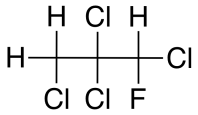
HCFC-241aa

Molecular Formula: CH_2ClCCl_2CHClF
Name: 1,2,2,3-Tetrachloro-1-fluoropropane
CAS number: –
Molecular Weight: 199.87



Global Atmospheric Lifetime (years): 1.43
  Tropospheric Atmospheric Lifetime (years): 1.52
  Stratospheric Atmospheric Lifetime (years): 23.5
Ozone Depletion Potential (ODP): 0.035

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.145	0.116
Global Warming Potential (GWP_H):		
GWP_{20}	234	187
GWP_{100}	63	51
Global Temperature Potentials (GTP_H)		
GTP_{20}		64
GTP_{50}		9
GTP_{100}		7

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 3.85 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 2.46 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 1.48$ years
$\tau^{OH}_{Trop} = 1.52$ years
$\tau^{OH}_{Strat} = 49.3$ years

Fractional Atmospheric Loss: 0.968

O(^{1}D) Reactivity

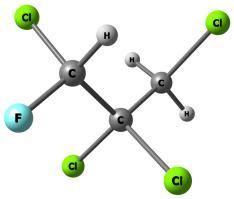
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 2.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)} = 185$ years
Fractional Atmospheric Loss: 0.008

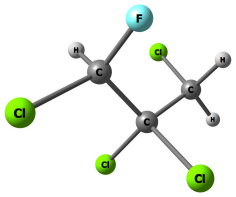
UV Photolysis

UV Spectrum: *No Recommendation*
$\tau_{hv} = 60$ years
Fractional Atmospheric Loss: 0.024

Molecular Structure and Infrared Spectrum (4 conformers)



E = 0
Population = 0.523



$\Delta E = 0.27$ kcal mol^{-1}
Population = 0.332

Optimized Coordinates (Angstroms)

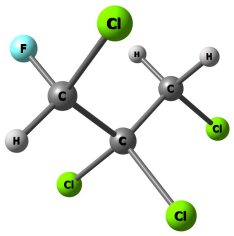
Atom	X	Y	Z
C	1.082876496788	-0.331446709999	1.022931527164
C	0.074665616736	0.443578926276	0.174038915706
C	-0.727867475108	-0.412771159014	-0.830497732789
Cl	2.251218946100	-1.281428310778	0.036295601348
H	1.656157999160	0.368884192894	1.626928999606
H	0.552295859041	-1.036649371669	1.659917075286
Cl	0.918667764220	1.701026573978	-0.805007851582
Cl	-1.046364365211	1.251009486699	1.325014482693
H	-0.047509606785	-0.852758895812	-1.560113714827
Cl	-1.561085618821	-1.787050171505	-0.019278011656
F	-1.645242616121	0.347088438930	-1.451346290950

Atom	X	Y	Z
C	-1.485764369632	0.307043344414	0.783847813114
C	-0.110267347198	0.407428715339	0.108338515456
C	0.581620601971	-0.972992738205	0.037144712546
Cl	-2.609710935971	-0.822774775123	-0.054448737537
H	-1.353636433566	-0.066576740236	1.797396382083
H	-1.955927188048	1.287820961394	0.796149079761
Cl	0.842470799797	1.526484669002	1.148150789480
Cl	-0.261461046981	1.074645165737	-1.544072183559
H	0.014265437142	-1.625739047664	-0.627251215973
Cl	2.249625003097	-0.910404216093	-0.593095797276
F	0.595491479389	-1.498863338566	1.285592641905

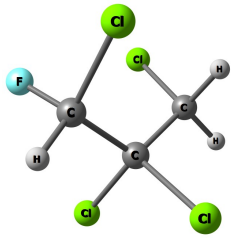
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
70.8727	0.118
104.3113	0.160
140.0884	0.0401
179.9163	0.248
221.2600	0.347
241.9431	0.176
278.0219	0.245
323.1870	0.218
367.2753	0.0320
395.8140	0.493
560.4768	3.41
625.3617	6.13
701.0682	20.1
744.0640	8.29
798.3542	6.46
924.4593	8.42
1018.3638	0.536
1108.3623	5.41
1162.8232	13.1
1231.8197	1.21
1276.8635	2.56
1304.6680	2.19
1367.2555	1.34
1459.3297	2.18
3116.9572	0.498
3128.2933	0.426
3186.8449	0.0296

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
72.9294	0.139
97.0410	0.210
142.4201	0.0722
181.0518	0.0714
190.0276	0.236
245.1487	0.0843
298.4788	0.671
319.8796	0.0461
375.8777	0.0459
424.7851	0.956
498.0325	4.55
629.6776	7.68
734.5892	13.4
744.5185	2.81
841.1548	13.8
933.2478	7.50
1009.6863	4.31
1094.3462	3.26
1119.4256	13.9
1234.2892	0.335
1285.0533	2.60
1302.7328	2.73
1358.8825	1.46
1457.1060	1.24
3118.4520	0.520
3125.0118	0.456
3190.5412	0.0728



ΔE = 1.15 kcal mol^{-1}
Population = 0.075



ΔE = 1.37 kcal mol^{-1}
Population = 0.052

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-0.685823470342	-0.553184736777	-0.978760487059
C	-0.076924294027	0.221106650936	0.191572312421
C	1.421127022443	0.535679965140	-0.062182493295
Cl	-2.436718135178	-0.865827849777	-0.814297046703
H	-0.532926155285	0.023158964603	-1.890844546415
H	-0.188587866332	-1.518470097973	-1.061797399773
Cl	-0.218143417879	-0.679116911494	1.731745409435
Cl	-0.874969857134	1.829282808271	0.369253099785
H	1.838292115651	1.089388925367	0.779028572420
Cl	2.415805151483	-0.952695484529	-0.253329881202
F	1.529040906599	1.260190766233	-1.197780539613

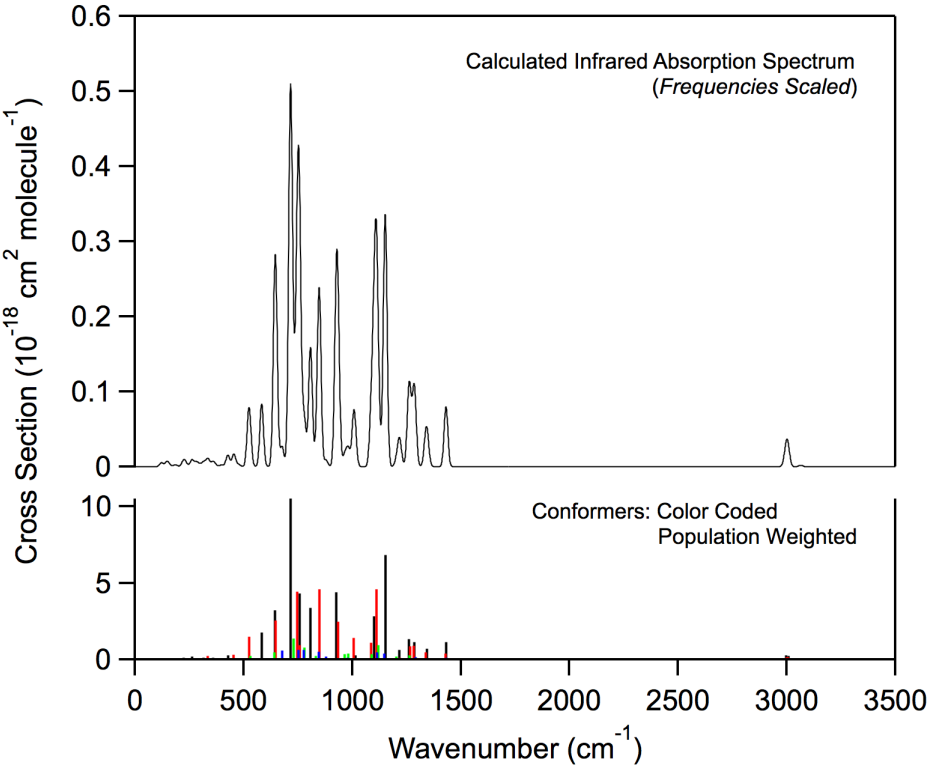
Atom	X	Y	Z
C	-0.794443844094	-0.030681278222	1.205415172106
C	-0.005577762870	0.563123984533	0.036110734915
C	0.789519426743	-0.421962680534	-0.860779382351
Cl	-2.061624275505	-1.203045943541	0.716657866844
H	-0.106252769597	-0.553762803128	1.867335373244
H	-1.285789299170	0.778837634957	1.741735032202
Cl	1.194079202250	1.696316811360	0.773425876891
Cl	-1.083527039412	1.496556845780	-1.057878109231
H	1.460988247110	0.140706822377	-1.510762471119
Cl	1.824879105298	-1.523894300449	0.118028670485
F	-0.046989990753	-1.167731093133	-1.602838763986

Infrared Absorption Spectrum (unscaled frequencies)

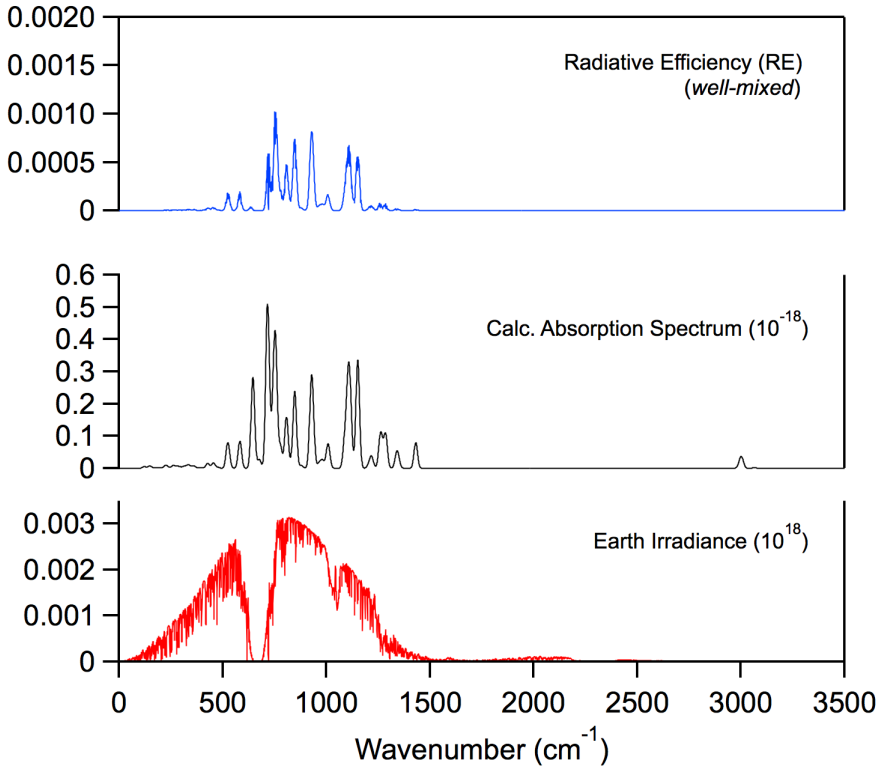
Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
82.1026	0.0258
90.4180	0.220
132.9101	0.177
164.6048	0.0961
211.6358	0.247
241.4114	0.104
291.5375	0.136
326.4989	0.230
358.1251	0.188
427.1608	0.529
506.1077	3.39
622.8584	6.30
716.4404	18.5
769.7031	10.5
823.6500	3.25
965.5345	4.66
983.1285	5.41
1097.5592	4.83
1129.7304	12.7
1218.0544	2.55
1279.9715	3.68
1313.3320	1.44
1359.2828	1.07
1463.3536	0.765
3105.3558	0.672
3129.4906	0.402
3172.6298	0.0385

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
59.5729	0.0329
116.5401	0.132
141.1489	0.0290
175.9079	0.0448
234.9815	0.0796
258.9776	1.11
271.7262	0.109
335.6722	0.586
357.4655	0.283
396.3155	1.35
448.8442	1.19
660.0029	11.1
740.6155	12.3
764.9454	12.5
837.8238	9.64
874.1151	3.68
980.4792	2.09
1122.4742	9.04
1157.1495	7.55
1242.5520	1.41
1278.0815	1.57
1310.0293	3.28
1378.7237	0.825
1459.2120	2.09
3113.3976	0.497
3119.1078	0.688
3180.9303	0.0201

Infrared Spectrum

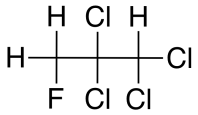


Radiative Efficiency



HCFC-241ab

Molecular Formula: $CH_2FCCl_2CHCl_2$
Name: 1,1,2,2-Tetrachloro-3-fluoropropane
CAS number: –
Molecular Weight: 199.87



Global Atmospheric Lifetime (years): 0.765
  Tropospheric Atmospheric Lifetime (years): 0.803
  Stratospheric Atmospheric Lifetime (years): 20
Ozone Depletion Potential (ODP): 0.020

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.135	0.094
Global Warming Potential (GWP_H):		
GWP_{20}	117	81
GWP_{100}	32	22
Global Temperature Potentials (GTP_H)		
GTP_{20}		25
GTP_{50}		4
GTP_{100}		3

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 7.30 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 4.66 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 0.780$ years
$\tau^{OH}_{Trop} = 0.803$ years
$\tau^{OH}_{Strat} = 27.7$ years

Fractional Atmospheric Loss: 0.981

O(^{1}D) Reactivity

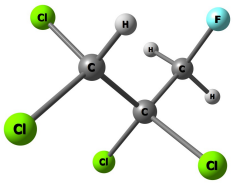
k_{Rec}(T), *No recommendation*

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

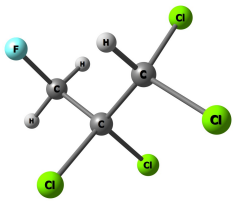
UV Photolysis

UV Spectrum: *No Recommendation*
$\tau_{hv} = 50$ years
Fractional Atmospheric Loss: 0.015

Molecular Structure and Infrared Spectrum (5 conformers)



E = 0
Population = 0.445



E = 0
Population = 0.445

Optimized Coordinates (Angstroms)

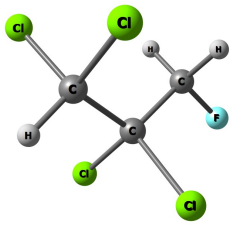
Atom	X	Y	Z
C	-1.376501768343	1.341986808963	0.129317259477
C	-0.596548076144	0.020109199739	0.193538831588
C	0.729093080648	0.094826623086	-0.600511182907
F	-1.533284690117	1.704975463928	-1.184812358136
H	-2.355592004003	1.197618601971	0.592880679231
H	-0.819448100150	2.120662895016	0.655686552451
Cl	-1.609778693932	-1.258364567577	-0.576632047899
Cl	-0.335029637895	-0.357096096806	1.921493500340
H	0.481764171744	0.312258312607	-1.636513346711
Cl	1.754189377669	1.454307719050	-0.029913649280
Cl	1.654242340524	-1.424987959978	-0.572893238155

Atom	X	Y	Z
C	-1.377859052887	1.340371835548	-0.130558463312
C	-0.596479649445	0.019296746124	-0.193953619773
C	0.728785704715	0.095742609004	0.600558932930
F	-1.535515802508	1.703726266325	1.183365666378
H	-0.821436010605	2.119425221459	-0.657036409051
H	-2.356623064244	1.194776888961	-0.594427038147
Cl	-0.333918168291	-0.358330871822	-1.921657824435
Cl	-1.608639911134	-1.259938734149	0.576359212462
H	0.480840528354	0.313330950393	1.636380877682
Cl	1.655557076083	-1.423100527568	0.573900675704
Cl	1.752651349963	1.456079615726	0.029791989564

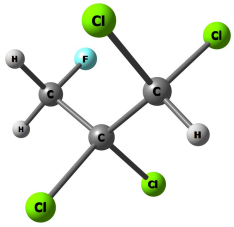
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
65.5739	0.0742
106.4286	0.270
161.5769	0.0599
171.8923	0.0692
201.1404	0.291
238.0538	0.0123
278.1049	0.585
330.2169	0.213
346.7702	0.454
393.9358	0.00890
510.7181	4.79
622.2262	4.61
690.1610	15.2
774.9692	9.45
822.6341	10.5
960.9406	6.24
1059.5821	1.54
1105.9600	10.7
1134.9667	2.01
1229.8788	2.48
1266.7128	1.24
1281.4400	0.475
1411.3020	1.03
1495.3874	1.41
3073.1361	1.37
3134.6071	1.09
3159.7565	0.632

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
65.5739	0.0742
106.4289	0.270
161.5769	0.0599
171.8923	0.0692
201.1405	0.291
238.0538	0.0123
278.1050	0.585
330.2170	0.213
346.7703	0.454
393.9359	0.00890
510.7182	4.79
622.2263	4.61
690.1612	15.2
774.9693	9.45
822.6342	10.5
960.9408	6.24
1059.5823	1.54
1105.9595	10.7
1134.9668	2.01
1229.8788	2.48
1266.7128	1.24
1281.4400	0.475
1411.3019	1.03
1495.3873	1.41
3073.1361	1.37
3134.6073	1.09
3159.7566	0.632



$\Delta E = 1.58$ kcal mol^{-1}
Population = 0.031



$\Delta E = 1.58$ kcal mol^{-1}
Population = 0.031

Optimized Coordinates (Angstroms)

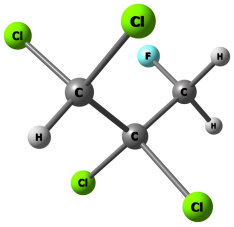
Atom	X	Y	Z
C	-1.596389705398	-0.304230941175	0.000000000000
C	-0.076157242376	-0.497418647439	0.000000000000
C	0.732023855217	0.823749703262	0.000000000000
F	-2.215913153322	-1.519260991945	0.000000000000
H	-1.884501060030	0.253007900006	0.896351341813
H	-1.884501060030	0.253007900006	-0.896351341813
Cl	0.405465864309	-1.442754909147	-1.455965751500
Cl	0.405465864309	-1.442754909147	1.455965751500
H	1.794335325079	0.595172986006	0.000000000000
Cl	0.405330156117	1.808599454798	-1.463921741398
Cl	0.405330156117	1.808599454798	1.463921741398

Atom	X	Y	Z
C	-0.696570757673	-0.213083013796	-1.546379756880
C	-0.655319516360	0.037345933653	-0.032450302251
C	0.746608469339	0.224434219533	0.607023911297
F	-0.132065919402	-1.417203478968	-1.856727232127
H	-1.742769141896	-0.206942321174	-1.864409505344
H	-0.150059183332	0.589287880909	-2.051659249225
Cl	-1.485910829553	-1.304112985068	0.826351333887
Cl	-1.585993411697	1.559886945179	0.249374889282
H	0.623613843784	0.481581345967	1.655781457277
Cl	1.745800908866	-1.255030818164	0.543378823169
Cl	1.638218537923	1.583406291929	-0.157350369085

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
69.9584	0.0724
104.9506	0.294
157.7743	0.310
162.4964	0.0776
222.6373	0.0001
244.4878	0.334
266.2724	0.0957
293.4464	0.207
341.0035	0.207
359.8423	0.121
549.3970	3.56
628.5031	3.88
703.3316	26.5
724.7854	7.43
773.1823	4.88
987.6648	1.46
1073.5301	2.54
1096.4513	0.722
1141.9153	12.5
1220.9306	2.14
1282.9295	1.40
1294.5291	0.236
1419.1373	0.406
1499.1768	0.548
3059.2839	1.66
3118.2041	0.987
3161.8904	0.441

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
58.3792	0.0620
117.5472	0.222
158.5574	0.0256
183.9578	0.146
222.9332	0.00407
256.0069	1.19
267.4651	0.115
302.7038	0.464
327.0605	0.273
399.9215	0.112
422.4618	2.31
665.9195	11.4
717.7686	6.16
759.1602	23.2
839.2741	4.95
885.0075	0.116
1056.6422	2.34
1122.0814	9.89
1156.0949	1.20
1224.4257	2.28
1285.1332	1.31
1301.2235	0.387
1421.7527	0.906
1494.0408	1.14
3060.9152	1.42
3119.6040	1.22
3157.4916	0.414



$\Delta E = 1.58$ kcal mol^{-1}
Population = 0.031

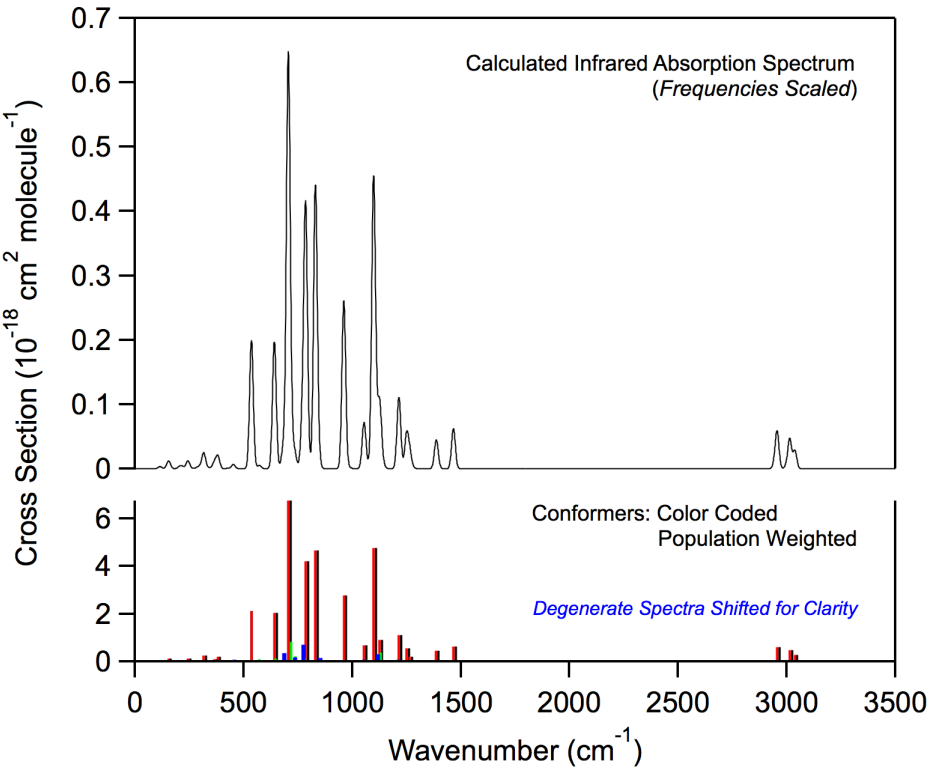
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-0.695873423952	0.211291228228	-1.547056606133
C	-0.655337859533	-0.037687847282	-0.032868609279
C	0.746287118164	-0.224171882722	0.607445739010
F	-0.131214798518	1.415110613782	-1.858291004854
H	-0.149128501707	-0.591566324058	-2.051309540616
H	-1.741921699923	0.204851900024	-1.865573822872
Cl	-1.586154142029	-1.559952818239	0.249975775934
Cl	-1.486325587730	1.304597848165	0.824255986181
H	0.622796143319	-0.480313811079	1.656390917595
Cl	1.638249046983	-1.583880656237	-0.155205930150
Cl	1.745518704926	1.255225749418	0.542855095183

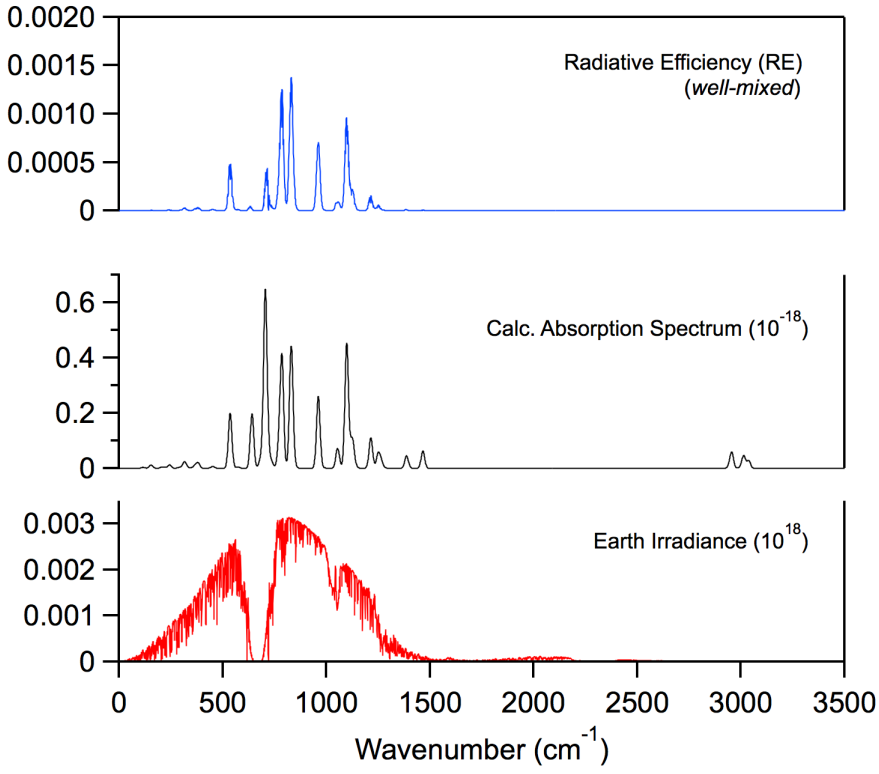
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
58.3789	0.0620
117.5470	0.222
158.5574	0.0256
183.9578	0.146
222.9333	0.00407
256.0067	1.19
267.4652	0.115
302.7039	0.464
327.0606	0.273
399.9215	0.112
422.4618	2.31
665.9195	11.4
717.7686	6.16
759.1601	23.2
839.2740	4.95
885.0074	0.116
1056.6424	2.34
1122.0818	9.89
1156.0949	1.20
1224.4265	2.28
1285.1340	1.31
1301.2242	0.387
1421.7533	0.906
1494.0416	1.14
3060.9153	1.42
3119.6042	1.22
3157.4916	0.414

Infrared Spectrum

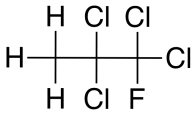


Radiative Efficiency



HCFC-241ac

Molecular Formula:	$CH_3CCl_2CCl_2F$
Name:	1,1,2,2-Tetrachloro-1-fluoropropane
CAS number:	7126-06-9
Molecular Weight:	199.87



Global Atmospheric Lifetime (years):	5.18
Tropospheric Atmospheric Lifetime (years):	6.18
Stratospheric Atmospheric Lifetime (years):	32.1
Ozone Depletion Potential (ODP):	0.112

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.207	0.191
Global Warming Potential (GWP_H):		
GWP_{20}	1181	1091
GWP_{100}	327	302
Global Temperature Potentials (GTP_H)		
GTP_{20}		610
GTP_{50}		65
GTP_{100}		42

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 9.49 \times 10^{-15}$; $k_{SAR}(272\ K) \approx 6.05 \times 10^{-15}$ cm^3 $molecule^{-1}$ s^{-1}

τ^{OH}_{Global} = 5.97 years
τ^{OH}_{Trop} = 6.18 years
τ^{OH}_{Strat} = 174.1 years

Fractional Atmospheric Loss: 0.868

O(^{1}D) Reactivity

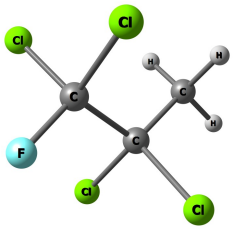
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 2.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)}$ = 185 years
Fractional Atmospheric Loss: 0.028

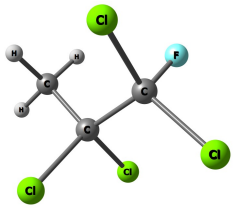
UV Photolysis

UV Spectrum: *No Recommendation*
τ_{hv} = 50 years
Fractional Atmospheric Loss: 0.104

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.432



$\Delta E = 0.25$ kcal mol^{-1}
Population = 0.284

Optimized Coordinates (Angstroms)

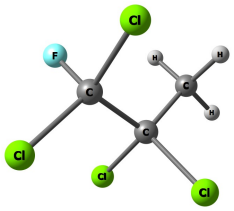
Atom	X	Y	Z
C	0.726156817856	-0.003436557328	1.858224789529
C	0.723907360468	-0.001897811396	0.338563955923
C	-0.701853255614	0.000379165777	-0.311980409808
H	0.219835269200	-0.894952054065	2.232026349558
H	1.758611452440	-0.004945450000	2.208770692353
H	0.221828801501	0.888451075239	2.233829206328
Cl	1.593490002992	-1.460836844091	-0.273157113250
Cl	1.596803217396	1.456294958057	-0.270208299510
Cl	-1.635618628579	-1.456032742934	0.175094882284
Cl	-1.632295327435	1.457938725161	0.178014988937
F	-0.596143710225	0.001586535580	-1.637954042342

Atom	X	Y	Z
C	1.004450817247	1.374599140858	1.305349588982
C	0.734164744275	0.359537341891	0.198966134565
C	-0.696268673978	-0.271524072607	0.324069937377
H	2.038080109539	1.712499195664	1.229157060007
H	0.337711788154	2.231461704596	1.203021683264
H	0.850390166992	0.904220527526	2.278323793004
Cl	1.927035144279	-0.987821644737	0.359840704175
Cl	0.927606189484	1.131998777953	-1.406162860918
Cl	-1.964102372034	1.002497373201	0.249834854281
Cl	-1.036883703772	-1.503653533592	-0.917822491813
F	-0.778865210185	-0.850857810753	1.529886597076

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
76.9941	0.0109
162.4739	0.0535
212.6745	0.163
222.9149	0.0194
244.0813	0.0591
273.9984	0.0262
283.7036	0.143
292.2973	0.143
340.9734	0.134
384.5919	0.0244
385.2506	0.0273
450.0113	0.691
565.9051	0.739
683.8827	13.4
705.9012	25.5
825.8651	18.8
929.1090	10.0
1086.9194	5.75
1098.1985	5.36
1148.8801	5.06
1192.6982	9.59
1413.9092	2.21
1480.6680	0.529
1481.6983	1.14
3071.3018	0.237
3156.9348	0.326
3160.7260	0.317

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
76.8194	0.0595
169.9252	0.0407
176.2412	0.101
229.8512	0.0247
245.5719	0.0648
279.1944	0.00689
295.8568	0.201
314.9759	0.204
347.3140	0.318
381.3306	0.0498
390.6248	0.0972
469.2774	1.72
508.9190	1.53
685.1540	16.6
759.5923	11.4
829.0166	27.3
948.8970	10.5
1077.2773	3.68
1101.3171	8.10
1115.5135	12.2
1169.9093	3.60
1409.7427	1.38
1480.5808	0.464
1483.9912	1.11
3071.9484	0.338
3157.8425	0.299
3164.0164	0.329



$\Delta E = 0.25$ kcal mol^{-1}
Population = 0.284

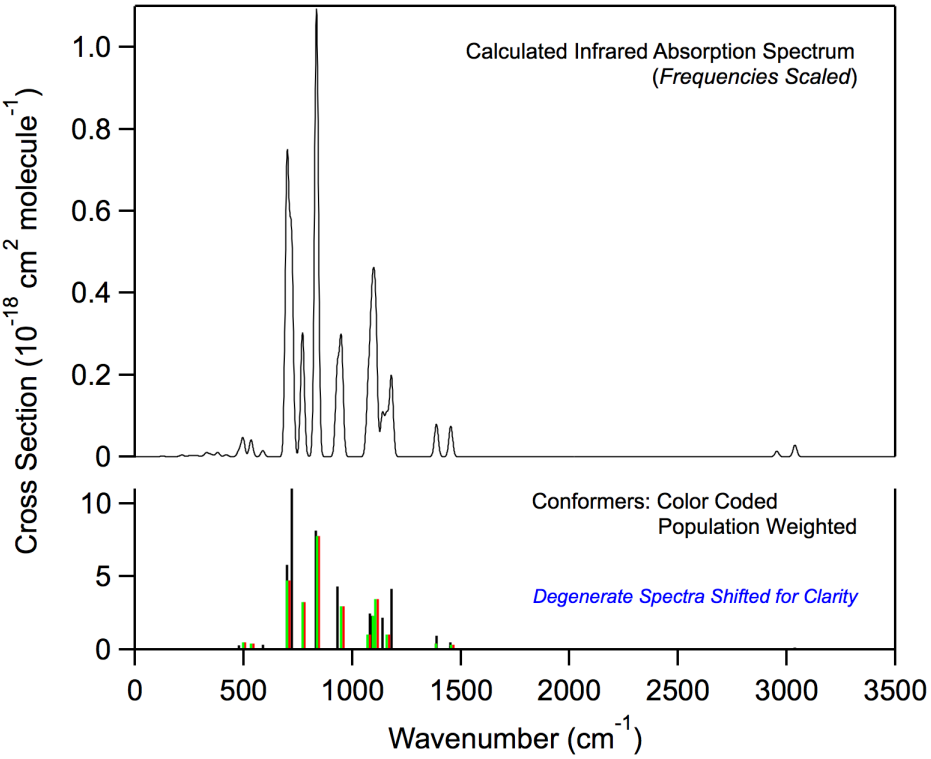
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	0.999143964761	-1.413212552704	1.264576367946
C	0.732252919103	-0.368925017972	0.184889352971
C	-0.696930223682	0.261805514924	0.325043082524
H	2.032112451352	-1.751287955649	1.180599161867
H	0.845077660357	-0.968139595325	2.249382538546
H	0.330642520794	-2.265623286111	1.139169094835
Cl	0.925713751420	-1.099504836154	-1.439727513743
Cl	1.927891212193	0.971118022208	0.382201714225
Cl	-1.033528967698	1.526799758646	-0.884481223579
Cl	-1.967465090283	-1.007025746698	0.216174592536
F	-0.779544198317	0.809529694834	1.545541831871

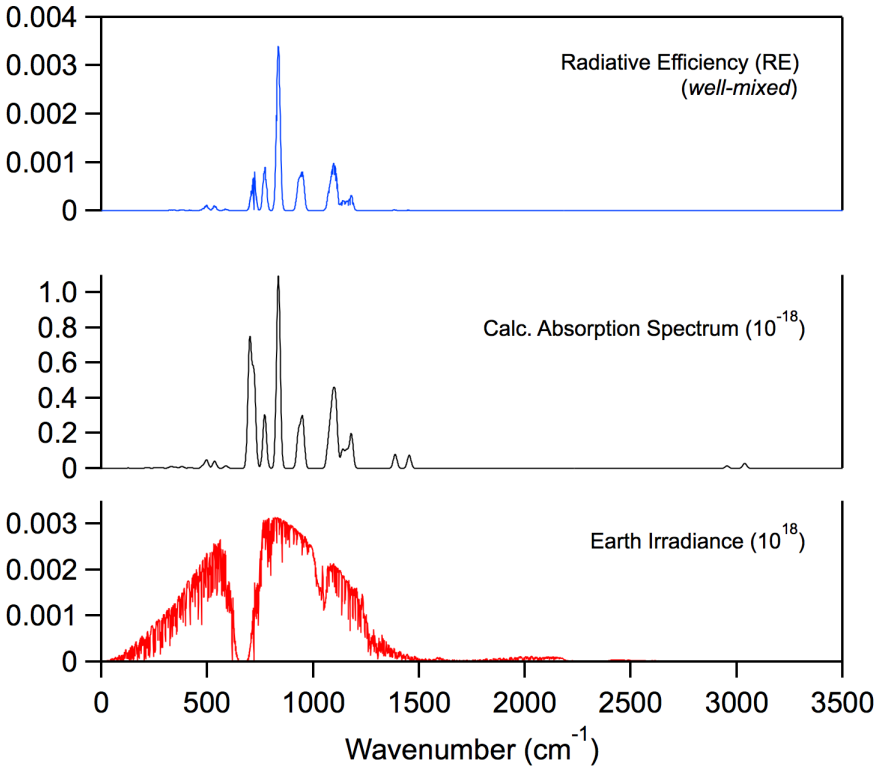
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
76.8193	0.0595
169.9253	0.0407
176.2414	0.101
229.8510	0.0247
245.5717	0.0648
279.1927	0.00689
295.8565	0.201
314.9762	0.204
347.3137	0.318
381.3306	0.0498
390.6249	0.0972
469.2773	1.72
508.9187	1.53
685.1534	16.6
759.5923	11.4
829.0165	27.3
948.8969	10.5
1077.2761	3.68
1101.3170	8.10
1115.5126	12.2
1169.9091	3.60
1409.7428	1.38
1480.5812	0.464
1483.9916	1.11
3071.9489	0.338
3157.8426	0.299
3164.0173	0.329

Infrared Spectrum

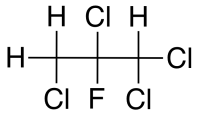


Radiative Efficiency



HCFC-241ba

Molecular Formula:	$CH_2ClCClFCHCl_2$
Name:	1,1,2,3-Tetrachloro-2-fluoropropane
CAS number:	3175-26-6
Molecular Weight:	199.87



Global Atmospheric Lifetime (years):	0.788
Tropospheric Atmospheric Lifetime (years):	0.826
Stratospheric Atmospheric Lifetime (years):	20
Ozone Depletion Potential (ODP):	0.020

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.174	0.121
Global Warming Potential (GWP_H):		
GWP_{20}	154	108
GWP_{100}	42	29
Global Temperature Potentials (GTP_H)		
GTP_{20}		34
GTP_{50}		5
GTP_{100}		4

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 7.10 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 4.53 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 0.802$ years

$\tau^{OH}_{Trop} = 0.826$ years

$\tau^{OH}_{Strat} = 28.4$ years

Fractional Atmospheric Loss: 0.982

O(^{1}D) Reactivity

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

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

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

Fractional Atmospheric Loss: 0.004

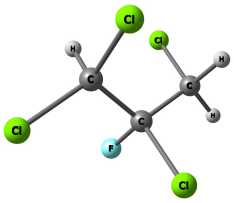
UV Photolysis

UV Spectrum: *No Recommendation*

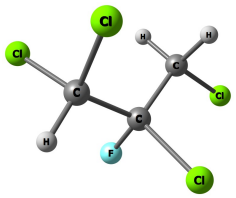
$\tau_{hv} = 60$ years

Fractional Atmospheric Loss: 0.014

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.748



$\Delta E = 1.07$ kcal mol^{-1}
Population = 0.123

Optimized Coordinates (Angstroms)

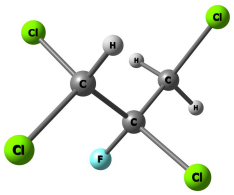
Atom	X	Y	Z
C	1.612285302478	-0.411047094877	0.575364005019
C	0.245340182136	-0.629984303808	-0.074829377619
C	-0.557869141828	0.665040021836	-0.335367339430
Cl	2.664067353615	0.652557668053	-0.429988193761
H	1.507107149827	0.049799574439	1.554056863429
H	2.111518617043	-1.374912511026	0.657559911901
Cl	-0.652971008773	-1.763297634398	1.005549925315
F	0.415130887083	-1.232577141429	-1.274052997471
H	0.036964609120	1.297015559019	-0.991221330976
Cl	-2.082780501866	0.325049847915	-1.188969090896
Cl	-0.833738448834	1.592670014277	1.165097624488

Atom	X	Y	Z
C	0.915234911387	-0.539085293093	-0.849908257211
C	0.273829879398	0.018911166639	0.418701969996
C	-1.275172700871	0.099990418732	0.358565496915
Cl	2.668027825598	-0.827905796245	-0.644154769534
H	0.452938071358	-1.498843662834	-1.082465323214
H	0.777996317661	0.151413386332	-1.678415224926
Cl	0.884705752540	1.681959937607	0.779366746695
F	0.576477448843	-0.762163936847	1.479442110865
H	-1.635840597894	0.577467457426	1.266055662896
Cl	-1.855473847222	1.064574650721	-1.026323195792
Cl	-1.981106060797	-1.548882328438	0.325792783310

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
57.3587	0.111
96.4925	0.257
155.5988	0.155
170.1100	0.0197
195.9686	0.359
258.0690	0.266
286.2876	0.128
339.9397	0.167
368.5391	0.204
435.6936	0.729
531.8859	4.92
620.3023	6.49
737.0171	11.8
798.1714	16.2
804.2768	3.91
900.6508	5.19
949.8013	10.8
1087.5523	4.27
1171.2815	6.29
1230.5941	3.15
1250.4835	1.11
1290.6129	2.38
1302.1106	1.51
1456.3216	2.03
3121.7027	0.562
3150.0894	0.440
3196.3008	0.0362

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
68.5291	0.0006
78.2452	0.312
140.1421	0.256
169.6135	0.0634
206.6130	0.160
239.1129	0.0420
294.3706	0.220
334.3536	0.217
379.2314	0.0440
421.2476	0.760
534.0086	4.46
640.8587	7.76
730.9320	14.0
792.5946	13.1
807.1225	5.45
875.2235	4.07
979.0247	7.44
1102.6876	5.00
1141.2033	6.07
1223.0350	4.71
1236.4515	1.70
1297.9891	1.48
1321.6162	0.700
1463.1340	1.19
3107.4783	0.808
3157.8694	0.492
3183.0037	0.0883



$\Delta E = 1.10$ kcal mol^{-1}
Population = 0.116

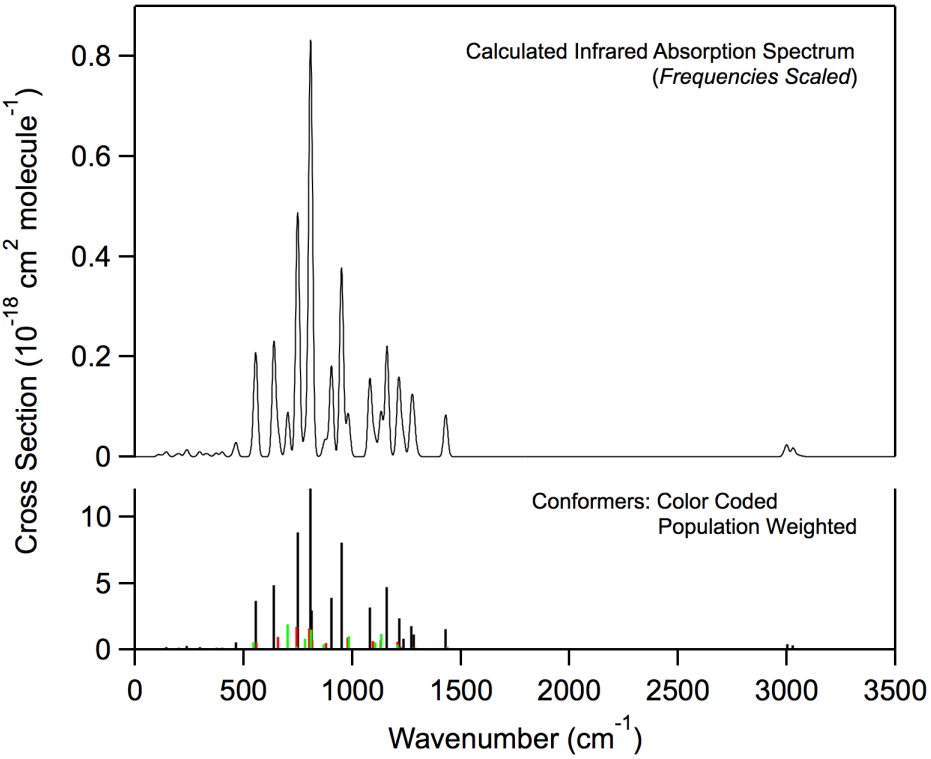
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.506612988227	0.446178463606	-0.792907984842
C	0.227267764556	-0.357903176858	-0.531277468132
C	-0.765351352303	0.296686146429	0.454867782520
Cl	2.411226630696	0.855110320650	0.697704081013
H	2.158474241613	-0.146522645098	-1.432666666255
H	1.240818371767	1.379811894585	-1.285821637553
Cl	0.666172887392	-1.991846174955	0.104051496569
F	-0.369818844108	-0.517258308656	-1.735245425858
H	-0.319131553979	0.366970449360	1.442318592876
Cl	-1.140108724355	1.973325427837	-0.074702868008
Cl	-2.269671409505	-0.646449396900	0.591649097668

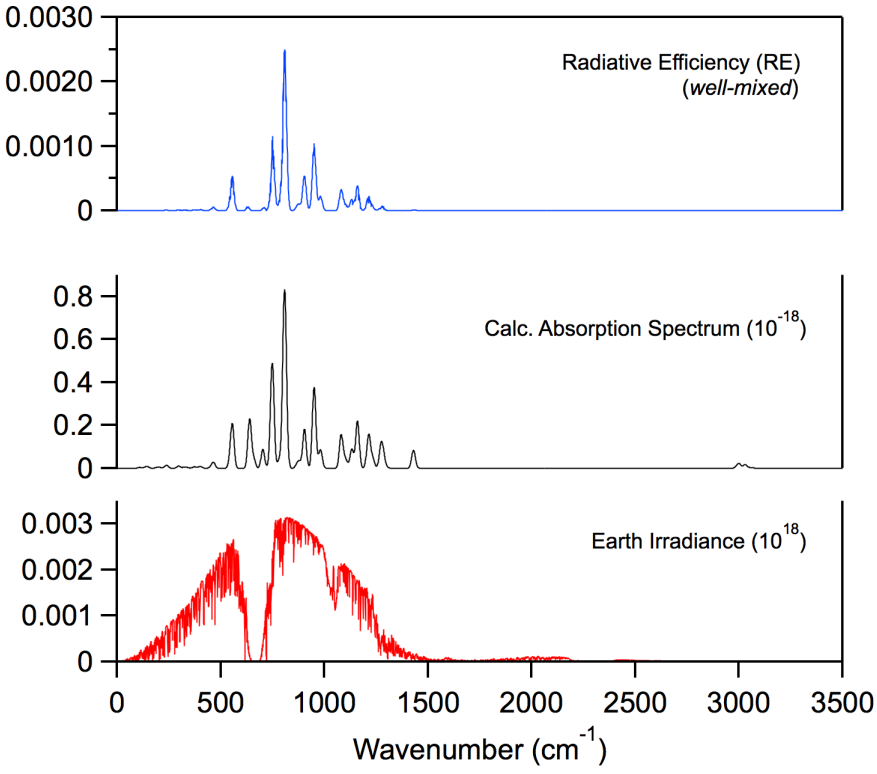
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
56.1611	0.0536
83.6805	0.176
148.9631	0.0838
186.1400	0.302
216.3809	0.0376
257.1712	0.144
301.0687	0.496
325.7327	0.0854
365.1014	0.426
430.8844	0.297
519.8713	4.74
687.9942	16.2
730.6275	1.78
771.9739	7.07
799.8211	12.9
863.6044	3.44
984.9933	8.70
1114.8235	4.79
1143.1695	10.0
1223.0561	3.09
1227.0936	1.12
1289.6719	0.668
1312.1062	1.02
1464.3316	1.86
3111.7035	0.693
3174.2230	0.540
3179.9197	0.00515

Infrared Spectrum

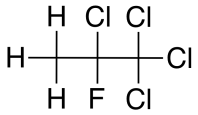


Radiative Efficiency



HCFC-241bb

Molecular Formula:	$CH_3CClFCCl_3$
Name:	1,1,1,2-Tetrachloro-2-fluoropropane
CAS number:	3175-25-5
Molecular Weight:	199.87



Global Atmospheric Lifetime (years):	7.76
Tropospheric Atmospheric Lifetime (years):	10.0
Stratospheric Atmospheric Lifetime (years):	34.3
Ozone Depletion Potential (ODP):	0.163

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.202	0.191
Global Warming Potential (GWP_H):		
GWP_{20}	1633	1543
GWP_{100}	479	452
Global Temperature Potentials (GTP_H)		
GTP_{20}		1049
GTP_{50}		131
GTP_{100}		64

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

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

OH Reactivity

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

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

τ^{OH}_{Global} = 9.67 years

τ^{OH}_{Trop} = 10.0 years

τ^{OH}_{Strat} = 269.2 years

Fractional Atmospheric Loss: 0.803

O(^{1}D) Reactivity

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

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

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

Fractional Atmospheric Loss: 0.042

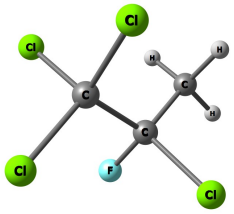
UV Photolysis

UV Spectrum: *No Recommendation*

τ_{hv} = 50 years

Fractional Atmospheric Loss: 0.155

Molecular Structure and Infrared Spectrum (1 conformer)



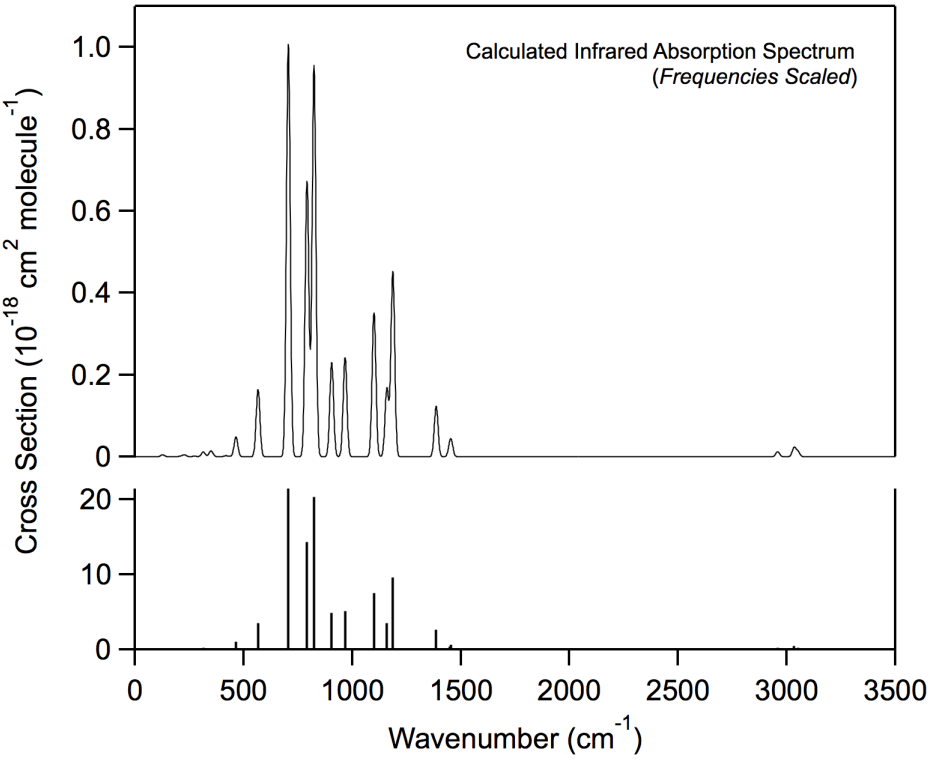
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.099163009507	1.797511505729	0.705906116629
C	0.843322758103	0.584095794957	-0.172000486599
C	-0.553439030155	-0.108589686493	0.041574017224
H	2.073424040186	2.206483453821	0.433367293956
H	0.331298688477	2.552240096744	0.528488878236
H	1.108064108975	1.522756509000	1.759809400386
Cl	2.158774136957	-0.630374622141	0.099926344644
F	0.890544516296	0.948740355263	-1.474895926558
Cl	-0.751495285156	-1.481931362541	-1.076840312090
Cl	-0.736704456138	-0.664879887973	1.727473320876
Cl	-1.838417487051	1.098311843635	-0.320241646705

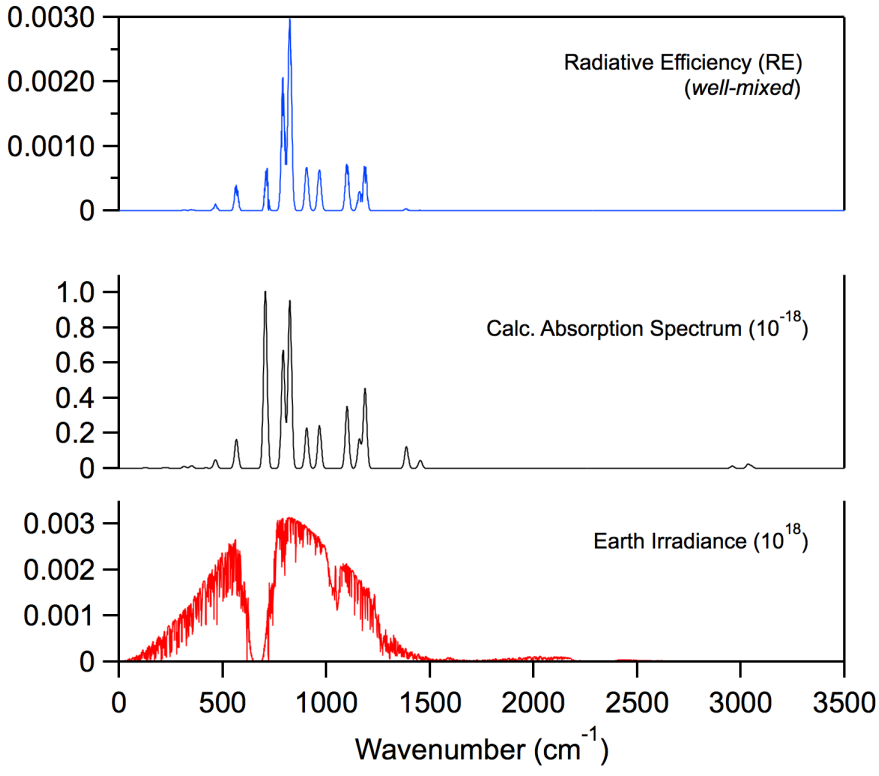
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
77.6810	0.103
166.5168	0.0334
184.8137	0.0965
215.5898	0.00125
233.7704	0.0276
267.3326	0.0111
276.0975	0.235
310.6933	0.167
317.1599	0.153
385.6158	0.0478
402.4459	0.0140
435.3368	1.02
542.9021	3.51
690.5563	21.5
781.5073	14.3
815.7473	20.4
901.8165	4.89
966.9454	5.15
1108.0518	7.51
1170.8183	3.54
1199.8540	9.65
1411.1100	2.63
1478.7111	0.385
1484.2810	0.607
3075.8978	0.266
3155.7940	0.467
3174.6006	0.260

Infrared Spectrum

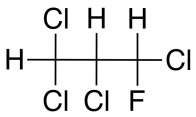


Radiative Efficiency



HCFC-241da

Molecular Formula:	$CHCl_2CHClCHClF$
Name:	1,1,2,3-Tetrachloro-3-fluoropropane
CAS number:	21981-25-9
Molecular Weight:	199.87



Global Atmospheric Lifetime (years):	0.558
Tropospheric Atmospheric Lifetime (years):	0.581
Stratospheric Atmospheric Lifetime (years):	20
Ozone Depletion Potential (ODP):	0.014

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.160	0.100
Global Warming Potential (GWP_H):		
GWP_{20}	100	63
GWP_{100}	27	17
Global Temperature Potentials (GTP_H)		
GTP_{20}		19
GTP_{50}		3
GTP_{100}		2

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 1.01 \times 10^{-13}$; $k_{SAR}(272\ K) \approx 0.644 \times 10^{-13}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 0.566$ years

$\tau^{OH}_{Trop} = 0.581$ years

$\tau^{OH}_{Strat} = 20.7$ years

Fractional Atmospheric Loss: 0.988

$O(^1D)$ Reactivity

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

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

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

Fractional Atmospheric Loss: 0.003

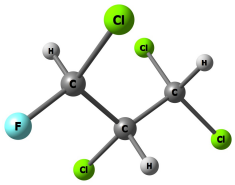
UV Photolysis

UV Spectrum: *No Recommendation*

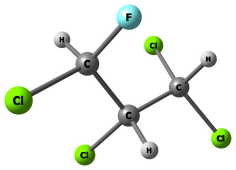
$\tau_{hv} = 60$ years

Fractional Atmospheric Loss: 0.009

Molecular Structure and Infrared Spectrum (8 conformers)



E = 0
Population = 0.349



$\Delta E = 0.26$ kcal mol^{-1}
Population = 0.226

Optimized Coordinates (Angstroms)

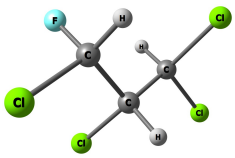
Atom	X	Y	Z
C	-0.828977614567	-0.645588281263	0.266500446794
C	0.168571962221	0.510776543445	0.377123272704
C	1.543480442194	0.203532734608	-0.230606530489
Cl	-2.342930128143	-0.273227502003	1.142020383223
Cl	-1.159392454937	-1.108669114668	-1.433100951069
H	-0.408891934116	-1.526673504579	0.744629047150
H	0.304149113804	0.737548028785	1.436482724539
Cl	-0.443439710680	2.013597668452	-0.396205239853
H	1.490923923317	-0.016469894622	-1.296903512321
F	2.370358910081	1.243359035519	-0.012112961150
Cl	2.259829490826	-1.258429713674	0.565973320473

Atom	X	Y	Z
C	1.130871127741	-0.468650481538	-0.439589474160
C	-0.184989184149	0.316254182336	-0.347171609341
C	-1.358383019569	-0.619662520747	-0.015428391843
Cl	2.455248277630	0.565209345376	-1.048218888220
Cl	1.577096372347	-1.254319485411	1.107630381072
H	1.004938220018	-1.270958814318	-1.161999285467
H	-0.359953862632	0.772541307389	-1.323356942826
Cl	-0.116646156163	1.643569984618	0.848698075149
H	-1.348226906023	-0.939046434811	1.026566471235
Cl	-2.932133007553	0.188788022636	-0.306729172568
F	-1.278208861646	-1.709375105529	-0.826194163032

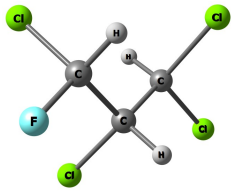
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
53.5725	0.0971
77.8880	0.118
132.6287	0.118
169.2435	0.107
179.6394	0.173
251.3438	0.225
293.4426	0.146
345.7788	0.0705
411.5043	0.782
419.3690	2.81
583.9952	3.00
660.9626	6.12
735.7807	22.8
773.2069	15.0
813.2777	2.09
1029.8839	2.18
1064.5081	3.63
1140.3788	17.4
1208.9081	3.58
1229.5281	1.69
1262.3058	2.07
1292.6376	2.41
1306.0234	2.47
1391.4080	1.64
3108.1439	0.375
3134.0154	0.450
3157.4643	0.296

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
60.1716	0.0815
65.7969	0.110
132.2399	0.171
169.8043	0.0307
184.8948	0.208
213.0552	0.0359
316.6100	0.389
341.2576	0.153
412.0475	1.40
454.7538	1.70
565.5689	5.71
659.9147	4.74
724.0064	18.9
821.6453	3.61
842.3091	12.8
1011.8020	3.93
1063.8615	7.67
1104.6701	13.8
1209.2706	1.36
1229.0960	0.894
1257.5501	3.03
1294.4960	4.07
1326.4524	2.92
1371.4156	1.37
3107.2299	0.511
3134.2040	0.481
3157.4399	0.282



$\Delta E = 0.61$ kcal mol^{-1}
Population = 0.125



$\Delta E = 0.69$ kcal mol^{-1}
Population = 0.108

Optimized Coordinates (Angstroms)

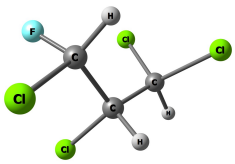
Atom	X	Y	Z
C	-1.211417855704	-0.158341110024	-0.308285579498
C	0.142515143570	0.232265419052	0.310364536086
C	1.258166300149	-0.719339074906	-0.143037697546
Cl	-1.607745205844	-1.874153385745	0.087307710713
Cl	-2.528573568030	0.898443422550	0.269150187827
H	-1.180661444043	-0.086481849296	-1.392392953104
H	0.072526757135	0.218449564919	1.398010161414
Cl	0.535084370596	1.913138404757	-0.191005660795
H	1.032492479351	-1.742996478023	0.155056777956
F	1.388075126660	-0.665624374621	-1.488850419707
Cl	2.825374896161	-0.319852538664	0.634481936655

Atom	X	Y	Z
C	1.036127816440	-0.218867162480	0.299783981503
C	-0.114278498174	0.357013005100	-0.532616619729
C	-1.370152485648	-0.527316699527	-0.566139236071
Cl	1.406740694938	-1.898812425013	-0.243157187533
Cl	2.506080533230	0.787089879825	0.165804730509
H	0.774887754760	-0.279356078210	1.352884309595
H	0.213864691635	0.480998653778	-1.567301025490
Cl	-0.540959060585	1.994896809096	0.069093787705
H	-1.141002148130	-1.502072670237	-0.997058151924
Cl	-2.032422301498	-0.855951560638	1.076016417406
F	-2.314045996968	0.081056248306	-1.312968005972

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
49.5933	0.0681
65.4734	0.207
138.8513	0.202
187.8924	0.143
201.7643	0.201
222.0940	0.0544
283.6628	0.121
330.9518	0.373
391.2857	0.406
405.8915	2.22
621.1715	7.47
694.9622	14.6
732.0040	15.6
798.4601	2.29
844.0649	6.39
955.9456	4.68
1045.2226	2.58
1135.7110	14.2
1197.1023	2.38
1226.8984	2.91
1263.6709	1.38
1286.0612	1.07
1339.5722	2.87
1376.1122	2.52
3126.4060	0.223
3132.4432	0.553
3163.1738	0.275

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
52.4388	0.0601
74.0252	0.135
143.4302	0.104
176.9016	0.306
200.2139	0.0357
243.9526	0.333
284.8383	0.219
331.6220	0.233
393.4567	0.931
442.1592	0.893
595.4476	8.00
666.9049	8.07
723.3065	11.0
766.2770	12.1
821.7612	5.82
1021.8545	6.60
1073.6769	1.08
1134.7052	15.7
1204.2611	2.29
1226.0692	3.11
1244.7626	3.36
1300.9286	5.98
1335.6460	0.679
1375.5650	2.09
3100.1232	0.247
3126.7170	0.691
3165.6897	0.333



$\Delta E = 0.92$ kcal mol^{-1}
Population = 0.074

$\Delta E = 1.14$ kcal mol^{-1}
Population = 0.051

Optimized Coordinates (Angstroms)

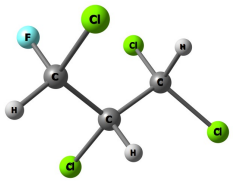
Atom	X	Y	Z
C	-1.312607724088	0.086486669259	0.532333632895
C	0.219218402643	0.077061102464	0.657805294919
C	0.953462033584	-0.634543697912	-0.486603014910
Cl	-1.923840694753	0.793031610059	-0.986211982648
Cl	-1.925898551791	-1.599021462803	0.744873309639
H	-1.739988750237	0.667856626821	1.344793536709
H	0.452578170055	-0.442269327998	1.587437399013
Cl	0.805888669061	1.762543226339	0.853489926234
H	0.458287809162	-1.578823840206	-0.722589547572
F	1.013536509497	0.131522542159	-1.590847849896
Cl	2.629254126867	-1.066655448182	0.018799295617

Atom	X	Y	Z
C	1.290035075286	0.236875793944	-0.441964136953
C	-0.241532031110	0.213786621708	-0.589404189249
C	-0.993048655090	-0.517282354430	0.533675579883
Cl	1.823966819975	0.670474166540	1.213419359308
Cl	2.007588555710	-1.320969642284	-0.969313062486
H	1.701234785178	0.995323169005	-1.101919187779
H	-0.478314967963	-0.242273674340	-1.550982543378
Cl	-0.828478568153	1.915766955960	-0.664501502842
H	-0.997569741815	0.061679552141	1.457119610557
Cl	-2.713695310338	-0.773909545886	0.073589482802
F	-0.423041961680	-1.722015042357	0.754260590136

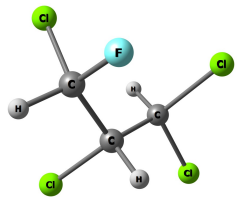
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
50.5095	0.152
74.2707	0.0455
146.4663	0.194
157.8137	0.131
196.0373	0.0185
219.7428	0.135
269.5287	0.0717
332.2479	0.238
379.2764	0.694
515.6170	5.82
620.2092	6.09
670.5906	4.46
723.7213	16.0
795.5019	4.09
831.0011	14.1
946.9508	2.36
1040.2074	7.68
1152.5611	11.7
1212.7755	1.86
1249.7315	1.39
1252.8170	3.42
1287.8470	4.67
1352.5873	1.54
1377.4018	2.37
3105.9963	0.602
3123.9277	0.574
3158.0072	0.259

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
54.6360	0.0572
70.5264	0.0240
139.3558	0.0473
167.5223	0.0847
195.0079	0.178
225.6582	0.129
317.4170	0.0671
352.4266	0.514
363.2287	2.62
442.7706	0.611
530.4348	5.97
678.9947	2.70
738.6459	20.4
817.9685	16.9
825.6382	4.86
963.1657	2.59
1097.1458	7.32
1131.3332	12.9
1204.9292	1.91
1225.8739	0.990
1262.9455	2.62
1280.9924	4.92
1338.2804	1.10
1390.9577	1.11
3121.0884	0.601
3134.2984	0.385
3160.0730	0.297



$\Delta E = 1.15$ kcal mol^{-1}
Population = 0.050



$\Delta E = 1.84$ kcal mol^{-1}
Population = 0.016

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	0.703466335728	-0.682945402408	-0.266473467824
C	-0.103543427183	0.604998653621	-0.473351893946
C	-1.571997958020	0.541113755538	-0.032533497178
Cl	2.239883012431	-0.598303699584	-1.192688544812
Cl	1.014226863930	-1.084566274391	1.442182997158
H	0.144877021902	-1.516682673921	-0.686140637638
H	-0.100233928565	0.815766282825	-1.543655828823
Cl	0.646586750203	2.032672943087	0.321542101500
H	-2.070465146140	1.484413288266	-0.261033444087
Cl	-2.445654908285	-0.722089877612	-1.000684805558
F	-1.710745616002	0.263414004579	1.273565021208

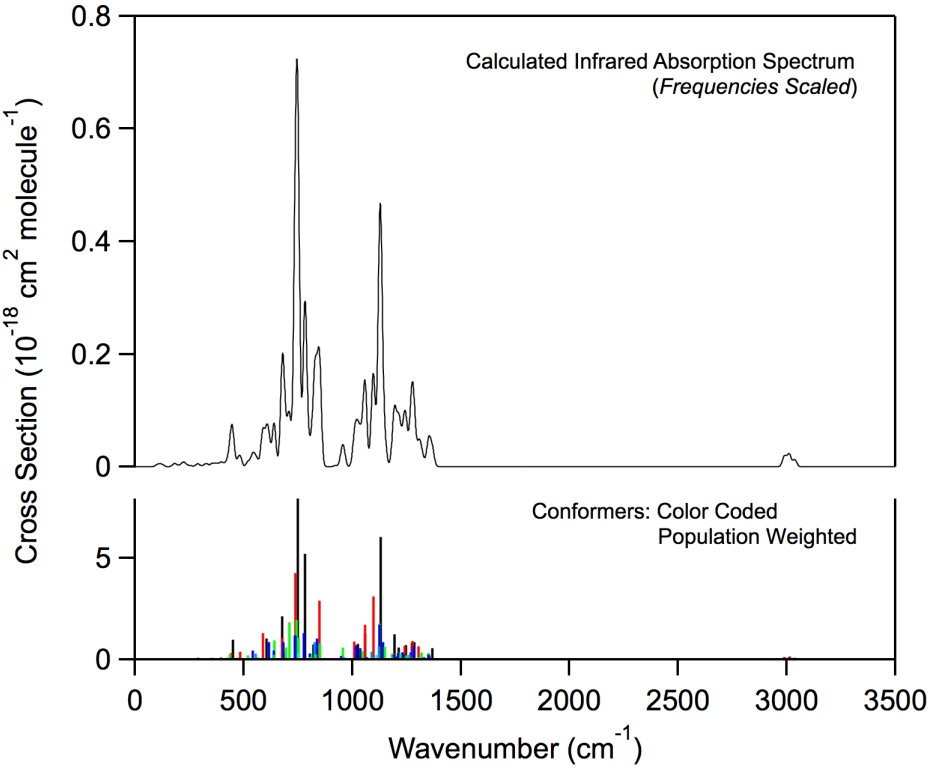
Atom	X	Y	Z
C	-0.904652098707	-0.183097703571	-0.392503440413
C	0.069253966054	0.394227843635	0.642244397572
C	1.496252509578	-0.190597100766	0.654299548989
Cl	-1.028317080785	-1.963942772794	-0.228094313663
Cl	-2.530607442846	0.548944205394	-0.210728589454
H	-0.570934224742	0.022746412614	-1.405695577182
H	-0.339239595323	0.253670043256	1.645106250113
Cl	0.230573598329	2.172211319219	0.385817149601
H	2.156811862844	0.480719021245	1.204385832078
F	1.500152007363	-1.401354224878	1.251541286851
Cl	2.207762498235	-0.338439043353	-0.994158544493

Infrared Absorption Spectrum (unscaled frequencies)

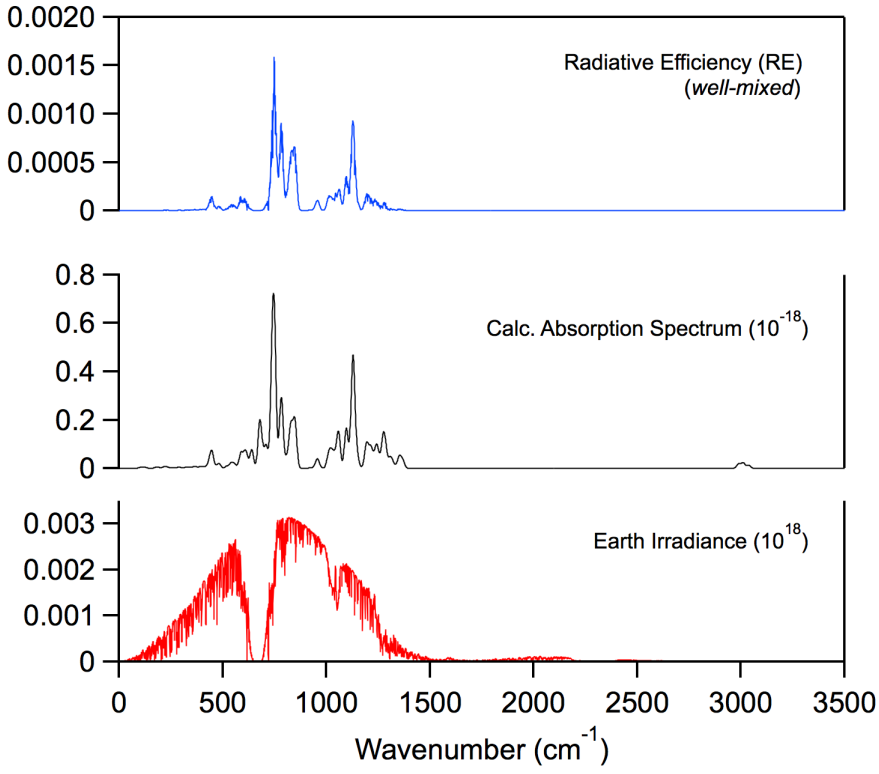
Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
41.1461	0.142
87.2115	0.0463
144.8535	0.274
166.3728	0.0709
171.8180	0.0363
250.9708	0.0274
282.7575	0.365
293.1972	0.319
388.3406	0.301
494.2331	3.87
621.7442	4.98
677.8436	11.8
739.0153	21.5
804.1896	2.56
822.1348	5.43
919.9566	0.828
1051.6097	8.03
1162.3191	12.7
1220.7564	0.781
1236.8018	5.51
1270.0234	4.39
1295.1232	1.27
1325.9866	2.10
1400.7529	1.44
3111.4543	1.17
3119.0851	0.138
3147.5048	0.271

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
49.5401	0.0476
76.5016	0.0512
146.8143	0.116
175.5105	0.0366
207.2834	0.200
252.7208	0.136
292.2238	1.01
341.7669	0.352
368.7670	1.34
432.2184	0.223
542.3004	7.27
687.7002	5.87
740.4548	19.6
794.4380	7.75
829.5726	1.82
964.6009	4.98
1098.1737	5.22
1120.0647	14.9
1203.0545	1.19
1221.7054	1.15
1245.0351	3.78
1289.7715	6.03
1363.4115	2.62
1377.3143	0.517
3107.4944	0.419
3117.3009	0.671
3167.2466	0.315

Infrared Spectrum

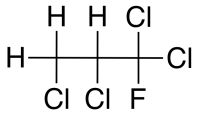


Radiative Efficiency



HCFC-241db

Molecular Formula:	$CH_2ClCHClCCl_2F$
Name:	1,1,2,3-Tetrachloro-1-fluoropropane
CAS number:	666-27-3
Molecular Weight:	199.87



Global Atmospheric Lifetime (years):	0.528
Tropospheric Atmospheric Lifetime (years):	0.549
Stratospheric Atmospheric Lifetime (years):	20
Ozone Depletion Potential (ODP):	0.014

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.193	0.119
Global Warming Potential (GWP_H):		
GWP_{20}	115	71
GWP_{100}	31	19
Global Temperature Potentials (GTP_H)		
GTP_{20}		22
GTP_{50}		3
GTP_{100}		3

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 1.07 \times 10^{-13}$; $k_{SAR}(272\ K) \approx 0.682 \times 10^{-13}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 0.534$ years

$\tau^{OH}_{Trop} = 0.549$ years

$\tau^{OH}_{Strat} = 20$ years

Fractional Atmospheric Loss: 0.988

$O(^1D)$ Reactivity

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

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

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

Fractional Atmospheric Loss: 0.003

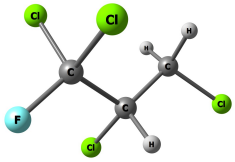
UV Photolysis

UV Spectrum: *No Recommendation*

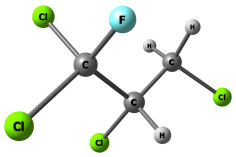
$\tau_{hv} = 60$ years

Fractional Atmospheric Loss: 0.009

Molecular Structure and Infrared Spectrum (5 conformers)



E = 0
Population = 0.526



$\Delta E = 0.58$ kcal mol^{-1}
Population = 0.196

Optimized Coordinates (Angstroms)

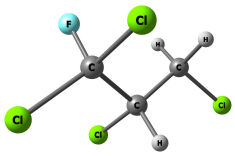
Atom	X	Y	Z
C	1.185683906591	-0.771560294058	0.532274952124
C	0.406992602758	0.073441166361	-0.469412186512
C	-1.123259303472	0.017779664213	-0.266954687703
Cl	2.886334470159	-1.006974675767	0.000316730616
H	1.210702047459	-0.295287988193	1.510500943701
H	0.741535423091	-1.763213166997	0.612806960105
H	0.590765719527	-0.273045764434	-1.487549339922
Cl	0.944750388780	1.790032648686	-0.420805008927
Cl	-1.700155417943	-1.654364488393	-0.641706918536
Cl	-1.619058018300	0.459383108735	1.397232219019
F	-1.726122818649	0.844952789847	-1.120596663965

Atom	X	Y	Z
C	1.450907425893	-0.855305085389	-0.073350917927
C	0.405985814442	0.222053744527	-0.361904681024
C	-1.022973071829	-0.368758760706	-0.323704770026
Cl	3.091518627088	-0.320499943693	-0.573875284877
H	1.491499093501	-1.092294353478	0.988069997048
H	1.220600720249	-1.752176700765	-0.647405348706
H	0.540531080603	0.610105532955	-1.373190884431
Cl	0.578665732539	1.612255764037	0.750715752293
Cl	-1.444253700278	-1.052604309638	1.278450571437
Cl	-2.245774556250	0.839457344879	-0.814184716485
F	-1.061035165959	-1.372737232729	-1.222456717302

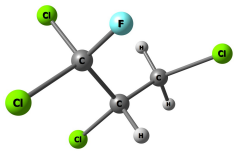
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
65.6876	0.0202
72.8042	0.323
147.8188	0.253
179.3175	0.205
220.1786	0.241
241.1715	0.117
279.6148	0.203
344.8266	0.0164
381.1716	0.165
431.8577	1.23
490.7744	0.624
631.4899	9.72
690.4954	11.4
765.3526	8.06
807.5024	27.7
940.5204	3.08
1040.2784	10.1
1067.5342	2.10
1160.7171	10.3
1193.1815	3.96
1272.1670	4.89
1281.3607	2.41
1345.7514	2.09
1467.9063	0.994
3107.6611	1.18
3116.1161	0.241
3176.8908	0.0108

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
63.1838	0.0130
79.0305	0.413
138.3416	0.296
169.9590	0.0699
213.4327	0.0749
252.3481	0.375
283.0084	0.0667
362.2043	0.245
382.3455	0.0182
426.1817	1.84
492.6877	0.391
608.5949	10.1
724.7032	8.62
750.0902	12.0
856.8215	19.5
948.3614	3.98
1024.5835	12.1
1068.1977	6.55
1122.2123	12.8
1179.4269	0.411
1269.4067	3.77
1284.7835	1.67
1343.0125	2.16
1469.2801	0.755
3106.7966	1.08
3111.4042	0.111
3177.4284	0.0302



$\Delta E = 0.66$ kcal mol^{-1}
Population = 0.173



$\Delta E = 1.14$ kcal mol^{-1}
Population = 0.077

Optimized Coordinates (Angstroms)

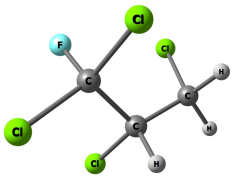
Atom	X	Y	Z
C	1.405114793923	-0.795920248201	0.358013292197
C	0.392506590489	0.150813576492	-0.289862219949
C	-1.046047361759	-0.158682981764	0.183880527824
Cl	3.025433852749	-0.638316758804	-0.400140050223
H	1.512018546940	-0.577569482430	1.419371556240
H	1.097620347344	-1.830957030981	0.220519440534
H	0.420343370005	0.072172997374	-1.375718133028
Cl	0.805782314805	1.853237467903	0.126248301395
Cl	-2.246082994887	0.977013364622	-0.494924604138
Cl	-1.499267679970	-1.831530469188	-0.339554605313
F	-1.112901779639	-0.112768435024	1.518979494460

Atom	X	Y	Z
C	1.637346894887	0.803815683341	0.210429205892
C	0.261306115456	0.704602310931	-0.455009773443
C	-0.549882054397	-0.559727946421	-0.082261728539
Cl	2.849143625842	-0.305473060782	-0.531993828403
H	2.020231471584	1.812445740981	0.071405878643
H	1.582997982430	0.576997080841	1.274306302011
H	0.364743416209	0.697154353922	-1.541019252075
Cl	-0.654389629176	2.194606737319	-0.032711642971
Cl	-0.887712609782	-0.666136969144	1.676992183533
Cl	-2.091069162245	-0.620490151223	-0.999079149965
F	0.165711949192	-1.637588779765	-0.427116194681

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
54.5152	0.0361
73.1322	0.399
152.9961	0.436
178.3397	0.0570
237.2189	0.160
251.6200	0.0403
279.4648	0.347
303.1598	0.143
378.5747	0.134
435.3377	1.84
453.3695	0.596
682.4343	12.9
701.1347	11.0
785.2852	18.3
839.8702	10.9
933.4030	5.79
967.4884	6.42
1055.1176	3.91
1165.1044	10.8
1182.4152	3.40
1277.1287	2.85
1280.0064	1.61
1343.0473	3.12
1470.6960	0.931
3110.6211	0.728
3138.9024	0.296
3178.3125	0.0149

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
37.5938	0.115
104.4024	0.302
163.4776	0.113
173.8309	0.181
198.7934	0.189
251.3776	0.0108
295.8135	0.0786
360.2072	1.00
372.5474	0.00252
412.0936	2.91
487.3318	0.579
557.2346	4.75
736.1236	12.6
793.2188	24.7
829.7692	6.71
905.7220	9.99
1021.7326	5.36
1086.4548	7.78
1145.0174	13.6
1188.0094	2.28
1226.3921	1.06
1309.9030	3.60
1350.0600	0.717
1473.9352	1.55
3111.7401	0.242
3118.9428	0.503
3179.7610	0.0236



$\Delta E = 1.82$ kcal mol^{-1}
Population = 0.024

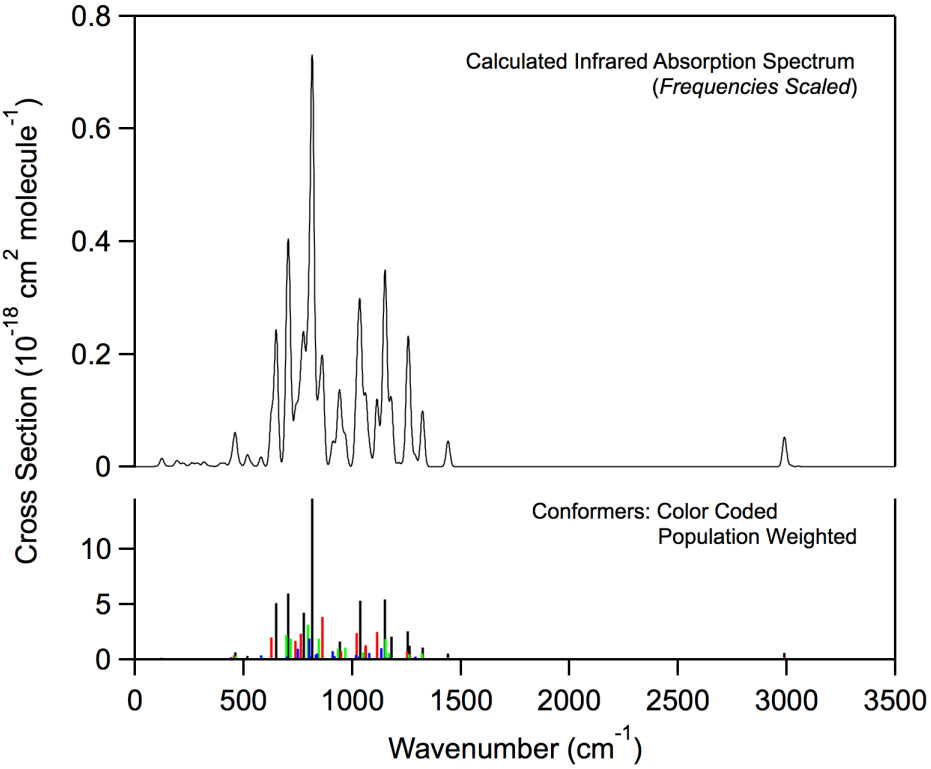
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.538229646839	-0.415385158057	-0.983749409776
C	0.272169496202	0.409226410411	-0.751758168238
C	-0.792346561424	-0.215270383352	0.179462193612
Cl	2.504619830447	-0.765033694202	0.488148046425
H	1.276790386961	-1.374142299117	-1.429493153697
H	2.184669206666	0.138413085597	-1.663661350745
H	-0.203928221682	0.547433130073	-1.724514892040
Cl	0.693354570335	2.054793308412	-0.156152833516
Cl	-2.316269041762	0.735818141898	0.125085544422
Cl	-1.161350529741	-1.897085716685	-0.372002258189
F	-0.378173782842	-0.271172824979	1.440770281742

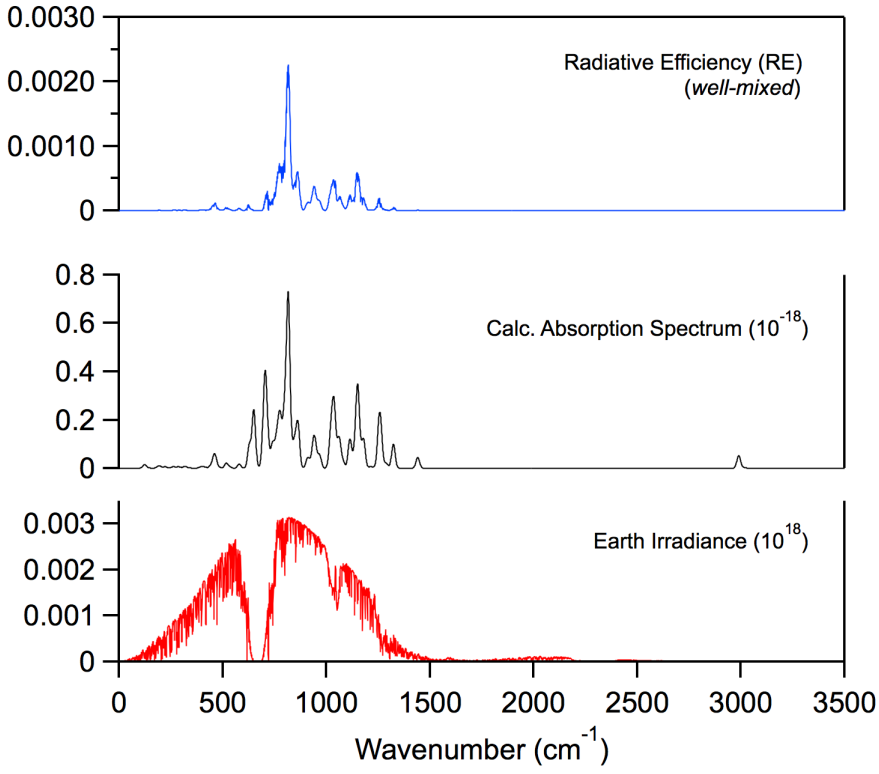
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
47.7241	0.0680
88.8574	0.0573
156.7245	0.0339
182.6552	0.130
224.6712	0.0541
255.9594	0.139
310.1086	0.347
325.3366	0.329
379.4161	0.156
430.1056	1.17
510.0930	4.61
666.0393	3.00
682.6800	10.9
796.0152	14.4
823.9333	17.4
916.0814	12.4
967.7365	1.10
1034.9429	10.3
1171.1477	6.17
1229.4967	2.77
1249.0819	3.71
1304.3800	6.78
1350.2668	1.84
1463.1671	2.11
3100.7840	0.766
3110.4223	0.529
3166.3388	0.0516

Infrared Spectrum

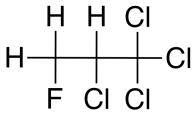


Radiative Efficiency



HCFC-241dc

Molecular Formula:	$CH_2FCHClCCl_3$
Name:	1,1,1,2-Tetrachloro-3-fluoropropane
CAS number:	84816-05-7
Molecular Weight:	199.87



Global Atmospheric Lifetime (years):	0.750
Tropospheric Atmospheric Lifetime (years):	0.786
Stratospheric Atmospheric Lifetime (years):	20
Ozone Depletion Potential (ODP):	0.019

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.167	0.115
Global Warming Potential (GWP_H):		
GWP_{20}	141	97
GWP_{100}	38	26
Global Temperature Potentials (GTP_H)		
GTP_{20}		31
GTP_{50}		5
GTP_{100}		4

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

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

OH Reactivity

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

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

τ^{OH}_{Global} = 0.764 years
τ^{OH}_{Trop} = 0.786 years
τ^{OH}_{Strat} = 27.2 years

Fractional Atmospheric Loss: 0.981

O(^{1}D) Reactivity

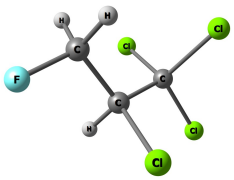
k_{Rec}(T), *No recommendation*

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

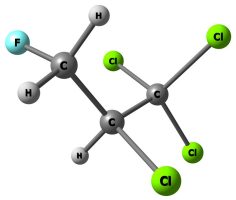
UV Photolysis

UV Spectrum: *No Recommendation*
τ_{hv} = 50 years
Fractional Atmospheric Loss: 0.015

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.520



$\Delta E = 0.31$ kcal mol^{-1}
Population = 0.308

Optimized Coordinates (Angstroms)

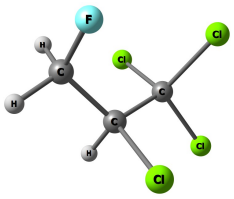
Atom	X	Y	Z
C	1.627624145704	-1.169273535530	0.181867002681
C	0.788959932530	-0.046711585384	-0.437384053118
C	-0.702839112812	-0.071620532548	-0.036745237810
H	1.158752178340	-2.139073922174	-0.008903132018
F	2.864535177658	-1.151227704970	-0.409496198530
H	1.737751209862	-1.017086822433	1.258951986059
H	0.826830796652	-0.129124548710	-1.524875244102
Cl	1.548317862425	1.532629172296	-0.029044593510
Cl	-1.594861088282	1.272010646639	-0.805779313034
Cl	-1.414447463973	-1.619420952702	-0.639181090381
Cl	-0.914283638105	0.011031785515	1.738313873764

Atom	X	Y	Z
C	1.898722697223	-0.886188350270	0.056589905415
C	0.878627348430	0.102645749985	-0.529728024108
C	-0.568358797433	-0.003042504162	0.013512729262
H	1.845635857627	-0.892862132619	1.149381432586
F	1.683671701660	-2.152963712816	-0.423445999504
H	2.895010155243	-0.559087576089	-0.254158625519
H	0.819644128709	-0.029764748833	-1.611201289314
Cl	1.542926947085	1.753010062256	-0.241112170961
Cl	-1.615623559470	1.216018110087	-0.783111015059
Cl	-1.218906230209	-1.628556413293	-0.377759831118
Cl	-0.630216248866	0.236750515753	1.787334888320

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
67.7960	0.0941
93.9647	0.547
157.0533	0.202
166.5394	0.0440
231.3341	0.0897
244.6000	0.406
272.1186	0.101
284.5407	0.123
328.2864	0.376
401.9578	0.0385
445.4429	2.41
628.8874	6.80
692.3582	14.2
766.8037	11.8
777.6176	20.2
1004.6688	3.05
1032.4104	2.84
1098.8908	1.34
1112.9363	13.4
1245.6536	0.822
1280.5462	1.25
1306.6271	1.76
1425.5395	1.04
1506.2180	0.435
3061.3206	2.35
3110.1600	0.363
3124.2623	1.54

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
39.5696	0.140
121.1703	0.570
164.9146	0.00990
189.7330	0.159
207.2041	0.222
230.5113	0.0448
273.6027	0.0940
301.5543	0.154
346.6010	0.530
396.1907	0.184
439.0628	4.03
550.0937	3.74
745.3945	24.3
765.0575	19.5
832.3887	1.66
915.8560	1.24
1075.8238	8.32
1084.7144	1.97
1111.0423	9.98
1217.6709	0.622
1270.1529	0.340
1346.2845	0.814
1423.6482	1.32
1505.1367	0.885
3060.1516	1.92
3109.7550	1.62
3123.0582	0.570



$\Delta E = 0.66$ kcal mol^{-1}
Population = 0.172

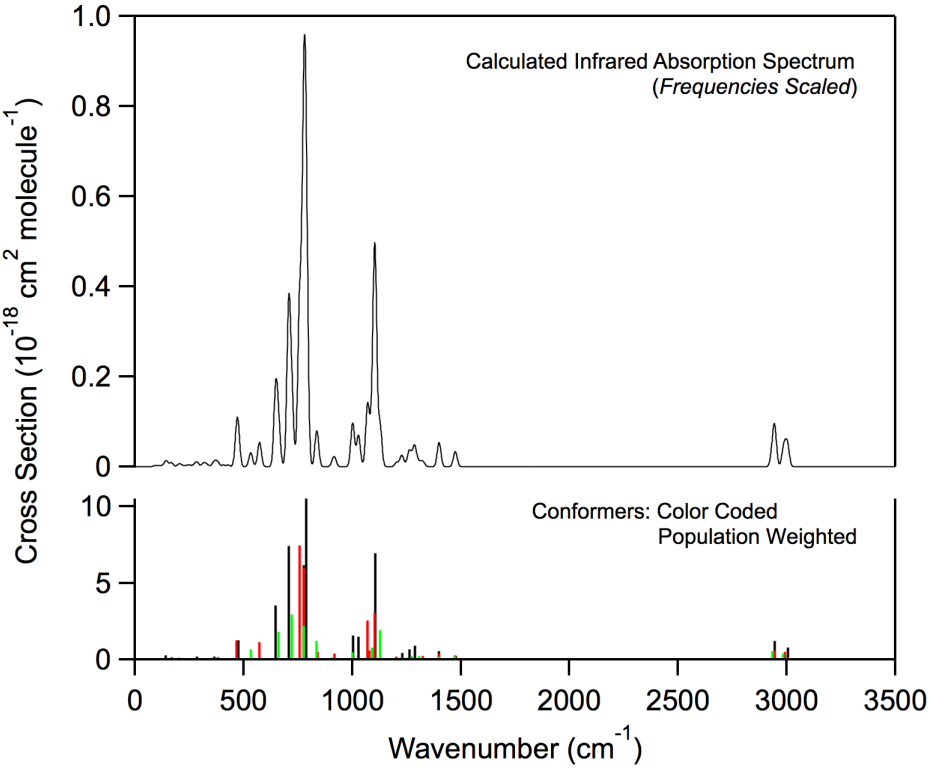
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.609835396749	-1.120513474812	-0.801363833190
C	0.723210545597	0.127071193411	-0.759786849538
C	-0.631461540615	-0.017780740767	-0.019920557442
H	2.439630805633	-0.912825141158	-1.485764599185
F	2.118136692521	-1.431487309480	0.429043126973
H	1.035487228358	-1.972155757296	-1.179118621936
H	0.473391583008	0.394455551508	-1.788746552161
Cl	1.676021439875	1.500523609255	-0.094538867123
Cl	-1.588729216316	1.489189141979	-0.194558553064
Cl	-1.557370285246	-1.345307124007	-0.827859514627
Cl	-0.445541649563	-0.405170948633	1.705614821292

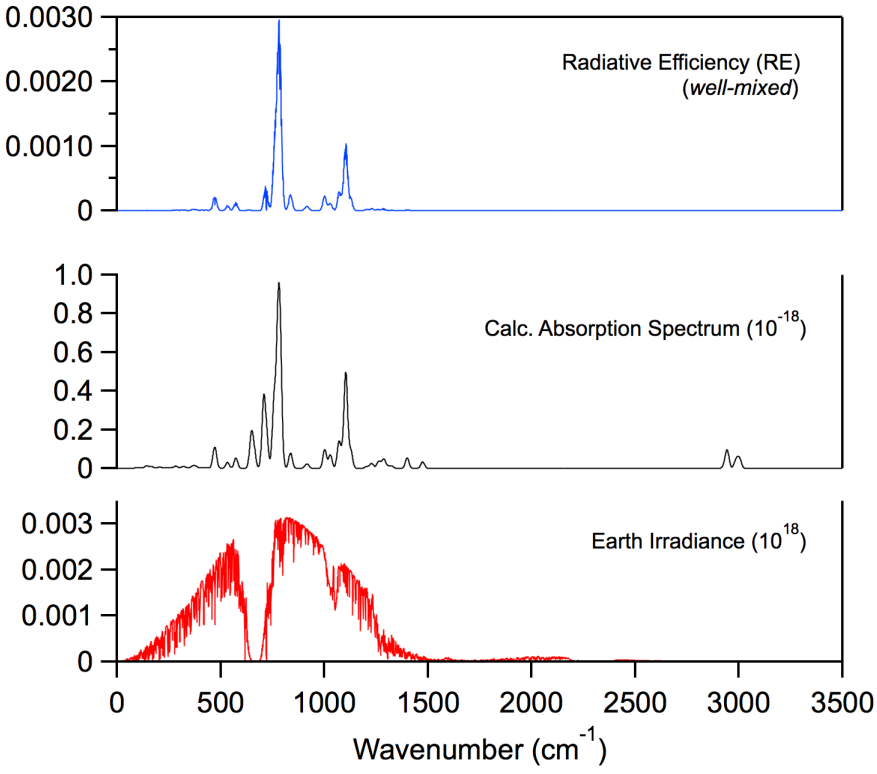
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
54.9095	0.197
109.7914	0.214
168.2764	0.150
174.2676	0.0677
218.0515	0.0621
240.3354	0.0338
284.0191	0.506
294.4992	0.0302
337.8594	0.554
374.0050	0.421
507.1803	3.79
643.0398	10.5
707.8015	17.1
765.9371	12.8
828.1760	7.11
906.4135	0.947
1001.9912	2.83
1100.6062	4.51
1137.4827	11.3
1236.6954	0.910
1294.0542	1.30
1327.0335	1.33
1427.4901	1.26
1500.9677	1.35
3048.3586	3.13
3101.7176	2.41
3103.8908	0.120

Infrared Spectrum

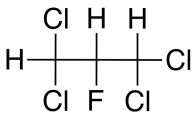


Radiative Efficiency



HCFC-241ea

Molecular Formula:	$CHCl_2CHFCHCl_2$
Name:	1,1,3,3-Tetrachloro-2-fluoropropane
CAS number:	–
Molecular Weight:	199.87



Global Atmospheric Lifetime (years):	0.416
Tropospheric Atmospheric Lifetime (years):	0.429
Stratospheric Atmospheric Lifetime (years):	20
Ozone Depletion Potential (ODP):	0.011

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.144	0.081
Global Warming Potential (GWP_H):		
GWP_{20}	68	38
GWP_{100}	18	10
Global Temperature Potentials (GTP_H)		
GTP_{20}		12
GTP_{50}		2
GTP_{100}		1

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 1.37 \times 10^{-13}$; $k_{SAR}(272\ K) \approx 0.872 \times 10^{-13}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 0.420$ years

$\tau^{OH}_{Trop} = 0.429$ years

$\tau^{OH}_{Strat} = 20$ years

Fractional Atmospheric Loss: 0.990

$O(^1D)$ Reactivity

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

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

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

Fractional Atmospheric Loss: 0.002

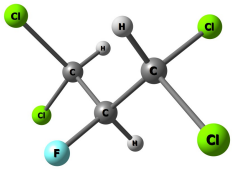
UV Photolysis

UV Spectrum: *No Recommendation*

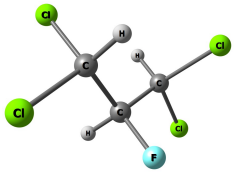
$\tau_{hv} = 50$ years

Fractional Atmospheric Loss: 0.008

Molecular Structure and Infrared Spectrum (2 conformers)



E = 0
Population = 0.500



E = 0
Population = 0.500

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.230866902566	-0.315416989899	0.284099795507
C	0.013066246578	0.583279219108	0.265675769620
C	1.278760842041	-0.132983253635	-0.231680678704
Cl	-2.606181455812	0.594071989258	0.980795914249
Cl	-1.627269318860	-0.913651613521	-1.359028490751
H	-1.075430145304	-1.187613327445	0.911913149159
H	0.185337060198	0.944240707188	1.286047022403
F	-0.216867300366	1.647792214075	-0.556710465752
H	1.149803594952	-0.520931938519	-1.238736669349
Cl	2.642585462785	1.018939121774	-0.278255761932
Cl	1.654521916354	-1.526705128382	0.834846415548

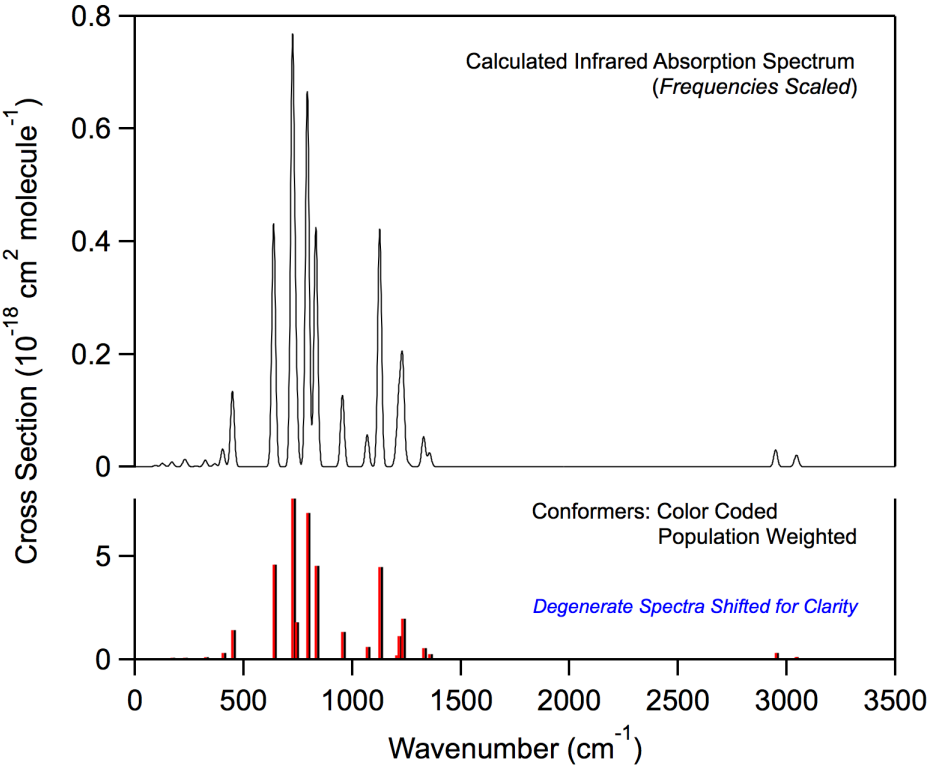
Atom	X	Y	Z
C	-1.279539474419	-0.132989095143	-0.242617425950
C	-0.015674401188	0.567957200414	0.280542802517
C	1.230278680972	-0.328030214043	0.267600886365
Cl	-1.652583454888	-1.564639438698	0.773430042368
Cl	-2.645948484840	1.016793688481	-0.248822437029
H	-1.149290208690	-0.484547569533	-1.262782965314
H	-0.189187882084	0.891995177338	1.313025604036
F	0.212199343903	1.661571256241	-0.503331459679
H	1.076555485102	-1.222355539585	0.863912744526
Cl	1.628707955623	-0.866544601930	-1.395573704807
Cl	2.603244440508	0.559189136458	0.996881912967

Infrared Absorption Spectrum (unscaled frequencies)

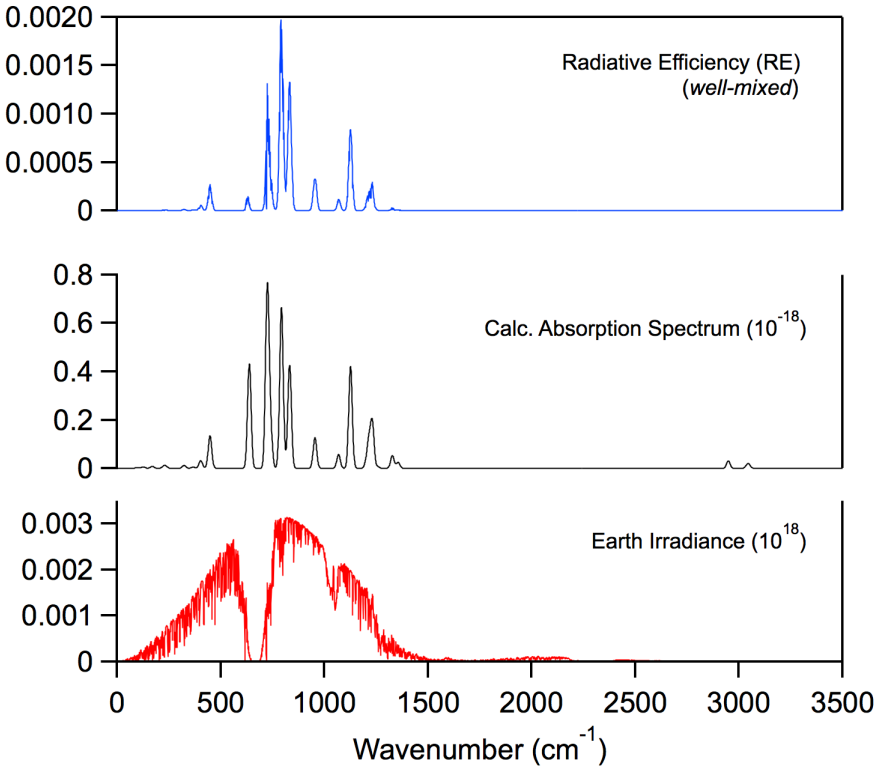
Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
43.5898	0.0491
76.8703	0.128
122.8285	0.178
183.6760	0.204
192.5584	0.111
241.4946	0.0221
285.6361	0.245
331.8208	0.110
370.3562	0.672
417.9621	2.87
618.8994	9.21
710.4310	15.6
726.4470	3.60
783.1102	14.2
824.6936	9.06
954.1455	2.71
1074.7120	1.21
1135.8259	8.99
1216.5238	0.436
1229.6458	2.29
1246.9986	3.95
1273.9407	0.153
1349.7336	1.13
1378.7838	0.522
3065.7007	0.645
3162.8293	0.229
3170.9705	0.256

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
43.5913	0.0491
76.8714	0.128
122.8284	0.178
183.6764	0.204
192.5589	0.111
241.4946	0.0221
285.6359	0.245
331.8204	0.110
370.3577	0.672
417.9610	2.87
618.8995	9.21
710.4304	15.6
726.4479	3.60
783.1101	14.2
824.6933	9.06
954.1466	2.71
1074.7130	1.21
1135.8259	8.99
1216.5229	0.436
1229.6448	2.29
1246.9967	3.95
1273.9395	0.153
1349.7332	1.13
1378.7825	0.522
3065.6990	0.645
3162.8294	0.229
3170.9718	0.256

Infrared Spectrum

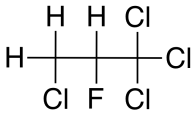


Radiative Efficiency



HCFC-241eb

Molecular Formula: $CH_2ClCHFCCl_3$
Name: 1,1,1,3-Tetrachloro-2-fluoropropane
CAS number: –
Molecular Weight: 199.87



Global Atmospheric Lifetime (years): 1.05
  Tropospheric Atmospheric Lifetime (years): 1.11
  Stratospheric Atmospheric Lifetime (years): 20
Ozone Depletion Potential (ODP): 0.027

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.166	0.125
Global Warming Potential (GWP_H):		
GWP_{20}	196	147
GWP_{100}	53	40
Global Temperature Potentials (GTP_H)		
GTP_{20}		48
GTP_{50}		7
GTP_{100}		6

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

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

OH Reactivity

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

k_{SAR}(298 K) = 5.28×10^{-14}; k_{SAR}(272 K) ≈ 3.37×10^{-14} cm^3 $molecule^{-1}$ s^{-1}

τ^{OH}_{Global} = 1.08 years
τ^{OH}_{Trop} = 1.11 years
τ^{OH}_{Strat} = 37.1 years

Fractional Atmospheric Loss: 0.973

O(^{1}D) Reactivity

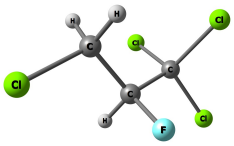
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 2.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)}$ = 185 years
Fractional Atmospheric Loss: 0.006

UV Photolysis

UV Spectrum: *No Recommendation*
τ_{hv} = 50 years
Fractional Atmospheric Loss: 0.021

Molecular Structure and Infrared Spectrum (1 conformer)



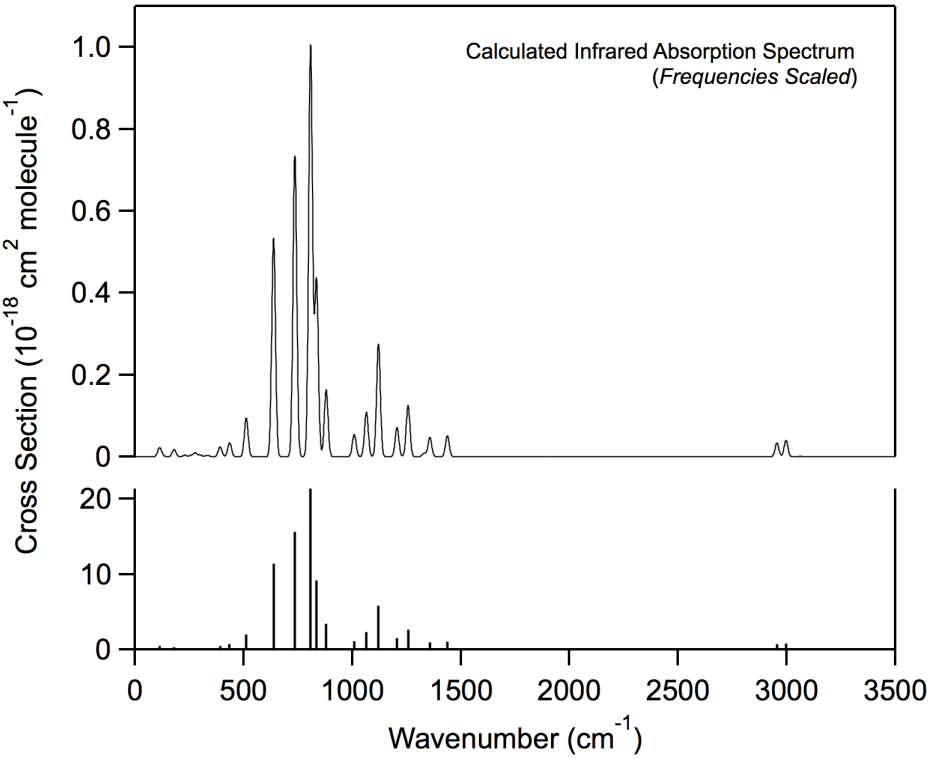
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.621823411015	0.539858676243	0.332035195940
C	-0.582132359299	-0.314985864567	-0.383281721531
C	0.884057487791	0.070757463693	-0.051128415807
Cl	-3.263056582538	0.149466796748	-0.294541202812
H	-1.622671456925	0.325099358370	1.399352059396
H	-1.452588129453	1.600673418379	0.160786708909
H	-0.691216883519	-0.223772542333	-1.469275053123
F	-0.757705421822	-1.622096545573	-0.027178495185
Cl	1.980630883556	-1.058803260996	-0.898704692322
Cl	1.198035473272	1.738988245671	-0.633101963324
Cl	1.188957399952	-0.025817745636	1.709688579859

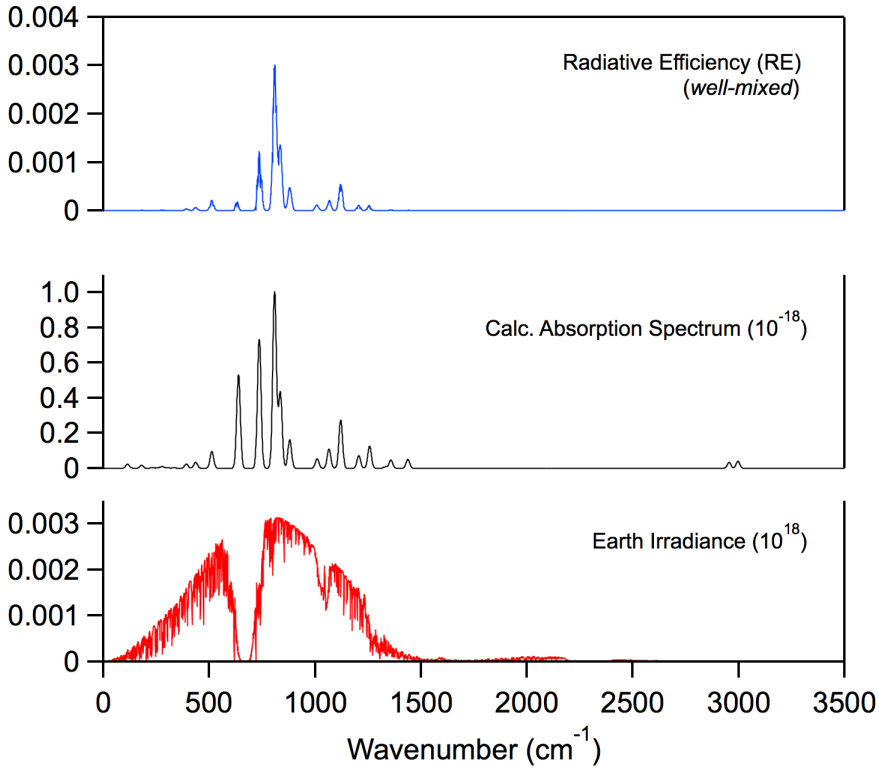
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
62.9864	0.472
78.0210	0.0404
133.6423	0.372
186.6612	0.0792
217.5965	0.0743
237.9374	0.197
262.3662	0.0802
295.6959	0.0778
357.9075	0.514
404.3347	0.728
485.2908	2.01
618.7343	11.4
722.3685	15.7
798.9665	21.4
827.6605	9.19
874.8815	3.48
1011.6137	1.16
1071.0209	2.32
1129.8695	5.86
1220.2428	1.52
1274.1531	2.68
1352.4645	0.174
1380.4899	0.998
1465.6813	1.09
3072.2592	0.713
3116.4824	0.853
3186.0748	0.0178

Infrared Spectrum

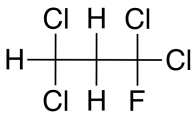


Radiative Efficiency



HCFC-241fa

Molecular Formula:	$CHCl_2CH_2CCl_2F$
Name:	1,1,3,3-Tetrachloro-1-fluoropropane
CAS number:	175897-94-6
Molecular Weight:	199.87



Global Atmospheric Lifetime (years):	0.533
Tropospheric Atmospheric Lifetime (years):	0.555
Stratospheric Atmospheric Lifetime (years):	20
Ozone Depletion Potential (ODP):	0.014

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.190	0.117
Global Warming Potential (GWP_H):		
GWP_{20}	114	70
GWP_{100}	31	19
Global Temperature Potentials (GTP_H)		
GTP_{20}		22
GTP_{50}		3
GTP_{100}		2

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 1.06 \times 10^{-13}$; $k_{SAR}(272\ K) \approx 0.674 \times 10^{-13}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 0.540$ years
$\tau^{OH}_{Trop} = 0.555$ years
$\tau^{OH}_{Strat} = 20$ years

Fractional Atmospheric Loss: 0.986

O(^{1}D) Reactivity

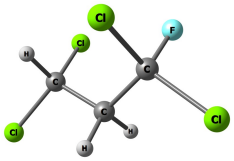
k_{Rec}(T), *No recommendation*

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

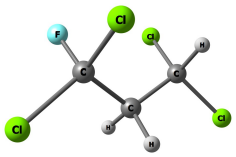
UV Photolysis

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

Molecular Structure and Infrared Spectrum (2 conformers)



E = 0
Population = 0.500



E = 0
Population = 0.500

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.360508601040	0.040930692194	0.319181708638
C	0.117265388856	0.743638807959	-0.226893780146
C	-1.188912207305	-0.047625146353	-0.119984986916
Cl	1.862867225098	-1.354743235038	-0.686055948419
Cl	2.697908397402	1.241922059593	0.425392369028
H	1.212506723778	-0.339328491668	1.326122206738
H	0.268426500969	0.993677125424	-1.280120759036
H	-0.018420407426	1.673103730760	0.328655419981
Cl	-1.542975182739	-0.507602420152	1.590167956134
Cl	-2.538178102923	0.975908665791	-0.738915390889
F	-1.163107936749	-1.167404788509	-0.845859795114

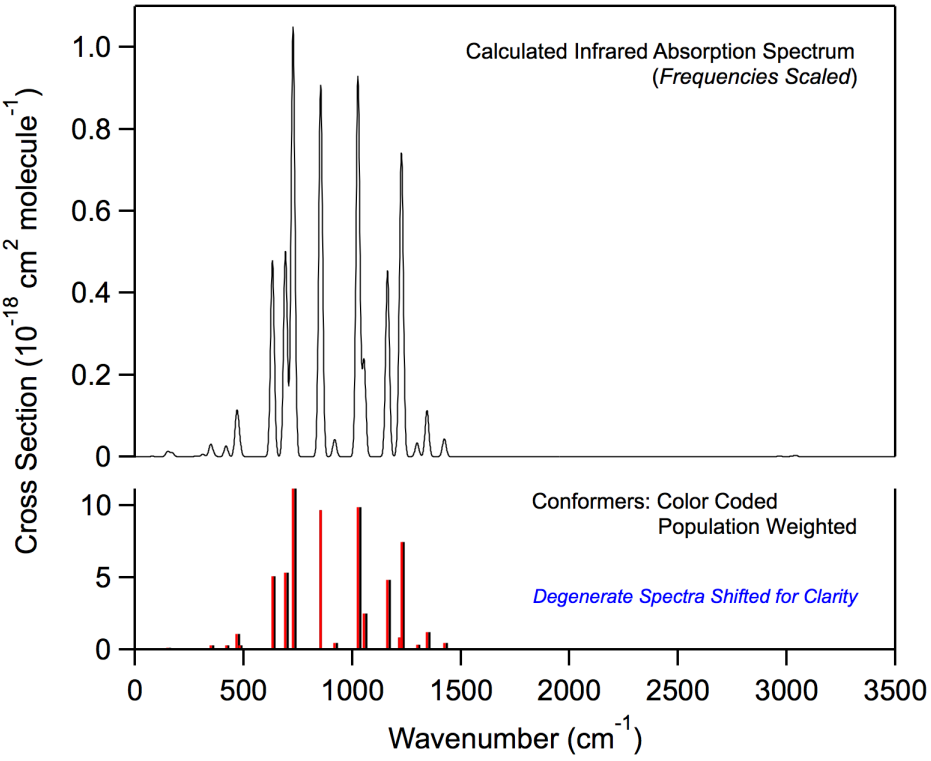
Atom	X	Y	Z
C	1.362323256990	-0.020810780017	0.337437368601
C	0.122119804010	-0.763083595772	-0.161138579141
C	-1.185869570565	0.031030371552	-0.114524487183
Cl	2.701637091128	-1.208438236252	0.532579842408
Cl	1.865215407663	1.301097756941	-0.762757183385
H	1.210447798304	0.429599256359	1.314420495553
H	-0.013557278421	-1.651091690743	0.458525925038
H	0.277045345463	-1.086868697692	-1.193522879914
Cl	-2.531265874862	-1.036646024191	-0.663331745513
Cl	-1.546143461079	0.610390211742	1.557631643441
F	-1.159897518631	1.096562428072	-0.917913399906

Infrared Absorption Spectrum (unscaled frequencies)

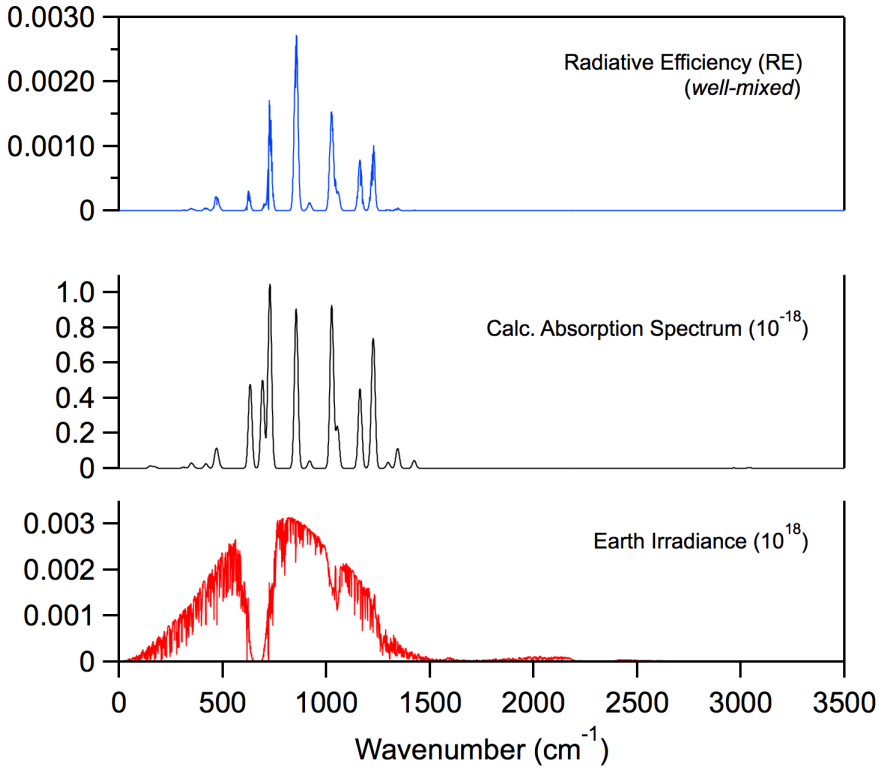
Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
28.0098	0.0237
102.5541	0.282
124.7297	0.198
189.5550	0.0116
240.2851	0.0309
273.1659	0.125
311.7866	0.605
325.3624	0.122
386.9372	0.558
439.3935	2.18
451.4575	0.582
612.9835	10.2
676.4630	10.7
713.4340	22.4
848.0825	19.4
916.3366	0.897
1029.7289	19.8
1059.0975	5.01
1173.9129	9.67
1232.0216	1.66
1242.4222	14.9
1318.0734	0.711
1366.3423	2.39
1450.8123	0.931
3084.1912	0.0427
3141.0059	0.0191
3163.2122	0.0761

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
28.0089	0.0237
102.5540	0.282
124.7293	0.198
189.5551	0.0116
240.2852	0.0309
273.1660	0.125
311.7869	0.605
325.3624	0.122
386.9375	0.558
439.3933	2.18
451.4575	0.582
612.9836	10.2
676.4639	10.7
713.4337	22.4
848.0832	19.4
916.3372	0.897
1029.7299	19.8
1059.0973	5.01
1173.9133	9.67
1232.0235	1.66
1242.4229	14.9
1318.0743	0.711
1366.3431	2.39
1450.8132	0.931
3084.1905	0.0427
3141.0051	0.0191
3163.2096	0.0761

Infrared Spectrum

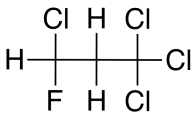


Radiative Efficiency



HCFC-241fb

Molecular Formula:	$CHClFCH_2CCl_3$
Name:	1,1,1,3-Tetrachloro-3-fluoropropane
CAS number:	23153-22-2
Molecular Weight:	199.87



Global Atmospheric Lifetime (years):	1.48
Tropospheric Atmospheric Lifetime (years):	1.59
Stratospheric Atmospheric Lifetime (years):	22.2
Ozone Depletion Potential (ODP):	0.037

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.189	0.152
Global Warming Potential (GWP_H):		
GWP_{20}	316	254
GWP_{100}	86	69
Global Temperature Potentials (GTP_H)		
GTP_{20}		87
GTP_{50}		12
GTP_{100}		10

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 3.69 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 2.36 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 1.54$ years

$\tau^{OH}_{Trop} = 1.59$ years

$\tau^{OH}_{Strat} = 51.1$ years

Fractional Atmospheric Loss: 0.962

O(^{1}D) Reactivity

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

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

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

Fractional Atmospheric Loss: 0.008

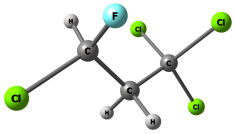
UV Photolysis

UV Spectrum: *No Recommendation*

$\tau_{hv} = 50$ years

Fractional Atmospheric Loss: 0.030

Molecular Structure and Infrared Spectrum (1 conformer)



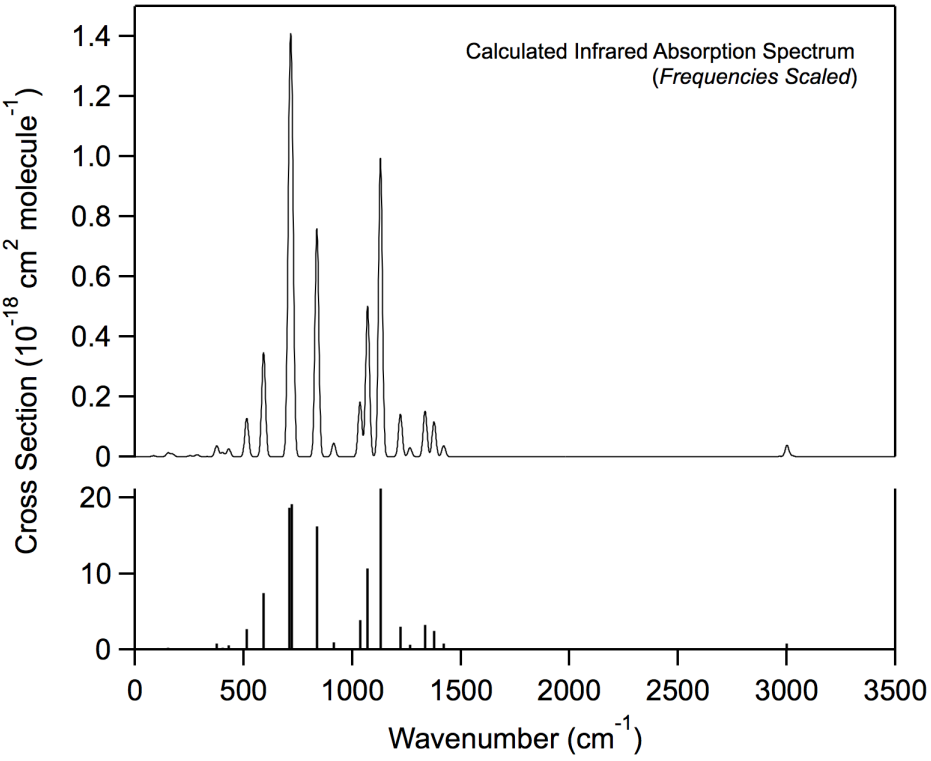
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.612272508757	0.162288267461	0.309804014367
C	0.472885589379	-0.586859268240	-0.375551301704
C	-0.945500284702	-0.118320946208	-0.018755275503
Cl	3.155604528948	-0.735331805007	0.003111444884
F	1.744736323882	1.414216947324	-0.180600608472
H	1.505881717728	0.209560176191	1.394036472113
H	0.538168814857	-1.641485527875	-0.102416252814
H	0.598325591864	-0.502964869106	-1.457923520832
Cl	-2.112187178190	-1.195093181605	-0.866818415921
Cl	-1.226685302945	-0.259744934560	1.755365831636
Cl	-1.254699309577	1.568568141624	-0.524126387755

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
33.7498	0.0677
104.5775	0.274
126.5890	0.185
210.6551	0.0500
213.2823	0.0244
245.8877	0.145
294.7702	0.0215
341.5441	0.787
369.9898	0.288
399.8935	0.554
487.7271	2.73
569.9786	7.41
695.8372	18.6
708.0349	19.2
829.7558	16.2
911.6431	0.961
1039.9755	3.87
1076.8980	10.7
1139.5911	21.2
1236.6379	3.02
1283.2448	0.641
1357.0653	3.25
1400.6197	2.48
1447.8301	0.783
3084.5813	0.0231
3121.1753	0.809
3145.1757	0.0791

Infrared Spectrum



Radiative Efficiency