWP ₁₀₀	144	123
Global Temperature Potentials (GTP _H):		
GTP ₂₀		176
GTP ₅₀		22
GTP ₁₀₀		17

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

Atmospheric Loss Processes *****

OH Reactivity

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

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

$$\tau_{\text{Global}}^{\text{OH}} = 2.47 \text{ years}$$

$$\tau_{\text{Trop}}^{\text{OH}} = 2.55 \text{ years}$$

$$\tau_{\text{Strat}}^{\text{OH}} = 78.5 \text{ years}$$

Fractional Atmospheric Loss: 0.941

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: 0.013

UV Photolysis

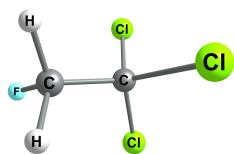
UV Spectrum: *No Recommendation*

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

Fractional Atmospheric Loss: 0.046



Molecular Structure and Infrared Spectrum (1 conformer)



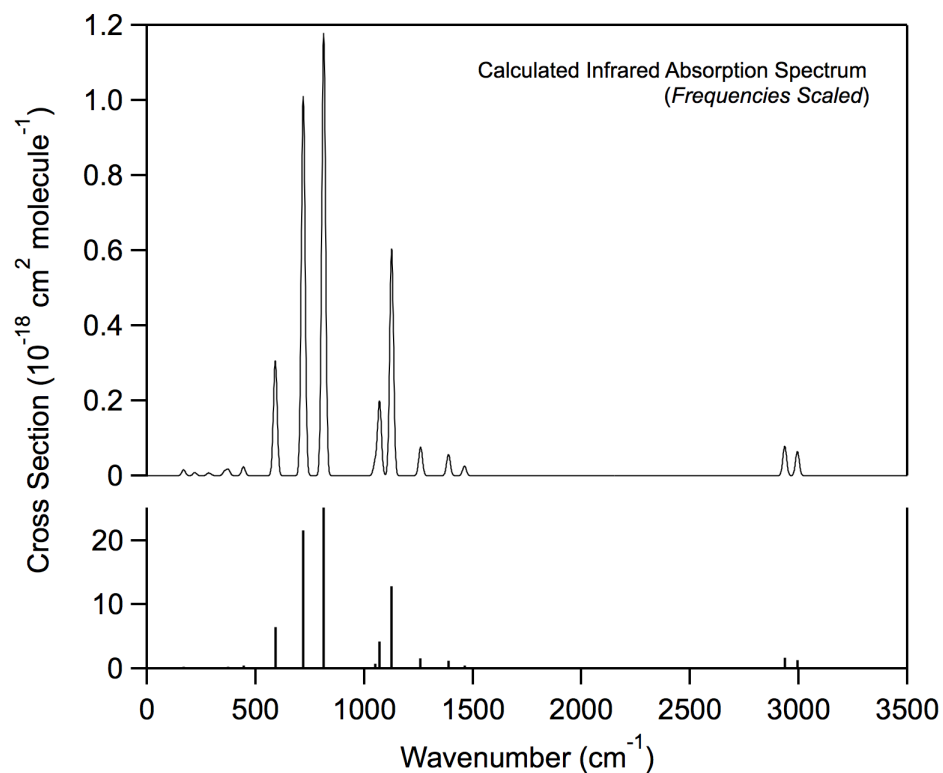
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	0.113346274700	0.000129548200	0.064864440500
C	-0.786215074000	-0.011746826700	1.306949041000
H	-0.576527311100	-0.922600870400	1.876847199900
H	-0.556211493900	0.873329477100	1.908733340400
F	-2.095585452800	0.009730044100	0.932815894000
Cl	1.812792633600	-0.029274703400	0.636797513600
Cl	-0.182830635300	1.480356505800	-0.892643229800
Cl	-0.215875941100	-1.438151174800	-0.944446199700

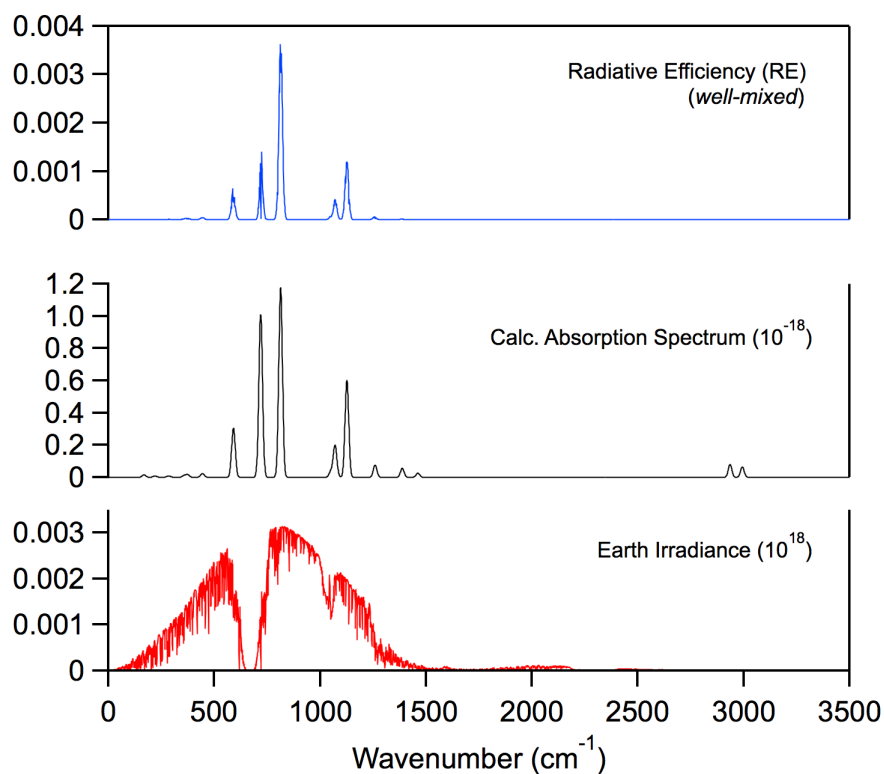
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
121.4857	0.333
175.9288	0.181
242.4902	0.144
256.3584	0.0375
321.3903	0.236
339.1743	0.336
413.3197	0.500
568.4174	6.53
704.6062	21.5
804.2348	25.1
1055.6124	0.755
1076.5407	4.22
1135.5702	12.9
1276.6969	1.63
1412.4618	1.21
1490.7237	0.541
3051.7259	1.68
3113.3278	1.37

Infrared Spectrum

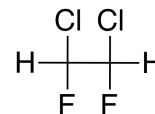


Radiative Efficiency



HCFC-132

Molecular Formula: CHClFCHClF
 Name: 1,2-Dichloro-1,2-difluoroethane
 CAS number: 431-06-1
 Molecular Weight: 134.94



Global Atmospheric Lifetime (years): 1.73
 Tropospheric Atmospheric Lifetime (years): 1.81
 Stratospheric Atmospheric Lifetime (years): 39.1
 Ozone Depletion Potential (ODP): 0.025

	<i>Well-mixed</i>	<i>Lifetime adjusted</i>
Radiative Efficiency (RE):	0.184	0.152
Global Warming Potential (GWP _H):		
GWP ₂₀	531	438
GWP ₁₀₀	144	119
Global Temperature Potentials (GTP _H):		
GTP ₂₀		156
GTP ₅₀		21
GTP ₁₀₀		17

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

Atmospheric Loss Processes *****

OH Reactivity

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

$$k_{\text{SAR}}(298 \text{ K}) = 3.23 \times 10^{-14}; k_{\text{SAR}}(272 \text{ K}) \approx 2.06 \times 10^{-14} \quad \text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$\tau_{\text{Global}}^{\text{OH}} = 1.76 \text{ years}$$

$$\tau_{\text{Trop}}^{\text{OH}} = 1.81 \text{ years}$$

$$\tau_{\text{Strat}}^{\text{OH}} = 57.7 \text{ years}$$

Fractional Atmospheric Loss: 0.986

O(¹D) Reactivity

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

$$k_{\text{Est}}(T) = 1.4 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$\tau_{\text{O}(\text{1D})} = 264 \text{ years}$$

Fractional Atmospheric Loss: 0.007

UV Photolysis

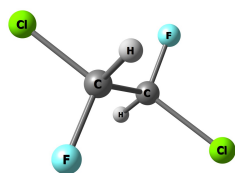
UV Spectrum: *No Recommendation*

$$\tau_{\text{hv}} = 225 \text{ years}$$

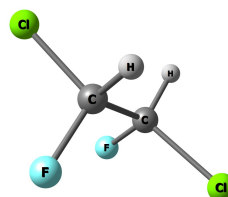
Fractional Atmospheric Loss: 0.008



Molecular Structure and Infrared Spectrum (6 conformers)



$E = 0$
Population = 0.626



$\Delta E = 0.86 \text{ kcal mol}^{-1}$
Population = 0.146

Optimized Coordinates (Angstroms)

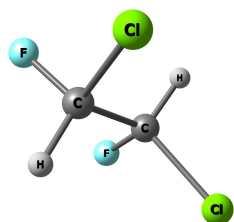
Atom	X	Y	Z
C	0.242178225313	0.724867108618	0.382329435266
C	-0.242178099887	-0.724867195934	0.317543936800
H	1.332361807120	0.781346036690	0.370755200028
Cl	-0.350670080216	1.600424074602	-1.074046356515
F	-0.250787750161	1.315957860034	1.486559631879
H	-1.332361764021	-0.781346797155	0.329115319675
F	0.250789884618	-1.315957593185	-0.786685146273
Cl	0.350667777234	-1.600423493669	1.773921979139

Atom	Z	Z	Z
C	-0.212246981563	0.734250061221	-0.238157071412
C	0.212246981563	-0.734250061221	-0.238157071412
H	0.166836677966	1.255245447354	-1.118817329024
Cl	-2.012427021137	0.814858131719	-0.318520050576
F	0.212219986288	1.338893782489	0.884264451012
H	-0.166836677966	-1.255245447354	-1.118817329024
Cl	2.012427021137	-0.814858131719	-0.318520050576
F	-0.212219986288	-1.338893782489	0.884264451012

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
70.8792	0.122
168.3834	0.188
264.6711	0.0
364.8257	0.0
365.3279	4.17
393.6975	0.275
517.2822	0.0
741.7271	39.0
797.3019	0.0
1076.5764	0.0
1140.3537	0.0
1155.3607	38.5
1221.5009	6.70
1300.6297	0.0
1330.8680	2.90
1403.4294	0.0
3107.4745	0.0
3119.9393	1.99

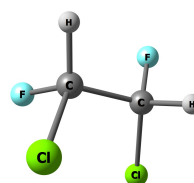
Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
73.0704	0.0923
179.4672	0.500
238.7362	0.135
273.0438	0.0869
377.8738	0.498
398.4238	0.297
728.4639	30.9
757.2816	13.7
790.3349	0.0112
908.7515	3.59
1112.8593	18.8
1191.6621	17.9
1253.0008	2.87
1290.3591	0.362
1371.7622	0.612
1397.1971	2.78
3111.4869	0.789
3119.2024	1.51



$\Delta E = 1.05 \text{ kcal mol}^{-1}$
Population = 0.107

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	0.246269480860	0.726085402521	0.426374935205
C	-0.246269480860	-0.726085402521	0.426374935205
H	1.333798945964	0.779878130351	0.347070578961
Cl	-0.448548232238	1.630349753718	-0.955311961008
F	-0.161629924723	1.295916442241	1.581613446853
H	-1.333798945964	-0.779878130351	0.347070578961
Cl	0.448548232238	-1.630349753718	-0.955311961008
F	0.161629924723	-1.295916442241	1.581613446853



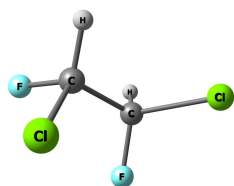
$\Delta E = 1.59 \text{ kcal mol}^{-1}$
Population = 0.043

Atom	Z	Z	Z
C	0.702490000000	0.233144000000	0.628147000000
C	-0.635920000000	0.726903000000	0.070960000000
H	0.588693000000	-0.132049000000	1.650233000000
Cl	1.380848000000	-1.101815000000	-0.347435000000
F	1.558964000000	1.283749000000	0.607644000000
H	-0.931872000000	1.628520000000	0.615052000000
F	-0.530640000000	1.007229000000	-1.238999000000
Cl	-1.924731000000	-0.490073000000	0.345510000000

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
75.0014	0.0993
161.4156	0.0826
310.4120	0.209
324.7999	1.61
381.5060	0.986
433.9766	1.82
447.6843	0.539
799.2918	17.6
812.9205	14.8
1066.0596	7.91
1111.1273	3.48
1140.3213	34.4
1221.4027	5.43
1287.3170	1.49
1348.3597	0.992
1396.5674	1.60
3106.3961	0.0631
3119.0229	2.00

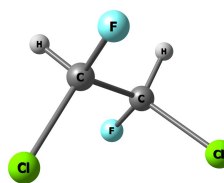
Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
74.8901	0.117
172.3437	0.262
224.0106	0.246
319.5644	0.132
381.0736	0.496
438.0025	0.533
614.2075	10.3
783.5652	5.98
808.7583	16.8
971.4502	6.21
1102.7267	19.6
1167.6899	20.0
1258.6551	1.74
1287.9964	3.44
1367.8909	0.550
1383.6687	4.50
3085.3371	1.41
3113.9666	1.40



$\Delta E = 1.59 \text{ kcal mol}^{-1}$
Population = 0.043

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	0.636454000	0.726490000	0.071804000
C	-0.702316000	0.232524000	0.627942000
H	0.932572000	1.627302000	0.617137000
Cl	1.924722000	-0.491318000	0.345212000
F	0.531692000	1.008523000	-1.237830000
H	-0.588977000	-0.134011000	1.649599000
F	-1.558390000	1.283475000	0.608505000
Cl	-1.380866000	-1.100940000	-0.349549000



$\Delta E = 1.70 \text{ kcal mol}^{-1}$
Population = 0.036

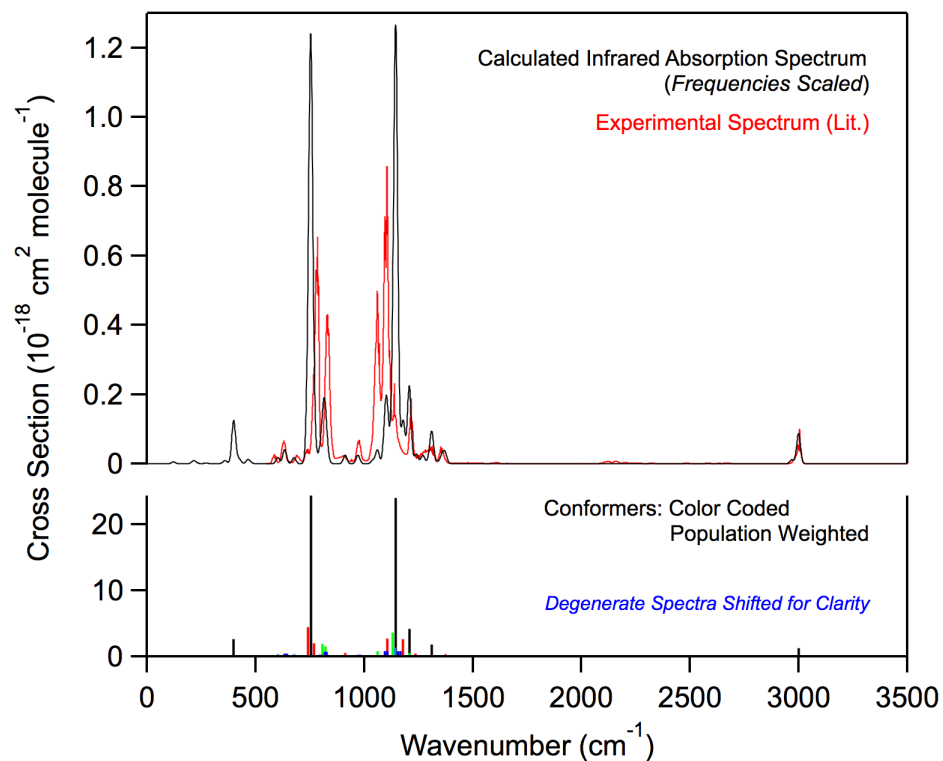
Atom	Z	Z	Z
C	-0.112744525657	0.757634507621	-0.691047301118
C	0.112744525657	-0.757634507621	-0.691047301118
H	-0.689060399976	1.030049675432	-1.580146279104
Cl	-1.072117810384	1.300914714040	0.715928987471
F	1.082108320443	1.382113601488	-0.714650407247
H	0.689060399976	-1.030049675432	-1.580146279104
Cl	1.072117810384	-1.300914714040	0.715928987471
F	-1.082108320443	-1.382113601488	-0.714650407247

Infrared Absorption Spectrum (unscaled frequencies)

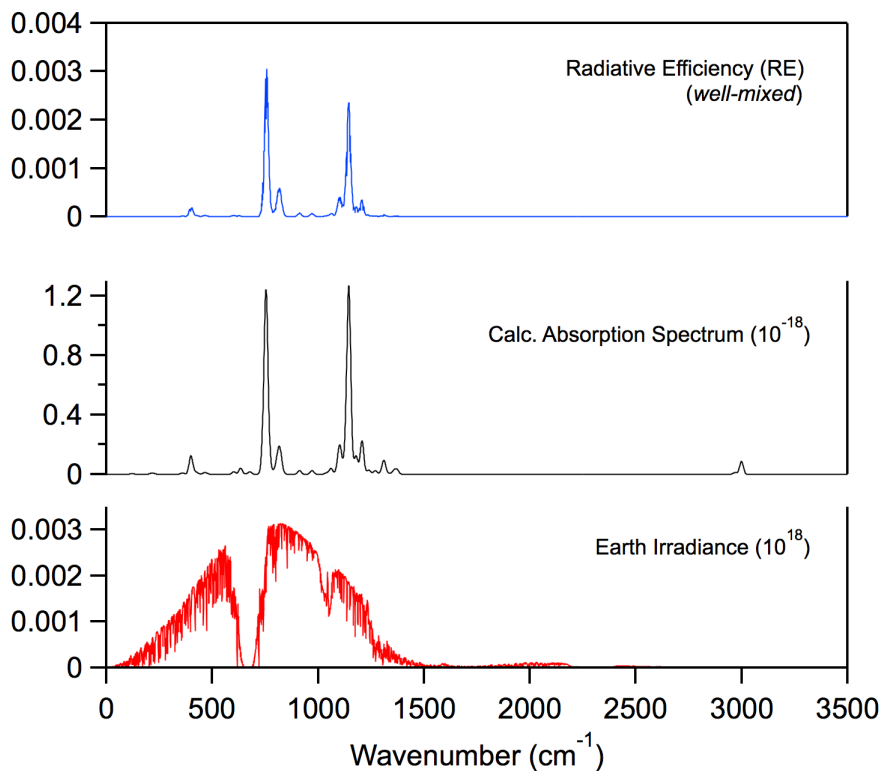
Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
74.8902	0.117
172.3436	0.262
224.0104	0.246
319.5645	0.132
381.0736	0.496
438.0025	0.533
614.2074	10.3
783.5651	5.98
808.7583	16.8
971.4503	6.21
1102.7267	19.6
1167.6901	20.0
1258.6551	1.74
1287.9965	3.44
1367.8908	0.550
1383.6689	4.50
3085.3370	1.41
3113.9665	1.40

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
80.2056	0.0842
174.3067	0.0841
197.8367	0.249
345.2726	0.0795
387.5003	0.430
521.1364	0.001
580.7132	10.4
660.0322	10.5
824.4772	7.51
1043.5754	5.98
1131.9645	1.96
1153.1116	37.3
1266.3666	1.93
1316.4138	5.44
1330.6899	3.40
1382.6678	2.87
3077.7103	0.548
3087.6043	3.01

Infrared Spectrum

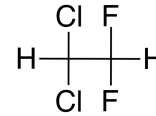


Radiative Efficiency



HCFC-132a

Molecular Formula: CHCl₂CHF₂
 Name: 1,1-Dichloro-2,2-difluoroethane
 CAS number: 471-43-2
 Molecular Weight: 134.94



Global Atmospheric Lifetime (years): 1.12
 Tropospheric Atmospheric Lifetime (years): 1.18
 Stratospheric Atmospheric Lifetime (years): 23.9
 Ozone Depletion Potential (ODP): 0.020

	<i>Well-mixed</i>	<i>Lifetime adjusted</i>
Radiative Efficiency (RE):	0.172	0.131
Global Warming Potential (GWP _H):		
GWP ₂₀	323	246
GWP ₁₀₀	87	67
Global Temperature Potentials (GTP _H):		
GTP ₂₀		81
GTP ₅₀		12
GTP ₁₀₀		9

* RE units: W m² ppb⁻¹

* GWP and GTP: Relative to CO₂

Atmospheric Loss Processes *****

OH Reactivity

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

$$k_{\text{SAR}}(298 \text{ K}) = 4.97 \times 10^{-14}; k_{\text{SAR}}(272 \text{ K}) \approx 3.17 \times 10^{-14} \quad \text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

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

$$\tau_{\text{Trop}}^{\text{OH}} = 1.18 \text{ years}$$

$$\tau_{\text{Strat}}^{\text{OH}} = 39.1 \text{ years}$$

Fractional Atmospheric Loss: 0.982

O(¹D) Reactivity

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

$$k_{\text{Est}}(T) = 1.4 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$\tau_{\text{O}(\text{1D})} = 264 \text{ years}$$

Fractional Atmospheric Loss: 0.004

UV Photolysis

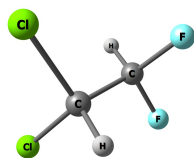
UV Spectrum: *No Recommendation*

$$\tau_{\text{hv}} = 80 \text{ years}$$

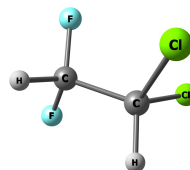
Fractional Atmospheric Loss: 0.014



Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.546



$\Delta E = 0.52 \text{ kcal mol}^{-1}$
Population = 0.227

Optimized Coordinates (Angstroms)

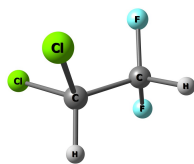
Atom	X	Y	Z
C	1.123520643016	-0.009037592750	-0.320975074188
C	-0.239903305341	-0.002051980046	0.384171390659
F	1.815741114873	1.081528460311	0.067724762543
F	1.808575224211	-1.101330189075	0.075494638637
H	1.019647759326	-0.012578554171	-1.411563427442
H	-0.098932251459	0.001326414887	1.463543699420
Cl	-1.137294930516	1.476236261745	-0.055793635331
Cl	-1.146992254111	-1.477509820901	-0.045282354299

Atom	Z	Z	Z
C	0.923593661849	-0.801411792494	0.207999179951
C	-0.268244335056	0.101632625671	0.548963949605
F	1.036875263368	-0.966321138273	-1.119416630008
F	2.050508135981	-0.217052726475	0.669774795018
H	0.804386969336	-1.781701898768	0.686813818173
H	-0.294211484327	0.283147933508	1.621488830870
Cl	-0.118952010027	1.682183904280	-0.258004242812
Cl	-1.786969201124	-0.736614907448	0.112922299203

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
74.3325	0.118
178.3261	0.152
244.9172	0.0466
338.9521	1.45
391.1349	0.429
393.2525	2.18
573.3082	1.27
787.8993	5.14
797.1977	22.7
1067.4197	2.22
1131.2765	19.7
1142.0664	23.5
1222.0019	3.02
1249.2504	0.380
1389.4629	1.45
1408.2278	5.44
3077.0838	3.31
3144.4973	0.490

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
79.7208	0.153
191.3058	0.311
204.3616	0.0891
271.0764	0.185
379.6343	0.305
537.7603	1.76
648.3566	11.3
738.1225	1.35
806.4554	16.4
970.6956	2.19
1131.7089	22.4
1185.6419	15.0
1226.2470	2.79
1279.7620	1.94
1381.8815	6.17
1407.4827	3.79
3053.4664	3.91
3144.2125	0.440



$\Delta E = 0.52 \text{ kcal mol}^{-1}$
Population = 0.227

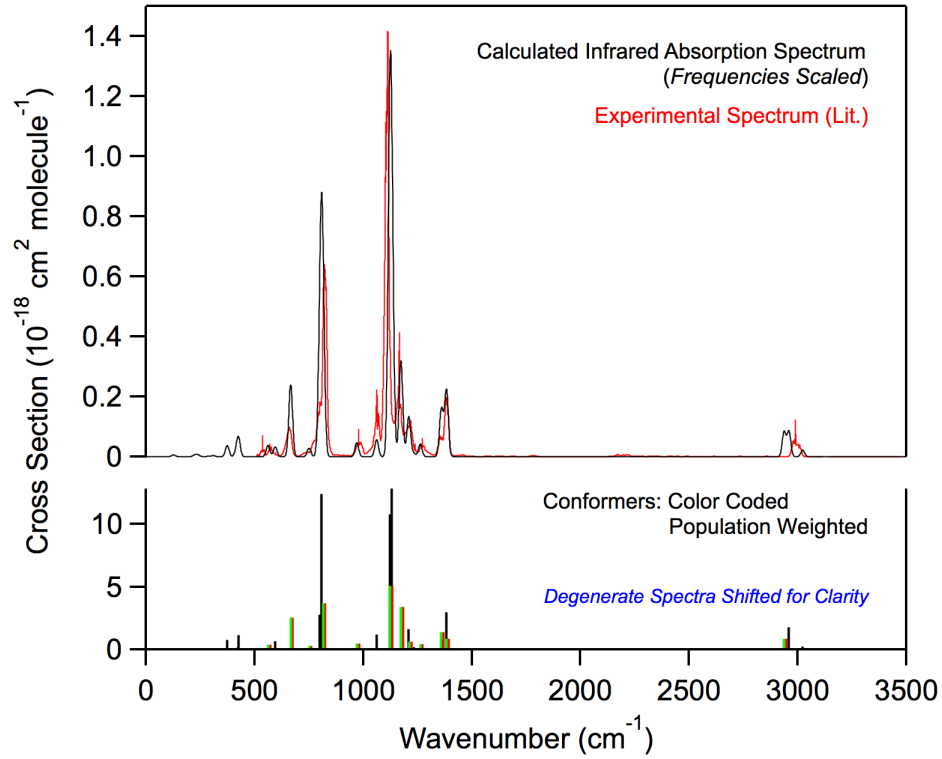
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-0.921667205173	-0.803985975527	0.205345847601
C	0.268666562400	0.100152352769	0.548657643183
F	-2.049194554031	-0.224226746599	0.671403547816
F	-1.036530532345	-0.963140169815	-1.122636449944
H	-0.799587108502	-1.786164734833	0.679543819848
H	0.295805440754	0.276871779303	1.621954187239
Cl	1.788602776531	-0.732738388258	0.106613126944
Cl	0.114689620366	1.684001882961	-0.250929722686

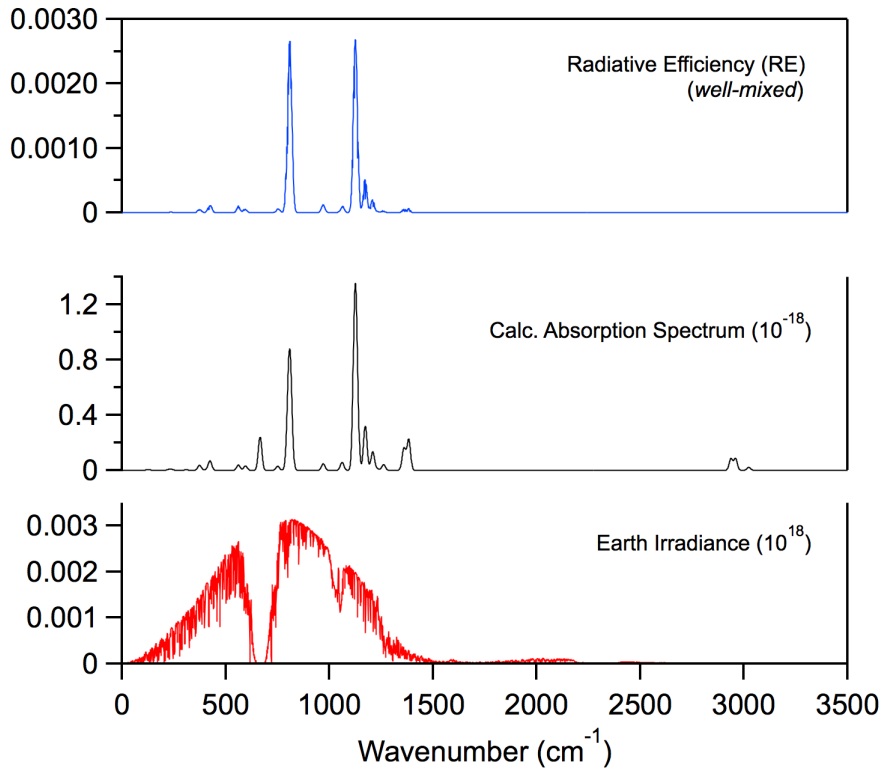
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength ($10^{-18} \text{ cm}^2 \text{ molecule}^{-1} \text{ cm}^{-1}$)
79.7209	0.153
191.3059	0.311
204.3617	0.0891
271.0764	0.185
379.6343	0.305
537.7603	1.76
648.3566	11.3
738.1226	1.35
806.4554	16.4
970.6957	2.19
1131.7088	22.4
1185.6418	15.0
1226.2470	2.79
1279.7620	1.94
1381.8815	6.17
1407.4826	3.79
3053.4664	3.91
3144.2124	0.440

Infrared Spectrum

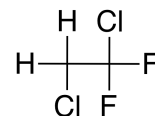


Radiative Efficiency



HCFC-132b

Molecular Formula: CH₂ClCClF₂
 Name: 1,2-Dichloro-1,1-difluoroethane
 CAS number: 1649-08-7
 Molecular Weight: 134.94



Global Atmospheric Lifetime (years): 4.84
 Tropospheric Atmospheric Lifetime (years): 5.21
 Stratospheric Atmospheric Lifetime (years): 67.0
 Ozone Depletion Potential (ODP): 0.048

	<i>Well-mixed</i>	<i>Lifetime adjusted</i>
Radiative Efficiency (RE):	0.219	0.202
Global Warming Potential (GWP _H):		
GWP ₂₀	1741	1602
GWP ₁₀₀	479	441
Global Temperature Potentials (GTP _H):		
GTP ₂₀		864
GTP ₅₀		92
GTP ₁₀₀		62

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

Atmospheric Loss Processes *****

OH Reactivity

$$k_{\text{Rec}}(T) = 3.6 \times 10^{-12} \exp(-1600/T); k_{\text{Rec}}(272 \text{ K}) = 1.0 \times 10^{-14} \quad \text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$k_{\text{SAR}}(298 \text{ K}) = 1.12 \times 10^{-14}; k_{\text{SAR}}(272 \text{ K}) \approx 0.718 \times 10^{-14} \quad \text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$\tau_{\text{Global}}^{\text{OH}} = 5.04 \text{ years}$$

$$\tau_{\text{Trop}}^{\text{OH}} = 5.21 \text{ years}$$

$$\tau_{\text{Strat}}^{\text{OH}} = 149.4 \text{ years}$$

Fractional Atmospheric Loss: 0.960

O(¹D) Reactivity

$$k_{\text{Rec}}(T) = 0.90 \times 1.6 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$k_{\text{Est}}(T) = 1.4 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$\tau_{\text{O}(\text{1D})} = 264 \text{ years}$$

Fractional Atmospheric Loss: 0.018

UV Photolysis

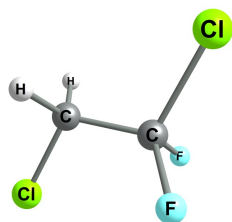
UV Spectrum: *No Recommendation*

$$\tau_{\text{hv}} = 225 \text{ years}$$

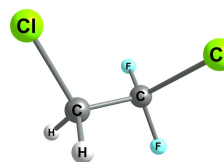
Fractional Atmospheric Loss: 0.022



Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.833



$\Delta E = 1.36 \text{ kcal mol}^{-1}$
Population = 0.084

Optimized Coordinates (Angstroms)

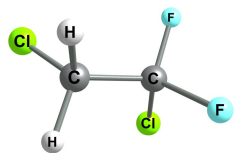
Atom	X	Y	Z
C	-0.421109158700	0.249626973700	-0.001297622600
C	0.618697834100	-0.861484627400	-0.024339953200
H	0.500804656400	-1.487565900000	0.858163471900
H	0.497789549500	-1.453340941700	-0.929751498900
Cl	2.276798209400	-0.177691089500	-0.014062121800
Cl	-2.067005465900	-0.514902330100	-0.013139309600
F	-0.322434038400	1.043010584200	-1.066218253000
F	-0.318749586400	1.001665330700	1.092856287300

Atom	X	Y	Z
C	-0.597420586000	0.415174957000	-0.028732088900
C	0.731006362700	0.664038007000	0.679835526800
H	0.935270719500	1.734599520100	0.622928633400
H	0.651897657200	0.351434640800	1.719527597100
Cl	2.093232710000	-0.200913772900	-0.079824166000
Cl	-1.148245496900	-1.291466051200	0.107981241700
F	-0.531180569000	0.739422099900	-1.319146802800
F	-1.520765797600	1.199456599300	0.549978058700

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
98.1018	0.531
166.9066	0.225
274.8232	0.201
320.7200	0.189
408.9020	0.000
413.5796	0.529
557.9070	2.24
744.7987	24.2
783.6838	1.66
911.9910	1.06
940.9220	31.1
1120.2754	12.8
1250.2676	17.0
1291.7684	15.0
1311.6245	4.33
1457.9132	1.62
3116.4686	0.898
3186.5502	0.00404

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
92.3713	0.312
169.3108	0.172
306.1704	0.312
321.0361	0.00928
415.4673	0.260
428.1017	0.323
576.2724	4.09
650.5902	8.10
804.9932	8.01
900.1583	3.98
1019.6028	26.6
1148.7972	27.9
1192.7586	12.2
1266.2412	18.6
1317.0896	0.640
1461.0087	1.28
3096.2423	1.15
3171.0222	0.0573



$\Delta E = 1.36 \text{ kcal mol}^{-1}$
Population = 0.084

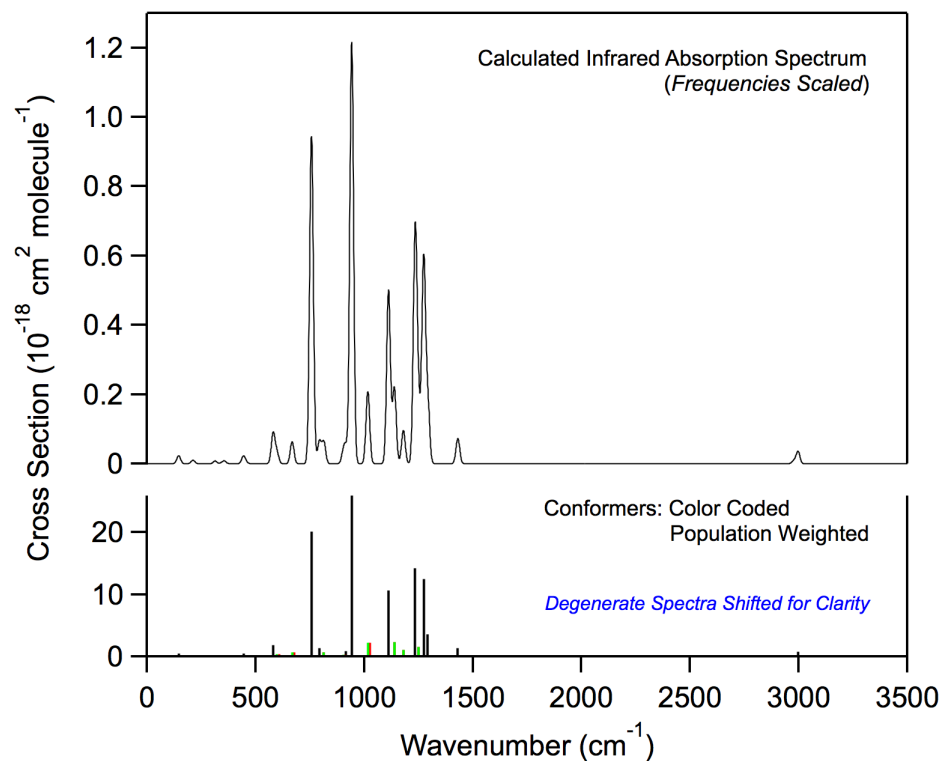
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-0.600914922900	-0.415026560000	-0.029751666800
C	0.729491243100	-0.677884082900	0.669971101300
H	0.657550063100	-0.373457295100	1.712604398200
H	0.926882076800	-1.749157355100	0.603131223600
Cl	2.093198194500	0.185034598200	-0.089385194100
Cl	-1.140553328200	1.293754985900	0.123875376500
F	-1.526132311400	-1.198449173100	0.547110705900
F	-0.543132015000	-0.728914117900	-1.323135944500

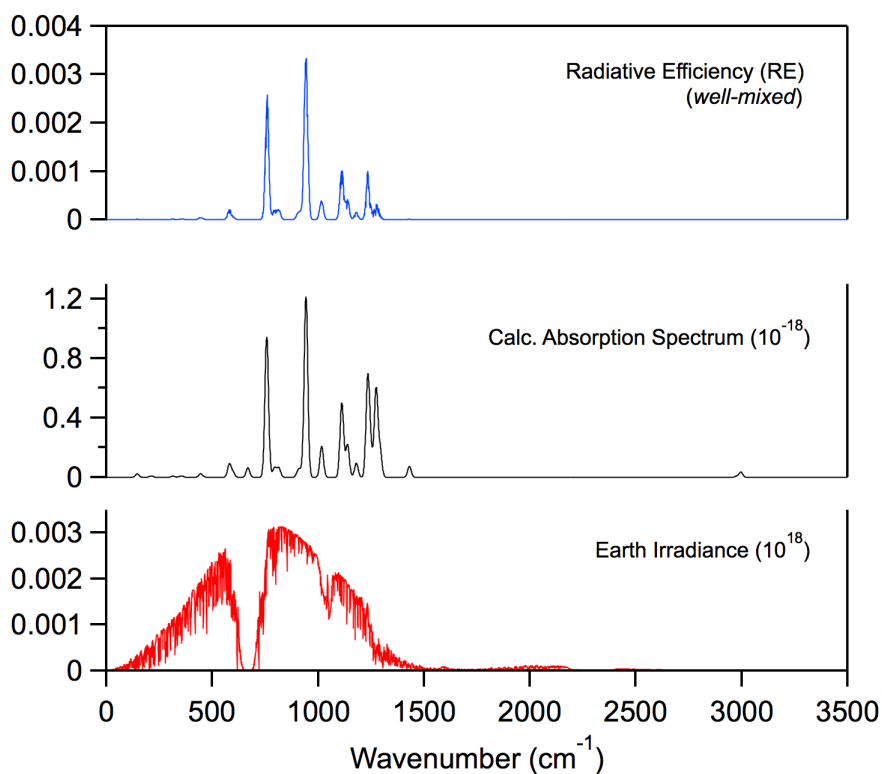
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
92.3726	0.312
169.3115	0.172
306.1639	0.312
321.0367	0.00927
415.4672	0.260
428.0956	0.323
576.2716	4.09
650.5843	8.10
804.9715	8.01
900.1576	3.98
1019.6020	26.6
1148.8173	27.9
1192.7655	12.2
1266.2335	18.6
1317.0846	0.640
1461.0015	1.28
3096.2646	1.15
3171.0468	0.0572

Infrared Spectrum

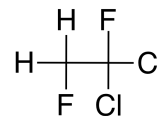


Radiative Efficiency



HCFC-132c

Molecular Formula: CH₂FCCL₂F
 Name: 1,1-Dichloro-1,2-difluoroethane
 CAS number: 1842-05-3
 Molecular Weight: 134.94



Global Atmospheric Lifetime (years): 3.76
 Tropospheric Atmospheric Lifetime (years): 4.14
 Stratospheric Atmospheric Lifetime (years): 40.8
 Ozone Depletion Potential (ODP): 0.054

	<i>Well-mixed</i>	<i>Lifetime adjusted</i>	
Radiative Efficiency (RE):	0.212	0.191	0.17 #
Global Warming Potential (GWP _H):			
GWP ₂₀	1322	1194	1230 #
GWP ₁₀₀	360	325	338 #
Global Temperature Potentials (GTP _H):			
GTP ₂₀		566	624 #
GTP ₅₀		63	67 #
GTP ₁₀₀		45	47 #

* RE units: W m² ppb⁻¹

* GWP and GTP: Relative to CO₂

Value taken from WMO (2014)

Atmospheric Loss Processes *****

OH Reactivity

$$k_{\text{Rec}}(T) = 8.2 \times 10^{-13} \exp(-1250/T); k_{\text{Rec}}(272 \text{ K}) = 8.28 \times 10^{-15} \quad \text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$k_{\text{SAR}}(298 \text{ K}) = 1.42 \times 10^{-14}; k_{\text{SAR}}(272 \text{ K}) \approx 0.904 \times 10^{-14} \quad \text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$\tau_{\text{Global}}^{\text{OH}} = 4.01 \text{ years}$$

$$\tau_{\text{Trop}}^{\text{OH}} = 4.14 \text{ years}$$

$$\tau_{\text{Strat}}^{\text{OH}} = 121.4 \text{ years}$$

Fractional Atmospheric Loss: 0.939

O(¹D) Reactivity

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

$$k_{\text{Est}}(T) = 1.4 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$\tau_{\text{O}(\text{1D})} = 264 \text{ years}$$

Fractional Atmospheric Loss: 0.014

UV Photolysis

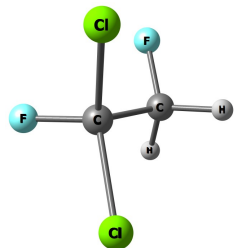
UV Spectrum: No Recommendation

$$\tau_{\text{hv}} = 80 \text{ years}$$

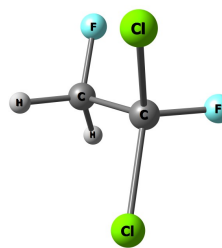
Fractional Atmospheric Loss: 0.047



Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.396



E = 0 kcal mol⁻¹
Population = 0.396

Optimized Coordinates (Angstroms)

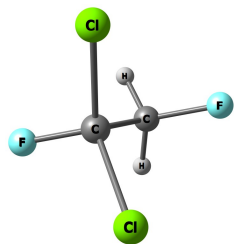
Atom	X	Y	Z
C	0.087996612951	-0.093265673584	0.194057267054
C	-0.841580136825	-1.047805606538	-0.554258034831
F	-0.034612519604	-0.268982809507	1.513567530640
Cl	1.781755830854	-0.468621986258	-0.281865506860
Cl	-0.300096264102	1.613821230059	-0.182967248570
H	-0.705810447910	-0.921694930477	-1.631475200117
H	-0.581765602524	-2.069947891370	-0.256598429211
F	-2.132899472839	-0.781464332325	-0.203391378105

Atom	Z	Z	Z
C	-0.088610181709	-0.092992513366	0.194246025611
C	0.840123663633	-1.048666748761	-0.553668038003
F	0.034118013459	-0.268003666358	1.513838993196
Cl	0.300665814372	1.613580850689	-0.183881335162
Cl	-1.782734271412	-0.467391123324	-0.281132399147
H	0.579615130780	-2.070438041930	-0.255341906941
H	0.704244022828	-0.923105825016	-1.630935571141
F	2.131704808049	-0.783062931933	-0.203205768413

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
118.2750	0.543
185.6388	0.290
248.9472	0.111
326.7550	0.172
355.1382	0.308
393.7687	0.358
450.1568	1.03
632.4204	12.1
832.8038	36.6
953.0757	12.5
1087.7723	6.49
1128.2909	9.02
1205.0578	15.8
1286.9835	4.82
1417.7890	0.895
1490.0727	0.454
3052.6034	1.81
3120.9295	1.53

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
118.2749	0.543
185.6386	0.290
248.9472	0.111
326.7550	0.172
355.1383	0.308
393.7688	0.358
450.1568	1.03
632.4205	12.1
832.8038	36.6
953.0758	12.5
1087.7724	6.49
1128.2909	9.02
1205.0580	15.8
1286.9840	4.82
1417.7890	0.895
1490.0724	0.454
3052.6030	1.81
3120.9296	1.53



$$\Delta E = 0.38 \text{ kcal mol}^{-1}$$

$$\text{Population} = 0.208$$

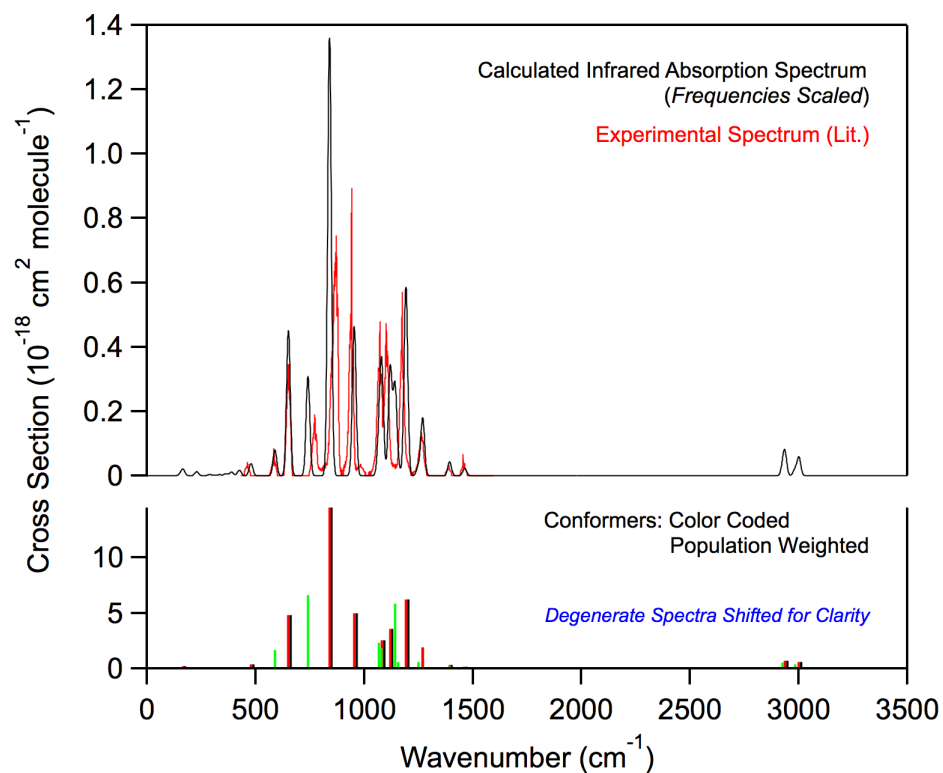
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	0.022629177089	0.156327308772	0.377767466984
C	-0.177565872622	-1.333666613046	0.660214507742
F	0.112392524972	0.790828000655	1.556078547125
Cl	1.536149518537	0.432430692091	-0.540690516407
Cl	-1.369707066753	0.824776373853	-0.530594658630
H	0.683238166054	-1.684882933981	1.240155634158
H	-1.096717908824	-1.444560106426	1.246329066794
F	-0.276066538453	-2.033370721917	-0.501265047766

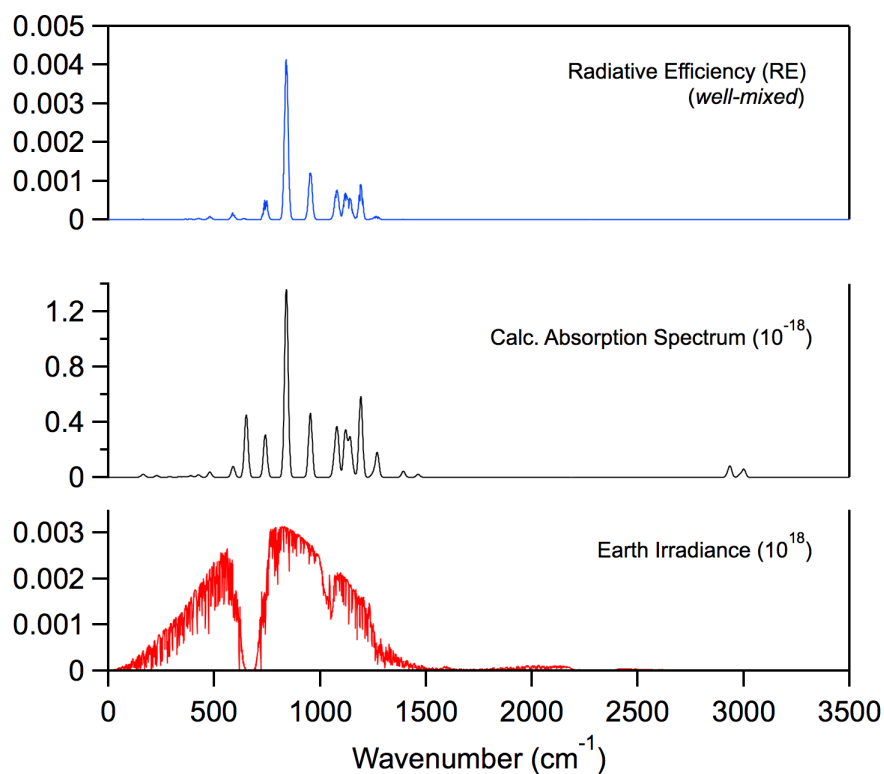
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
104.7938	0.376
182.4018	0.174
272.4327	0.0935
296.6726	0.328
387.0193	0.228
395.9757	0.259
544.1487	0.0696
566.6570	8.20
727.6269	31.6
1074.1347	11.2
1085.8779	8.98
1151.4103	28.2
1167.2426	2.82
1265.6302	2.84
1418.8646	0.993
1495.9410	0.588
3042.1694	2.57
3101.6287	2.01

Infrared Spectrum

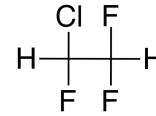


Radiative Efficiency



HCFC-133

Molecular Formula: CHClFCH₂F
 Name: 1-Chloro-1,2,2-trifluoroethane
 CAS number: 431-07-2
 Molecular Weight: 118.49



Global Atmospheric Lifetime (years): 3.07
 Tropospheric Atmospheric Lifetime (years): 3.21
 Stratospheric Atmospheric Lifetime (years): 67.8
 Ozone Depletion Potential (ODP): 0.017

	<i>Well-mixed</i>	<i>Lifetime adjusted</i>
Radiative Efficiency (RE):	0.195	0.173
Global Warming Potential (GWP _H):		
GWP ₂₀	1137	1008
GWP ₁₀₀	308	273
Global Temperature Potentials (GTP _H):		
GTP ₂₀		434
GTP ₅₀		51
GTP ₁₀₀		38

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

Atmospheric Loss Processes *****

OH Reactivity

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

$$k_{\text{SAR}}(298 \text{ K}) = 1.83 \times 10^{-14}; k_{\text{SAR}}(272 \text{ K}) \approx 1.17 \times 10^{-14} \quad \text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$\tau_{\text{Global}}^{\text{OH}} = 3.11 \text{ years}$$

$$\tau_{\text{Trop}}^{\text{OH}} = 3.21 \text{ years}$$

$$\tau_{\text{Strat}}^{\text{OH}} = 96.5 \text{ years}$$

Fractional Atmospheric Loss: 0.987

O(¹D) Reactivity

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

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

$$\tau_{\text{O}(\text{1D})} = 463 \text{ years}$$

Fractional Atmospheric Loss: 0.007

UV Photolysis

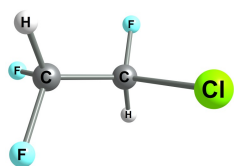
UV Spectrum: *No Recommendation*

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

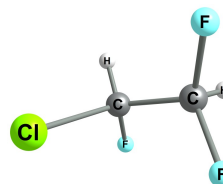
Fractional Atmospheric Loss: 0.006



Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.710



$\Delta E = 0.87 \text{ kcal mol}^{-1}$
Population = 0.165

Optimized Coordinates (Angstroms)

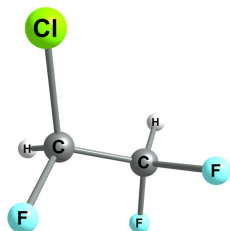
Atom	X	Y	Z
C	-0.939889382300	-0.240071163900	0.320943768600
C	0.257050229400	0.424868847400	-0.363105488000
H	0.147243439800	0.398812625600	-1.449802227900
F	0.343202430700	1.700555899600	0.067354579100
Cl	1.762360328500	-0.456885087700	0.049538527900
H	-0.831167171100	-0.249204832100	1.411686681900
F	-1.077338721300	-1.498252589400	-0.138507137600
F	-2.044310153600	0.462684300500	-0.016182704000

Atom	X	Y	Z
C	-1.101471266700	0.231510504500	-0.170587159200
C	0.366525906000	0.424952354300	-0.560056648500
H	0.492210915500	0.320739426700	-1.640272190100
F	0.748912483200	1.661731719100	-0.168985821400
Cl	1.405042623300	-0.809944758100	0.211131192100
H	-1.704249756200	1.049208289400	-0.589870026400
F	-1.238227841600	0.229393174700	1.166185039300
F	-1.541027063600	-0.944353710500	-0.662851385800

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
77.4324	0.193
180.7726	0.192
312.9368	0.275
376.9684	2.74
405.6339	2.36
472.5491	0.363
589.4160	1.18
811.5938	17.5
1091.0769	4.64
1127.8835	7.54
1144.1797	15.9
1163.5461	40.0
1256.8815	1.94
1334.4734	2.84
1390.0860	1.80
1431.4156	3.09
3070.2004	3.12
3105.9206	2.53

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
77.8617	0.159
190.6858	0.264
228.7732	0.346
359.3367	0.196
456.1312	0.614
568.5606	2.33
647.8518	13.0
785.1209	4.74
978.8730	1.85
1121.0585	9.79
1161.9957	35.1
1195.7440	14.1
1296.7988	3.17
1336.8552	2.13
1406.2208	5.84
1411.5740	3.17
3037.5523	5.26
3100.1601	2.34



$\Delta E = 1.03 \text{ kcal mol}^{-1}$
Population = 0.125

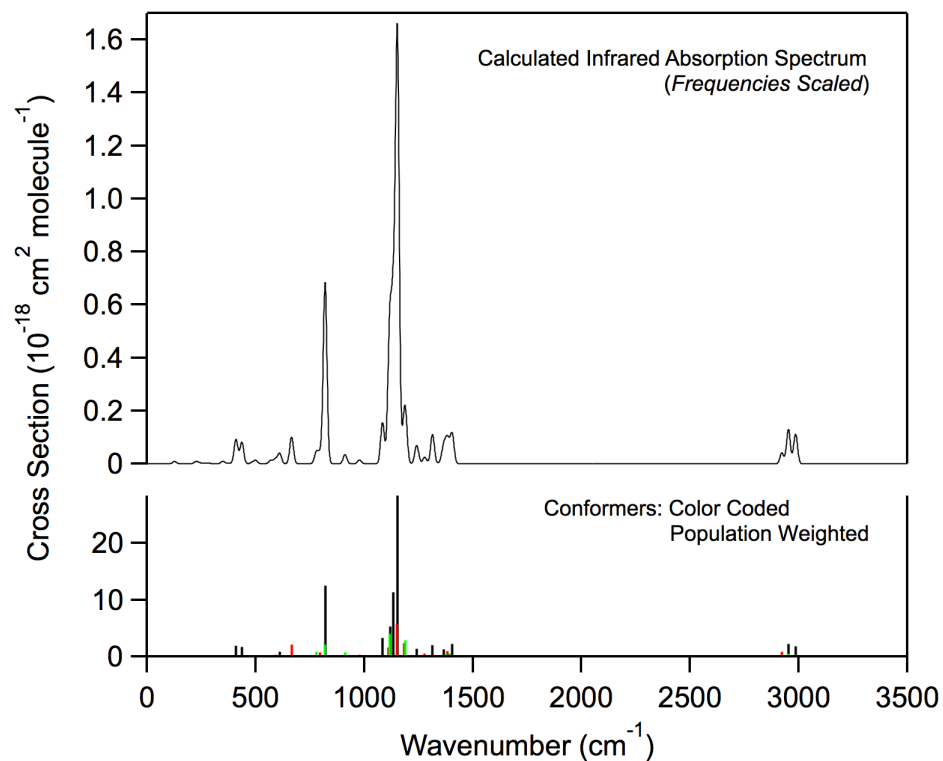
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-0.908776251800	-0.441340994400	-0.354333917400
C	0.256230603200	0.552372164500	-0.330787086600
H	0.288531846900	1.131747716100	-1.256414174000
F	0.117214976400	1.376454571500	0.724408461700
Cl	1.810131889400	-0.341242844100	-0.214201418500
H	-0.795731096400	-1.176693343800	-1.159298366900
F	-2.045336639000	0.267946890600	-0.550421659600
F	-0.998200328700	-1.072089160400	0.828807161400

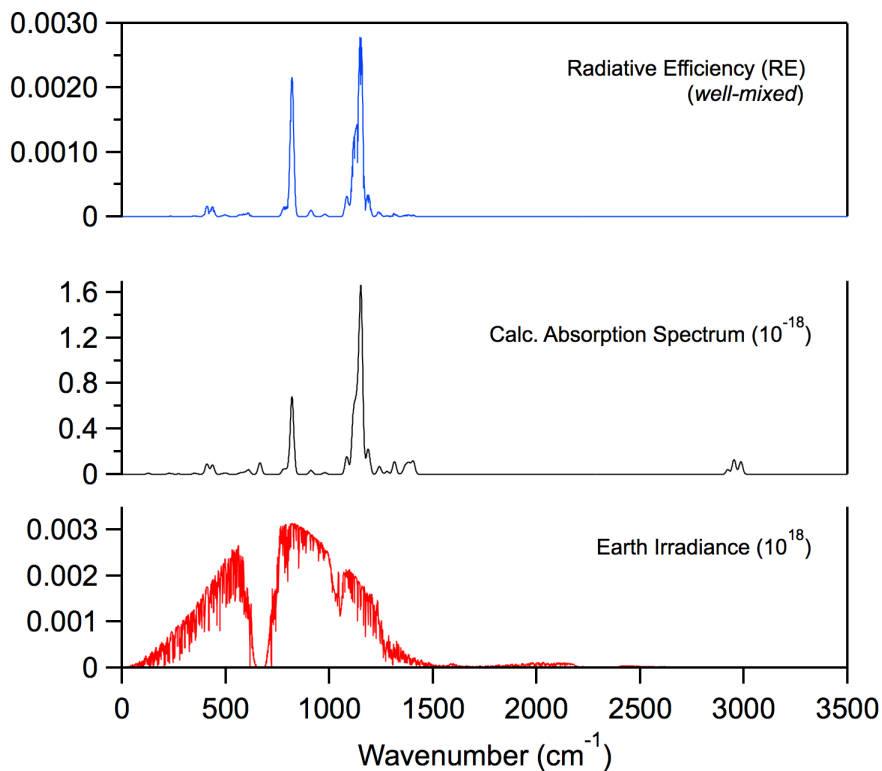
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
75.4615	0.119
197.1321	0.478
246.2558	0.272
334.3506	0.289
399.7188	0.534
546.1657	2.10
767.7814	6.99
808.9809	17.4
908.2208	5.87
1125.8449	32.1
1130.3737	3.16
1203.5489	22.9
1266.7938	1.40
1378.2013	1.69
1402.3806	3.56
1419.4894	4.10
3067.1489	4.38
3101.0286	2.27

Infrared Spectrum

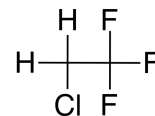


Radiative Efficiency



HCFC-133a

Molecular Formula: CH₂ClCF₃
 Name: 2-Chloro-1,1,1-trifluoroethane
 CAS number: 75-88-7
 Molecular Weight: 118.49



Global Atmospheric Lifetime (years): 9.82 4.45 #
 Tropospheric Atmospheric Lifetime (years): 10.6 4.65 #
 Stratospheric Atmospheric Lifetime (years): 126.5 103 #
 Ozone Depletion Potential (ODP): 0.026

	<i>Well-mixed</i>	<i>Lifetime adjusted</i>	
Radiative Efficiency (RE):	0.154	0.147	0.16 #
Global Warming Potential (GWP _H):			
GWP ₂₀	2502	2386	
GWP ₁₀₀	779	743	380 #
Global Temperature Potentials (GTP _H):			
GTP ₂₀		1782	
GTP ₅₀		280	
GTP ₁₀₀		107	

* RE units: W m² ppb⁻¹
 * GWP and GTP: Relative to CO₂
 # McGillen et al. (2015)

Atmospheric Loss Processes *****

OH Reactivity

$$k_{\text{Rec}}(T) = 9.4 \times 10^{-13} \exp(-1300/T); k_{\text{Rec}}(272 \text{ K}) = 7.9 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$k_{\text{SAR}}(298 \text{ K}) = 5.51 \times 10^{-15}; k_{\text{SAR}}(272 \text{ K}) \approx 3.52 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

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

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

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

Fractional Atmospheric Loss: 0.957

O(¹D) Reactivity

$$k_{\text{Rec}}(T) = 0.80 \times 1.2 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

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

$$\tau_{\text{O}(\text{1D})} = 463 \text{ years}$$

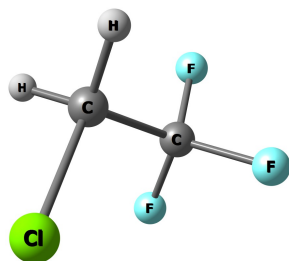
Fractional Atmospheric Loss: 0.021

UV Photolysis

UV Spectrum: *Recommendation Available*
 $\tau_{\text{hv}} = 450 \text{ years}$
 Fractional Atmospheric Loss: 0.022



Molecular Structure and Infrared Spectrum (1 conformer)



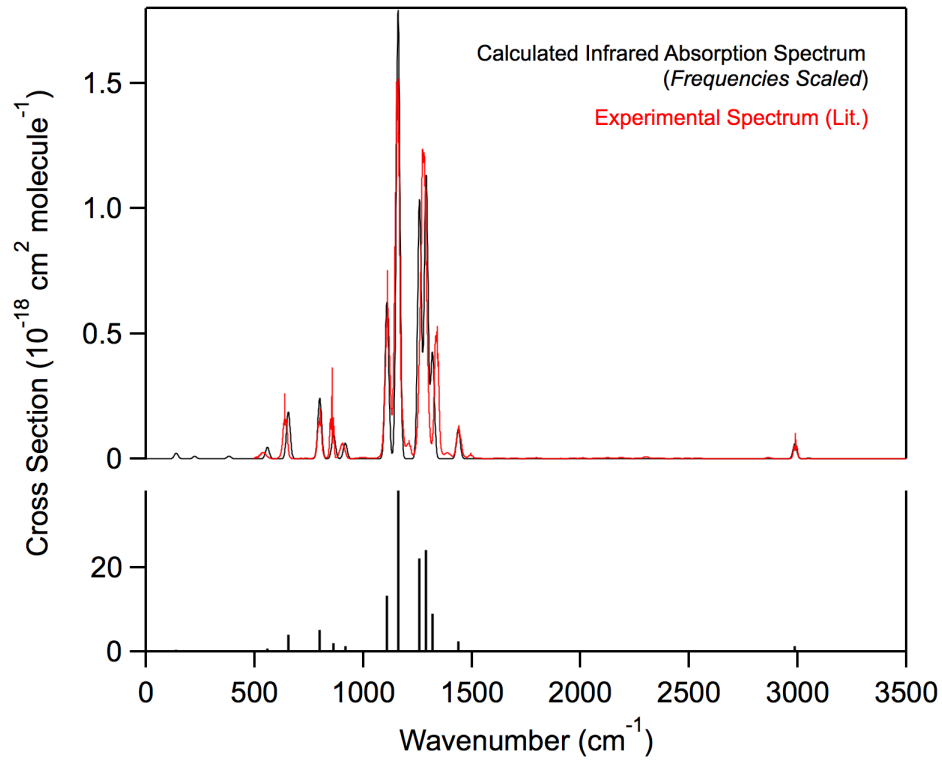
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	0.787239363274	0.004663257591	-0.000040150750
C	-0.446223163804	-0.887078548185	-0.001405574673
F	0.836798104046	0.788700337183	1.077612864857
F	1.877474706749	-0.780554609686	0.007685673178
F	0.845664530757	0.779745491085	-1.083710011713
Cl	-1.954407773824	0.071720356581	-0.011562900844
H	-0.429237318460	-1.514109462973	-0.892091631506
H	-0.436565448646	-1.506708821689	0.894553709055

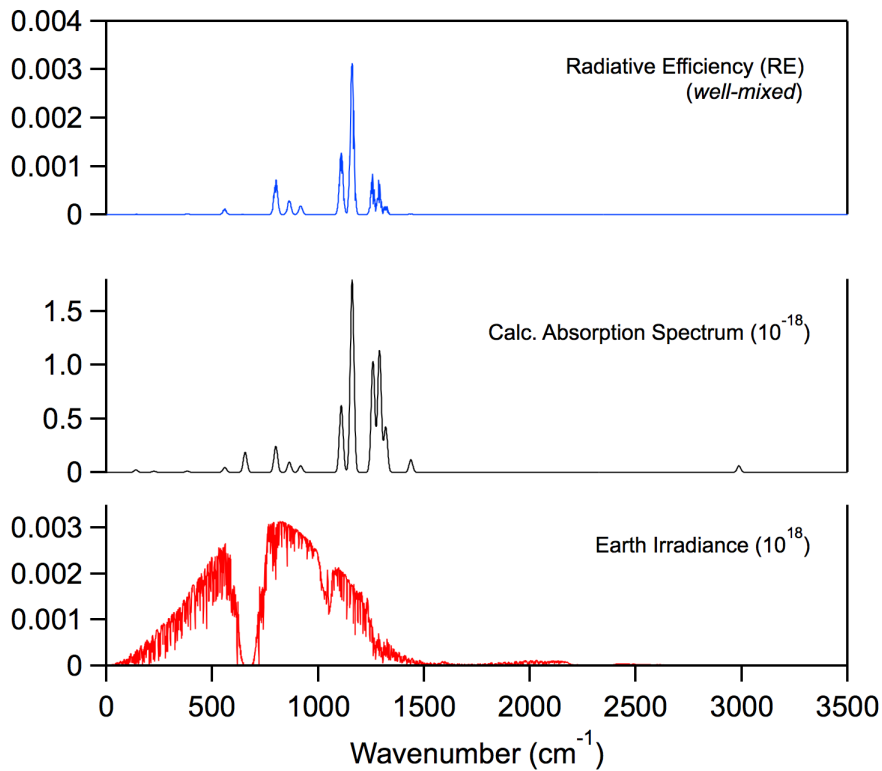
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
90.3567	0.474
180.4775	0.207
346.7595	0.188
351.3988	0.0411
532.7797	0.213
535.3757	0.763
636.9466	4.00
790.0443	5.16
857.5694	2.03
914.3240	1.33
1117.4174	13.3
1171.8497	38.2
1276.1437	22.0
1308.6176	24.1
1339.6245	9.01
1465.6051	2.52
3106.1847	1.28
3173.5333	0.0511

Infrared Spectrum

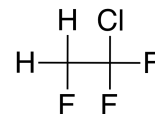


Radiative Efficiency



HCFC-133b

Molecular Formula: CH₂FCClF₂
Name: 1-Chloro-1,1,2-trifluoroethane
CAS number: 421-04-5
Molecular Weight: 118.49



Global Atmospheric Lifetime (years): 7.21
Tropospheric Atmospheric Lifetime (years): 7.71
Stratospheric Atmospheric Lifetime (years): 110.0
Ozone Depletion Potential (ODP): 0.024

	<i>Well-mixed</i>	<i>Lifetime adjusted</i>
Radiative Efficiency (RE):	0.218	0.206
Global Warming Potential (GWP _H):		
GWP ₂₀	2805	2640
GWP ₁₀₀	810	762
Global Temperature Potentials (GTP _H):		
GTP ₂₀		1736
GTP ₅₀		206
GTP ₁₀₀		108

* RE units: W m² ppb⁻¹

* GWP and GTP: Relative to CO₂

Atmospheric Loss Processes *****

OH Reactivity

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

$k_{\text{SAR}}(298 \text{ K}) = 7.60 \times 10^{-15}$; $k_{\text{SAR}}(272 \text{ K}) \approx 4.85 \times 10^{-15}$ cm³ molecule⁻¹ s⁻¹

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

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

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

Fractional Atmospheric Loss: 0.968

O(¹D) Reactivity

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

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

$\tau_{\text{O}(\text{1D})} = 463$ years

Fractional Atmospheric Loss: 0.016

UV Photolysis

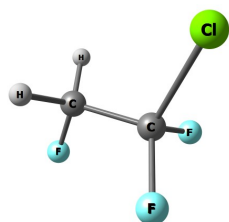
UV Spectrum: *No Recommendation*

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

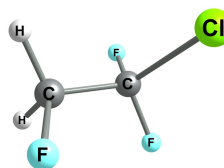
Fractional Atmospheric Loss: 0.016



Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.479



$\Delta E = 0.36 \text{ kcal mol}^{-1}$
Population = 0.260

Optimized Coordinates (Angstroms)

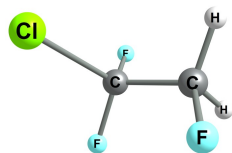
Atom	X	Y	Z
C	0.041536956800	-0.235455207800	0.001080482100
C	-0.967347929000	0.905606858600	0.054716246000
H	-0.820097293100	1.555522587700	-0.812852227200
F	-2.223298840700	0.364675794000	0.029898403200
H	-0.819467458400	1.471857031600	0.978961442100
Cl	1.713035387100	0.453493145400	0.032630338400
F	-0.105500817000	-0.953987971500	-1.112801104900
F	-0.104717005600	-1.054648238200	1.043290420200

Atom	X	Y	Z
C	0.116597469900	0.433763413400	-0.010186994000
C	-1.245611689700	0.127400684600	0.604081152600
H	-1.847367704900	1.042338272400	0.538778505600
F	-1.853126352400	-0.876385856800	-0.087853454300
H	-1.110090987600	-0.157342843300	1.651553977800
Cl	1.194496877400	-1.006224432400	0.010812623500
F	0.693601092700	1.415587601300	0.694965365400
F	-0.012587705500	0.844316160700	-1.273502176600

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
113.9311	0.743
193.6651	0.386
317.6176	0.184
332.8123	0.331
411.0742	0.00945
420.8601	0.895
567.3647	2.95
803.3340	10.9
953.1314	43.0
989.8715	7.93
1113.6800	8.06
1203.0952	11.7
1264.1852	24.2
1309.2273	10.5
1428.8059	1.28
1491.9528	0.376
3062.1226	1.71
3122.6618	1.89

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
103.5275	0.548
194.7403	0.306
314.7775	0.290
346.9790	0.125
421.6154	0.282
457.9432	0.555
608.6884	6.12
660.4792	10.4
936.0356	16.0
1098.6786	16.7
1144.8538	17.7
1186.3549	25.5
1239.3964	9.88
1288.9960	12.2
1430.4112	0.592
1495.5423	0.508
3042.0480	2.92
3109.4603	2.27



$\Delta E = 0.36 \text{ kcal mol}^{-1}$
Population = 0.260

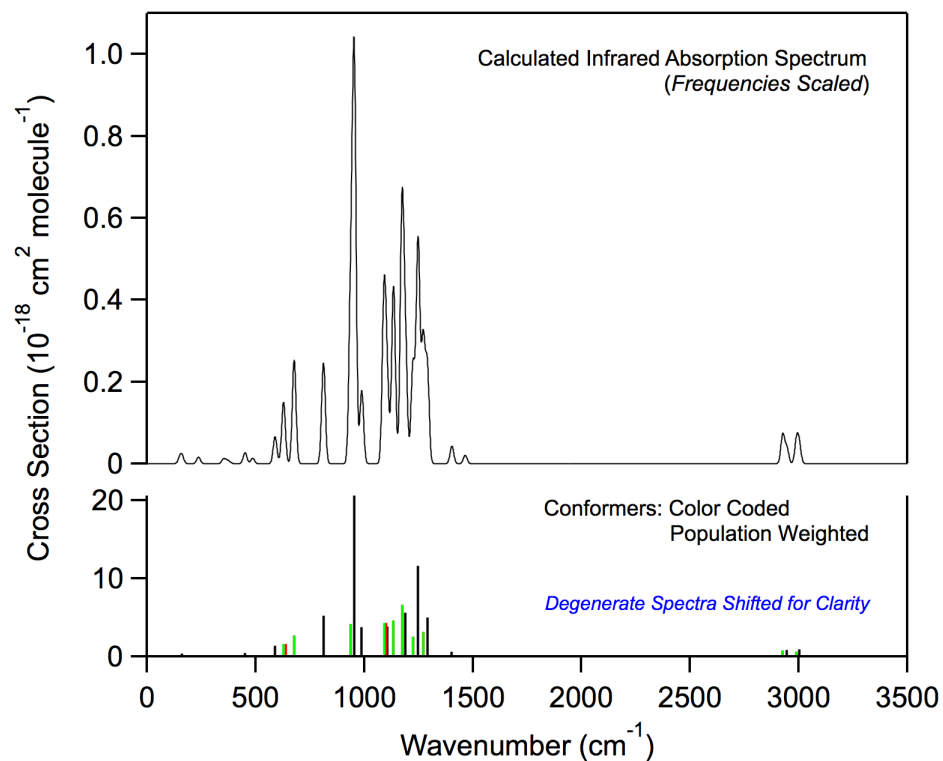
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	0.130765191800	0.439269326900	0.014933350200
C	-1.261111851800	0.192728013000	-0.558387698500
H	-1.171075090700	-0.070384429000	-1.616360555000
F	-1.877858976900	-0.807458184200	0.130596532200
H	-1.829344106500	1.124918215300	-0.450595991400
Cl	1.158574065200	-1.034115613200	-0.077532365000
F	0.058558491900	0.822576668900	1.291284347500
F	0.715871277000	1.418849002400	-0.686674619900

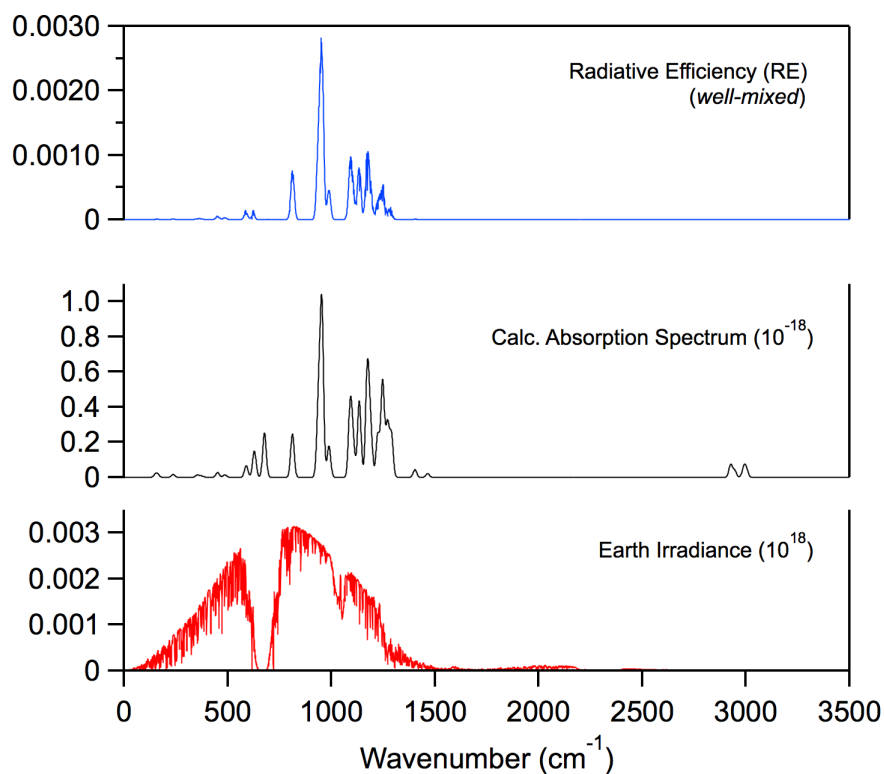
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength ($10^{-18} \text{ cm}^2 \text{ molecule}^{-1} \text{ cm}^{-1}$)
103.5344	0.548
194.7426	0.306
314.7838	0.290
346.9795	0.125
421.6253	0.282
457.9419	0.555
608.6896	6.11
660.4898	10.4
936.0433	16.0
1098.6805	16.7
1144.8376	17.7
1186.3266	25.4
1239.3890	9.88
1288.9861	12.2
1430.4044	0.592
1495.5434	0.508
3042.0518	2.92
3109.4699	2.27

Infrared Spectrum

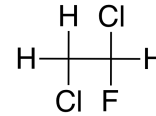


Radiative Efficiency



HCFC-141

Molecular Formula: CH₂ClCHClF
 Name: 1,2-Dichloro-1-fluoroethane
 CAS number: 430-57-9
 Molecular Weight: 116.95



Global Atmospheric Lifetime (years): 1.14
 Tropospheric Atmospheric Lifetime (years): 1.19
 Stratospheric Atmospheric Lifetime (years): 29.5
 Ozone Depletion Potential (ODP): 0.022

	<i>Well-mixed</i>	<i>Lifetime adjusted</i>
Radiative Efficiency (RE):	0.101	0.077
Global Warming Potential (GWP _H):		
GWP ₂₀	222	170
GWP ₁₀₀	60	46
Global Temperature Potentials (GTP _H):		
GTP ₂₀		56
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*

$k_{\text{SAR}}(298 \text{ K}) = 4.94 \times 10^{-14}$; $k_{\text{SAR}}(272 \text{ K}) \approx 3.15 \times 10^{-14}$ cm³ molecule⁻¹ s⁻¹

$\tau_{\text{Global}}^{\text{OH}} = 1.15$ years

$\tau_{\text{Trop}}^{\text{OH}} = 1.19$ years

$\tau_{\text{Strat}}^{\text{OH}} = 39.4$ years

Fractional Atmospheric Loss: 0.990

O(¹D) Reactivity

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

$k_{\text{Est}}(T) = 1.5 \times 10^{-10}$ cm³ molecule⁻¹ s⁻¹

$\tau_{\text{O}(\text{1D})} = 247$ years

Fractional Atmospheric Loss: 0.005

UV Photolysis

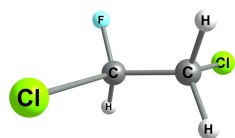
UV Spectrum: *No Recommendation*

$\tau_{\text{hv}} = 225$ years

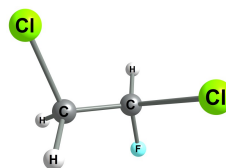
Fractional Atmospheric Loss: 0.005



Molecular Structure and Infrared Spectrum (2 conformers)



E = 0
Population = 0.905



$\Delta E = 1.51 \text{ kcal mol}^{-1}$
Population = 0.070

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	0.448242677000	0.264189477600	0.329745506500
C	-0.555838015100	-0.673268872000	-0.311284952900
H	-0.441753093300	-0.662755577900	-1.394942376200
H	-0.434417645000	-1.684345288700	0.073057069500
Cl	-2.231288012000	-0.134675586300	0.075007656800
H	0.342429270100	0.323372802400	1.414333750600
F	0.359316469200	1.499621117900	-0.200730951600
Cl	2.109477349000	-0.392115073100	0.014647297300

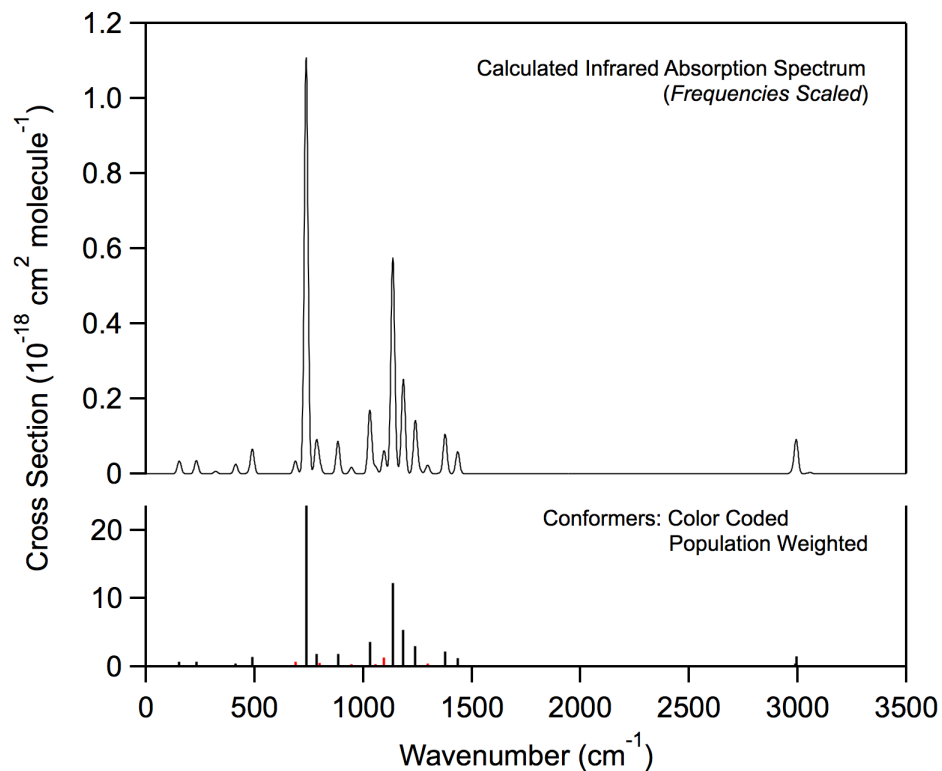
Atom	X	Y	Z
C	0.639886516900	-0.480131611000	-0.372716141100
C	-0.643661743900	-0.855172234500	0.352417970800
H	-0.883470225500	-1.891524542700	0.108427574800
H	-0.524129698500	-0.743197987300	1.429596587400
Cl	-2.023528457200	0.158913364100	-0.173925655200
H	0.503524047200	-0.407660947600	-1.453211467200
F	1.565485814400	-1.432438593700	-0.092594732700
Cl	1.272320746600	1.116372552900	0.165975863100

Infrared Absorption Spectrum (unscaled frequencies)

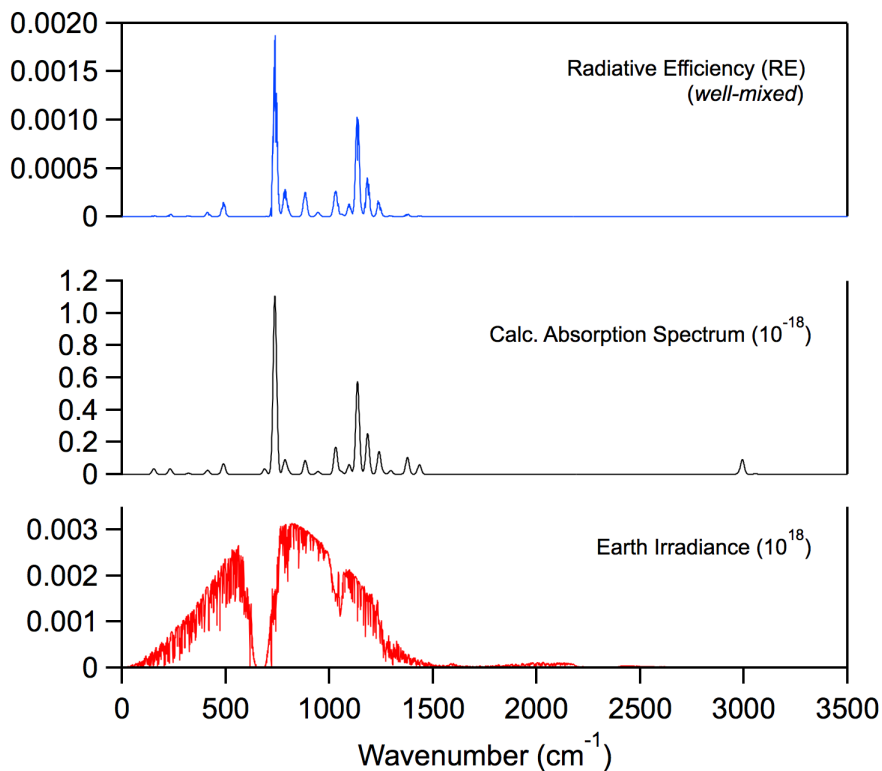
Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
105.7049	0.776
188.5383	0.770
282.7118	0.145
380.6329	0.459
461.5069	1.54
723.8450	26.1
774.2723	2.01
878.7175	2.03
1034.3185	3.98
1146.2223	13.6
1197.5453	5.93
1256.0682	3.32
1310.7272	0.105
1401.0959	2.48
1461.9893	1.33
3106.9656	0.511
3113.9089	1.64
3180.0556	0.0703

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
98.5304	0.510
190.3707	0.701
347.1943	0.0894
378.8996	1.73
444.5040	0.737
671.5555	10.2
789.4108	7.12
944.3518	5.15
1062.0477	5.45
1103.3696	18.6
1167.8953	2.10
1276.3860	3.22
1316.8207	5.92
1375.8655	0.457
1469.3556	1.09
3090.8524	1.31
3109.3743	1.41
3162.7270	0.217

Infrared Spectrum

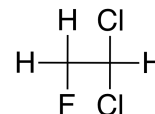


Radiative Efficiency



HCFC-141a

Molecular Formula: CH₂FCHCl₂
Name: 1,1-Dichloro-2-fluoroethane
CAS number: 430-53-5
Molecular Weight: 116.95



Global Atmospheric Lifetime (years): 0.494
Tropospheric Atmospheric Lifetime (years): 0.51
Stratospheric Atmospheric Lifetime (years): 20
Ozone Depletion Potential (ODP): 0.011

	<i>Well-mixed</i>	<i>Lifetime adjusted</i>
Radiative Efficiency (RE):	0.099	0.059
Global Warming Potential (GWP _H):		
GWP ₂₀	94	56
GWP ₁₀₀	25	15
Global Temperature Potentials (GTP _H):		
GTP ₂₀		17
GTP ₅₀		3
GTP ₁₀₀		2

* RE units: W m² ppb⁻¹

* GWP and GTP: Relative to CO₂

Atmospheric Loss Processes *****

OH Reactivity

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

$k_{\text{SAR}}(298 \text{ K}) = 1.15 \times 10^{-13}$; $k_{\text{SAR}}(272 \text{ K}) \approx 0.734 \times 10^{-13}$ cm³ molecule⁻¹ s⁻¹

$\tau_{\text{Global}}^{\text{OH}} = 0.498$ years

$\tau_{\text{Trop}}^{\text{OH}} = 0.51$ years

$\tau_{\text{Strat}}^{\text{OH}} = 20$ years

Fractional Atmospheric Loss: 0.992

O(¹D) Reactivity

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

$k_{\text{Est}}(\text{T}) = 1.5 \times 10^{-10}$ cm³ molecule⁻¹ s⁻¹

$\tau_{\text{O}(\text{1D})} = 247$ years

Fractional Atmospheric Loss: 0.002

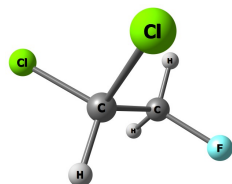
UV Photolysis

UV Spectrum: *No Recommendation*

$\tau_{\text{hv}} = 80$ years

Fractional Atmospheric Loss: 0.006

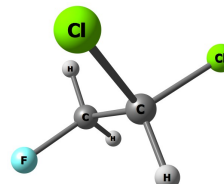
Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.460

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-0.095286774700	0.096848790800	-0.400521304300
C	0.816180037700	1.119027900500	0.265551319200
H	0.513268072700	2.122665805800	-0.054709879500
H	0.735799518200	1.039693094500	1.354333366000
F	2.109015024100	0.889401675400	-0.123698688100
H	-0.012832605300	0.129115286400	-1.484751147800
Cl	-1.795363591700	0.489699893500	0.015893758200
Cl	0.337024318900	-1.567038446800	0.095796576300



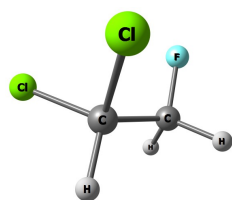
E = 0
Population = 0.460

Atom	X	Y	Z
C	-0.092791370800	0.097344318300	0.397152911200
C	0.824096955800	1.110080507200	-0.275874008400
H	0.744994643100	1.022177726600	-1.364093214700
H	0.525063614100	2.117607578000	0.035695720800
F	2.115335284900	0.878058512800	0.117222927000
H	-0.011811564700	0.138117748500	1.481207247500
Cl	0.332992347300	-1.572397543500	-0.084912412900
Cl	-1.790533909700	0.494161152200	-0.025033170500

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
127.2108	0.797
203.6759	0.732
260.6783	0.194
375.6595	0.223
414.7744	1.96
666.6801	8.73
774.8125	17.1
1003.2965	2.92
1079.8356	3.28
1113.6628	11.9
1222.9731	2.04
1247.6936	0.351
1310.3583	3.13
1421.2701	1.27
1498.5525	0.373
3043.2950	2.58
3102.2308	1.91
3148.2182	0.601

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
127.2028	0.797
203.6752	0.732
260.6788	0.194
375.6597	0.223
414.7722	1.96
666.6916	8.73
774.7980	17.1
1003.2951	2.92
1079.8349	3.27
1113.6689	11.9
1222.9670	2.04
1247.6929	0.351
1310.3565	3.13
1421.2698	1.27
1498.5539	0.373
3043.3022	2.58
3102.2269	1.91
3148.2200	0.601



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

$$\text{Population} = 0.081$$

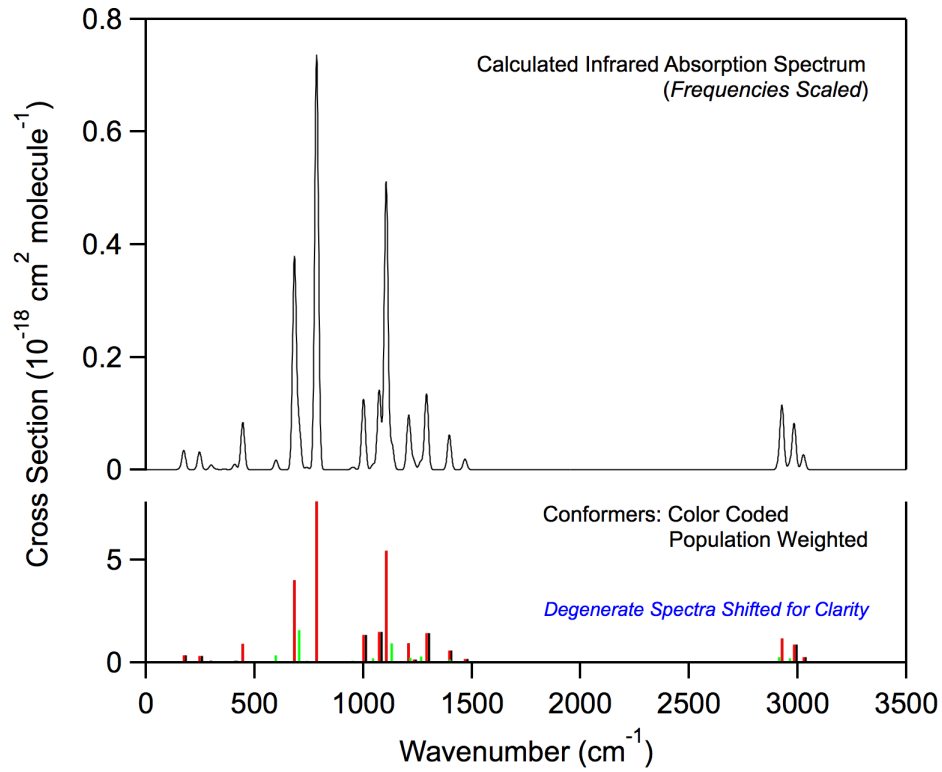
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-0.014996826700	-0.137758386500	0.629246476200
C	0.099673680600	1.378012537900	0.593219280000
H	-0.771278693400	1.807778514700	1.103139123900
H	1.016220175800	1.672924558700	1.118806828400
F	0.145473742400	1.836008076300	-0.690594542100
H	-0.050666661400	-0.490960299000	1.658481106900
Cl	1.415529365000	-0.904157923900	-0.134273911200
Cl	-1.530750782300	-0.681884078200	-0.160120362000

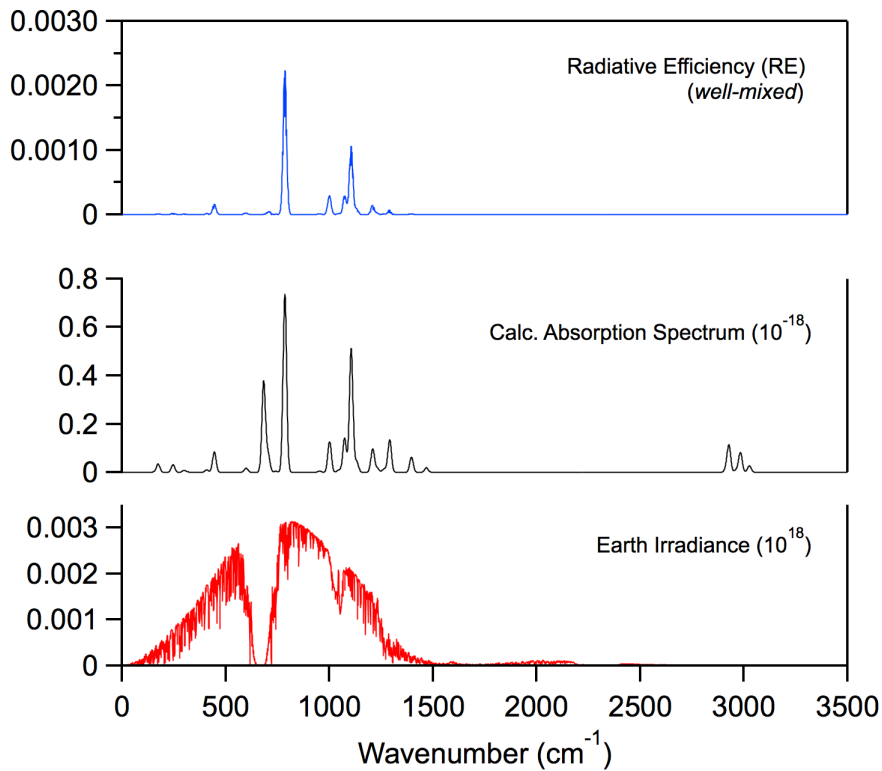
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
104.9562	0.264
196.0267	0.0427
283.1262	0.278
324.6537	0.302
576.6687	4.56
689.5648	19.5
726.9209	1.11
951.7803	1.24
1050.1027	2.49
1142.0639	11.6
1230.2617	3.08
1278.4034	0.310
1282.9713	3.56
1423.5072	1.88
1495.2607	0.784
3028.4859	3.39
3081.0511	2.76
3134.5768	0.597

Infrared Spectrum

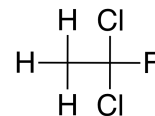


Radiative Efficiency



HCFC-141b

Molecular Formula: CH₃CCl₂F
 Name: 1,1-Dichloro-1-fluoroethane
 CAS number: 1717-00-6
 Molecular Weight: 116.95



Global Atmospheric Lifetime (years): 8.33 9.4 #
 Tropospheric Atmospheric Lifetime (years): 10.0 10.7 #
 Stratospheric Atmospheric Lifetime (years): 49.3 72.3 #
 Ozone Depletion Potential (ODP): 0.122

	<i>Well-mixed</i>	<i>Lifetime adjusted</i>	
Radiative Efficiency (RE):	0.164	0.156	0.16 #
Global Warming Potential (GWP _H):			
GWP ₂₀	2395	2269	2550 #
GWP ₁₀₀	713	676	782 #
Global Temperature Potentials (GTP _H):			
GTP ₂₀		1589	1850 #
GTP ₅₀		211	271 #
GTP ₁₀₀		96	111 #

* RE units: W m² ppb⁻¹

* GWP and GTP: Relative to CO₂

Value taken from WMO (2014)

Atmospheric Loss Processes *****

OH Reactivity

$$k_{\text{Rec}}(T) = 1.25 \times 10^{-12} \exp(-1600/T); k_{\text{Rec}}(272 \text{ K}) = 3.48 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$k_{\text{SAR}}(298 \text{ K}) = 5.85 \times 10^{-15}; k_{\text{SAR}}(272 \text{ K}) \approx 3.73 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$\tau_{\text{Global}}^{\text{OH}} = 9.67 \text{ years}$$

$$\tau_{\text{Trop}}^{\text{OH}} = 10.0 \text{ years}$$

$$\tau_{\text{Strat}}^{\text{OH}} = 269.2 \text{ years}$$

Fractional Atmospheric Loss: 0.862

O(¹D) Reactivity

$$k_{\text{Rec}}(T) = 0.69 \times 2.60 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$k_{\text{Est}}(T) = 1.5 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$\tau_{\text{O}(\text{1D})} = 247 \text{ years}$$

Fractional Atmospheric Loss: 0.034

UV Photolysis

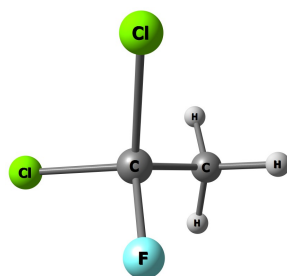
UV Spectrum: *Recommendation Available*

$$\tau_{\text{hv}} = 80 \text{ years}$$

Fractional Atmospheric Loss: 0.104



Molecular Structure and Infrared Spectrum (1 conformer)



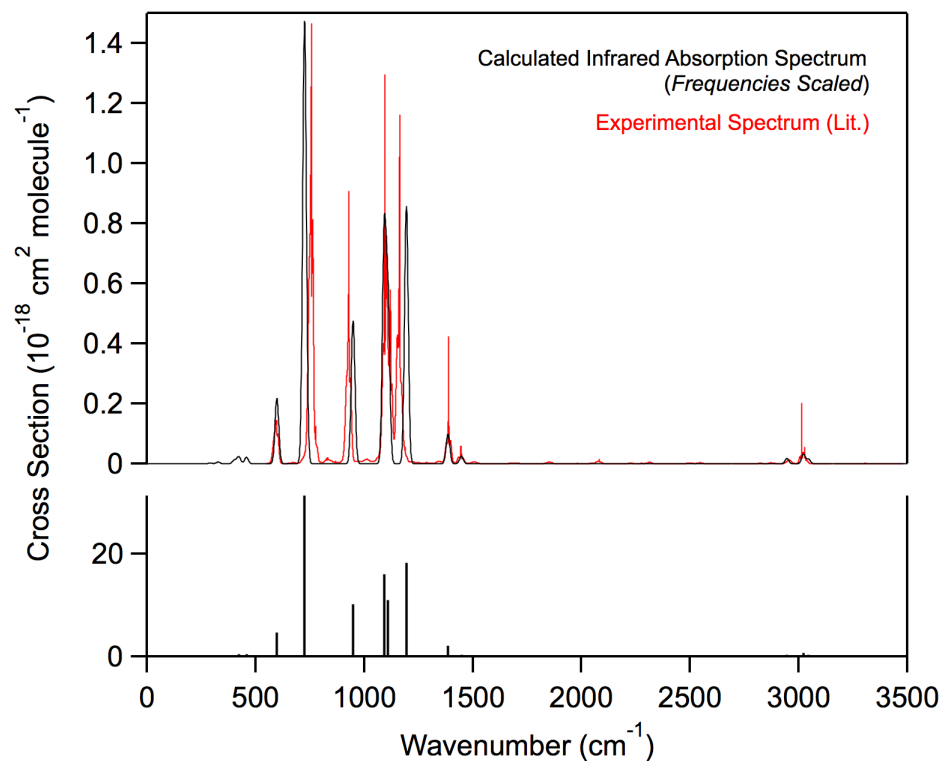
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	0.000257379673	1.513057735147	0.850747674752
C	0.000187623550	0.336096135094	-0.100643221973
H	-0.892595660299	2.115097899080	0.666181379534
H	0.000462066201	1.166522014703	1.883818535592
H	0.892949633304	2.115241984052	0.665874851846
F	-0.000064965480	0.756354248224	-1.373579919925
Cl	1.469923468089	-0.685338116166	0.136281258082
Cl	-1.469302545038	-0.685573900135	0.136786442094

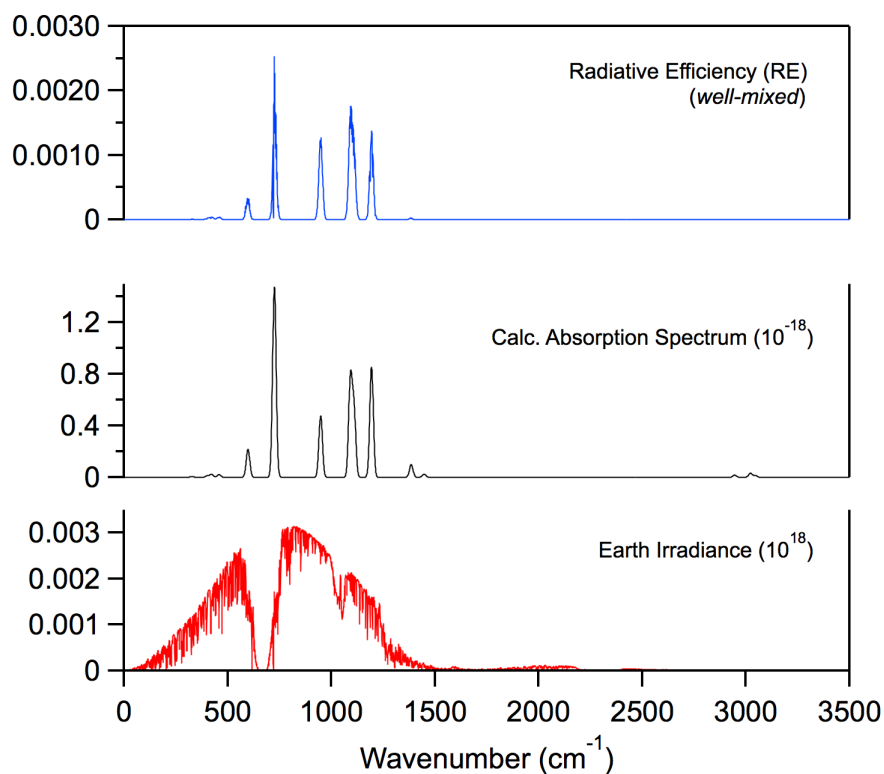
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
251.0517	0.0411
259.8453	0.00400
289.5528	0.115
368.4740	0.260
390.3623	0.507
427.9039	0.454
576.2923	4.64
711.1273	31.4
947.6138	10.1
1099.4229	16.1
1117.8861	11.1
1207.5254	18.2
1410.0493	2.10
1475.1579	0.148
1476.1756	0.391
3062.3062	0.363
3143.0555	0.691
3167.7017	0.326

Infrared Spectrum

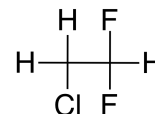


Radiative Efficiency



HCFC-142

Molecular Formula: CH₂ClCHF₂
 Name: 2-Chloro-1,1-difluoroethane
 CAS number: 338-65-8
 Molecular Weight: 100.49



Global Atmospheric Lifetime (years): 2.61
 Tropospheric Atmospheric Lifetime (years): 2.73
 Stratospheric Atmospheric Lifetime (years): 60.1
 Ozone Depletion Potential (ODP): 0.019

	<i>Well-mixed</i>	<i>Lifetime adjusted</i>
Radiative Efficiency (RE):	0.126	0.110
Global Warming Potential (GWP _H):		
GWP ₂₀	738	643
GWP ₁₀₀	200	174
Global Temperature Potentials (GTP _H):		
GTP ₂₀		259
GTP ₅₀		32
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*

$k_{\text{SAR}}(298 \text{ K}) = 2.15 \times 10^{-14}$; $k_{\text{SAR}}(272 \text{ K}) \approx 1.37 \times 10^{-14}$ cm³ molecule⁻¹ s⁻¹

$\tau_{\text{Global}}^{\text{OH}} = 2.64$ years

$\tau_{\text{Trop}}^{\text{OH}} = 2.73$ years

$\tau_{\text{Strat}}^{\text{OH}} = 83.4$ years

Fractional Atmospheric Loss: 0.988

O(¹D) Reactivity

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

$k_{\text{Est}}(T) = 0.9 \times 10^{-10}$ cm³ molecule⁻¹ s⁻¹

$\tau_{\text{O}(\text{¹D})} = 411$ years

Fractional Atmospheric Loss: 0.006

UV Photolysis

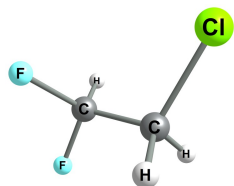
UV Spectrum: *No Recommendation*

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

Fractional Atmospheric Loss: 0.006



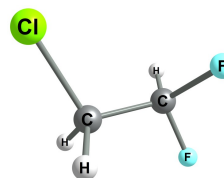
Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.441

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	0.895406330000	0.035319879800	0.334387909700
C	-0.256892103700	-0.764299916500	-0.250819719300
H	-0.156622755400	-0.807828727300	-1.335756355900
H	-0.261181443400	-1.770375660200	0.167627444700
Cl	-1.829991307000	0.005941076100	0.139240961200
F	0.987331545900	1.239679349500	-0.267813277300
F	2.040910109100	-0.650154984700	0.081034945900
H	0.802667624600	0.186836983300	1.416337091200



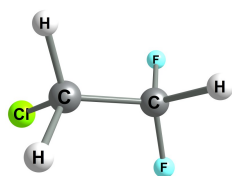
E = 0
Population = 0.441

Atom	X	Y	Z
C	0.883940716800	0.032878616500	-0.323897778000
C	-0.267936979500	-0.718086707700	0.323327866200
H	-0.290911075200	-1.745865086300	-0.037859513700
H	-0.150334474700	-0.702142363900	1.407281608000
Cl	-1.838064421200	0.048957611500	-0.084476600000
F	2.025285425200	-0.651825478200	-0.050510378200
F	0.999932703600	1.267779333000	0.208218864800
H	0.775258105100	0.124813075000	-1.411055069100

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
103.2545	0.749
203.6280	0.688
371.1185	0.191
456.1758	2.38
565.8545	0.717
786.8285	7.05
875.7647	1.12
1045.9590	2.82
1111.7709	25.8
1148.2456	14.9
1222.1643	5.05
1280.7392	1.23
1396.9749	1.88
1424.4242	5.71
1467.6146	2.14
3062.3125	5.21
3098.2475	1.63
3167.3351	0.358

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
103.2334	0.749
203.6180	0.688
371.1220	0.191
456.1702	2.38
565.8576	0.717
786.8719	7.05
875.7580	1.12
1045.9630	2.82
1111.7879	25.8
1148.2453	14.9
1222.1782	5.05
1280.7594	1.23
1396.9823	1.88
1424.4258	5.71
1467.6179	2.13
3062.2986	5.21
3098.2236	1.63
3167.3014	0.359



$\Delta E = 0.78 \text{ kcal mol}^{-1}$
 Population = 0.118

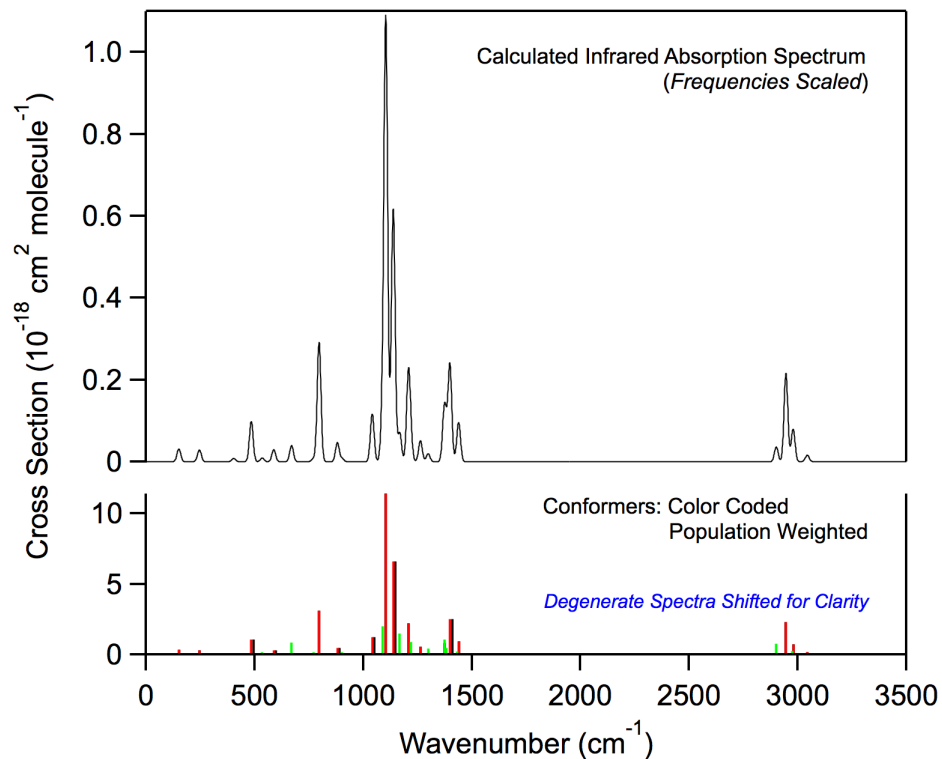
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.051821708400	-0.014790012100	-0.364367127400
C	-0.341677683900	-0.098259190800	-0.961540037100
H	-0.495346655700	0.733556999200	-1.649861733700
H	-0.456373882800	-1.043858614500	-1.492576912800
Cl	-1.614634726700	-0.014704573500	0.298338402000
F	1.265432078200	-1.033240740700	0.497410016400
F	1.217499056000	1.147418132200	0.304414256600
H	1.808310106600	-0.068768999700	-1.161811864200

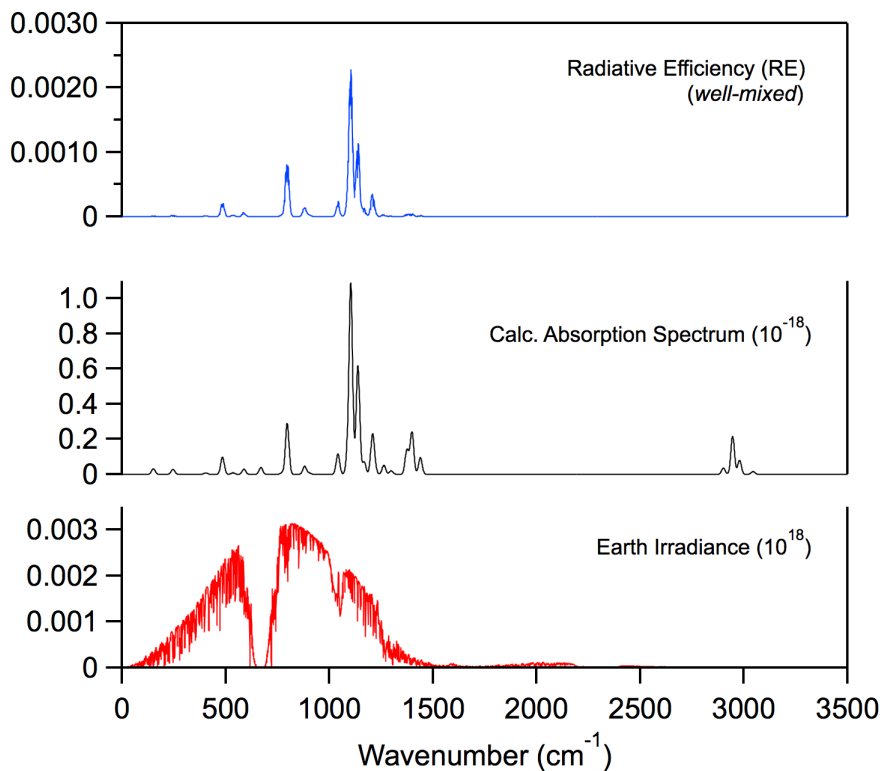
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
101.0268	0.0694
190.2128	0.158
362.4959	0.0599
509.7115	1.57
652.6125	7.10
760.0245	1.46
898.9297	1.40
942.8625	0.0570
1095.7796	17.0
1179.6680	12.8
1233.1620	7.77
1318.2632	3.57
1398.8225	9.23
1407.9616	4.05
1460.4738	1.74
3015.2438	6.54
3093.8510	2.39
3156.6903	0.338

Infrared Spectrum

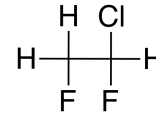


Radiative Efficiency



HCFC-142a

Molecular Formula: CH₂FCHClF
 Name: 1-Chloro-1,2-difluoroethane
 CAS number: 338-64-7
 Molecular Weight: 100.49



Global Atmospheric Lifetime (years): 1.58
 Tropospheric Atmospheric Lifetime (years): 1.64
 Stratospheric Atmospheric Lifetime (years): 42.3
 Ozone Depletion Potential (ODP): 0.015

	<i>Well-mixed</i>	<i>Lifetime adjusted</i>
Radiative Efficiency (RE):	0.139	0.113
Global Warming Potential (GWP _H):		
GWP ₂₀	491	399
GWP ₁₀₀	133	108
Global Temperature Potentials (GTP _H):		
GTP ₂₀		139
GTP ₅₀		19
GTP ₁₀₀		15

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

Atmospheric Loss Processes *****

OH Reactivity

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

$$k_{\text{SAR}}(298 \text{ K}) = 3.57 \times 10^{-14}; k_{\text{SAR}}(272 \text{ K}) \approx 2.28 \times 10^{-14} \quad \text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$\tau_{\text{Global}}^{\text{OH}} = 1.59 \text{ years}$$

$$\tau_{\text{Trop}}^{\text{OH}} = 1.64 \text{ years}$$

$$\tau_{\text{Strat}}^{\text{OH}} = 52.7 \text{ years}$$

Fractional Atmospheric Loss: 0.993

O(¹D) Reactivity

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

$$k_{\text{Est}}(T) = 0.9 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$\tau_{\text{O}(\text{1D})} = 411 \text{ years}$$

Fractional Atmospheric Loss: 0.004

UV Photolysis

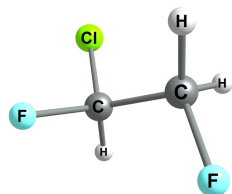
UV Spectrum: *No Recommendation*

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

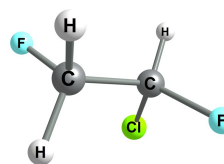
Fractional Atmospheric Loss: 0.003



Molecular Structure and Infrared Spectrum (3 conformers)



$E = 0$
Population = 0.714



$\Delta E = 0.72 \text{ kcal mol}^{-1}$
Population = 0.212

Optimized Coordinates (Angstroms)

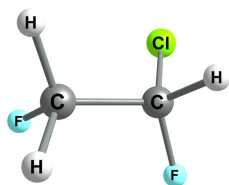
Atom	X	Y	Z
C	-0.030548679500	0.255281619200	0.351944394100
C	0.981053139300	-0.714828443100	-0.230737913900
H	0.807772034200	-1.719924509300	0.166221618000
H	0.888864646600	-0.725670502600	-1.322132874000
F	2.237196087500	-0.286551637000	0.122548327500
Cl	-1.692766603800	-0.358788984000	-0.000133761200
F	0.124604100700	1.476904530400	-0.201495801500
H	0.050255275100	0.339430926500	1.438039011000

Atom	X	Y	Z
C	-0.131861625200	-0.495471171900	-0.369993325700
C	1.237231094600	-0.389750435500	0.284417043600
H	1.124913407300	-0.345498026800	1.372897975400
H	1.815956009400	-1.281595606500	0.011474560500
F	1.880443240600	0.728788517600	-0.168375730700
Cl	-1.181995557200	0.885535712000	0.111634809700
F	-0.705464763200	-1.657207053000	0.025414538000
H	-0.073280806400	-0.462978935800	-1.460179870700

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
123.5595	0.979
216.7426	0.970
329.9041	0.223
402.1081	0.584
470.6342	2.06
787.1789	18.5
917.3277	5.12
1090.6990	14.3
1119.3396	1.17
1149.2204	20.1
1247.0197	1.57
1282.1304	1.47
1389.6575	2.00
1432.1417	1.72
1495.4527	0.367
3050.8965	2.05
3097.0531	0.931
3115.5327	4.08

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
114.4504	0.796
212.7543	0.869
359.5555	0.390
415.3201	2.82
496.2461	0.0373
676.0554	13.0
1010.0994	3.57
1096.9786	3.56
1127.9737	0.386
1133.8465	32.0
1245.5308	0.159
1318.3964	7.09
1339.7429	1.42
1435.8439	0.491
1503.3329	0.450
3031.6454	4.06
3088.6231	0.415
3107.3366	4.80



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

$$\text{Population} = 0.074$$

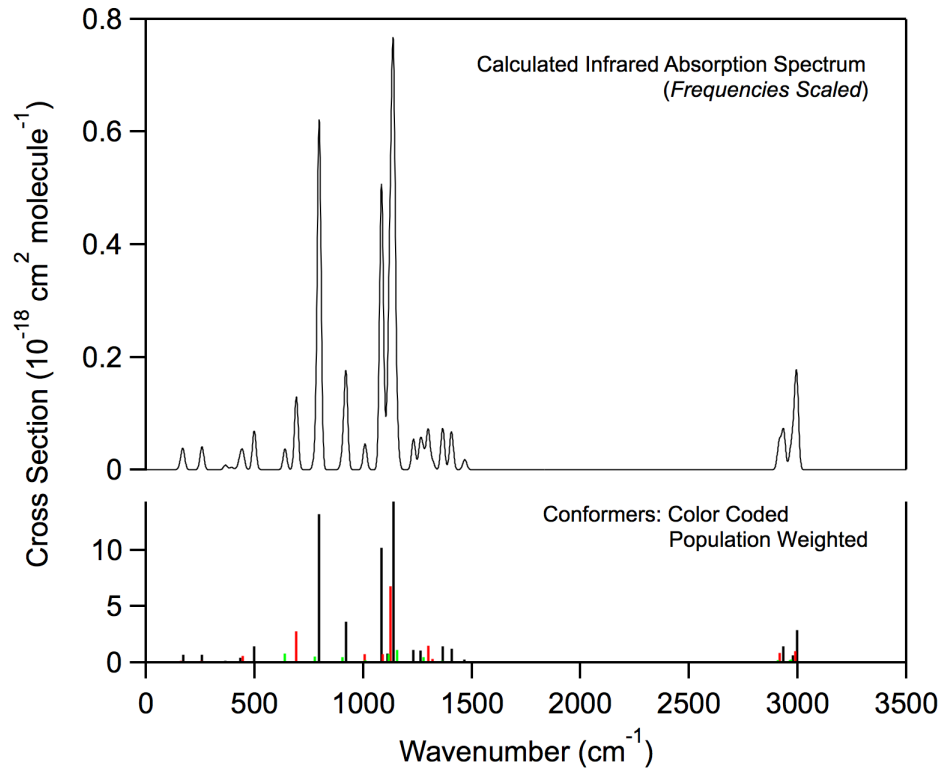
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-0.079629692200	0.532400515500	0.482028295700
C	1.204969302500	-0.264662736100	0.613855495500
H	1.996438353800	0.422456267100	0.942523784200
H	1.072278924200	-1.053955399900	1.362036363100
F	1.556829734300	-0.812585390400	-0.586325649200
Cl	-1.427363857300	-0.508262319200	-0.112727440000
F	0.094858882100	1.558676528400	-0.381935856300
H	-0.399323647400	0.921796534600	1.452815006900

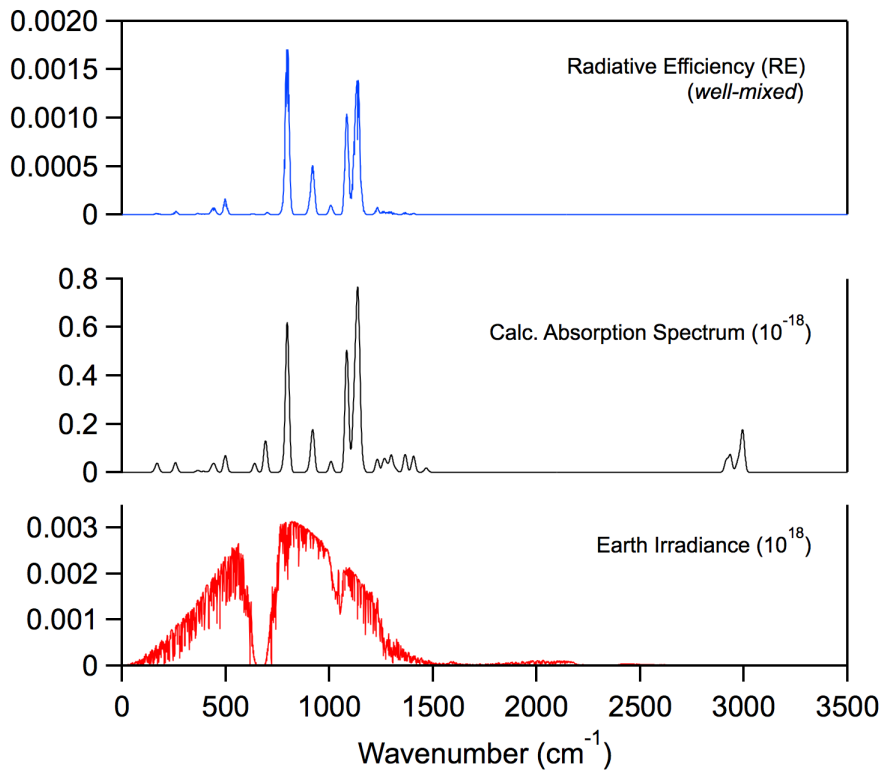
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength ($10^{-18} \text{ cm}^2 \text{ molecule}^{-1} \text{ cm}^{-1}$)
107.3344	0.302
210.3441	0.127
337.7985	0.248
380.8723	0.374
620.5992	10.7
766.8059	7.16
900.7699	6.65
1012.4327	2.99
1125.7978	9.92
1167.6685	15.3
1272.0942	1.26
1297.0370	6.54
1385.6838	2.10
1428.1459	1.57
1494.1304	0.711
3024.5756	3.30
3081.9945	3.05
3086.9361	3.85

Infrared Spectrum

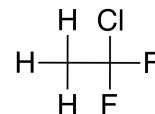


Radiative Efficiency



HCFC-142b

Molecular Formula: CH₃CClF₂
 Name: 1-Chloro-1,1-difluoroethane
 CAS number: 75-68-3
 Molecular Weight: 100.49



Global Atmospheric Lifetime (years): 16.6 18 #
 Tropospheric Atmospheric Lifetime (years): 18.7 19.3 #
 Stratospheric Atmospheric Lifetime (years): 147.6 212 #
 Ozone Depletion Potential (ODP): 0.041

	<i>Well-mixed</i>	<i>Lifetime adjusted</i>	
Radiative Efficiency (RE):	0.197	0.191	0.19 #
Global Warming Potential (GWP _H):			
GWP ₂₀	5131	4969	5020 #
GWP ₁₀₀	1978	1916	1980 #
Global Temperature Potentials (GTP _H):			
GTP ₂₀		4319	4390 #
GTP ₅₀		1291	1370 #
GTP ₁₀₀		336	356 #

* RE units: W m² ppb⁻¹

* GWP and GTP: Relative to CO₂

Value taken from WMO (2014)

Atmospheric Loss Processes *****

OH Reactivity

$$k_{\text{Rec}}(T) = 1.3 \times 10^{-12} \exp(-1770/T); k_{\text{Rec}}(272 \text{ K}) = 1.94 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$k_{\text{SAR}}(298 \text{ K}) = 3.14 \times 10^{-15}; k_{\text{SAR}}(272 \text{ K}) \approx 2.00 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$\tau_{\text{Global}}^{\text{OH}} = 17.9 \text{ years}$$

$$\tau_{\text{Trop}}^{\text{OH}} = 18.7 \text{ years}$$

$$\tau_{\text{Strat}}^{\text{OH}} = 471.3 \text{ years}$$

Fractional Atmospheric Loss: 0.923

O(¹D) Reactivity

$$k_{\text{Rec}}(T) = 0.65 \times 2.0 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$k_{\text{Est}}(T) = 0.9 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$\tau_{\text{O}(\text{1D})} = 411 \text{ years}$$

Fractional Atmospheric Loss: 0.040

UV Photolysis

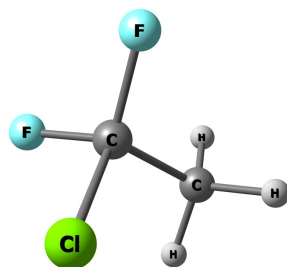
UV Spectrum: *Recommendation Available*

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

Fractional Atmospheric Loss: 0.037



Molecular Structure and Infrared Spectrum (1 conformer)



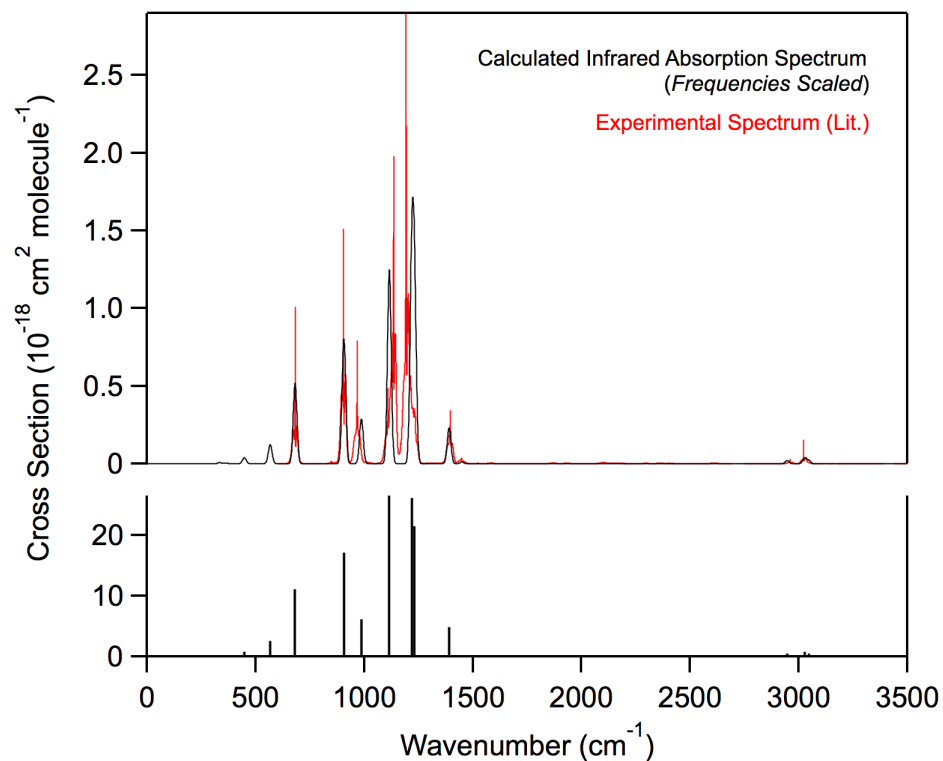
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.071031745107	1.261991497871	-0.000507328541
C	0.359088593728	-0.069777027260	0.000473162176
H	0.796745188491	1.830140650731	0.888747961022
H	2.148373884993	1.073853341867	0.002316092321
H	0.800807012966	1.826653190093	-0.893220691054
Cl	-1.446003465381	0.140656995425	-0.004021025473
F	0.683012212864	-0.795520020219	-1.077691996863
F	0.678121827233	-0.791315628507	1.082909826411

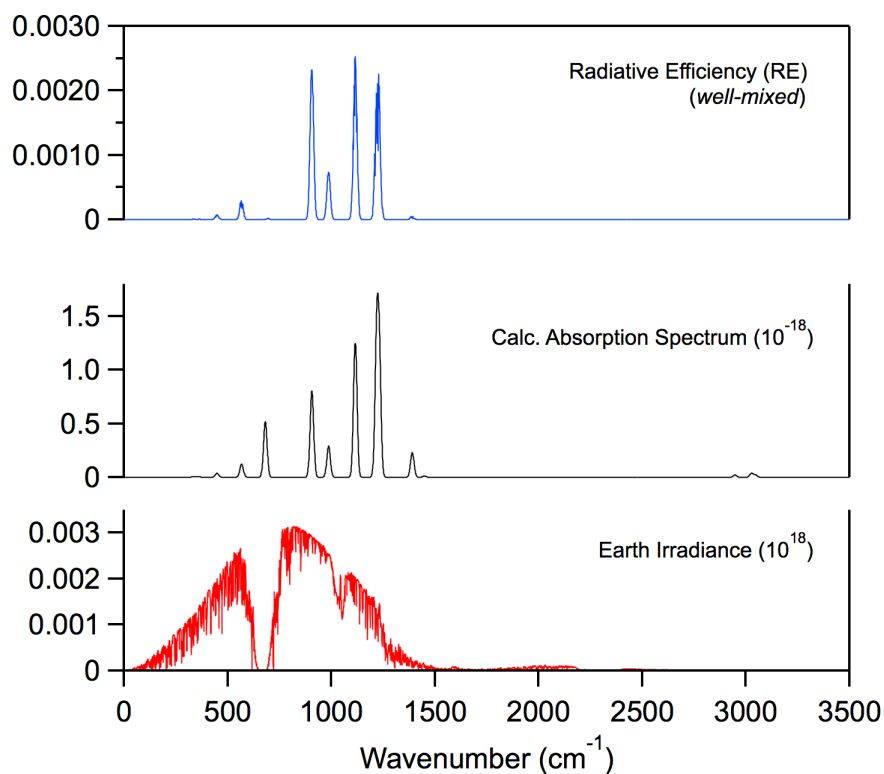
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
238.2855	0.000
297.6295	0.149
327.0328	0.0934
417.7560	0.811
423.6611	0.000
543.6296	2.61
664.9037	11.1
902.7462	17.1
988.1298	6.15
1124.3827	26.6
1233.9103	26.2
1247.2207	21.6
1415.4821	4.89
1477.6065	0.189
1478.8512	0.0523
3064.2190	0.447
3148.2913	0.781
3168.9394	0.447

Infrared Spectrum

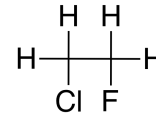


Radiative Efficiency



HCFC-151

Molecular Formula: CH₂ClCH₂F
 Name: 1-Chloro-2-fluoroethane
 CAS number: 762-50-5
 Molecular Weight: 82.5



Global Atmospheric Lifetime (years): 0.487
 Tropospheric Atmospheric Lifetime (years): 0.500
 Stratospheric Atmospheric Lifetime (years): 20
 Ozone Depletion Potential (ODP): 0.008

	<i>Well-mixed</i>	<i>Lifetime adjusted</i>
Radiative Efficiency (RE):	0.051	0.031
Global Warming Potential (GWP _H):		
GWP ₂₀	68	41
GWP ₁₀₀	18	11
Global Temperature Potentials (GTP _H):		
GTP ₂₀		12
GTP ₅₀		2
GTP ₁₀₀		2

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

Atmospheric Loss Processes *****

OH Reactivity

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

$$k_{\text{SAR}}(298 \text{ K}) = 1.17 \times 10^{-13}; k_{\text{SAR}}(272 \text{ K}) \approx 0.749 \times 10^{-13} \quad \text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$\tau_{\text{Global}}^{\text{OH}} = 0.488 \text{ years}$$

$$\tau_{\text{Trop}}^{\text{OH}} = 0.50 \text{ years}$$

$$\tau_{\text{Strat}}^{\text{OH}} = 20 \text{ years}$$

Fractional Atmospheric Loss: 0.998

O(¹D) Reactivity

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

$$k_{\text{Est}}(T) = 1.0 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$\tau_{\text{O}(\text{1D})} = 370 \text{ years}$$

Fractional Atmospheric Loss: 0.001

UV Photolysis

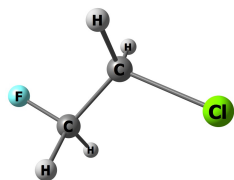
UV Spectrum: *No Recommendation*

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

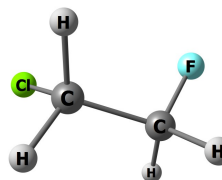
Fractional Atmospheric Loss: 0.001



Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.393



$\Delta E = 0.15 \text{ kcal mol}^{-1}$
Population = 0.304

Optimized Coordinates (Angstroms)

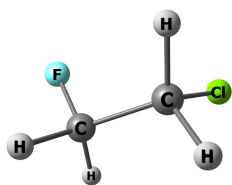
Atom	X	Y	Z
C	-0.019227741500	0.614989001800	0.014070479300
C	1.023020749500	-0.492149723400	0.021867697900
H	0.924306482100	-1.111162247800	0.920242093000
H	0.917989216300	-1.129666617000	-0.862744383300
F	2.269692638200	0.096153383400	0.011341205500
Cl	-1.670540662500	-0.108042344500	0.027424117200
H	0.063749863100	1.228070603600	-0.883558516200
H	0.070065454800	1.246563943900	0.898170306600

Atom	X	Y	Z
C	-0.076307724000	-0.881369567200	0.271941773000
C	1.236605934400	-0.413198733100	-0.317048596600
H	2.003163497300	-1.174765678100	-0.113142467400
H	1.151245989400	-0.275877906300	-1.400925649500
F	1.627208412200	0.771521978900	0.254627602100
Cl	-1.433100699300	0.234325861100	-0.143669933100
H	-0.021613843500	-0.918597391000	1.360564309100
H	-0.337677566400	-1.866947564300	-0.116952037600

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
126.0634	1.38
239.2686	1.64
379.5078	0.317
765.3531	7.48
792.9304	0.101
1055.2108	0.299
1064.5426	0.557
1082.3553	17.7
1220.7100	0.240
1273.9987	2.17
1298.5772	0.00237
1425.7217	0.932
1490.6197	0.674
1519.9385	0.195
3042.8134	3.48
3092.6832	3.55
3095.0818	2.45
3160.8226	1.36

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
128.7771	0.271
280.5790	0.148
464.0313	1.94
671.0638	5.08
858.3704	1.12
965.5094	0.834
1062.7127	2.08
1119.2049	10.6
1218.2060	0.894
1271.4892	0.147
1327.0476	5.26
1430.1149	2.30
1462.5161	1.24
1501.4635	0.515
3011.4905	5.34
3072.9572	2.41
3089.1363	3.70
3151.2185	0.949



$\Delta E = 0.15 \text{ kcal mol}^{-1}$
Population = 0.304

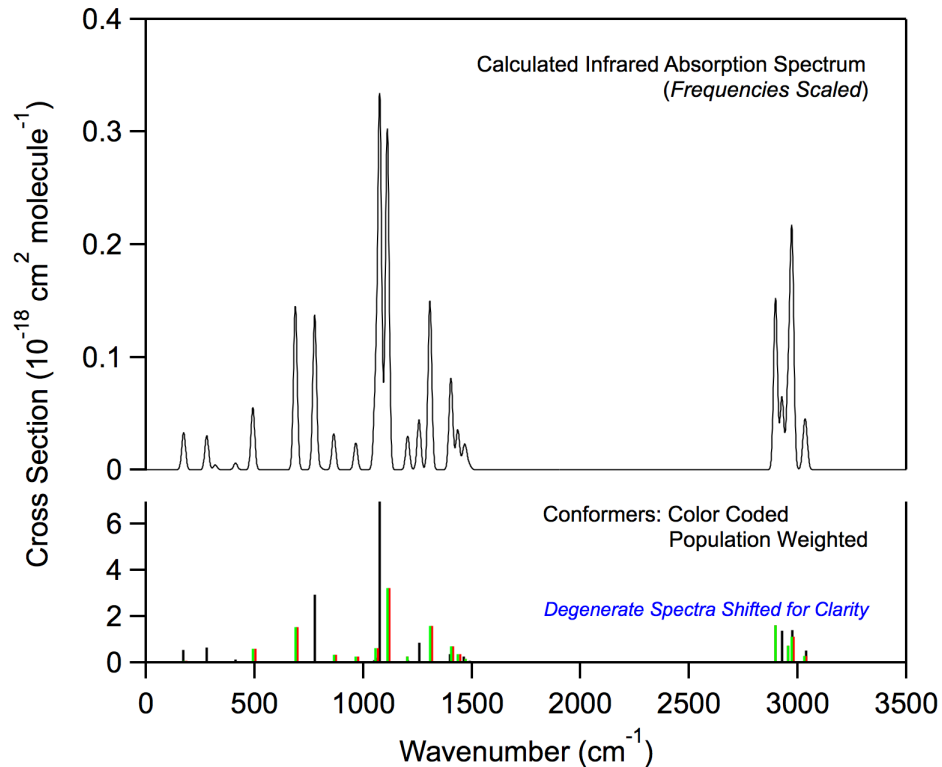
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-0.078732567300	-0.857713241700	-0.288192713000
C	1.216949761200	-0.408038337300	0.351209183100
H	1.091116084300	-0.266989088500	1.430656946300
H	1.979307697000	-1.181529397800	0.178907297800
F	1.647630806200	0.769360687200	-0.206637752500
Cl	-1.433779856400	0.279199004300	0.071908330400
H	-0.370041977700	-1.838378493700	0.091745016200
H	0.018109052700	-0.898195132400	-1.373761308300

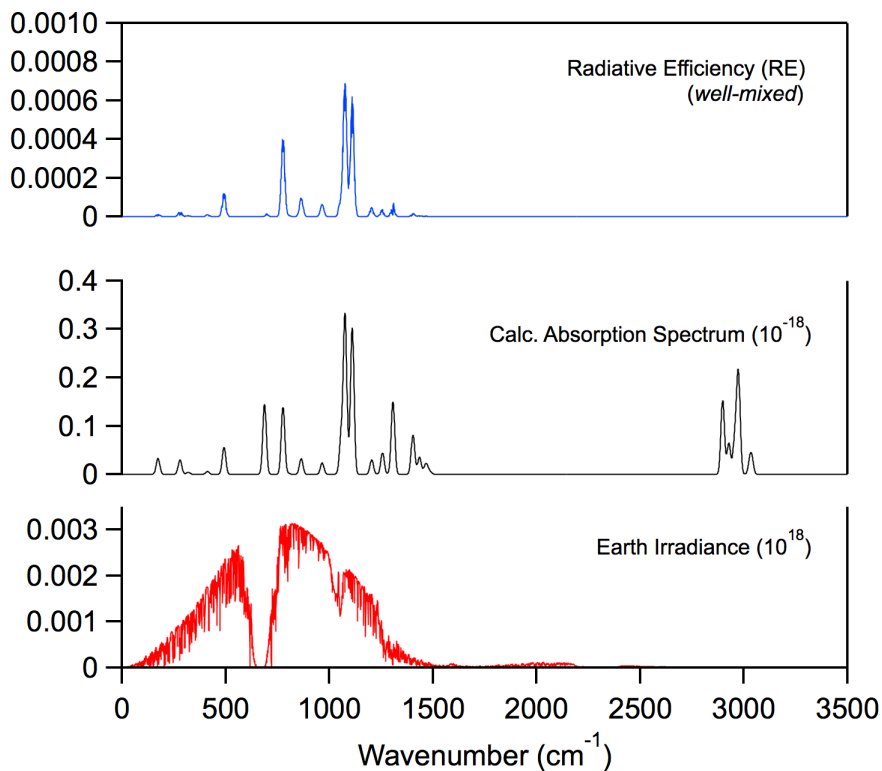
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength ($10^{-18} \text{ cm}^2 \text{ molecule}^{-1} \text{ cm}^{-1}$)
128.7721	0.271
280.5824	0.148
464.0282	1.94
671.0628	5.08
858.3715	1.12
965.5087	0.834
1062.7131	2.08
1119.2053	10.6
1218.2020	0.894
1271.4922	0.147
1327.0462	5.26
1430.1159	2.30
1462.5169	1.24
1501.4618	0.515
3011.5096	5.34
3072.9491	2.41
3089.1331	3.70
3151.2153	0.949

Infrared Spectrum

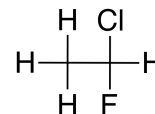


Radiative Efficiency



HCFC-151a

Molecular Formula: CH₃CHClF
Name: 1-Chloro-1-fluoroethane
CAS number: 1615-75-4
Molecular Weight: 82.5



Global Atmospheric Lifetime (years): 1.16
Tropospheric Atmospheric Lifetime (years): 1.20
Stratospheric Atmospheric Lifetime (years): 33.2
Ozone Depletion Potential (ODP): 0.015

	<i>Well-mixed</i>	<i>Lifetime adjusted</i>
Radiative Efficiency (RE):	0.082	0.063
Global Warming Potential (GWP _H):		
GWP ₂₀	259	199
GWP ₁₀₀	70	54
Global Temperature Potentials (GTP _H):		
GTP ₂₀		66
GTP ₅₀		9
GTP ₁₀₀		7

* RE units: W m² ppb⁻¹

* GWP and GTP: Relative to CO₂

Atmospheric Loss Processes *****

OH Reactivity

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

$k_{\text{SAR}}(298 \text{ K}) = 4.89 \times 10^{-14}$; $k_{\text{SAR}}(272 \text{ K}) \approx 3.12 \times 10^{-14}$ cm³ molecule⁻¹ s⁻¹

$\tau_{\text{Global}}^{\text{OH}} = 1.16$ years

$\tau_{\text{Trop}}^{\text{OH}} = 1.20$ years

$\tau_{\text{Strat}}^{\text{OH}} = 39.7$ years

Fractional Atmospheric Loss: 0.994

O(¹D) Reactivity

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

$k_{\text{Est}}(T) = 1.0 \times 10^{-10}$ cm³ molecule⁻¹ s⁻¹

$\tau_{\text{O}(\text{1D})} = 370$ years

Fractional Atmospheric Loss: 0.003

UV Photolysis

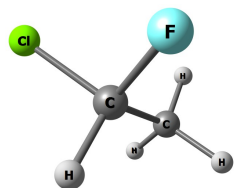
UV Spectrum: *No Recommendation*

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

Fractional Atmospheric Loss: 0.003



Molecular Structure and Infrared Spectrum (1 conformer)



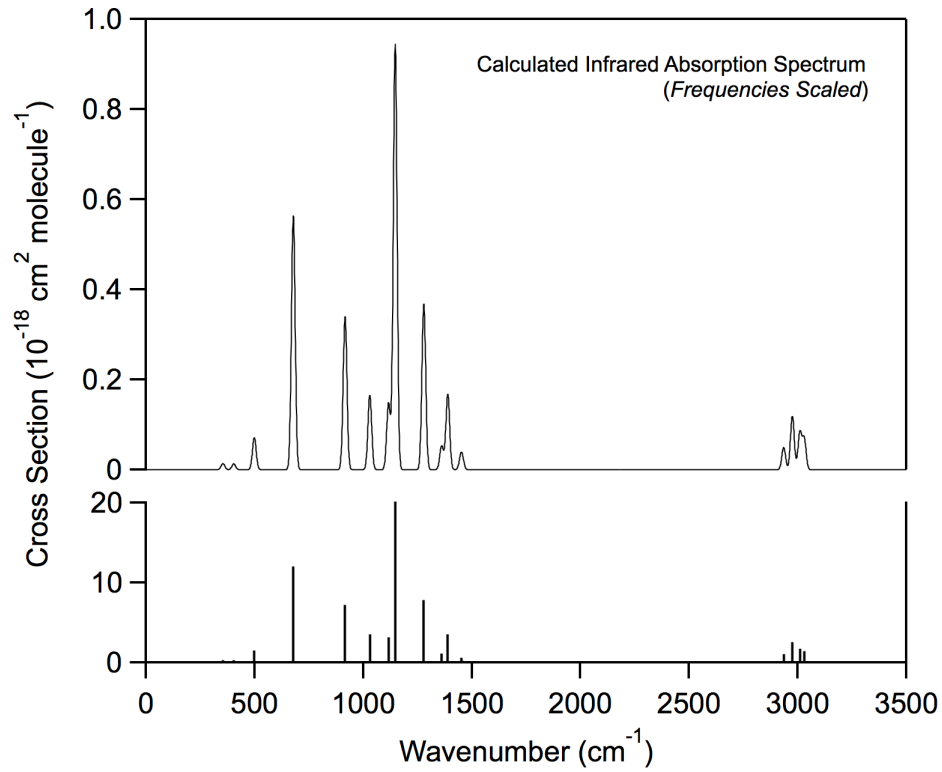
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	0.421891997300	0.114214074900	0.384543973700
C	1.267140844400	-1.035556596900	-0.110729120000
H	0.943947377300	-1.971943195000	0.347753405100
H	1.185814021300	-1.120254038900	-1.196557194400
H	2.311900740800	-0.847519735200	0.156484175700
Cl	-1.327110939900	-0.139099995100	-0.043431683600
F	0.831524343900	1.278998652600	-0.175729567200
H	0.432313614800	0.224981833600	1.471097010600

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm ⁻¹)	Band Strength (10 ⁻¹⁸ cm ² molecule ⁻¹ cm ⁻¹)
246.9374	0.0106
318.3283	0.294
370.8012	0.279
471.0427	1.52
661.1632	12.0
913.3329	7.25
1034.0651	3.53
1125.3330	3.16
1157.7892	20.1
1297.2953	7.84
1384.2152	1.13
1414.0938	3.57
1479.1232	0.621
1485.4169	0.253
3051.4780	1.05
3093.7237	2.53
3130.3705	1.75
3151.5466	1.46

Infrared Spectrum



Radiative Efficiency

