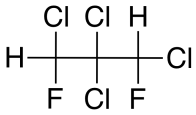
HCFC-232aa

Molecular Formula:	$CHClFCCl_2CHClF$
Name:	1,2,2,3-Tetrachloro-1,3-difluoropropane
CAS number:	–
Molecular Weight:	217.86



Global Atmospheric Lifetime (years): 1.65
Tropospheric Atmospheric Lifetime (years): 1.77
Stratospheric Atmospheric Lifetime (years): 24.9
Ozone Depletion Potential (ODP): 0.036

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.217	0.177
Global Warming Potential (GWP_H):		
GWP_{20}	370	303
GWP_{100}	100	82
Global Temperature Potentials (GTP_H)		
GTP_{20}		107
GTP_{50}		14
GTP_{100}		11

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 3.32 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 2.12 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 1.71$ years
$\tau^{OH}_{Trop} = 1.77$ years
$\tau^{OH}_{Strat} = 56.4$ years

Fractional Atmospheric Loss: 0.963

O(^{1}D) Reactivity

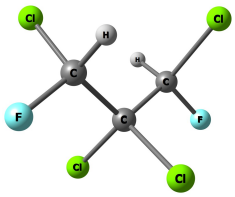
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 2.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)} = 185$ years
Fractional Atmospheric Loss: 0.009

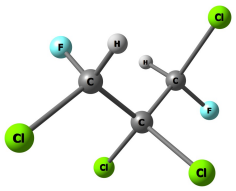
UV Photolysis

UV Spectrum: *No Recommendation*
$\tau_{hv} = 59$ years
Fractional Atmospheric Loss: 0.028

Molecular Structure and Infrared Spectrum (9 conformers)



E = 0
Population = 0.283



$\Delta E = 0.20$ kcal mol^{-1}
Population = 0.202

Optimized Coordinates (Angstroms)

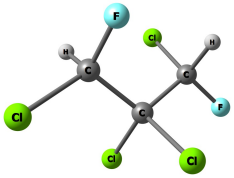
Atom	X	Y	Z
C	1.047115777398	-0.421082980440	0.757480209624
C	-0.006379128901	0.422463611571	0.003803305249
C	-1.055790367434	-0.414385514158	-0.762936507355
Cl	1.853720731194	-1.607854955105	-0.330940270520
F	1.978684300469	0.388176867991	1.285767364019
H	0.562953336277	-1.000713447360	1.543403471898
Cl	0.803547373628	1.468279921193	-1.207785230949
Cl	-0.821314819279	1.445382770918	1.231472124930
H	-0.568842847874	-0.979356826225	-1.557762650547
Cl	-1.856568402821	-1.621859541949	0.306857469320
F	-1.991311952658	0.398443093565	-1.278610285669

Atom	X	Y	Z
C	-0.896668539999	-0.916877417032	0.223769675262
C	0.003638532200	0.316244280551	-0.021218079247
C	1.406119907869	0.098093283490	0.607359766874
Cl	-2.585099358830	-0.678884957225	-0.294339480942
H	-0.509027731622	-1.767458316863	-0.336798985860
F	-0.867456844925	-1.196398156837	1.550596180053
Cl	-0.672124282314	1.755298902420	0.813338929517
Cl	0.148600864647	0.612909653374	-1.771301114747
H	1.302982966244	-0.027649393644	1.685134538320
Cl	2.196635580715	-1.399928617428	-0.006932196252
F	2.196606906015	1.146532739194	0.333595767022

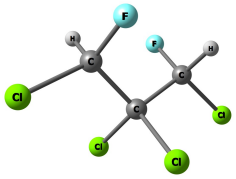
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
72.7972	0.0940
93.2896	0.124
128.7781	0.00782
176.6883	0.0193
184.7322	0.415
229.5362	0.000
229.6238	0.0359
295.5789	0.0536
319.7613	0.250
366.0779	0.174
396.1757	0.444
458.1176	0.0625
613.9439	8.74
629.2788	6.69
753.2543	24.3
763.3646	17.7
846.7160	2.95
1050.5184	0.330
1053.1400	5.35
1159.0588	17.8
1169.3120	16.2
1269.3474	2.93
1277.0142	3.31
1363.3621	0.00
1369.3316	2.45
3131.9380	0.852
3132.2613	0.00133

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
72.9745	0.133
83.6733	0.110
126.7925	0.0238
172.9093	0.0655
190.8898	0.228
202.9256	0.0631
245.2861	0.111
290.4177	0.162
324.8197	0.160
376.6004	0.144
411.0349	0.767
440.0548	0.101
607.8530	7.64
642.2623	7.54
750.1328	23.6
796.0025	11.8
864.5287	9.24
1028.8905	4.34
1063.9685	6.58
1116.6758	11.9
1165.8039	17.9
1274.1084	3.30
1286.8681	3.05
1356.4448	1.35
1363.8780	1.94
3131.6996	0.0215
3131.9721	0.733



$\Delta E = 0.20$ kcal mol^{-1}
Population = 0.202



$\Delta E = 0.35$ kcal mol^{-1}
Population = 0.157

Optimized Coordinates (Angstroms)

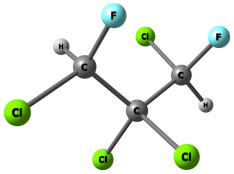
Atom	X	Y	Z
C	-1.398977156331	0.105016521541	0.620738224193
C	-0.001326650295	0.310545107101	-0.022676457990
C	0.900952425521	-0.917487312562	0.239984033699
Cl	-2.193956335827	-1.404921951871	0.042435628184
H	-1.287658499507	0.000775144550	1.699991832506
F	-2.191636621455	1.147820062139	0.332133013119
Cl	0.680572492790	1.765915162616	0.777900783848
Cl	-0.159599167901	0.572286519340	-1.777172281229
H	0.509159718324	-1.779046966027	-0.300574585422
Cl	2.585377376673	-0.689935710942	-0.295562083733
F	0.881840418009	-1.170529575886	1.572296892825

Atom	X	Y	Z
C	-1.242778068209	0.803390920627	-0.142749890414
C	-0.000053190974	-0.116758159395	0.001329363498
C	1.241887157301	0.805829727532	0.136292033748
Cl	-2.784969610598	-0.084969559879	-0.209575306941
F	-1.262130488923	1.653123806480	0.914275254936
H	-1.157860885058	1.374992418563	-1.067150701429
Cl	0.127318618010	-1.122272176551	-1.465575312002
Cl	-0.126575641663	-1.107816700467	1.478111896988
H	1.156478297551	1.386478928438	1.054991001548
Cl	2.784834486607	-0.080512340899	0.211902473353
F	1.260522325957	1.645076135549	-0.929090813285

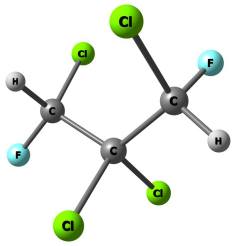
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
72.9750	0.133
83.6732	0.110
126.7919	0.0238
172.9092	0.0655
190.8897	0.228
202.9251	0.0631
245.2854	0.111
290.4182	0.162
324.8193	0.160
376.6002	0.144
411.0346	0.767
440.0551	0.101
607.8535	7.64
642.2633	7.54
750.1337	23.6
796.0025	11.8
864.5294	9.24
1028.8909	4.34
1063.9695	6.58
1116.6777	11.9
1165.8034	17.9
1274.1079	3.30
1286.8682	3.05
1356.4450	1.35
1363.8761	1.94
3131.7009	0.0216
3131.9734	0.733

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
75.7078	0.0887
79.2830	0.144
123.0156	0.0483
178.0798	0.0486
191.1666	0.00689
208.2118	0.360
242.7731	0.00609
259.3731	0.0611
346.5177	0.0575
382.0635	0.111
427.6935	0.694
444.1066	0.0183
587.5329	10.4
659.0490	6.25
726.2449	20.7
864.8626	0.663
873.3378	15.3
1021.4665	4.61
1051.2526	11.5
1111.1054	14.0
1118.6945	15.0
1282.6122	6.76
1282.7363	0.0191
1356.1075	2.85
1356.8944	0.489
3128.8183	0.00251
3129.5069	0.655



$\Delta E = 1.02$ kcal mol^{-1}
Population = 0.051



$\Delta E = 1.22$ kcal mol^{-1}
Population = 0.036

Optimized Coordinates (Angstroms)

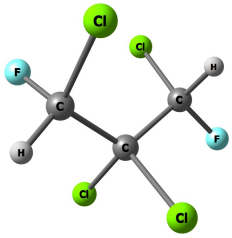
Atom	X	Y	Z
C	0.710946294570	-0.214453514500	-0.951760843306
C	0.018617695909	0.100624901838	0.396191510465
C	-1.476703873244	-0.334490795183	0.418803303043
Cl	2.442111153848	0.231054017950	-0.968746126675
F	0.588829988836	-1.534110506660	-1.201463136783
H	0.231236778820	0.358296808088	-1.746156403720
Cl	0.075840704455	1.862197365114	0.696047104402
Cl	0.812289012912	-0.785595017128	1.734345763167
H	-1.941688483156	0.036735508777	1.332981467933
Cl	-2.406101909319	0.371658316783	-0.955420598932
F	-1.579342363632	-1.672218085079	0.356614960405

Atom	X	Y	Z
C	1.164422823485	0.326318537561	-0.751669085257
C	-0.018317252422	-0.495212048134	-0.173192260753
C	-0.829416699156	0.170146294441	0.964010559168
Cl	2.226861721246	0.974876874100	0.552139692969
H	1.784877266599	-0.332232752142	-1.360828779388
F	0.722153931847	1.353629280273	-1.495240288479
Cl	0.682371908273	-2.003256415690	0.523510109496
Cl	-1.091438489732	-0.921111898248	-1.538886722812
H	-0.170887569113	0.370798766123	1.809201169447
Cl	-1.540208136244	1.740533408825	0.478565115352
F	-1.820057504784	-0.659838047109	1.340331490258

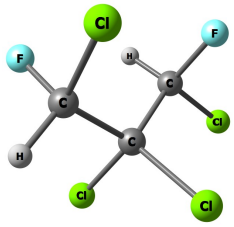
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
61.5972	0.0781
88.6864	0.0441
140.6315	0.0584
166.7923	0.0230
191.2501	0.131
212.6262	0.0684
246.3779	0.0302
301.0946	0.142
337.1664	0.0754
370.7702	0.286
413.4339	0.586
448.4336	0.464
536.2059	7.84
641.2278	9.83
754.2055	16.1
835.1503	11.2
879.7895	15.6
968.2673	0.278
1084.6061	8.06
1131.3801	2.77
1157.9991	26.0
1277.3258	4.76
1285.5044	2.28
1356.3833	1.55
1375.1454	1.71
3120.3553	0.465
3125.3598	0.447

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
62.1661	0.0648
97.6287	0.0304
140.0920	0.0539
171.4854	0.0999
183.4966	0.125
233.6248	0.0357
250.3619	0.151
284.0223	0.316
332.9687	0.266
356.9623	0.224
399.3054	0.609
436.5428	0.304
594.4561	5.78
655.5090	8.79
756.3869	17.0
773.5919	23.6
846.9856	5.17
984.8428	0.865
1096.6174	5.20
1143.7723	10.4
1166.3508	19.7
1275.6075	2.20
1284.9095	4.49
1364.4445	1.87
1376.7432	0.247
3120.5549	0.456
3129.4155	0.463



$\Delta E = 1.22$ kcal mol^{-1}
Population = 0.036



$\Delta E = 1.78$ kcal mol^{-1}
Population = 0.014

Optimized Coordinates (Angstroms)

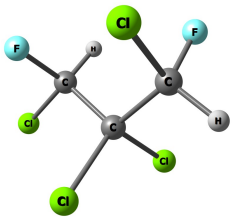
Atom	X	Y	Z
C	-0.827851664007	-0.165708177708	0.964284722622
C	-0.017355220698	0.491864961734	-0.177865908285
C	1.160337710369	-0.336757797190	-0.756525833282
Cl	-1.546452691555	-1.735064592955	0.487073378888
H	-0.167691214062	-0.365739199482	1.808349396919
F	-1.813999699240	0.669790070254	1.340203976123
Cl	0.691500065561	1.999751093876	0.510872473031
Cl	-1.092697354135	0.916792529770	-1.542115714589
H	1.781696402300	0.316856368783	-1.370065537969
Cl	2.223914734651	-0.984535544276	0.546742793563
F	0.711720930816	-1.365160712807	-1.494765747022

Atom	X	Y	Z
C	-0.736937583961	-0.626192483857	-0.768059139600
C	-0.057852749989	0.374519734329	0.201008136224
C	1.440939022087	0.607755896054	-0.154003735426
Cl	-2.498388371597	-0.775202866610	-0.498129285015
H	-0.596444641689	-0.274640667914	-1.791409202107
F	-0.174511577964	-1.841977686403	-0.620231148175
Cl	-0.200338002639	-0.148595770805	1.892945673567
Cl	-0.831387420751	1.986655425922	-0.023083872425
H	1.827015729607	1.424077897129	0.456851406417
Cl	2.508207945232	-0.798889642116	0.133064329539
F	1.511748651665	0.939187164271	-1.466258162999

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
62.1653	0.0648
97.6283	0.0304
140.0920	0.0539
171.4853	0.0999
183.4964	0.125
233.6249	0.0357
250.3618	0.151
284.0221	0.316
332.9686	0.266
356.9624	0.224
399.3054	0.609
436.5427	0.304
594.4561	5.78
655.5088	8.79
756.3871	17.0
773.5918	23.6
846.9855	5.17
984.8422	0.865
1096.6168	5.20
1143.7719	10.4
1166.3498	19.7
1275.6083	2.20
1284.9103	4.49
1364.4454	1.87
1376.7436	0.247
3120.5547	0.456
3129.4146	0.463

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
56.2510	0.0746
88.9508	0.0569
139.6771	0.0339
162.1988	0.0121
195.3701	0.140
209.6550	0.118
247.2620	0.130
275.1652	0.0512
355.4336	0.103
369.0335	0.297
420.1642	0.992
443.9957	0.110
535.2658	7.86
661.3578	6.97
761.9276	25.8
836.7466	7.83
857.0569	6.15
981.0184	5.48
1086.0091	9.24
1114.1210	13.3
1138.8809	13.4
1280.3628	4.30
1292.7139	4.28
1352.0232	0.579
1367.6897	2.21
3119.4382	0.336
3124.7000	0.442



$\Delta E = 1.78$ kcal mol^{-1}
Population = 0.014

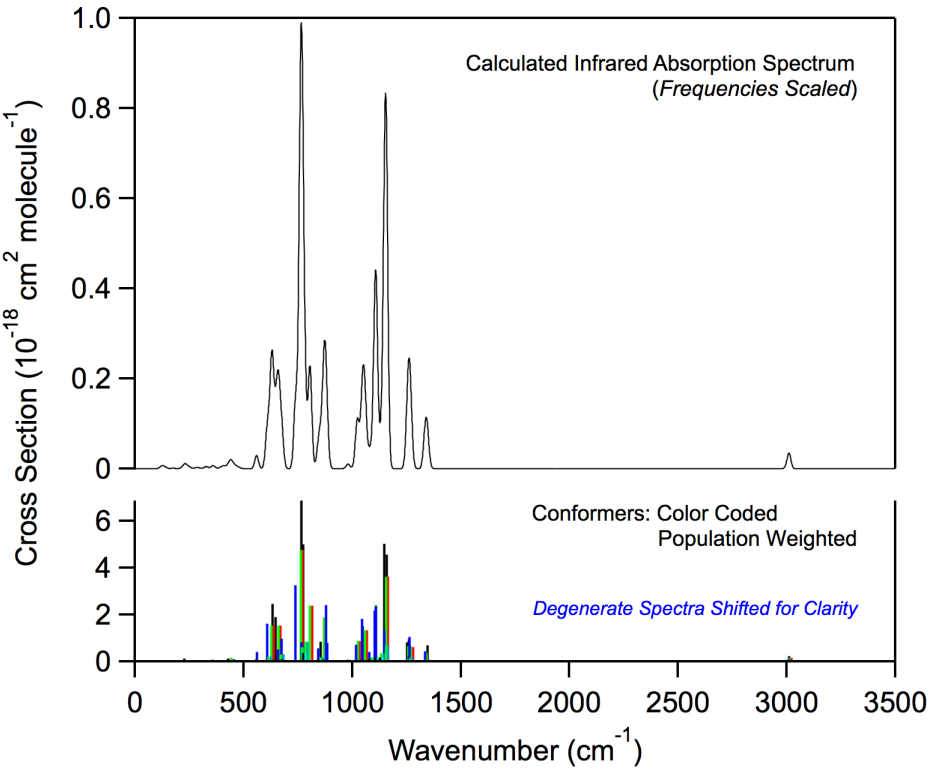
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.439989686581	0.614195041574	-0.151870703489
C	0.057037744643	0.372980442602	0.205266841034
C	0.728930371040	-0.640519614607	-0.755489731493
Cl	-2.517473615544	-0.782279026417	0.146477439586
H	-1.820186871203	1.438246963271	0.452255753387
F	-1.508269498822	0.935433958770	-1.466790392290
Cl	0.195553052082	-0.137333177371	1.901439137586
Cl	0.842293383125	1.977568260612	-0.031851670541
H	0.591092781373	-0.296331362261	-1.781699750320
Cl	2.489227193775	-0.800106310547	-0.484079886442
F	0.157676146111	-1.850941175627	-0.597821037018

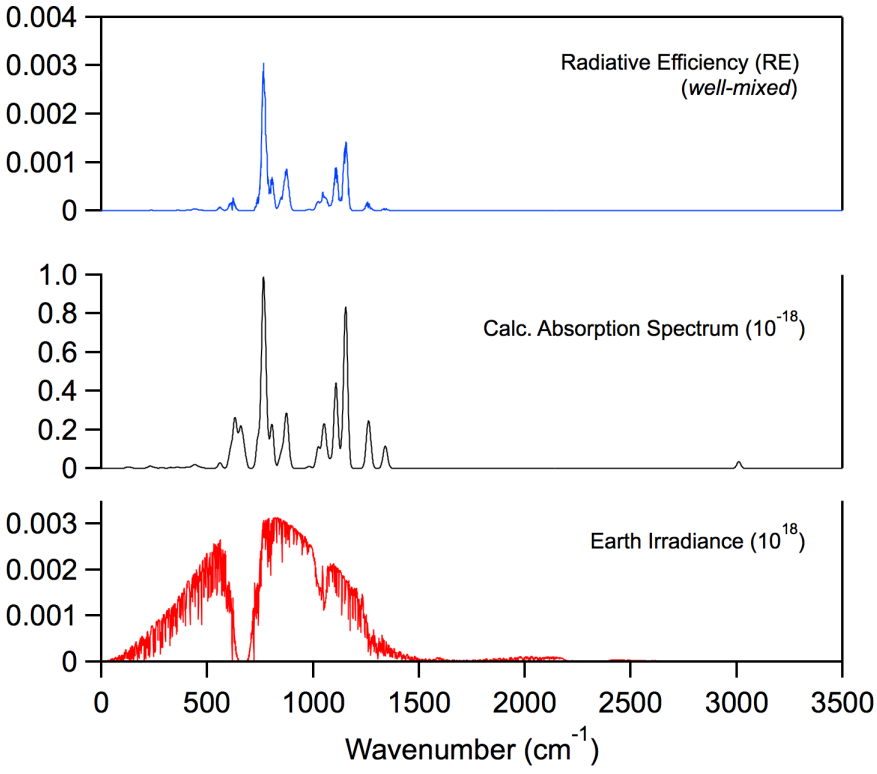
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
56.2500	0.0746
88.9484	0.0569
139.6767	0.0339
162.1983	0.0121
195.3705	0.140
209.6541	0.118
247.2605	0.130
275.1654	0.0512
355.4323	0.103
369.0334	0.297
420.1639	0.992
443.9952	0.110
535.2652	7.86
661.3573	6.97
761.9270	25.8
836.7448	7.83
857.0571	6.15
981.0123	5.48
1086.0049	9.24
1114.1219	13.3
1138.8779	13.4
1280.3614	4.30
1292.7130	4.28
1352.0244	0.579
1367.6890	2.21
3119.4401	0.336
3124.7022	0.442

Infrared Spectrum

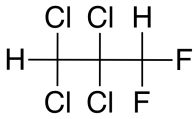


Radiative Efficiency



HCFC-232ab

Molecular Formula:	$CHCl_2CCl_2CHF_2$
Name:	1,1,2,2-Tetrachloro-3,3-difluoropropane
CAS number:	872817-81-7
Molecular Weight:	217.86



Global Atmospheric Lifetime (years):	1.01
Tropospheric Atmospheric Lifetime (years):	1.07
Stratospheric Atmospheric Lifetime (years):	20
Ozone Depletion Potential (ODP):	0.024

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.192	0.143
Global Warming Potential (GWP_H):		
GWP_{20}	202	150
GWP_{100}	55	41
Global Temperature Potentials (GTP_H)		
GTP_{20}		49
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*

$k_{SAR}(298\ K) = 5.47 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 3.49 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

τ^{OH}_{Global} = 1.04 years
τ^{OH}_{Trop} = 1.07 years
τ^{OH}_{Strat} = 35.9 years

Fractional Atmospheric Loss: 0.975

O(^{1}D) Reactivity

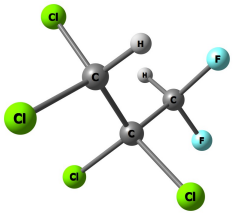
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 2.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)}$ = 185 years
Fractional Atmospheric Loss: 0.005

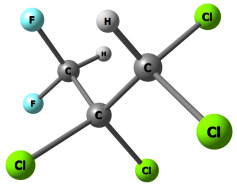
UV Photolysis

UV Spectrum: *No Recommendation*
τ_{hv} = 50 years
Fractional Atmospheric Loss: 0.020

Molecular Structure and Infrared Spectrum (6 conformers)



E = 0
Population = 0.417



E = 0
Population = 0.417

Optimized Coordinates (Angstroms)

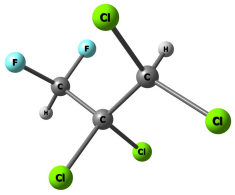
Atom	X	Y	Z
C	-0.952737871854	-0.160016405486	-0.590846553672
C	0.388106937724	0.162158306527	0.111234470861
C	1.442028652231	-0.943168576304	-0.178013808903
Cl	-1.551561912180	-1.791004843598	-0.131451157556
Cl	-2.206710378402	1.064109819082	-0.291188857049
H	-0.772459091925	-0.190507276650	-1.662289154807
Cl	0.210038552126	0.285792691133	1.882442954179
Cl	1.005699775185	1.701383434611	-0.571807311650
H	1.161011195043	-1.881650660403	0.306781738901
F	1.509272419219	-1.131020945063	-1.516281099377
F	2.647054722834	-0.554688543848	0.260364779072

Atom	X	Y	Z
C	-0.955047705940	0.195183932319	-0.575747656154
C	0.382500876822	-0.178295475141	0.106931465882
C	1.440998926803	0.940281396784	-0.104092276704
Cl	-2.214019402921	-1.041918433876	-0.362923994032
Cl	-1.549885410571	1.793613663599	-0.009223307091
H	-0.771298145763	0.297167074043	-1.642169210556
Cl	0.997114311155	-1.670168962436	-0.676486914753
Cl	0.198445800565	-0.420363253172	1.865254678508
H	1.161584963335	1.844946881309	0.442033592609
F	2.643342008041	0.518889372916	0.310612884092
F	1.513071778473	1.217651803657	-1.426454261800

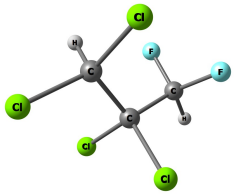
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
68.1967	0.0731
87.5512	0.183
140.4110	0.0316
167.2111	0.0293
200.4690	0.278
207.3494	0.0642
232.8320	0.0153
278.8016	0.200
307.4974	0.0841
352.6495	0.159
404.9486	0.166
551.7565	2.93
598.3935	3.68
653.9281	11.6
731.7665	9.55
778.6872	12.0
859.5147	12.8
1031.3345	2.05
1057.1697	2.22
1140.1990	18.1
1187.1544	20.7
1230.3062	2.74
1274.0896	1.06
1372.5972	5.33
1396.0207	1.32
3105.0770	1.69
3160.8319	0.649

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
68.1982	0.0731
87.5516	0.183
140.4115	0.0316
167.2120	0.0293
200.4695	0.278
207.3499	0.0642
232.8318	0.0153
278.8014	0.200
307.4975	0.0841
352.6496	0.159
404.9486	0.166
551.7562	2.93
598.3938	3.68
653.9283	11.6
731.7660	9.56
778.6871	12.0
859.5145	12.8
1031.3348	2.05
1057.1727	2.22
1140.1988	18.1
1187.1544	20.7
1230.3049	2.74
1274.0884	1.06
1372.5952	5.33
1396.0191	1.32
3105.0807	1.69
3160.8322	0.649



$\Delta E = 1.21$ kcal mol^{-1}
Population = 0.054



$\Delta E = 1.21$ kcal mol^{-1}
Population = 0.054

Optimized Coordinates (Angstroms)

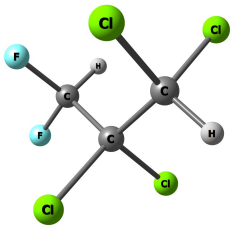
Atom	X	Y	Z
C	-0.785312140439	-0.228357895693	-0.628105565037
C	0.402415423542	0.348749292585	0.180567378450
C	1.752220149136	-0.375065563215	-0.115650275477
Cl	-1.065333650142	-1.957587820663	-0.273939429128
Cl	-2.290130464485	0.698408026555	-0.383532355684
H	-0.532587781982	-0.161530477155	-1.683078183077
Cl	0.120054873554	0.318605975135	1.936480086582
Cl	0.665435775894	2.045360882412	-0.378512259259
H	2.582014718844	0.231589940756	0.260003595485
F	1.800031448501	-1.590520748487	0.448739689889
F	1.869928647576	-0.524828612231	-1.454924682743

Atom	X	Y	Z
C	-0.779326942633	0.246080221567	-0.631238941697
C	0.392574622971	-0.362533716486	0.177423958832
C	1.750395551798	0.363070352976	-0.074455406670
Cl	-2.292294489912	-0.679926169843	-0.439846550365
Cl	-1.056633270695	1.964748805258	-0.227060099416
H	-0.510148802843	0.211201314831	-1.683678744804
Cl	0.656295806331	-2.042056370778	-0.430767057620
Cl	0.082433310185	-0.386246391502	1.928742197236
H	2.571170981135	-0.259527507465	0.294875871225
F	1.890133985921	0.554345759407	-1.406306835037
F	1.795069247744	1.559860702034	0.528744608316

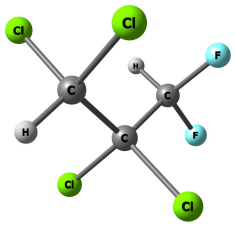
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
56.9171	0.0436
95.4767	0.115
150.5414	0.0736
162.5698	0.0314
200.2265	0.0862
211.9561	0.111
238.5992	0.0468
269.3624	0.0988
314.1731	0.430
378.1361	0.0898
393.7319	0.372
529.0844	5.91
574.2451	2.03
645.9167	5.95
749.7834	22.6
815.0616	7.95
851.6407	3.34
963.5251	4.27
1104.3044	3.54
1134.2259	17.8
1179.3497	17.2
1229.6565	4.99
1279.2152	1.28
1380.8704	4.07
1396.6542	2.51
3087.8266	2.40
3160.2952	0.585

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
56.9168	0.0436
95.4773	0.115
150.5409	0.0736
162.5692	0.0314
200.2266	0.0862
211.9560	0.111
238.5993	0.0468
269.3629	0.0988
314.1734	0.430
378.1363	0.0898
393.7323	0.372
529.0850	5.91
574.2453	2.03
645.9160	5.95
749.7835	22.6
815.0620	7.95
851.6408	3.34
963.5268	4.27
1104.3056	3.54
1134.2236	17.8
1179.3512	17.2
1229.6565	4.99
1279.2163	1.28
1380.8695	4.07
1396.6549	2.51
3087.8258	2.40
3160.2945	0.585



$\Delta E = 1.62$ kcal mol^{-1}
Population = 0.027



$\Delta E = 1.62$ kcal mol^{-1}
Population = 0.027

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.061272482770	0.177433877683	0.517038708343
C	0.464782834689	0.120456228645	0.233218106193
C	0.855024066406	-0.150312461626	-1.243698481762
Cl	-1.872505354015	1.396656731442	-0.526412347528
Cl	-1.883598877309	-1.397493096783	0.347663728005
H	-1.203659879051	0.501407592500	1.544604063906
Cl	1.204943130204	-1.124926944929	1.280700806786
Cl	1.146203247384	1.729688505611	0.669958437805
H	0.424681341884	0.615914899253	-1.895925765321
F	2.193497471164	-0.138920566091	-1.359127517926
F	0.408604501414	-1.363042765706	-1.618541738500

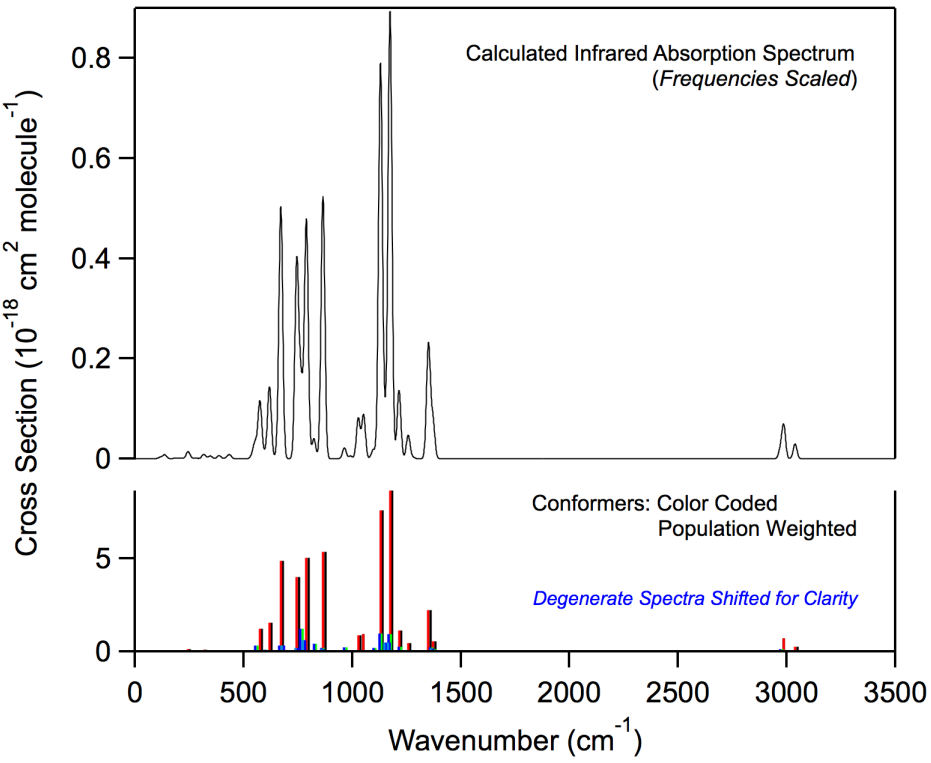
Atom	X	Y	Z
C	-1.063882992643	-0.166992806577	0.516532407474
C	0.462393414847	-0.126685068866	0.231036390777
C	0.854679206059	0.200825665354	-1.233797121324
Cl	-1.856312163276	1.429165391123	0.418369197855
Cl	-1.900430417628	-1.323880526956	-0.576715523839
H	-1.210305701418	-0.532739984521	1.529405768724
Cl	1.113851197479	-1.766098086148	0.595220782926
Cl	1.228381352306	1.057512659094	1.329661386959
H	0.408439293162	-0.527898397007	-1.917559283824
F	0.430722891119	1.437016473720	-1.554118793228
F	2.192449919994	0.169073680784	-1.353490212500

Infrared Absorption Spectrum (unscaled frequencies)

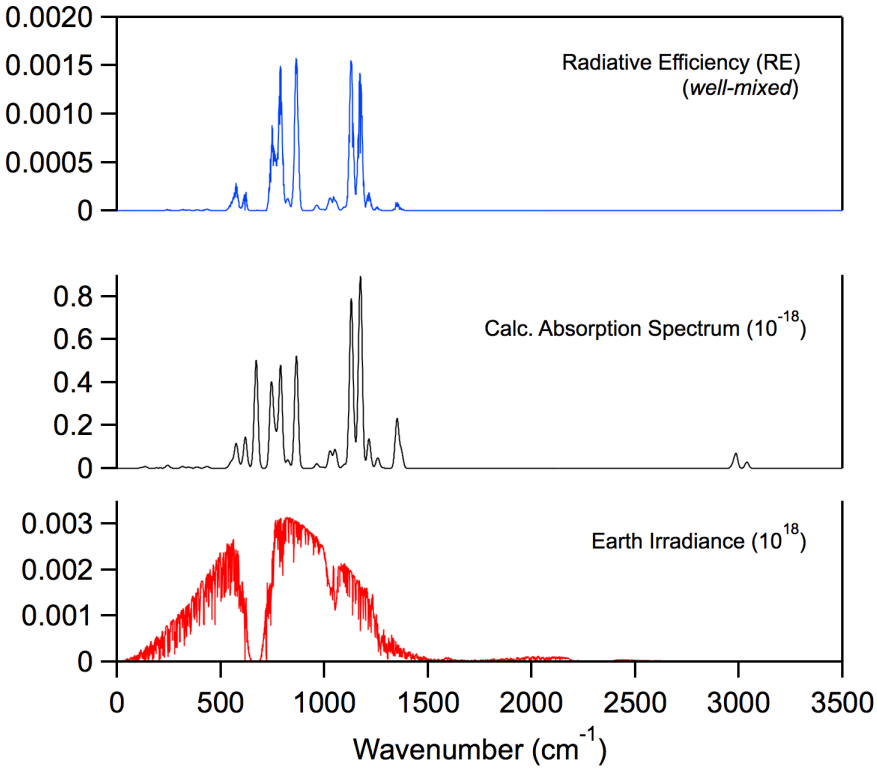
Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
56.1208	0.0924
89.1651	0.0667
149.6131	0.0433
163.1320	0.0249
198.0458	0.188
222.4693	0.00613
242.7067	0.168
277.0935	0.246
302.5636	0.161
341.1817	0.0499
396.0796	0.433
515.6401	2.81
631.0039	1.24
658.1782	11.8
725.2821	7.00
759.9644	22.9
852.3931	5.10
993.7395	2.13
1082.2241	0.152
1157.7251	17.4
1175.2194	18.1
1222.9959	2.20
1298.9166	0.985
1383.8762	5.49
1393.8093	1.54
3090.7397	1.81
3157.9219	0.485

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
56.1204	0.0924
89.1643	0.0667
149.6124	0.0433
163.1324	0.0249
198.0458	0.188
222.4690	0.00613
242.7063	0.168
277.0933	0.246
302.5634	0.161
341.1813	0.0499
396.0796	0.433
515.6398	2.81
631.0028	1.24
658.1784	11.8
725.2827	7.00
759.9659	22.9
852.3941	5.10
993.7367	2.13
1082.2208	0.152
1157.7248	17.4
1175.2180	18.1
1222.9966	2.20
1298.9159	0.985
1383.8753	5.49
1393.8085	1.54
3090.7400	1.81
3157.9243	0.485

Infrared Spectrum

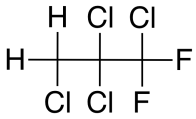


Radiative Efficiency



HCFC-232ac

Molecular Formula:	$CH_2ClCCl_2CClF_2$
Name:	1,2,2,3-Tetrachloro-1,1-difluoropropane
CAS number:	1538604-30-6
Molecular Weight:	217.86



Global Atmospheric Lifetime (years):	2.56
Tropospheric Atmospheric Lifetime (years):	2.80
Stratospheric Atmospheric Lifetime (years):	29.3
Ozone Depletion Potential (ODP):	0.053

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.256	0.222
Global Warming Potential (GWP_H):		
GWP_{20}	675	587
GWP_{100}	183	159
Global Temperature Potentials (GTP_H)		
GTP_{20}		235
GTP_{50}		29
GTP_{100}		22

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

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

OH Reactivity

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

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

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

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

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

Fractional Atmospheric Loss: 0.943

O(^{1}D) Reactivity

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

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

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

Fractional Atmospheric Loss: 0.014

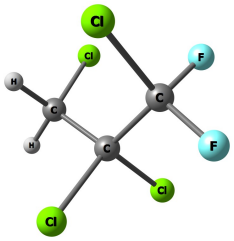
UV Photolysis

UV Spectrum: *No Recommendation*

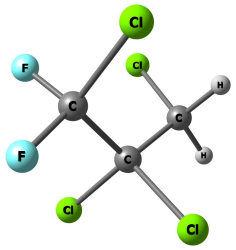
$\tau_{hv} = 59$ years

Fractional Atmospheric Loss: 0.043

Molecular Structure and Infrared Spectrum (7 conformers)



E = 0
Population = 0.200



E = 0
Population = 0.200

Optimized Coordinates (Angstroms)

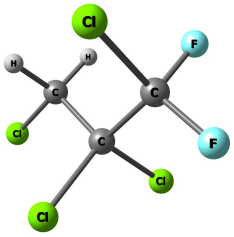
Atom	X	Y	Z
C	1.116510012692	0.050301202906	-1.156006760983
C	0.111400900739	-0.557586039302	-0.170958219563
C	-0.774037083988	0.459229892075	0.623894263771
Cl	2.341260321703	1.127378794337	-0.410288492042
H	1.650702758242	-0.766096329977	-1.638274607270
H	0.578229689167	0.633754610137	-1.900776729962
Cl	0.945592924375	-1.581325805876	1.042211229997
Cl	-0.980235935722	-1.587832804023	-1.165933832979
Cl	-1.575246266979	1.643275278345	-0.471362783937
F	-1.715652399366	-0.192028639223	1.298618526873
F	-0.031030920863	1.136011840599	1.493316406094

Atom	X	Y	Z
C	-1.117726478993	0.050373372575	-1.154758326074
C	-0.111479911418	-0.557773535555	-0.171032188482
C	0.774375525294	0.458857476698	0.623591806188
Cl	-2.342125751380	1.126593174452	-0.407227278814
H	-0.580347802744	0.634455153806	-1.899686864690
H	-1.652105859858	-0.765910756429	-1.637011355280
Cl	0.979552530100	-1.587056931368	-1.167666317794
Cl	-0.944178496346	-1.582522024381	1.042311512026
Cl	1.574149741394	1.643829675038	-0.471711724759
F	0.031971467858	1.134867829341	1.494127877163
F	1.716848036093	-0.192494434178	1.297027860516

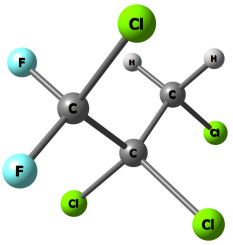
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
56.9182	0.0434
108.1670	0.0898
144.0220	0.0136
177.4956	0.0611
223.5180	0.204
241.4885	0.195
269.6156	0.252
291.7133	0.121
333.8931	0.118
355.1473	0.183
423.7420	0.213
430.1570	0.418
532.2990	2.98
653.2172	2.01
713.5476	16.1
749.4281	13.3
846.3798	7.49
907.4565	26.1
1014.5842	3.42
1086.8403	7.14
1188.8581	12.3
1215.9009	20.0
1255.5697	4.02
1312.9732	4.49
1459.0640	2.25
3115.0123	0.621
3182.5623	0.0218

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
56.9182	0.0434
108.1669	0.0898
144.0220	0.0136
177.4956	0.0611
223.5180	0.204
241.4885	0.195
269.6156	0.252
291.7133	0.121
333.8931	0.118
355.1473	0.183
423.7420	0.213
430.1570	0.418
532.2990	2.98
653.2172	2.01
713.5477	16.1
749.4281	13.3
846.3798	7.49
907.4565	26.1
1014.5843	3.42
1086.8402	7.14
1188.8582	12.3
1215.9009	20.0
1255.5698	4.02
1312.9733	4.49
1459.0641	2.25
3115.0123	0.621
3182.5623	0.0218



$\Delta E = 0.14$ kcal mol^{-1}
Population = 0.158



$\Delta E = 0.14$ kcal mol^{-1}
Population = 0.158

Optimized Coordinates (Angstroms)

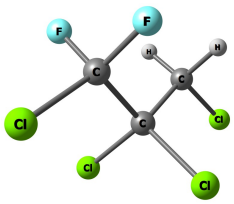
Atom	X	Y	Z
C	-0.967593893859	-0.750198255864	0.829702080787
C	-0.200522332278	0.190786712193	-0.106684610430
C	1.313919250486	0.233659558456	0.290104747760
Cl	-2.726324196864	-0.790971863414	0.523703382129
H	-0.592861580903	-1.764486965732	0.703573203035
H	-0.816396431935	-0.421179476937	1.857482150801
Cl	-0.802537366436	1.876115629248	0.068446197350
Cl	-0.338311657452	-0.323780209755	-1.811092723089
Cl	2.092223327518	-1.387402901650	0.193309079754
F	1.982717032164	1.065699479426	-0.494241840477
F	1.418176849560	0.659444294030	1.553178332380

Atom	X	Y	Z
C	-0.967095125803	0.750933567109	0.829354771122
C	-0.200364910932	-0.190948795366	-0.106409133242
C	1.314161032104	-0.233692418497	0.290072186255
Cl	-2.725889389310	0.791688404405	0.523721445363
H	-0.815708797405	0.422764486468	1.857378670051
H	-0.592253111398	1.765063887738	0.702281901074
Cl	-0.338471575312	0.322193425644	-1.811221022625
Cl	-0.802570027118	-1.876046531045	0.070285627007
Cl	2.092664176194	1.387181166553	0.191726772994
F	1.418647736238	-0.658421594451	1.553482202465
F	1.982666992742	-1.066487598559	-0.493721420463

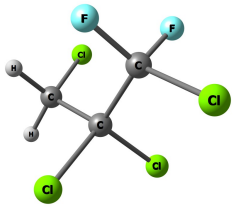
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
73.8041	0.00103
90.3942	0.218
129.7255	0.138
168.9456	0.107
206.6373	0.0464
236.1440	0.147
284.7707	0.111
294.7800	0.0627
333.8668	0.187
337.6468	0.119
424.0946	0.0973
444.9176	0.275
559.3850	2.51
624.9061	2.54
718.3122	20.6
772.8413	9.56
824.8720	13.5
970.9180	9.25
1001.0355	16.6
1068.4845	2.67
1179.4802	18.1
1222.4771	3.79
1230.2796	20.7
1313.9214	1.79
1463.2465	0.676
3106.2748	0.758
3175.1676	0.0388

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
73.8041	0.00103
90.3940	0.218
129.7255	0.138
168.9456	0.107
206.6373	0.0464
236.1440	0.147
284.7707	0.111
294.7800	0.0627
333.8668	0.187
337.6468	0.119
424.0946	0.0973
444.9176	0.275
559.3850	2.51
624.9060	2.54
718.3122	20.6
772.8413	9.56
824.8720	13.5
970.9181	9.25
1001.0355	16.6
1068.4843	2.67
1179.4802	18.1
1222.4773	3.79
1230.2796	20.7
1313.9215	1.79
1463.2468	0.676
3106.2748	0.758
3175.1676	0.0388



$\Delta E = 0.37$ kcal mol^{-1}
Population = 0.108



$\Delta E = 0.49$ kcal mol^{-1}
Population = 0.088

Optimized Coordinates (Angstroms)

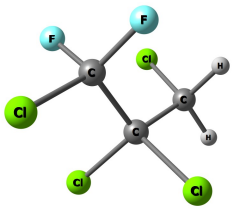
Atom	X	Y	Z
C	-1.637805699704	0.163740670111	0.000000000000
C	-0.138228791686	-0.182044081918	0.000000000000
C	0.652975411533	1.170815895449	0.000000000000
Cl	-2.707381590028	-1.264633543403	0.000000000000
H	-1.863802519316	0.745498939277	0.892483472126
H	-1.863802519316	0.745498939277	-0.892483472126
Cl	0.293789724148	-1.099937262410	-1.470704734004
Cl	0.293789724148	-1.099937262410	1.470704734004
Cl	2.423548453632	0.984693732248	0.000000000000
F	0.294144903300	1.875157486946	-1.080321705726
F	0.294144903300	1.875157486946	1.080321705726

Atom	X	Y	Z
C	-1.500991836673	-0.593240002213	0.695311473460
C	-0.122157471400	-0.543346485465	0.009714429575
C	0.628900573634	0.804870785972	0.271250970023
Cl	-2.715321734268	0.567254381534	0.067048527642
H	-1.909748991494	-1.591920621126	0.557541015672
H	-1.369279649448	-0.387748997400	1.756417717315
Cl	-0.254843615756	-0.823591527811	-1.743217133221
Cl	0.814398236855	-1.872598071248	0.786499253865
Cl	2.322868614522	0.805424499216	-0.301685718710
F	-0.013288406740	1.802802260336	-0.329323233577
F	0.621127280768	1.037939778206	1.589450697957

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
71.7858	0.00397
93.1829	0.265
124.8360	0.158
183.2303	0.148
188.8818	0.00780
246.7505	0.0261
261.6879	0.190
299.7324	0.0362
333.3215	0.145
361.6917	0.225
431.4336	0.00751
449.3866	0.511
550.3141	4.08
628.0557	2.46
727.4559	16.7
754.2085	11.9
869.5157	1.78
973.2837	9.78
1007.9867	19.7
1069.6164	14.4
1170.9283	14.8
1174.9766	20.0
1224.1494	4.81
1313.8797	1.63
1464.4545	0.687
3106.9592	0.529
3174.8979	0.0168

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
55.3584	0.0392
106.3927	0.141
146.5936	0.0436
180.9375	0.140
191.4686	0.111
242.9347	0.0837
273.1645	0.0276
291.9980	0.578
328.3046	0.0549
382.8513	0.253
424.8672	0.0293
448.7172	0.491
499.9778	5.90
628.0330	2.23
741.5831	16.7
755.8519	3.29
852.0989	10.6
938.2741	21.8
997.4467	10.1
1086.5976	13.6
1166.9594	17.3
1194.9883	15.3
1255.4619	1.34
1311.9474	5.59
1457.6438	1.21
3114.5002	0.640
3183.6707	0.0824



$\Delta E = 0.49$ kcal mol^{-1}
Population = 0.088

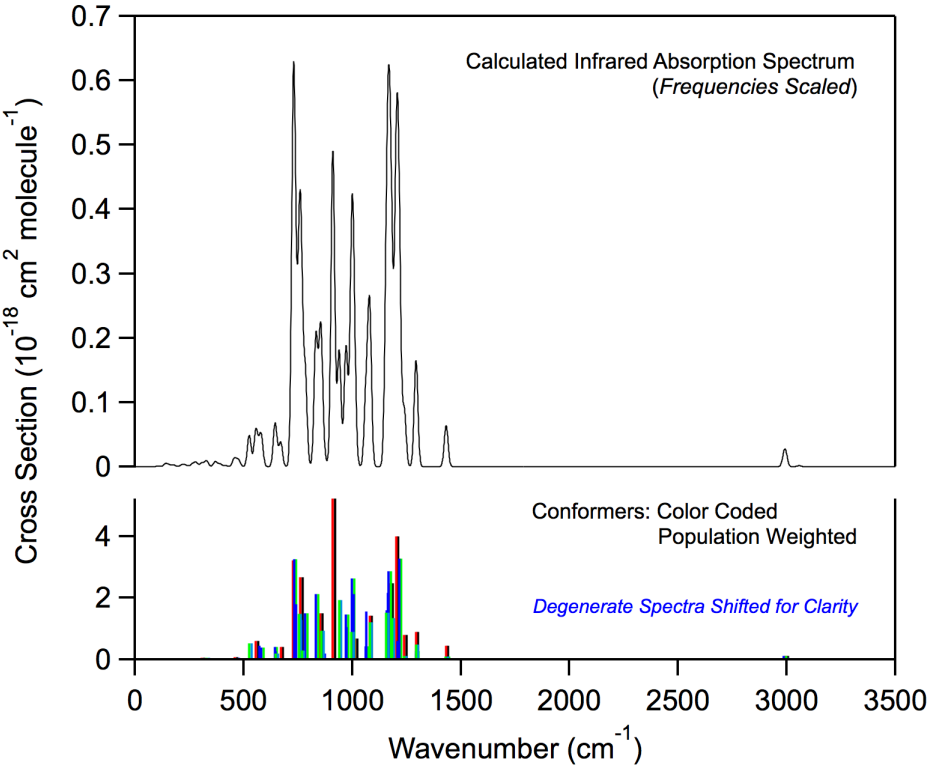
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.501152270482	-0.591892919120	-0.695875248421
C	-0.122470710904	-0.543288635001	-0.009878271760
C	0.629695601268	0.804439239675	-0.270752019536
Cl	-2.714764848733	0.569323472090	-0.067560349005
H	-1.368987288316	-0.386147516819	-1.756875873785
H	-1.910714742113	-1.590305317251	-0.558553256381
Cl	0.813280025078	-1.872998156599	-0.786849285913
Cl	-0.255860359287	-0.824020669844	1.742922128919
Cl	2.323503964935	0.803498921984	0.302655917886
F	0.622468553887	1.037957938127	-1.588875256441
F	-0.011893925331	1.802661642758	0.329979514438

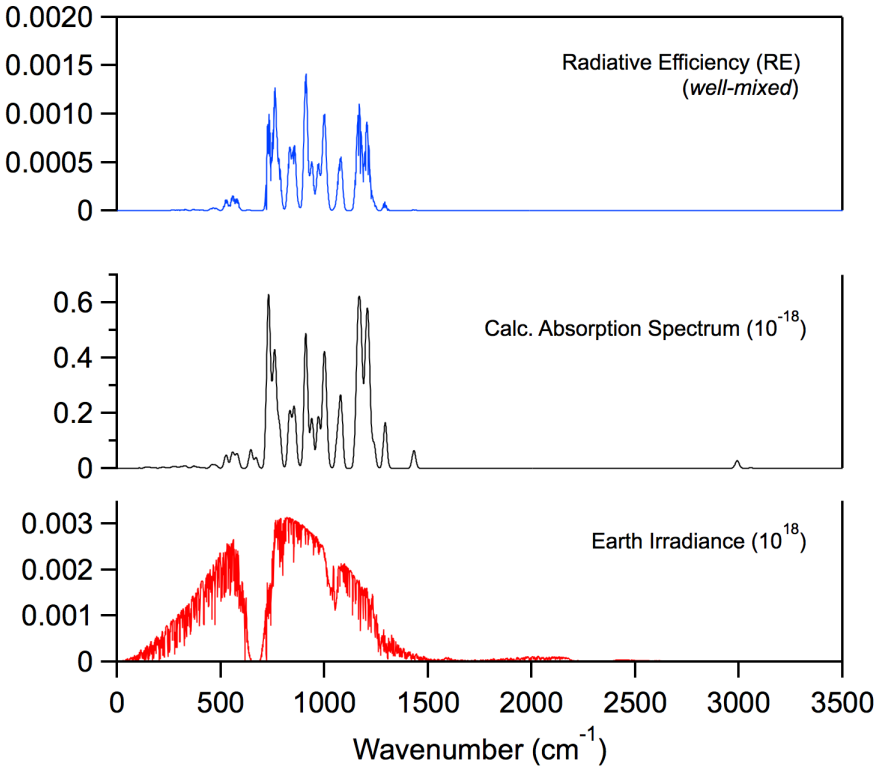
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
55.3588	0.0392
106.3928	0.141
146.5936	0.0436
180.9375	0.140
191.4688	0.111
242.9347	0.0837
273.1645	0.0276
291.9978	0.578
328.3047	0.0549
382.8512	0.253
424.8673	0.0293
448.7172	0.491
499.9777	5.90
628.0331	2.23
741.5831	16.7
755.8519	3.29
852.0990	10.6
938.2740	21.8
997.4465	10.1
1086.5978	13.6
1166.9598	17.3
1194.9884	15.3
1255.4614	1.34
1311.9471	5.59
1457.6434	1.21
3114.5004	0.640
3183.6708	0.0824

Infrared Spectrum

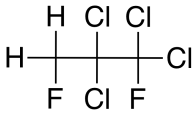


Radiative Efficiency



HCFC-232ad

Molecular Formula:	$CH_2FCCl_2CCl_2F$
Name:	1,1,2,2-Tetrachloro-1,3-difluoropropane
CAS number:	–
Molecular Weight:	217.86



Global Atmospheric Lifetime (years):	2.33
Tropospheric Atmospheric Lifetime (years):	2.55
Stratospheric Atmospheric Lifetime (years):	26.2
Ozone Depletion Potential (ODP):	0.050

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.248	0.213
Global Warming Potential (GWP_H):		
GWP_{20}	597	513
GWP_{100}	162	139
Global Temperature Potentials (GTP_H)		
GTP_{20}		198
GTP_{50}		25
GTP_{100}		19

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

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

OH Reactivity

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

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

$\tau^{OH}_{Global} = 2.47$ years

$\tau^{OH}_{Trop} = 2.55$ years

$\tau^{OH}_{Strat} = 78.5$ years

Fractional Atmospheric Loss: 0.941

O(^{1}D) Reactivity

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

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

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

Fractional Atmospheric Loss: 0.012

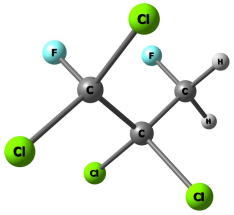
UV Photolysis

UV Spectrum: *No Recommendation*

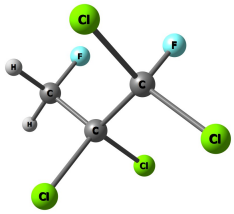
$\tau_{hv} = 50$ years

Fractional Atmospheric Loss: 0.047

Molecular Structure and Infrared Spectrum (9 conformers)



E = 0
Population = 0.188



E = 0
Population = 0.188

Optimized Coordinates (Angstroms)

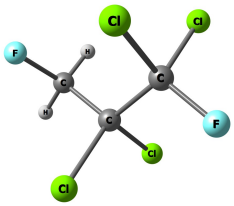
Atom	X	Y	Z
C	1.470106627378	1.236744566626	0.432281326376
C	0.667768024967	-0.066439504704	0.251498713897
C	-0.737847813459	0.157938842437	-0.410179785665
H	2.429213676541	0.974341626984	0.887475172980
F	1.680738424470	1.842476538654	-0.772707603587
H	0.917879454370	1.912181449096	1.090949286811
Cl	0.488398799526	-0.779160767486	1.881042743643
Cl	1.602860875827	-1.165279532016	-0.814408036309
Cl	-1.677959069442	-1.354566109568	-0.543667560592
Cl	-1.693857202258	1.363379755457	0.522787327935
F	-0.551859797919	0.648017134519	-1.636322585488

Atom	X	Y	Z
C	1.471580404347	-1.243237510755	0.418701997115
C	0.665872004111	0.060246297738	0.255958994187
C	-0.732532564676	-0.156304527676	-0.423373943763
H	0.915793571226	-1.933602911688	1.058631514562
F	1.696011619693	-1.824282544977	-0.795914570845
H	2.425288920999	-0.986276141633	0.888120853090
Cl	1.606677988243	1.183385436988	-0.779147087703
Cl	0.468298368461	0.740022150173	1.897432629157
Cl	-1.692566136209	-1.383485300796	0.476533946412
Cl	-1.677285352990	1.355002033553	-0.536024147613
F	-0.533033823206	-0.621411980926	-1.657096184600

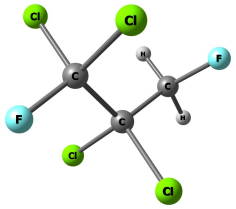
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
59.1178	0.0450
118.6638	0.220
163.3140	0.0183
176.9461	0.0849
204.8235	0.129
236.1556	0.0421
263.6660	0.138
291.0726	0.342
335.9750	0.565
352.6929	0.0802
386.3930	0.0602
405.3076	0.0620
484.9475	1.72
537.6074	6.03
691.1831	16.9
822.6905	24.2
880.9447	17.3
940.5896	7.66
1063.6701	2.73
1103.9187	0.476
1131.4141	12.3
1170.4198	17.3
1287.4460	0.828
1416.0729	1.59
1494.3442	1.48
3066.5177	1.40
3126.0497	1.14

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
59.1185	0.0450
118.6639	0.220
163.3143	0.0183
176.9457	0.0849
204.8220	0.129
236.1557	0.0421
263.6658	0.138
291.0723	0.342
335.9763	0.565
352.6927	0.0802
386.3934	0.0601
405.3063	0.0620
484.9475	1.72
537.6078	6.03
691.1837	16.9
822.6913	24.2
880.9425	17.3
940.5882	7.66
1063.6693	2.73
1103.9187	0.476
1131.4129	12.3
1170.4199	17.3
1287.4461	0.828
1416.0724	1.59
1494.3439	1.48
3066.5179	1.40
3126.0503	1.14



$\Delta E = 0.30$ kcal mol^{-1}
Population = 0.114



$\Delta E = 0.30$ kcal mol^{-1}
Population = 0.114

Optimized Coordinates (Angstroms)

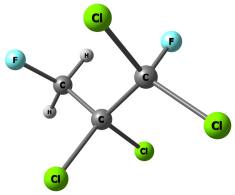
Atom	X	Y	Z
C	0.889152874759	-0.360118069450	-1.579079166503
C	0.716673927324	0.055653386424	-0.109266886388
C	-0.761412623326	0.177954049500	0.401447458442
H	1.953757057652	-0.288433629681	-1.817795976176
F	0.461917994308	-1.639684297247	-1.786999787500
H	0.319907864636	0.325566332819	-2.213497886202
Cl	1.486676251894	1.676013848586	0.041763165369
Cl	1.581169978130	-1.102515225533	0.950032746499
Cl	-1.689311751583	1.344974681890	-0.606923629520
Cl	-1.611377417566	-1.392491917809	0.379796987590
F	-0.751443156227	0.631134840503	1.654864974388

Atom	X	Y	Z
C	0.895185158718	0.368162607898	-1.571506892266
C	0.714326550258	-0.064355740576	-0.107545919050
C	-0.766105289744	-0.168843800780	0.400321612605
H	0.315236040442	-0.299365189041	-2.215522157968
F	0.489532274200	1.657346723574	-1.762558521142
H	1.958687029305	0.281951276269	-1.810332765434
Cl	1.596924797652	1.064929286406	0.967888140400
Cl	1.457082617341	-1.699204734100	0.022313822208
Cl	-1.589774210376	1.415699360086	0.399094344486
Cl	-1.712296464128	-1.306606755437	-0.624355757060
F	-0.764947503668	-0.638899034299	1.647548093220

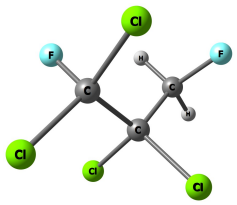
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
60.1179	0.0782
121.3362	0.234
160.0903	0.0191
183.3876	0.0751
221.7023	0.00807
236.6985	0.480
260.6740	0.0543
279.3590	0.305
295.8137	0.311
364.4210	0.0519
386.9198	0.0501
397.4249	0.0578
458.2311	1.20
602.2634	4.58
692.7508	15.6
792.2630	40.2
853.5806	4.36
932.2387	5.35
1068.5987	2.38
1125.8235	1.95
1131.3732	9.74
1176.9561	16.5
1294.7273	0.933
1420.0698	0.858
1493.8489	1.23
3064.2123	1.30
3123.1625	1.15

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
60.1185	0.0782
121.3368	0.234
160.0903	0.0191
183.3880	0.0751
221.7023	0.00807
236.6986	0.480
260.6740	0.0543
279.3589	0.305
295.8137	0.311
364.4210	0.0519
386.9200	0.0501
397.4248	0.0578
458.2313	1.20
602.2635	4.58
692.7512	15.6
792.2632	40.2
853.5812	4.36
932.2390	5.35
1068.5984	2.38
1125.8234	1.95
1131.3727	9.74
1176.9571	16.5
1294.7261	0.933
1420.0687	0.858
1493.8477	1.23
3064.2126	1.30
3123.1627	1.14



$\Delta E = 0.34$ kcal mol^{-1}
Population = 0.106



$\Delta E = 0.34$ kcal mol^{-1}
Population = 0.106

Optimized Coordinates (Angstroms)

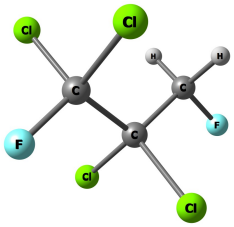
Atom	X	Y	Z
C	1.547891209515	-0.986720721209	-0.749431613305
C	0.727945718529	0.081495183910	0.007351280794
C	-0.793547973905	0.066492191980	-0.372900294687
H	2.605970906465	-0.756406257129	-0.601781325063
F	1.292730675265	-2.243651563033	-0.285660320213
H	1.297847138333	-0.926606626328	-1.813219601646
Cl	1.408099001332	1.657116510980	-0.545552070426
Cl	0.945907872422	-0.109980737637	1.762082826497
Cl	-1.563122785835	-1.491224863830	0.047112542574
Cl	-1.703601569607	1.397570229825	0.393853791642
F	-0.871235192513	0.214048652471	-1.705608216167

Atom	X	Y	Z
C	1.558952266101	0.977724058011	-0.735936861202
C	0.727104599345	-0.088180668793	0.011055216599
C	-0.792338313651	-0.059404994180	-0.376533636606
H	1.313700420928	0.925240673672	-1.801243214626
F	1.311171537025	2.234081202077	-0.266642453474
H	2.614491201002	0.738472370541	-0.584364648596
Cl	0.937891688189	0.092197641252	1.767838201294
Cl	1.397840615449	-1.666015070093	-0.547018365039
Cl	-1.716362324812	-1.387515437793	0.378568492664
Cl	-1.551974563959	1.501927655953	0.048122579700
F	-0.864595125616	-0.199209430646	-1.710382310715

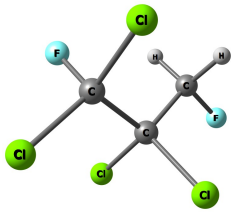
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
60.7324	0.0670
127.8544	0.343
163.9665	0.0194
173.4972	0.0786
208.6804	0.223
235.9649	0.0799
249.3042	0.224
287.6296	0.190
304.5131	0.440
380.4298	0.139
385.8658	0.0145
397.3621	0.0241
488.5614	1.53
535.3407	7.28
738.1005	9.99
790.8258	33.7
874.1734	9.07
937.9146	6.43
1063.8908	5.22
1100.9238	11.6
1132.9836	15.3
1149.5204	5.21
1297.4943	0.609
1415.2336	1.23
1494.1577	0.867
3062.8061	1.39
3124.2889	1.00

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
60.7316	0.0670
127.8545	0.343
163.9662	0.0194
173.4974	0.0786
208.6808	0.223
235.9650	0.0799
249.3043	0.224
287.6295	0.190
304.5126	0.440
380.4294	0.139
385.8656	0.0145
397.3617	0.0241
488.5612	1.53
535.3403	7.28
738.1004	9.99
790.8249	33.7
874.1728	9.07
937.9137	6.43
1063.8888	5.22
1100.9224	11.6
1132.9832	15.3
1149.5194	5.21
1297.4933	0.609
1415.2331	1.23
1494.1585	0.867
3062.8067	1.39
3124.2887	1.00



$\Delta E = 0.66$ kcal mol^{-1}
Population = 0.062



$\Delta E = 0.67$ kcal mol^{-1}
Population = 0.061

Optimized Coordinates (Angstroms)

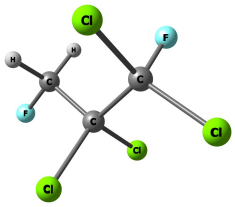
Atom	X	Y	Z
C	0.978655031317	0.005004597195	-1.473441511381
C	0.590207679867	-0.000184224222	0.012812888326
C	-0.956343928214	0.000967106890	0.252424928287
H	0.575725941238	0.904312565019	-1.947845240751
F	2.337565668886	0.003605571709	-1.583242303305
H	0.573322361972	-0.889549146558	-1.954736266802
Cl	1.282266777634	1.452672225656	0.810088014789
Cl	1.278363778110	-1.460971856125	0.798895676969
Cl	-1.720959063668	1.461799372365	-0.462530180757
Cl	-1.724862865934	-1.452276667347	-0.473722160570
F	-1.206745381207	-0.003711544583	1.557911155196

Atom	X	Y	Z
C	1.394274914816	1.061309667890	-0.765434314592
C	0.602744317412	-0.008941258870	0.013141415505
C	-0.907343878645	0.009084775599	-0.399844468122
H	1.042282184913	2.054470330387	-0.476285321727
F	2.719691327814	0.948917295122	-0.470654980990
H	1.239822680962	0.901446842610	-1.836902558464
Cl	0.784649047778	0.270249624764	1.766479339219
Cl	1.274203520522	-1.618035153229	-0.420108980094
Cl	-1.873224851883	-1.231428199400	0.432492707219
Cl	-1.633345473180	1.627453781128	-0.096792507509
F	-0.968617790509	-0.215860706001	-1.721277330445

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
71.4696	0.0264
105.5927	0.346
159.1190	0.229
162.3715	0.0742
221.4443	0.00219
228.4256	0.00694
250.1794	0.195
282.9992	0.0608
325.9811	0.323
335.6398	0.125
385.3787	0.0286
385.6945	0.130
495.3517	0.460
586.5952	4.10
715.9716	26.3
751.9670	18.6
824.9537	17.6
1021.9496	4.76
1067.8269	1.47
1077.1984	1.69
1139.8009	14.0
1189.2772	13.9
1284.9645	1.29
1418.3244	0.389
1499.4366	0.483
3062.2804	1.75
3122.9468	1.00

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
72.0806	0.0574
106.6540	0.356
151.4854	0.232
169.4522	0.0790
202.0311	0.0640
230.1013	0.0597
258.1441	0.0160
304.3856	0.303
320.5956	0.196
337.0568	0.302
381.4726	0.0376
389.7921	0.160
496.7704	0.427
581.3162	5.05
724.7810	23.3
780.6053	11.9
823.4287	25.7
1023.0368	4.02
1068.6831	6.95
1079.8990	5.02
1133.3121	11.0
1145.5699	12.9
1285.5989	1.79
1415.7737	0.554
1501.5935	0.368
3062.5399	1.66
3126.4018	1.06



$\Delta E = 0.67$ kcal mol^{-1}
Population = 0.061

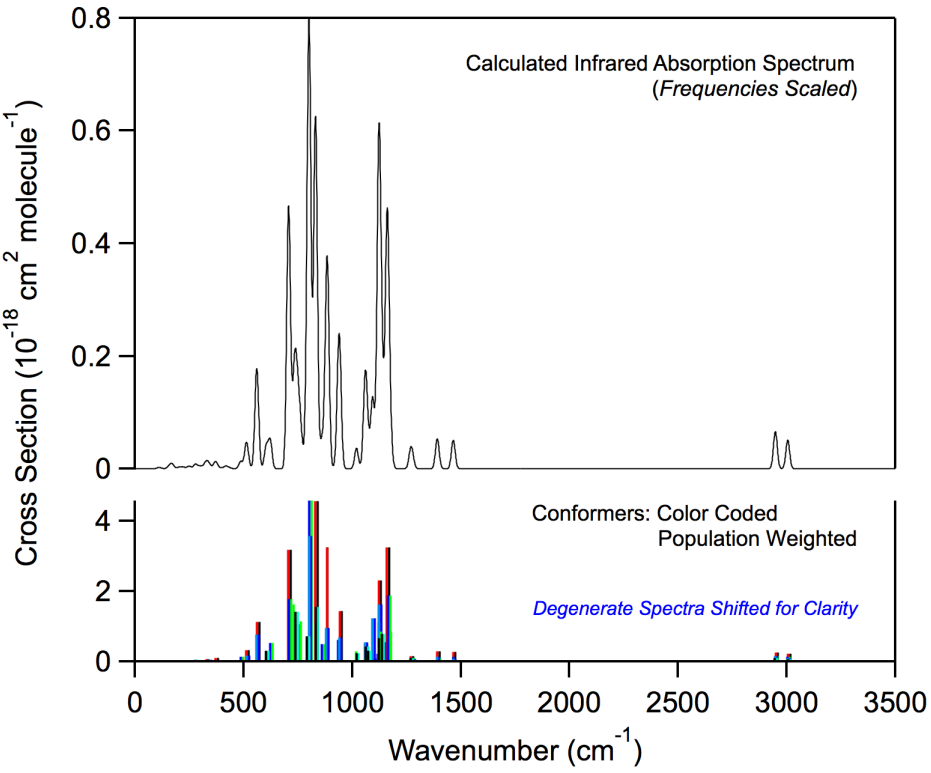
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.399012175619	-1.033727300249	-0.799945016641
C	0.604565285884	0.012078869741	0.008310552508
C	-0.905963067314	-0.000278771273	-0.403269791494
H	1.242631603345	-0.845414352536	-1.866499815464
F	2.724379191895	-0.924499350239	-0.503757530309
H	1.051006400645	-2.035657487919	-0.537452188160
Cl	1.269618648888	1.634795757492	-0.381868135316
Cl	0.789680522750	-0.313933152431	1.753211814611
Cl	-1.625678214219	-1.628941274957	-0.143451189204
Cl	-1.875313306407	1.213611197003	0.463572002426
F	-0.969716241086	0.260244865368	-1.718032702956

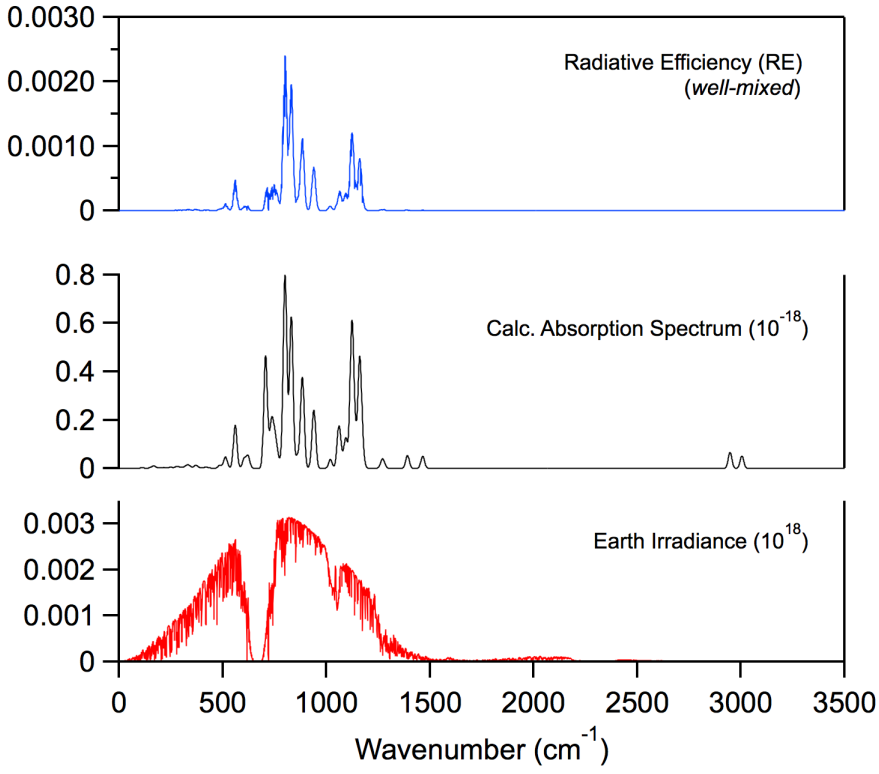
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
72.0801	0.0573
106.6542	0.356
151.4858	0.232
169.4522	0.0790
202.0317	0.0640
230.1016	0.0597
258.1443	0.0160
304.3859	0.303
320.5959	0.196
337.0572	0.302
381.4727	0.0376
389.7923	0.160
496.7705	0.427
581.3166	5.05
724.7816	23.3
780.6050	11.9
823.4280	25.7
1023.0376	4.02
1068.6854	6.95
1079.9000	5.02
1133.3132	11.0
1145.5702	12.9
1285.5996	1.79
1415.7749	0.554
1501.5943	0.368
3062.5391	1.66
3126.4006	1.06

Infrared Spectrum

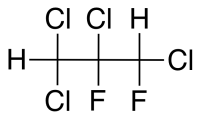


Radiative Efficiency



HCFC-232ba

Molecular Formula:	$CHCl_2CClFCHClF$
Name:	1,1,2,3-Tetrachloro-2,3-difluoropropane
CAS number:	–
Molecular Weight:	217.86



Global Atmospheric Lifetime (years):	0.988
Tropospheric Atmospheric Lifetime (years):	1.04
Stratospheric Atmospheric Lifetime (years):	20
Ozone Depletion Potential (ODP):	0.023

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.219	0.162
Global Warming Potential (GWP_H):		
GWP_{20}	224	165
GWP_{100}	61	45
Global Temperature Potentials (GTP_H)		
GTP_{20}		54
GTP_{50}		8
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*

$k_{SAR}(298\ K) = 5.64 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 3.60 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

τ^{OH}_{Global} = 1.01 years

τ^{OH}_{Trop} = 1.04 years

τ^{OH}_{Strat} = 35.0 years

Fractional Atmospheric Loss: 0.978

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: 0.005

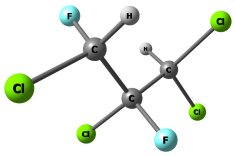
UV Photolysis

UV Spectrum: *No Recommendation*

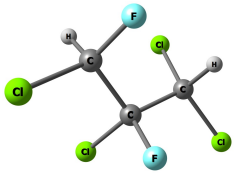
τ_{hv} = 59 years

Fractional Atmospheric Loss: 0.017

Molecular Structure and Infrared Spectrum (8 conformers)



E = 0
Population = 0.237



$\Delta E = 0.01$ kcal mol^{-1}
Population = 0.231

Optimized Coordinates (Angstroms)

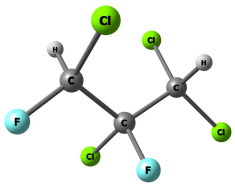
Atom	X	Y	Z
C	1.259400462514	-0.754006220167	-0.206385075890
C	0.139895708548	0.235190197271	0.200568391477
C	-1.221404018005	-0.176640136672	-0.416351658425
Cl	2.840338710079	-0.291206338934	0.474861637089
H	1.031037014557	-1.744162680004	0.187376677563
F	1.322588314157	-0.802050091087	-1.556212661500
Cl	0.539858415487	1.879214322852	-0.403399197537
F	0.054522076759	0.249381088988	1.541383495929
H	-1.158442591731	-0.137599554191	-1.499915619267
Cl	-1.622848223812	-1.874268436350	0.025936126116
Cl	-2.529561868554	0.907572848293	0.109454884445

Atom	X	Y	Z
C	1.324845255741	0.707322086130	-0.034799237713
C	0.163881049178	-0.309774212331	-0.174188204967
C	-1.174944362832	0.422206827769	-0.448229046836
Cl	2.910825475091	-0.104989842976	-0.099081381390
F	1.234784489112	1.582476480895	-1.070245166388
H	1.264284422885	1.245900426591	0.909358570020
Cl	0.091465374948	-1.321661129430	1.296584768133
F	0.395961399353	-1.092697390918	-1.249346349060
H	-1.047134147122	1.003623927911	-1.357872871814
Cl	-2.494424575663	-0.732265216890	-0.743191344337
Cl	-1.581844380692	1.575663043248	0.853589264354

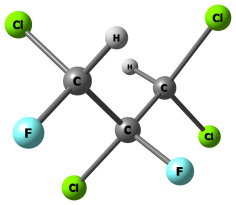
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
53.0254	0.0546
67.9023	0.157
127.7750	0.0615
187.6498	0.137
196.3356	0.204
217.5522	0.0478
239.3585	0.0244
270.2403	0.0109
324.2121	0.299
365.3109	0.0656
406.2049	0.310
502.8057	0.895
613.4094	10.7
694.9571	20.8
735.1528	7.82
755.2362	10.2
852.8531	5.90
958.5845	7.15
1089.2748	5.13
1137.0268	17.5
1189.0009	8.49
1225.9244	2.31
1281.8434	0.580
1301.1959	1.70
1358.6351	2.01
3132.9712	0.471
3171.3056	0.539

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
62.1820	0.0930
69.4209	0.0786
123.8446	0.0487
171.3471	0.0751
188.5127	0.232
215.3227	0.0316
251.6767	0.0319
308.7413	0.114
327.4598	0.233
370.0793	0.153
421.3519	0.828
451.9383	0.539
586.4093	6.98
698.7407	19.2
767.6887	4.52
817.1657	13.4
846.0421	10.9
963.2919	15.6
1079.2688	2.90
1093.7094	13.9
1184.1157	11.0
1238.2702	1.92
1269.7547	1.69
1292.7691	2.28
1361.3754	0.495
3146.0607	0.494
3158.2473	0.483



$\Delta E = 0.12$ kcal mol^{-1}
Population = 0.194



$\Delta E = 0.32$ kcal mol^{-1}
Population = 0.139

Optimized Coordinates (Angstroms)

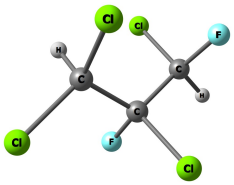
Atom	X	Y	Z
C	1.512181203324	0.053368119610	-0.432454960554
C	0.160077649942	0.473512828147	0.195149603513
C	-0.882629469543	-0.665014806526	0.256439207458
Cl	2.211002185785	-1.349982699830	0.458675864859
H	1.394166915335	-0.252812538414	-1.470589377406
F	2.365912781586	1.086436878948	-0.337420894921
Cl	-0.440126453969	1.874216836442	-0.757194017627
F	0.391198374004	0.877482541636	1.461502069557
H	-0.469663448084	-1.467451425680	0.862910684135
Cl	-2.375330476312	-0.127403951090	1.061684527496
Cl	-1.208989262067	-1.350634783245	-1.360385706509

Atom	X	Y	Z
C	1.395459469369	0.508866843097	-0.507589467291
C	0.116297304407	-0.358797779861	-0.383570033203
C	-1.013355767412	0.287641846254	0.446741227923
Cl	2.042357507324	0.998240841322	1.090886790084
F	2.324757958320	-0.190895744090	-1.180141994637
H	1.159945415944	1.424025787422	-1.051356275428
Cl	0.543349488753	-1.943090588842	0.344567732517
F	-0.310667441986	-0.562001860172	-1.649402720175
H	-0.709667169919	0.386285267334	1.484341968546
Cl	-1.356979202777	1.944183141096	-0.164395270885
Cl	-2.493796562024	-0.698930753561	0.393421042550

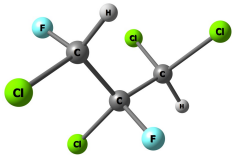
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
56.5336	0.0658
80.0993	0.106
127.3870	0.0383
170.9891	0.139
181.3612	0.180
235.4600	0.0422
257.4839	0.0617
289.7125	0.100
329.5687	0.0876
371.2667	0.198
412.2400	0.360
434.3139	1.27
592.4619	5.00
729.6101	20.9
756.5647	15.8
788.8538	10.6
810.5565	8.33
952.0894	8.98
1094.1580	7.94
1145.0315	8.97
1189.2973	15.4
1236.9469	1.72
1266.4196	2.88
1285.4293	0.386
1374.2566	0.893
3145.4536	0.449
3155.6838	0.459

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
58.0587	0.0375
77.6051	0.124
132.8632	0.0257
178.8338	0.353
199.5858	0.0249
214.3311	0.0431
260.0715	0.0291
298.3946	0.182
315.1538	0.138
366.0090	0.164
420.7371	0.607
431.0980	0.628
621.4376	10.5
720.1120	9.50
731.4866	7.97
775.3882	13.2
819.9915	14.5
973.4066	12.3
1080.0141	1.25
1162.3025	24.5
1172.1309	5.16
1224.6607	2.21
1264.9785	1.89
1292.7006	0.800
1370.6624	2.10
3128.9873	0.523
3176.8578	0.599



$\Delta E = 0.55$ kcal mol^{-1}
Population = 0.093



$\Delta E = 0.81$ kcal mol^{-1}
Population = 0.060

Optimized Coordinates (Angstroms)

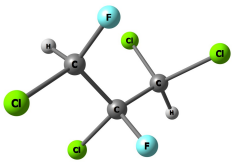
Atom	X	Y	Z
C	1.576601110058	-0.382641786511	0.289219928988
C	0.101022867944	-0.640184790523	-0.114670500489
C	-0.742144534252	0.612485185379	-0.445090422256
Cl	2.416113821585	0.604158842133	-0.964267368425
F	1.679841512417	0.226379376650	1.478187430692
H	2.087117993864	-1.347324749779	0.311722989716
Cl	-0.632092516652	-1.627057761553	1.191018723932
F	0.159549453266	-1.390980871324	-1.240610276801
H	-0.228120490044	1.160666988533	-1.231220085536
Cl	-2.330586339402	0.140686227579	-1.108299260477
Cl	-0.911122878782	1.715560339414	0.939478840656

Atom	X	Y	Z
C	0.927997661473	-0.491303272931	-0.735653794795
C	0.205736873480	-0.010858882112	0.546657096713
C	-1.344787100236	0.027537821098	0.447902426045
Cl	2.643081167093	-0.870749991181	-0.396654686362
H	0.466597640836	-1.416260197202	-1.087035124001
F	0.853213634187	0.450029419793	-1.693445256244
Cl	0.782012309996	1.617134600003	1.027134159441
F	0.490916703056	-0.877787917782	1.543719665543
H	-1.726855940125	0.361060836649	1.409874131300
Cl	-1.967448957971	1.134150265945	-0.794908132210
Cl	-1.977381991791	-1.636290682281	0.197083514569

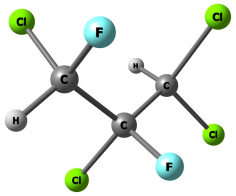
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
47.2724	0.0724
88.4438	0.0533
140.8960	0.144
168.7080	0.0111
175.9128	0.0622
226.9624	0.160
263.8974	0.100
276.1845	0.178
350.8840	0.210
376.3133	0.146
408.1069	0.230
505.2568	4.13
570.4584	3.90
620.2887	7.63
755.8758	24.7
808.6797	4.55
814.0332	15.8
970.8599	4.26
1124.3689	3.41
1136.5662	16.4
1179.3383	11.6
1233.0598	2.86
1279.3749	1.01
1292.2503	3.60
1371.9796	1.70
3111.9440	0.676
3152.2669	0.420

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
47.7117	0.102
76.6548	0.0433
139.6294	0.0669
167.0001	0.0447
195.0677	0.0872
207.5190	0.0962
252.3516	0.0896
306.2815	0.0607
345.4862	0.0605
371.4087	0.141
416.4542	0.846
523.8651	6.95
541.9253	0.299
636.3861	9.72
733.3532	13.7
810.5556	21.3
827.0453	6.18
982.5035	7.21
1113.8056	2.16
1140.1955	10.8
1153.9150	17.3
1224.3639	2.55
1289.7050	2.63
1299.4826	0.0519
1367.0306	2.18
3111.9100	0.559
3151.4217	0.564



$\Delta E = 1.31$ kcal mol^{-1}
Population = 0.026



$\Delta E = 1.49$ kcal mol^{-1}
Population = 0.019

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	0.954542185973	-0.451125933853	-0.714144869215
C	0.221745927679	0.202369572909	0.481756671797
C	-1.330718693511	0.215749086373	0.376879222321
Cl	2.696495302024	-0.649403737442	-0.359311946781
F	0.413952117566	-1.665185671091	-0.952440655347
H	0.870648509272	0.172762565830	-1.602681739868
Cl	0.760389064580	1.920639959853	0.604271375865
F	0.543735156929	-0.427101864612	1.625799049486
H	-1.711617577647	0.902905426851	1.127889911641
Cl	-1.880280787145	0.822167407974	-1.213250524851
Cl	-2.038014205721	-1.380956812791	0.743806504950

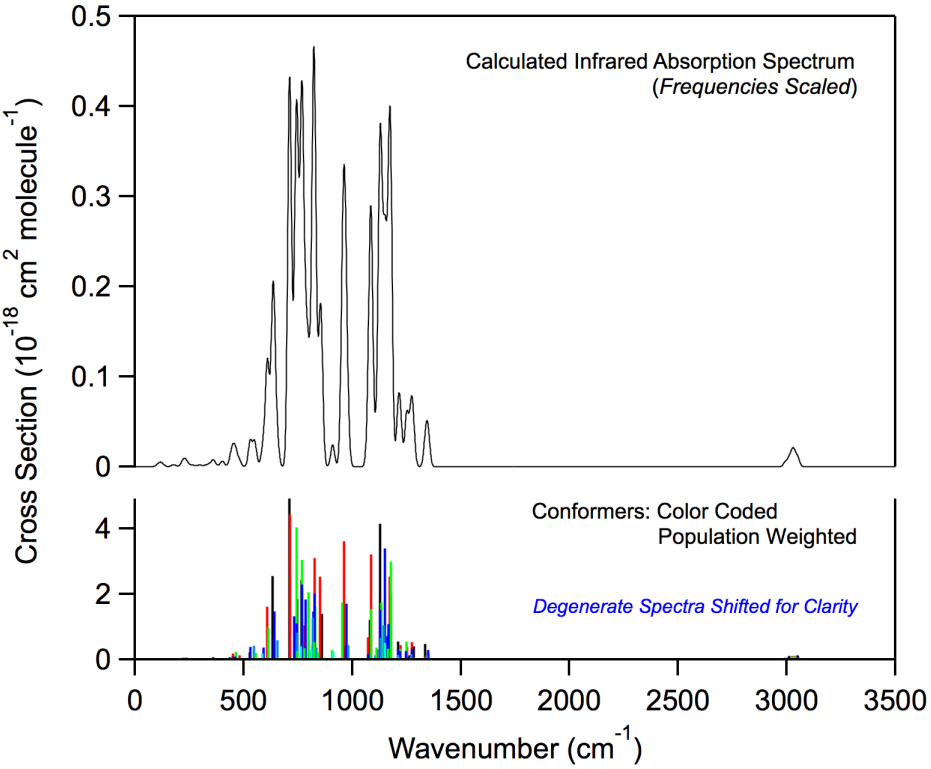
Atom	X	Y	Z
C	1.527755476032	-0.181710170632	0.556893596834
C	0.082769339939	0.394469969708	0.498830383734
C	-0.875741726401	-0.227995865807	-0.539743356076
Cl	2.269448284207	-0.320746754699	-1.071032784203
H	2.149862118267	0.506003887560	1.131870635586
F	1.519645564071	-1.384527602295	1.156636308322
Cl	0.255203866592	2.156109118750	0.139301556528
F	-0.424967173627	0.253077478972	1.738358194622
H	-0.502765427222	-0.046434096592	-1.542982018938
Cl	-0.991793985803	-2.000031950715	-0.325212554866
Cl	-2.498194336054	0.507948985749	-0.419824961543

Infrared Absorption Spectrum (unscaled frequencies)

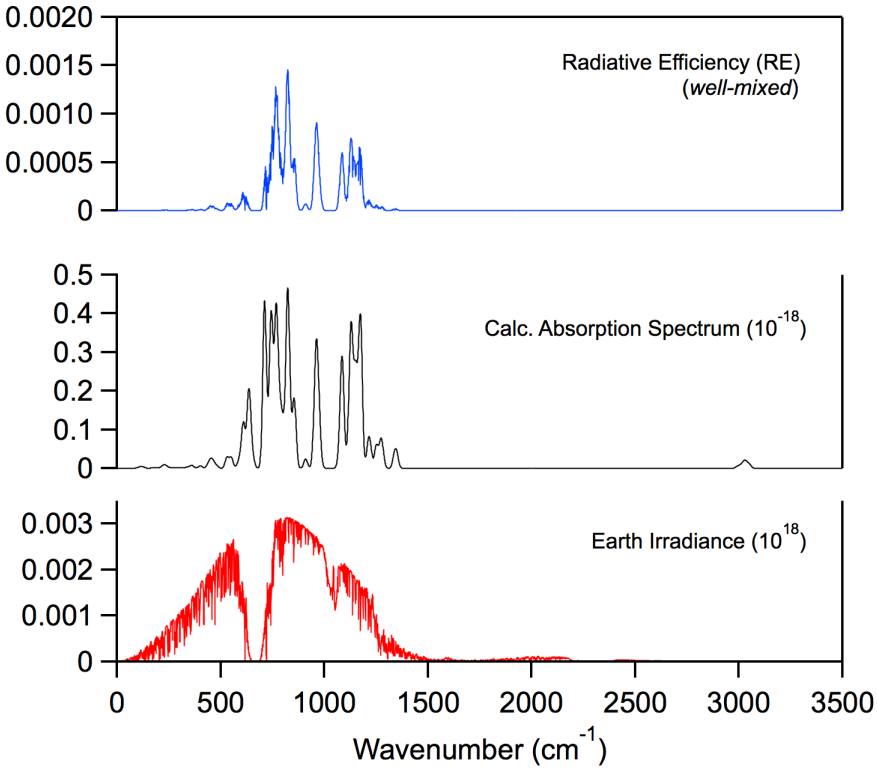
Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
51.5616	0.0489
72.2207	0.0284
137.0633	0.0155
172.5047	0.0645
195.0970	0.205
217.7126	0.0636
246.7919	0.0214
314.6947	0.166
333.2554	0.187
357.6347	0.0961
415.4537	1.02
451.3741	0.739
530.5511	7.70
733.7750	9.81
769.5415	13.1
816.7843	20.4
837.5625	8.59
904.3428	11.5
1102.9248	2.18
1119.7601	14.0
1176.1583	12.4
1232.9036	0.750
1286.6218	1.87
1305.1052	1.83
1376.2806	0.654
3142.1001	0.524
3155.7391	0.543

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
51.6400	0.0225
79.7733	0.0493
144.2474	0.110
177.0115	0.0390
204.1924	0.209
217.2274	0.0192
250.8899	0.101
309.4267	0.157
314.3941	0.278
372.4831	0.0947
409.6031	0.562
439.7141	0.740
563.2247	9.41
733.1004	1.84
751.5665	21.2
802.3529	16.2
833.5163	4.18
909.3762	12.2
1095.5866	0.377
1161.3790	27.1
1164.0814	3.71
1225.8594	3.38
1287.7204	2.23
1295.5034	0.829
1378.2357	1.74
3116.0611	0.637
3175.1467	0.541

Infrared Spectrum

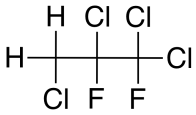


Radiative Efficiency



HCFC-232bb

Molecular Formula:	$CH_2ClCClFCCl_2F$
Name:	1,1,2,3-Tetrachloro-1,2-difluoropropane
CAS number:	1943659-44-6
Molecular Weight:	217.86



Global Atmospheric Lifetime (years): 2.56
- Tropospheric Atmospheric Lifetime (years): 2.80
- Stratospheric Atmospheric Lifetime (years): 29.3

Ozone Depletion Potential (ODP): 0.053

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.256	0.222
Global Warming Potential (GWP_H):		
GWP_{20}	675	587
GWP_{100}	183	159
Global Temperature Potentials (GTP_H)		
GTP_{20}		235
GTP_{50}		29
GTP_{100}		22

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

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

OH Reactivity

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

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

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

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

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

Fractional Atmospheric Loss: 0.943

O(^{1}D) Reactivity

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

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

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

Fractional Atmospheric Loss: 0.014

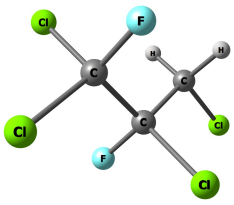
UV Photolysis

UV Spectrum: *No Recommendation*

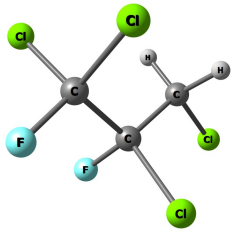
$\tau_{hv} = 59$ years

Fractional Atmospheric Loss: 0.043

Molecular Structure and Infrared Spectrum (5 conformers)



E = 0
Population = 0.344



$\Delta E = 0.20$ kcal mol^{-1}
Population = 0.245

Optimized Coordinates (Angstroms)

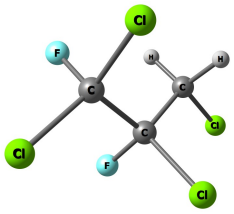
Atom	X	Y	Z
C	-1.373452621535	0.813913295762	-0.474819154522
C	-0.372931748841	-0.145295789242	0.181344179778
C	1.089580398479	0.149501736993	-0.302415683331
Cl	-3.036971895839	0.561821693854	0.128699568168
H	-1.098745965038	1.838750577589	-0.231906882348
H	-1.370174631183	0.669828719497	-1.553401473120
Cl	-0.775498875894	-1.842804829969	-0.260241024182
F	-0.400216448455	-0.020422047872	1.519019561121
Cl	1.545319920506	1.837707623877	0.127774094345
Cl	2.267385074229	-0.962177981885	0.432518744222
F	1.131927793573	0.031403001397	-1.633818930132

Atom	X	Y	Z
C	-1.138845517315	0.663493786850	-0.768782905239
C	-0.381807641782	-0.056061049247	0.348130529495
C	1.176855960062	-0.023120860644	0.162864710263
Cl	-2.877905521415	0.826850504079	-0.384960341209
H	-0.737272365381	1.670247649292	-0.881725038079
H	-1.046367484905	0.115652774799	-1.703173534167
Cl	-0.890718341775	-1.777732445425	0.466383438458
F	-0.625095717205	0.532621452959	1.537554205686
Cl	1.674573968140	-0.713197007351	-1.409436900201
Cl	1.760904830691	1.672376732847	0.290751777265
F	1.743247830883	-0.722468538159	1.142390057728

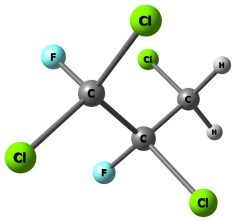
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
60.6701	0.0606
75.1421	0.356
132.8197	0.181
181.3306	0.0484
214.7959	0.0333
238.9771	0.155
253.3483	0.0869
287.8239	0.0109
317.7269	0.178
379.5657	0.0338
390.7334	0.107
431.9621	0.329
536.0902	1.40
627.2808	6.11
704.3429	22.7
780.8830	26.3
854.4220	12.0
898.7807	0.857
1003.3246	3.81
1080.4867	9.74
1160.8705	18.9
1181.6161	0.450
1254.6449	7.29
1315.2630	0.969
1464.1540	0.902
3115.7385	0.638
3184.3095	0.0188

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
68.2672	0.00619
74.7029	0.295
139.9146	0.172
169.2529	0.0357
206.8596	0.0590
235.2941	0.0318
275.9375	0.133
303.6226	0.343
332.1032	0.0994
369.7644	0.0134
391.9547	0.0347
430.6802	0.786
484.0931	0.683
629.4975	5.51
736.2881	26.2
792.3532	9.97
837.9667	22.3
911.5752	11.3
1007.5641	5.79
1054.6929	6.14
1177.8916	8.75
1188.7089	13.2
1241.4641	4.72
1317.3017	0.880
1463.6021	1.07
3112.0060	0.876
3186.2211	0.0849



$\Delta E = 0.32$ kcal mol^{-1}
Population = 0.200



$\Delta E = 0.68$ kcal mol^{-1}
Population = 0.109

Optimized Coordinates (Angstroms)

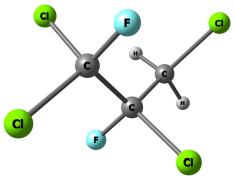
Atom	X	Y	Z
C	-1.404522966929	0.893900911238	0.222340038966
C	-0.381196255311	-0.247351676023	0.173783414272
C	1.077363213936	0.312583899325	0.331046205243
Cl	-3.077087276695	0.276854050680	0.352331415532
H	-1.209103299769	1.497904812631	1.107870966833
H	-1.335885008936	1.505823434540	-0.673486444935
Cl	-0.536277372753	-1.198685640208	-1.332628752899
F	-0.570073618908	-1.066485388858	1.230722056483
Cl	2.271161144706	-1.001799210258	0.433268998057
Cl	1.500966471824	1.445971761212	-0.985678777313
F	1.104842968834	0.991869045720	1.491254879762

Atom	X	Y	Z
C	-1.615768040364	-0.654556726864	-0.512081501252
C	-0.251262644557	-0.700318994229	0.187643617004
C	0.599028005862	0.616742840803	0.124751718287
Cl	-2.790979839016	0.457992961737	0.264066150471
H	-1.498795951310	-0.358516578378	-1.551880476487
H	-2.042355812297	-1.654554923927	-0.456143183775
Cl	0.653565710807	-2.052950476180	-0.589261149672
F	-0.414213984407	-0.981294425087	1.495023712878
Cl	2.166836365471	0.403462904142	0.953856315735
Cl	0.855518178592	1.151841432967	-1.563408571392
F	-0.074765988781	1.571300985015	0.771674368201

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
68.0079	0.0126
80.8468	0.362
129.1831	0.188
171.6131	0.0318
205.7087	0.0733
229.6933	0.0320
278.6827	0.104
304.3985	0.385
334.4462	0.0271
377.4874	0.108
395.1390	0.0344
426.1131	0.937
496.5925	0.720
620.7417	7.88
723.7219	17.3
824.4487	7.71
864.0097	25.7
908.8678	9.58
1003.7710	18.6
1066.6914	3.71
1131.2119	9.31
1169.4507	5.32
1242.6308	7.12
1316.4345	1.02
1463.6313	0.855
3113.3228	0.665
3187.6110	0.101

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
41.8010	0.0625
105.7799	0.171
163.1589	0.111
174.8636	0.0267
188.1598	0.231
246.2145	0.0451
281.7325	0.198
302.4628	0.285
320.2107	0.298
373.0769	0.153
388.3660	0.0675
434.5040	0.975
489.4812	1.28
562.3978	7.17
750.4314	14.5
827.0844	13.2
857.2408	24.9
914.2432	9.89
936.2811	17.7
1081.7582	2.70
1154.5329	15.2
1182.9882	4.12
1274.6485	3.26
1310.0878	4.08
1456.8191	1.96
3118.3817	0.676
3188.6508	0.0337



$\Delta E = 0.72$ kcal mol^{-1}
Population = 0.101

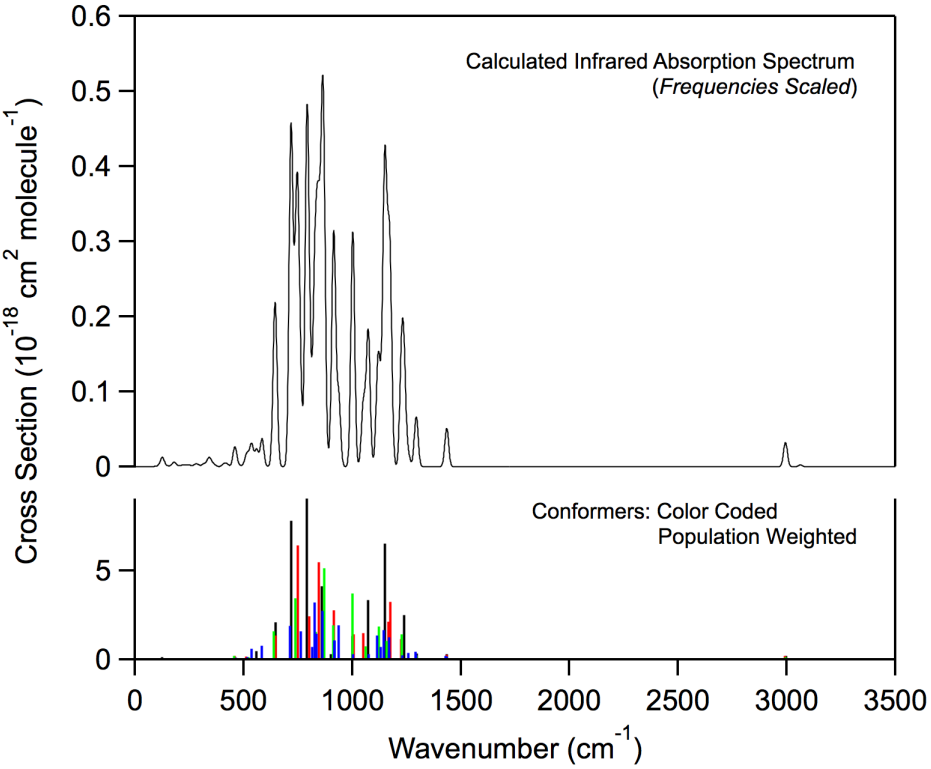
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.547635287414	0.367382545579	0.910699906126
C	-0.276511645288	-0.429852373765	0.583657517731
C	0.774259454645	0.285810300158	-0.331173733231
Cl	-2.548831563678	0.822072229999	-0.495817646860
H	-2.152467267395	-0.256664775035	1.567610584167
H	-1.262590844135	1.281451648756	1.428868021409
Cl	-0.706524956484	-2.004758083539	-0.164056069910
F	0.321379944796	-0.663532960432	1.775944698314
Cl	1.129187995058	1.923744690540	0.324987612436
Cl	2.294495114245	-0.650068751995	-0.394215869723
F	0.295694055649	0.419025529734	-1.564252020459

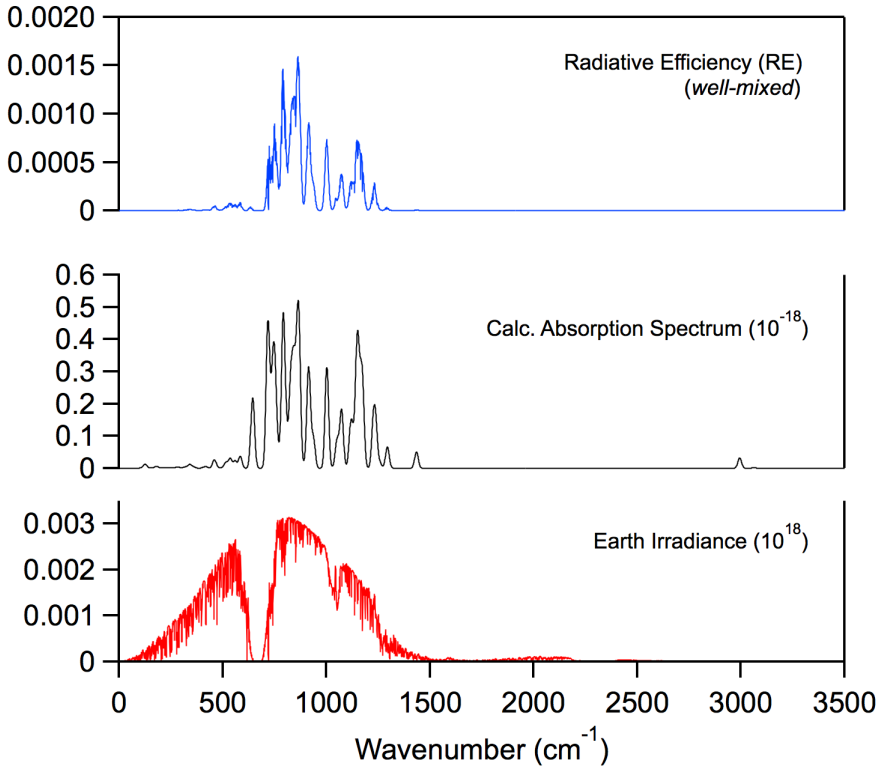
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
48.1056	0.0403
91.0296	0.102
152.5043	0.0481
183.2760	0.106
203.5631	0.0972
247.7182	0.0745
287.2305	0.148
300.4493	0.474
338.6473	0.0214
375.0995	0.163
387.5815	0.207
458.6281	0.306
511.9683	6.07
570.0313	0.0558
699.0367	18.7
806.7063	7.01
818.5857	31.7
916.2490	10.5
1006.3173	3.04
1123.7669	13.4
1141.6707	7.00
1180.9845	12.3
1244.6304	2.39
1313.8043	2.78
1463.5277	1.76
3108.2965	0.791
3174.7361	0.00724

Infrared Spectrum

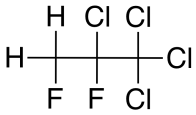


Radiative Efficiency



HCFC-232bc

Molecular Formula:	$CH_2FCClFCCl_3$
Name:	1,1,1,2-Tetrachloro-2,3-difluoropropane
CAS number:	–
Molecular Weight:	217.86



Global Atmospheric Lifetime (years):	3.64
Tropospheric Atmospheric Lifetime (years):	4.14
Stratospheric Atmospheric Lifetime (years):	29.7
Ozone Depletion Potential (ODP):	0.075

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.227	0.205
Global Warming Potential (GWP_H):		
GWP_{20}	851	766
GWP_{100}	231	208
Global Temperature Potentials (GTP_H)		
GTP_{20}		357
GTP_{50}		40
GTP_{100}		29

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

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

OH Reactivity

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

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

$\tau^{OH}_{Global} = 4.01$ years

$\tau^{OH}_{Trop} = 4.14$ years

$\tau^{OH}_{Strat} = 121.4$ years

Fractional Atmospheric Loss: 0.908

$O(^1D)$ 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: 0.020

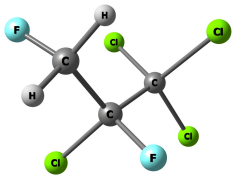
UV Photolysis

UV Spectrum: *No Recommendation*

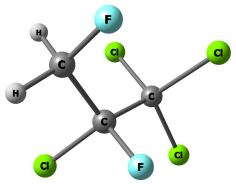
$\tau_{hv} = 50$ years

Fractional Atmospheric Loss: 0.072

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.392



$\Delta E = 0.10$ kcal mol^{-1}
Population = 0.331

Optimized Coordinates (Angstroms)

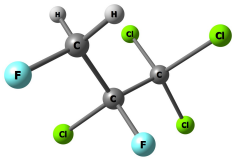
Atom	X	Y	Z
C	1.607929465656	1.071860962126	-0.722345597572
C	0.727069815780	-0.179988383246	-0.555813724147
C	-0.688208392816	0.051689306914	0.084442705632
H	1.025851307538	1.864015227419	-1.201608209232
F	2.098676419838	1.517472803122	0.467642613095
H	2.433535728099	0.773849368388	-1.376803667204
Cl	1.637029956224	-1.410734497409	0.379972323221
F	0.515570807595	-0.656424011742	-1.806095851689
Cl	-1.609381401648	-1.476974915326	0.101029889079
Cl	-0.552588216173	0.704249513441	1.731419201911
Cl	-1.580136490093	1.229474626313	-0.946833683093

Atom	X	Y	Z
C	1.811214792627	0.884560970317	0.420602608612
C	0.863970410635	-0.087750356410	-0.303197196266
C	-0.662518191788	0.007331605248	0.058752498395
H	2.826910623518	0.618389274855	0.112757561548
F	1.560232987385	2.177422884771	0.058286655706
H	1.710765583859	0.770134598892	1.502343988648
Cl	1.482260646864	-1.737763259730	0.090867587037
F	0.965968975536	0.104824844999	-1.633085556007
Cl	-1.577047147997	-1.239241429274	-0.837445145890
Cl	-0.901725533912	-0.213506747712	1.816633812803
Cl	-1.285659146727	1.612053614046	-0.423233814586

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
56.5720	0.117
110.3474	0.285
167.6215	0.0454
175.1372	0.0628
203.4653	0.203
235.6001	0.0334
263.8862	0.0503
278.0363	0.563
310.2415	0.216
334.9436	0.189
388.9191	0.207
404.0299	0.262
511.8793	2.18
557.3497	6.35
695.0177	20.8
778.1618	12.3
830.4054	20.7
916.9517	1.81
1068.0891	7.37
1135.1816	14.4
1155.5780	6.59
1161.1090	1.17
1283.6553	2.02
1420.1342	0.875
1500.0357	1.19
3057.8516	2.01
3117.4717	1.44

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
46.6873	0.107
122.1203	0.372
168.2479	0.0111
183.5081	0.128
201.5931	0.202
227.3037	0.0439
265.4372	0.0270
278.7786	0.400
312.8156	0.208
325.0784	0.237
381.4994	0.236
400.5895	0.0496
445.0500	1.25
571.8062	8.92
757.1781	30.4
800.2348	14.3
841.2216	8.22
923.8752	5.92
965.8923	8.00
1116.3637	6.86
1152.4915	2.02
1204.0420	11.7
1307.6055	1.82
1422.1786	0.918
1490.7343	1.04
3066.3726	1.41
3130.0564	1.21



$\Delta E = 0.21$ kcal mol^{-1}
Population = 0.276

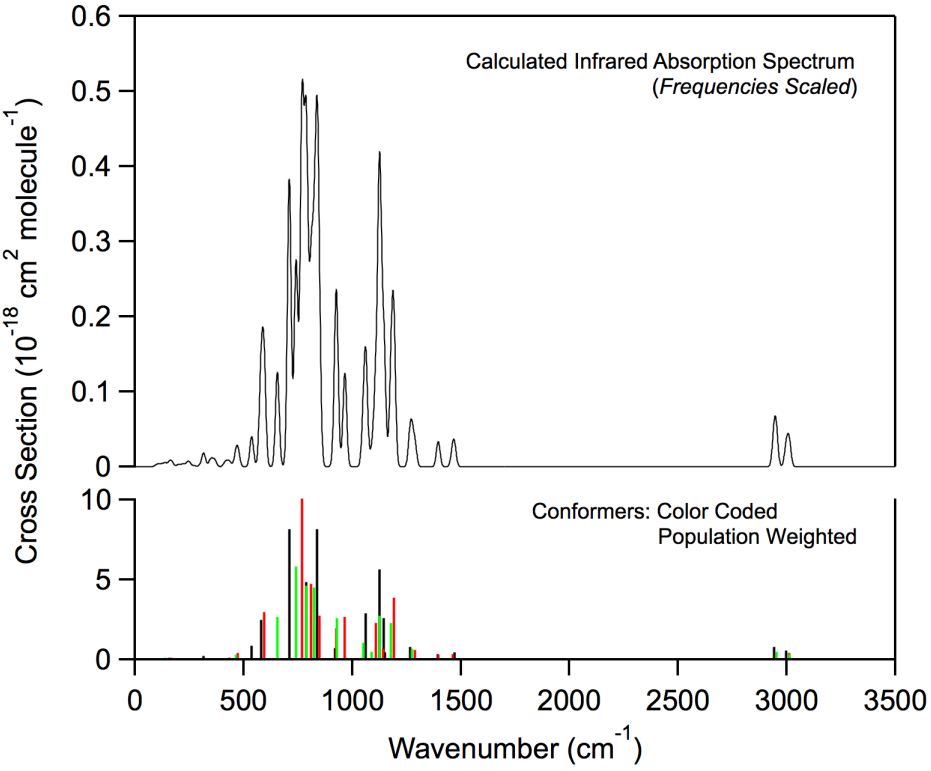
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.556196935486	1.128143611851	0.477037885814
C	0.753781454901	0.048112021626	-0.266975170016
C	-0.781495005748	0.054254654929	0.059504778164
H	1.466847506568	0.991203926363	1.556825240277
F	2.864147123707	1.024213278651	0.099355969312
H	1.177662934740	2.112377473308	0.187548331220
Cl	1.458411966399	-1.562407810062	0.110011209259
F	0.876216732790	0.257131690388	-1.595539204380
Cl	-1.622755480838	-1.185924499449	-0.901317972571
Cl	-1.062545025004	-0.224088941605	1.800606956047
Cl	-1.447243143001	1.665045593999	-0.390659023125

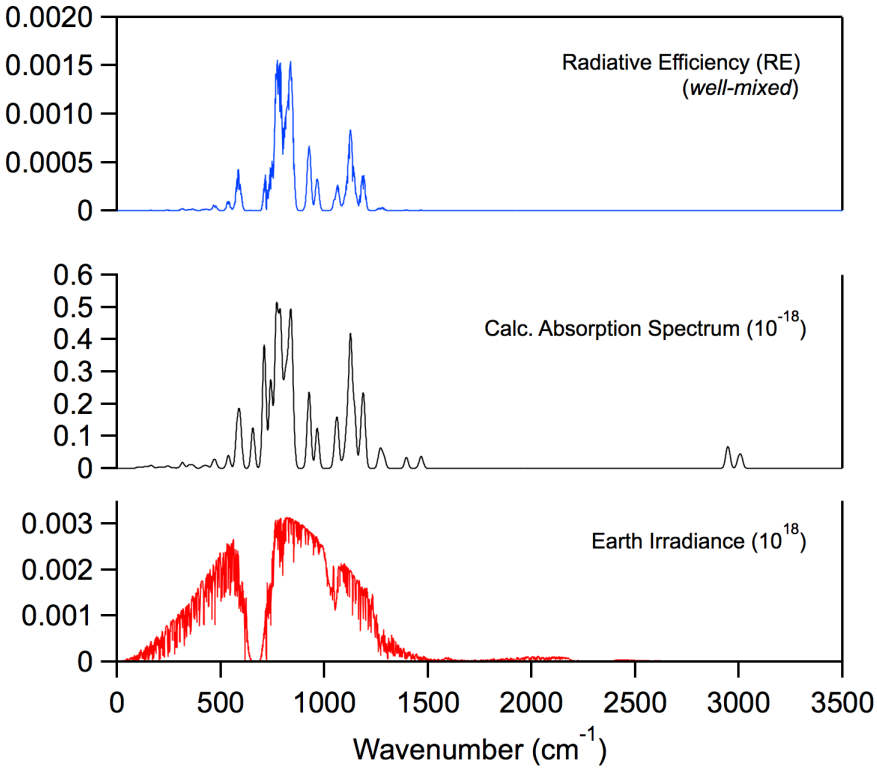
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
70.2434	0.238
89.0101	0.373
153.8999	0.209
167.9437	0.0289
213.5575	0.0882
228.2872	0.0141
257.1154	0.0471
274.2303	0.0971
310.1443	0.168
330.0781	0.270
382.8598	0.0210
403.2930	0.0875
434.6461	1.11
637.0400	9.71
728.2403	21.0
776.9771	16.7
815.1211	16.3
925.7363	9.42
1056.2515	3.85
1098.0851	1.73
1135.5694	9.90
1191.6773	8.32
1293.1884	2.49
1421.3301	0.271
1499.5890	0.293
3070.5037	1.73
3133.8860	1.19

Infrared Spectrum

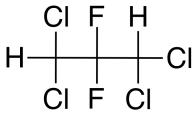


Radiative Efficiency



HCFC-232ca

Molecular Formula:	$CHCl_2CF_2CHCl_2$
Name:	1,1,3,3-Tetrachloro-2,2-difluoropropane
CAS number:	1112-14-7
Molecular Weight:	217.86



Global Atmospheric Lifetime (years):	0.704
Tropospheric Atmospheric Lifetime (years):	0.737
Stratospheric Atmospheric Lifetime (years):	20
Ozone Depletion Potential (ODP):	0.017

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.192	0.130
Global Warming Potential (GWP_H):		
GWP_{20}	140	95
GWP_{100}	38	26
Global Temperature Potentials (GTP_H)		
GTP_{20}		30
GTP_{50}		4
GTP_{100}		4

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 7.96 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 5.08 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 0.716$ years

$\tau^{OH}_{Trop} = 0.737$ years

$\tau^{OH}_{Strat} = 25.6$ years

Fractional Atmospheric Loss: 0.982

$O(^1D)$ 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: 0.004

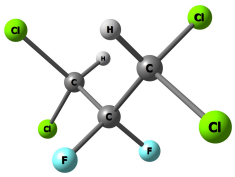
UV Photolysis

UV Spectrum: *No Recommendation*

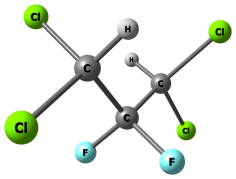
$\tau_{hv} = 50$ years

Fractional Atmospheric Loss: 0.014

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	-1.266912879479	-0.309934976798	0.294698931514
C	-0.002437828422	0.534784965888	0.003183398609
C	1.264193143125	-0.306105606405	-0.290038188072
Cl	-2.642444678325	0.769102661644	0.632852342194
Cl	-1.621169157643	-1.407395918760	-1.073344742691
H	-1.108995369672	-0.926426130616	1.174539156269
F	0.219141242647	1.319617450484	1.073201906156
F	-0.226026999520	1.321213169503	-1.065244043498
H	1.107849167565	-0.921220070276	-1.171122148240
Cl	2.636957767729	0.777128759565	-0.626011561972
Cl	1.621263591995	-1.405417304230	1.075785949730

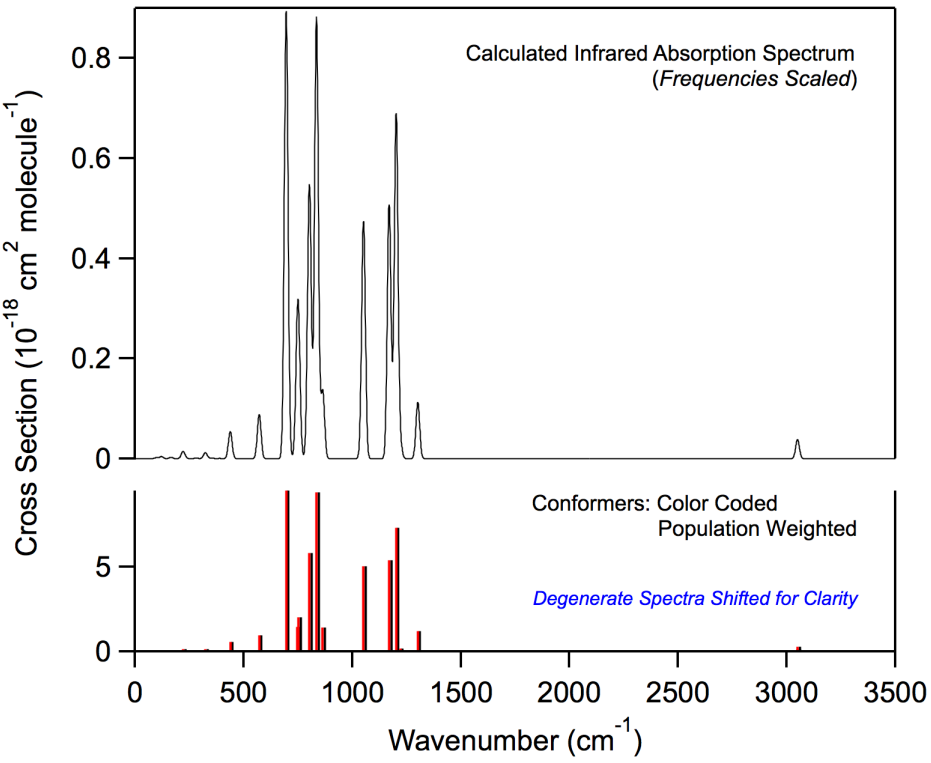
Atom	X	Y	Z
C	-1.264303929384	-0.314053171050	-0.290940461393
C	0.002192078978	0.527337057761	0.001428650836
C	1.266596647946	-0.316882841101	0.294693762335
Cl	-1.621809201760	-1.411275957701	1.076448872842
Cl	-2.636992414673	0.768610176669	-0.629058706835
H	-1.107628843162	-0.930516915847	-1.171021985420
F	-0.219793588395	1.313812433374	1.070155711303
F	0.226127610639	1.312122871121	-1.068133333869
H	1.108393379399	-0.932018731169	1.175430867828
Cl	1.621375061876	-1.416444874306	-1.071526386937
Cl	2.641969198537	0.762728952251	0.631661009310

Infrared Absorption Spectrum (unscaled frequencies)

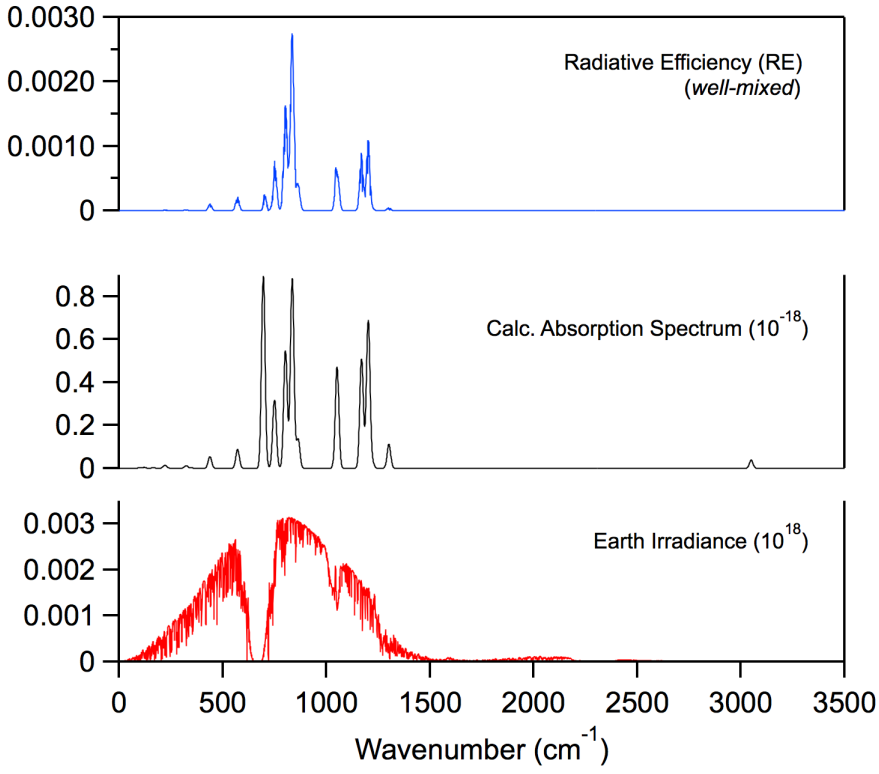
Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
45.8151	0.0398
71.4816	0.0914
118.4171	0.0621
177.3873	0.308
191.4904	0.0146
241.4986	0.0259
251.5400	0.00271
285.8930	0.255
316.6666	0.0321
355.5737	0.0139
407.3719	1.15
548.5924	1.89
680.1170	19.0
734.8112	2.94
739.3400	4.07
793.1839	11.7
827.7056	18.8
858.0707	2.88
1056.9138	10.1
1181.8296	10.8
1216.0128	14.6
1235.9818	0.243
1236.2560	0.349
1264.4651	0.001
1321.6659	2.41
3172.4296	0.552
3172.4467	0.268

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
45.8156	0.0398
71.4814	0.0914
118.4170	0.0621
177.3870	0.308
191.4905	0.0146
241.4984	0.0259
251.5397	0.00271
285.8927	0.255
316.6666	0.0321
355.5737	0.0139
407.3716	1.15
548.5927	1.89
680.1167	19.0
734.8109	2.94
739.3403	4.07
793.1837	11.7
827.7055	18.8
858.0707	2.88
1056.9136	10.1
1181.8292	10.8
1216.0124	14.6
1235.9815	0.243
1236.2559	0.349
1264.4645	0.001
1321.6656	2.41
3172.4294	0.552
3172.4465	0.268

Infrared Spectrum

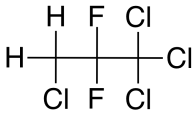


Radiative Efficiency



HCFC-232cb

Molecular Formula:	$CH_2ClCF_2CCl_3$
Name:	1,1,1,3-Tetrachloro-2,2-difluoropropane
CAS number:	677-54-3
Molecular Weight:	217.86



Global Atmospheric Lifetime (years):	4.47
Tropospheric Atmospheric Lifetime (years):	5.21
Stratospheric Atmospheric Lifetime (years):	31.2
Ozone Depletion Potential (ODP):	0.090

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.228	0.208
Global Warming Potential (GWP_H):		
GWP_{20}	1039	951
GWP_{100}	285	260
Global Temperature Potentials (GTP_H)		
GTP_{20}		492
GTP_{50}		53
GTP_{100}		37

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

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

OH Reactivity

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

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

$\tau^{OH}_{Global} = 5.04$ years

$\tau^{OH}_{Trop} = 5.21$ years

$\tau^{OH}_{Strat} = 149.4$ years

Fractional Atmospheric Loss: 0.887

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: 0.024

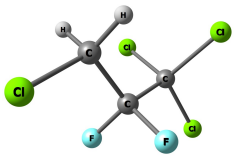
UV Photolysis

UV Spectrum: *No Recommendation*

$\tau_{hv} = 50$ years

Fractional Atmospheric Loss: 0.089

Molecular Structure and Infrared Spectrum (1 conformer)



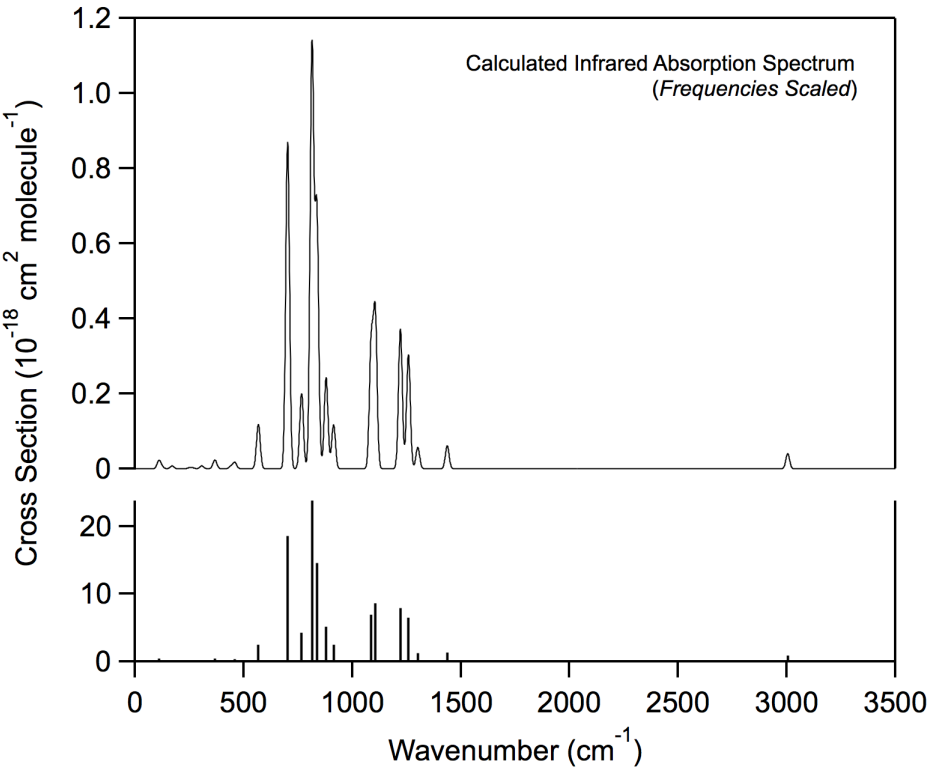
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.669009711725	0.475692272545	0.000000000000
C	0.149210080628	0.650212622616	0.000000000000
C	-0.650774891247	-0.705849319743	0.000000000000
Cl	2.474167318947	2.075385754820	0.000000000000
H	1.985999037888	-0.058228391120	0.892899556093
H	1.985999037888	-0.058228391120	-0.892899556093
F	-0.237271402638	1.339058420846	-1.089467455411
F	-0.237271402638	1.339058420846	1.089467455411
Cl	-2.393645714360	-0.339932167109	0.000000000000
Cl	-0.237613388092	-1.647550611295	-1.463462464783
Cl	-0.237613388092	-1.647550611295	1.463462464783

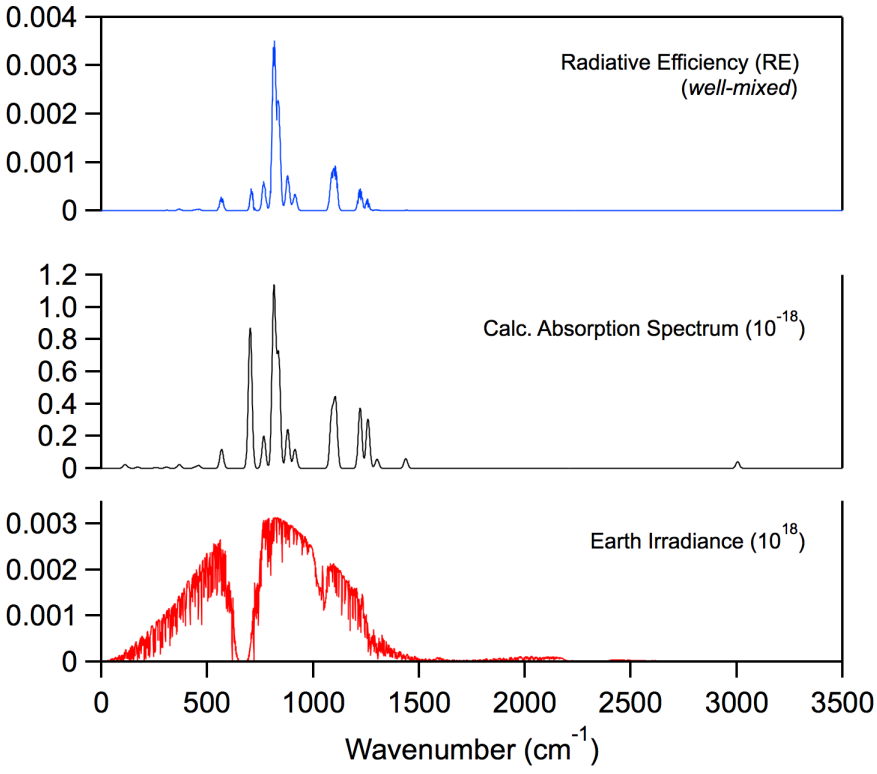
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
59.6882	0.446
73.6044	0.117
123.8521	0.159
180.8824	0.00511
210.1982	0.0651
225.0656	0.0395
265.7962	0.0204
268.7755	0.139
328.3584	0.106
333.7450	0.405
411.2492	0.151
429.7139	0.352
544.4200	2.51
687.1015	18.6
755.1086	4.27
805.6638	23.8
829.2018	14.6
874.5351	5.18
911.0093	2.50
1094.5692	6.95
1114.0120	8.66
1236.8145	7.94
1275.9459	6.50
1321.4577	1.22
1465.0557	1.30
3124.6511	0.860
3193.6012	0.00588

Infrared Spectrum

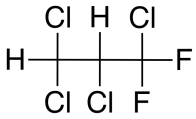


Radiative Efficiency



HCFC-232da

Molecular Formula:	$CHCl_2CHClCClF_2$
Name:	1,2,3,3-Tetrachloro-1,1-difluoropropane
CAS number:	67879-59-8
Molecular Weight:	217.86



Global Atmospheric Lifetime (years):	0.820
Tropospheric Atmospheric Lifetime (years):	0.859
Stratospheric Atmospheric Lifetime (years):	20
Ozone Depletion Potential (ODP):	0.019

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.252	0.178
Global Warming Potential (GWP_H):		
GWP_{20}	214	151
GWP_{100}	58	41
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*

$k_{SAR}(298\ K) = 6.82 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 4.36 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 0.835$ years

$\tau^{OH}_{Trop} = 0.859$ years

$\tau^{OH}_{Strat} = 29.4$ years

Fractional Atmospheric Loss: 0.982

$O(^1D)$ 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: 0.004

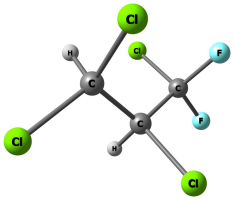
UV Photolysis

UV Spectrum: *No Recommendation*

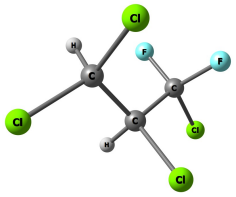
$\tau_{hv} = 59$ years

Fractional Atmospheric Loss: 0.014

Molecular Structure and Infrared Spectrum (5 conformers)



E = 0
Population = 0.509



$\Delta E = 0.29$ kcal mol^{-1}
Population = 0.311

Optimized Coordinates (Angstroms)

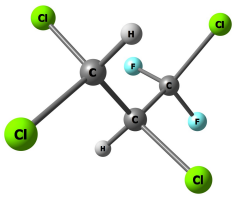
Atom	X	Y	Z
C	0.975424333642	0.645670699734	0.308248954398
C	-0.021455759038	-0.514808979823	0.434897353218
C	-1.464022930182	-0.189697701677	-0.010570183097
Cl	2.483968350319	0.247070324142	1.193002538632
Cl	1.326177656726	1.117015315701	-1.375152150284
H	0.563583581391	1.524437159900	0.797871010777
H	-0.081039748331	-0.777305806469	1.492066317053
Cl	0.519206430748	-1.985998449560	-0.431470730320
Cl	-2.096565081768	1.237052166919	0.916085947273
F	-1.560663075665	0.076062876369	-1.306239773774
F	-2.254371757841	-1.225809605235	0.267514716124

Atom	X	Y	Z
C	1.232639111596	0.360898314848	0.550842704985
C	-0.056051813095	-0.449352905150	0.324382766496
C	-1.306910422335	0.458917107582	0.255248304944
Cl	2.568088010610	-0.736763432315	1.023798050826
Cl	1.698725434611	1.379670818205	-0.836621471885
H	1.078099562189	1.032724550043	1.391432727381
H	-0.180254427587	-1.092009916686	1.196754712164
Cl	0.026613159208	-1.511826671078	-1.102966380128
Cl	-2.813185213657	-0.500103838164	0.460676623940
F	-1.243469581205	1.345098009286	1.265692427990
F	-1.385612820337	1.136376963429	-0.882594466711

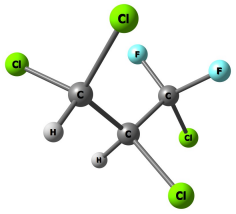
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
40.8930	0.0458
80.0538	0.0245
136.8361	0.188
171.4432	0.0290
173.4990	0.0658
245.3975	0.129
262.0042	0.134
281.3413	0.233
329.8784	0.123
392.9398	0.184
415.6489	0.426
573.7629	3.50
610.3344	3.74
671.8762	6.99
748.4221	18.1
785.5387	17.4
823.7914	4.20
959.0770	21.5
1038.0041	1.40
1171.3988	19.2
1221.7711	9.91
1228.1934	3.30
1259.8054	17.3
1295.8792	2.26
1337.0649	4.70
3118.6879	0.554
3155.8837	0.289

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
45.7774	0.0268
71.6437	0.0380
135.7041	0.227
169.7491	0.0102
184.7464	0.0983
205.1625	0.0298
254.1315	0.0192
314.0743	0.342
330.3259	0.0618
419.9267	0.0384
428.6401	0.323
566.4905	6.49
600.0143	2.77
668.0626	5.61
713.3610	18.9
822.2735	3.72
857.1280	4.51
958.3996	24.0
1036.9161	16.2
1140.7002	21.0
1221.5352	9.80
1227.8697	0.963
1257.0580	16.0
1299.1902	2.53
1328.6569	3.38
3119.5382	0.571
3154.4752	0.243



$\Delta E = 1.10$ kcal mol^{-1}
Population = 0.079



$\Delta E = 1.12$ kcal mol^{-1}
Population = 0.076

Optimized Coordinates (Angstroms)

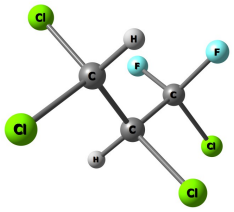
Atom	X	Y	Z
C	1.129740000651	0.172791201712	-0.376274129318
C	0.015650159986	-0.398552257106	0.516704551267
C	-1.366368781742	0.299724786181	0.413097939573
Cl	1.351137202855	1.934531039733	-0.135048473143
Cl	2.678541502028	-0.665916338592	-0.044102479913
H	0.900611286233	0.019973757476	-1.427504033664
H	0.311309297576	-0.331853465705	1.565829911513
Cl	-0.200679690128	-2.138198333109	0.129753583224
Cl	-1.924999432820	0.501192838390	-1.285178529673
F	-2.275347640489	-0.417767982032	1.072977767960
F	-1.315969904151	1.500996753052	0.991720892175

Atom	X	Y	Z
C	1.384778125960	-0.224054346479	0.507922193910
C	-0.146222532227	-0.260158246594	0.682738094388
C	-0.978557868071	0.508765169953	-0.372667810859
Cl	1.944976043612	-0.627544406778	-1.137836834069
Cl	2.046462866888	1.356046337087	1.054562546461
H	1.816818029613	-0.969201019140	1.170177272894
H	-0.367467993406	0.170744080835	1.658507035849
Cl	-0.683272107667	-1.971483643510	0.741602555247
Cl	-2.656696405431	0.778893182967	0.234519586616
F	-0.427519571385	1.702531067115	-0.603065470880
F	-1.052869587886	-0.144838175455	-1.526370169556

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
44.8001	0.0252
66.2909	0.0107
145.1976	0.0989
176.8055	0.0576
211.3560	0.0701
242.8983	0.234
263.5695	0.245
313.4753	0.0259
344.0127	0.184
390.6592	1.02
424.9243	0.569
450.7552	0.630
612.0285	8.74
663.6097	6.76
740.0675	14.0
763.1654	11.1
830.2671	3.01
1028.9595	27.4
1062.0159	2.98
1168.0942	18.3
1187.6656	17.1
1211.6211	4.05
1225.9003	6.03
1276.0167	8.03
1349.0011	3.09
3109.6919	0.344
3163.8256	0.364

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
45.4888	0.0182
75.1111	0.0197
142.7186	0.0645
161.9821	0.0738
193.3986	0.0513
210.4945	0.0684
259.7951	0.0909
309.2856	0.0331
348.1426	0.111
409.3859	0.364
422.9789	0.356
497.9283	7.07
597.8450	4.20
673.0038	2.76
734.6214	17.9
823.7224	2.54
854.5586	9.13
925.8928	28.5
1039.1888	15.8
1173.5466	22.0
1208.7093	8.59
1224.8043	1.12
1262.7476	7.15
1284.2579	8.09
1358.7144	2.11
3133.3174	0.563
3156.1569	0.386



$\Delta E = 2.00$ kcal mol^{-1}
Population = 0.017

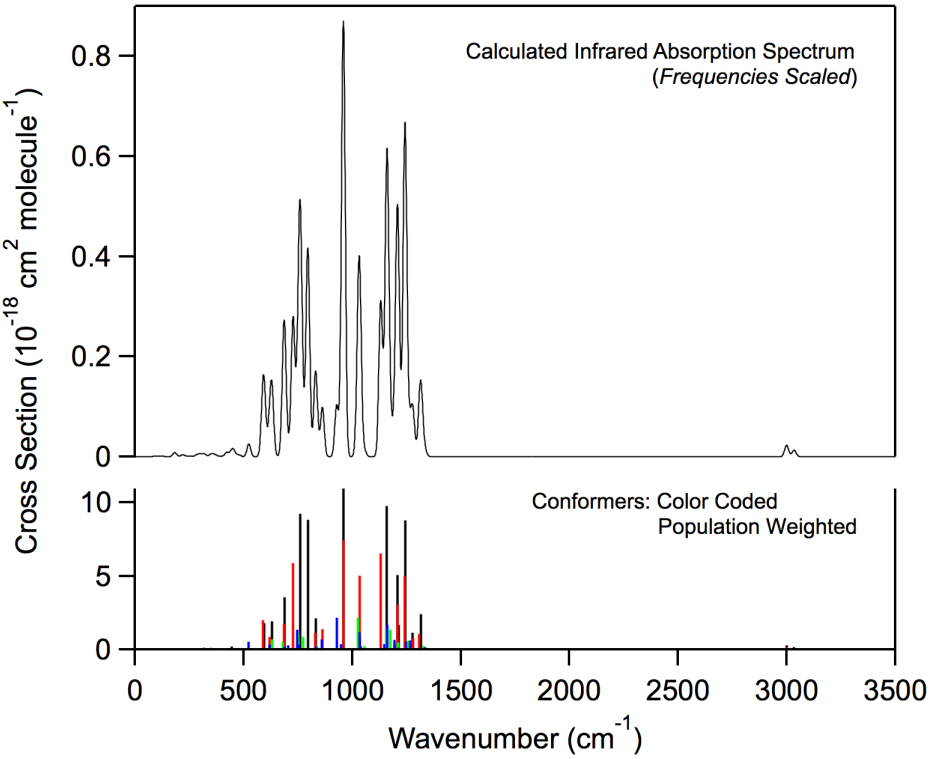
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.295449801086	0.102745430006	-0.331874687916
C	-0.035937546357	-0.338739380920	0.317361158467
C	-1.253148196005	0.509115707412	-0.139666650213
Cl	1.694314565770	1.819528575147	-0.005967760678
Cl	2.644228237638	-0.920835780008	0.255646217119
H	1.247669423390	-0.014145111885	-1.411543099932
H	0.034110883914	-0.288938597245	1.403619738460
Cl	-0.323408521381	-2.050390059573	-0.145220565114
Cl	-2.808044597713	-0.143213929601	0.483506128561
F	-1.150398056597	1.757963400980	0.318812846693
F	-1.304720993744	0.556154745687	-1.474295325447

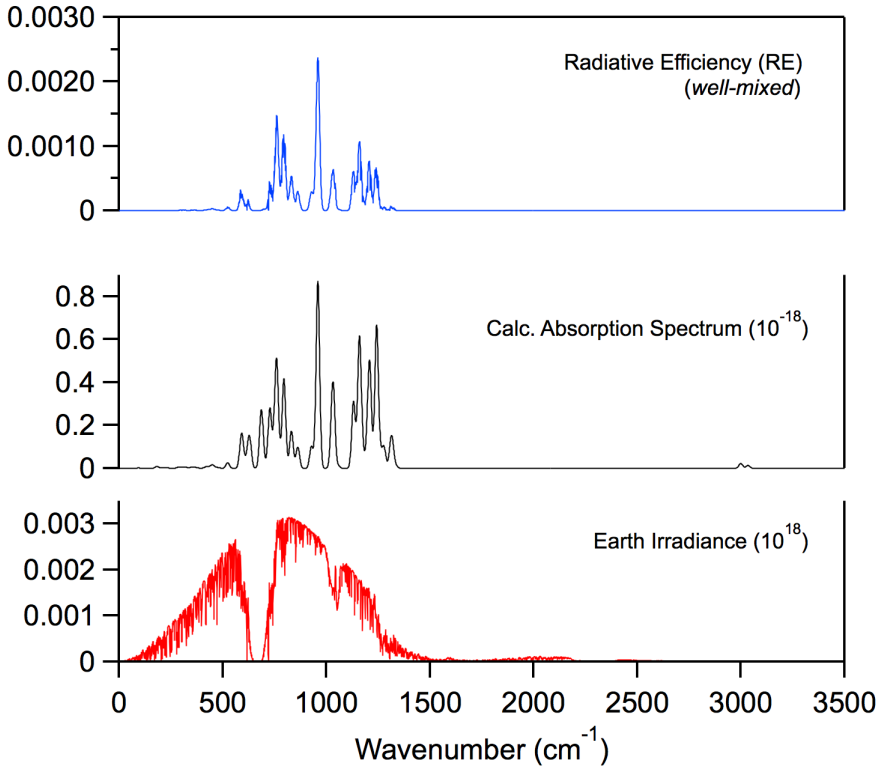
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
27.5786	0.0318
54.3076	0.0238
151.7833	0.0895
196.4364	0.0779
206.6064	0.261
223.4379	0.0877
255.3267	0.0719
320.3624	0.219
348.0477	0.161
377.7412	1.70
417.5378	0.0905
446.7801	1.55
601.4591	3.33
690.3537	16.7
743.6115	18.7
802.4334	1.79
853.6855	0.654
947.1241	21.2
1044.9599	12.2
1156.8701	21.0
1201.4554	0.656
1207.4331	16.8
1225.0047	7.09
1281.0887	4.62
1345.7207	3.23
3135.1965	0.285
3160.3419	0.302

Infrared Spectrum

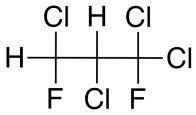


Radiative Efficiency



HCFC-232db

Molecular Formula:	$CHClFCHClCCl_2F$
Name:	1,1,2,3-Tetrachloro-1,3-difluoropropane
CAS number:	1943659-46-8
Molecular Weight:	217.86



Global Atmospheric Lifetime (years):	1.51
Tropospheric Atmospheric Lifetime (years):	1.61
Stratospheric Atmospheric Lifetime (years):	24.0
Ozone Depletion Potential (ODP):	0.033

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.249	0.200
Global Warming Potential (GWP_H):		
GWP_{20}	387	312
GWP_{100}	105	84
Global Temperature Potentials (GTP_H)		
GTP_{20}		108
GTP_{50}		15
GTP_{100}		12

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 3.65 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 2.33 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 1.56$ years

$\tau^{OH}_{Trop} = 1.61$ years

$\tau^{OH}_{Strat} = 51.7$ years

Fractional Atmospheric Loss: 0.967

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

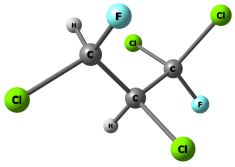
UV Photolysis

UV Spectrum: *No Recommendation*

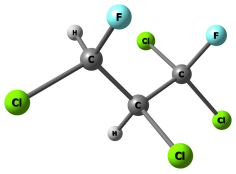
$\tau_{hv} = 59$ years

Fractional Atmospheric Loss: 0.025

Molecular Structure and Infrared Spectrum (9 conformers)



E = 0
Population = 0.281



$\Delta E = 0.03$ kcal mol^{-1}
Population = 0.268

Optimized Coordinates (Angstroms)

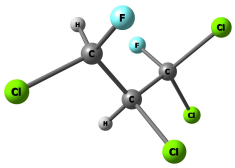
Atom	X	Y	Z
C	1.162561420038	-0.760517546930	0.295136189770
C	0.303354996150	0.177957564074	-0.565207368078
C	-1.221279412841	0.044853048695	-0.334163698726
Cl	2.813137656830	-0.904433225862	-0.410841896852
F	1.262535518602	-0.314798335775	1.560782145389
H	0.747941813164	-1.769771506917	0.295034779771
H	0.463337002834	-0.069046775073	-1.615125092466
Cl	0.801263826642	1.881766686089	-0.347294404906
Cl	-1.728218570045	-1.625288098557	-0.818924952948
Cl	-1.731545801524	0.358893927036	1.343564422250
F	-1.856197449850	0.899046263221	-1.139882123205

Atom	X	Y	Z
C	1.345367127821	-0.730848443871	0.084091667877
C	0.255944629834	0.252087512725	-0.381145321003
C	-1.149569380169	-0.157567952186	0.123401549785
Cl	2.896229854730	-0.394919633712	-0.763458264684
F	1.529373630494	-0.643890305441	1.415055466530
H	1.080215338928	-1.754727705025	-0.179964826676
H	0.231872517433	0.271928464774	-1.469420323661
Cl	0.642308860707	1.902964471708	0.193646795244
Cl	-2.408873621645	0.967003619166	-0.467751162981
Cl	-1.544138029411	-1.815356923229	-0.491142480663
F	-1.187867928722	-0.189733104909	1.453912900232

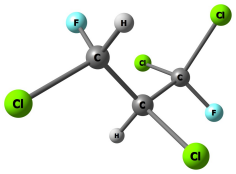
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
48.1797	0.0793
74.2327	0.0586
146.7751	0.230
160.5069	0.0791
197.6068	0.00794
220.5151	0.119
253.5683	0.0225
281.5185	0.243
343.2187	0.162
383.3877	0.174
403.9837	0.294
479.1740	1.17
624.2450	9.37
636.6475	7.60
759.0265	25.9
792.0444	13.0
835.7066	10.8
978.4309	4.08
1045.0466	14.1
1152.1392	12.7
1169.4220	19.3
1247.0599	2.50
1271.6153	1.16
1325.6581	4.89
1376.8515	2.49
3115.5510	0.481
3124.6302	0.775

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
43.8902	0.0790
71.8774	0.0592
140.8139	0.216
178.9325	0.0870
200.6029	0.0313
226.7967	0.0426
260.5779	0.00654
269.7608	0.283
325.8176	0.138
377.0159	0.209
394.5673	0.492
455.0321	0.648
618.6535	9.41
683.2805	19.9
771.8183	26.0
800.8240	3.22
867.3904	8.25
964.0903	3.56
973.6404	10.5
1147.1251	7.07
1187.2095	25.9
1245.7561	3.34
1277.8122	0.801
1319.6252	5.77
1377.0493	2.71
3125.9232	0.457
3144.8159	0.576



$\Delta E = 0.41$ kcal mol^{-1}
Population = 0.141



$\Delta E = 0.56$ kcal mol^{-1}
Population = 0.108

Optimized Coordinates (Angstroms)

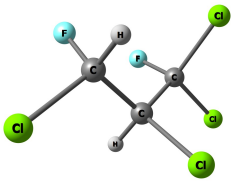
Atom	X	Y	Z
C	1.398255001361	-0.625751362847	-0.395208048309
C	0.277951421284	0.426026257322	-0.308300892837
C	-1.124565507431	-0.221300195693	-0.434777395564
Cl	2.958312777966	0.166874194602	-0.818394033598
F	1.542679616017	-1.294569768499	0.762900294975
H	1.188917505376	-1.330812082220	-1.201314313365
H	0.371941061608	1.088300748603	-1.169889706925
Cl	0.434015784973	1.422404642667	1.156690579952
Cl	-1.539907062420	-1.308152557942	0.914798910789
Cl	-2.382533474979	1.039694467136	-0.618868679681
F	-1.112126123755	-0.951642343129	-1.570969715438

Atom	X	Y	Z
C	-1.210807014118	0.547285961156	0.486679307210
C	-0.327466959191	-0.233996546485	-0.503187827635
C	1.199943887613	-0.077788877434	-0.279466413303
Cl	-2.906011311500	0.598999431110	-0.111823761637
H	-1.234344099248	0.060302937865	1.461689394277
F	-0.769041333371	1.815834474707	0.623818103523
H	-0.532942920267	0.083496964382	-1.525922181060
Cl	-0.766233967309	-1.969816649985	-0.389812628228
Cl	1.746933041535	1.530525406146	-0.859611812285
Cl	1.660825628472	-0.301933712658	1.439488698948
F	1.845105047385	-0.994462388803	-1.006219879810

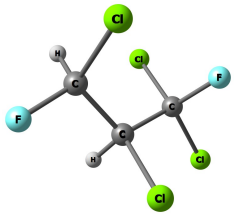
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
48.1446	0.0671
72.3707	0.0707
139.5168	0.211
168.7816	0.0847
193.0383	0.111
213.0850	0.0300
245.6549	0.0831
277.8241	0.00380
376.6972	0.110
380.9692	0.0123
400.4734	0.573
493.1676	0.441
609.5617	13.1
643.0818	7.70
729.1735	19.2
823.9806	2.60
879.7801	20.8
970.6074	3.78
1044.3526	18.3
1113.7070	12.1
1157.6399	20.4
1244.3884	3.04
1277.3009	0.653
1320.1873	4.56
1379.7632	2.53
3114.3810	0.203
3120.4228	0.779

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
52.2159	0.0623
66.1377	0.0155
142.6313	0.0993
171.7849	0.0468
198.5354	0.0569
226.8962	0.0723
267.8677	0.244
315.2148	0.476
343.3220	0.187
388.8337	0.0908
421.4236	1.03
453.5865	1.23
493.4331	1.78
636.5248	11.0
759.7252	24.8
798.3277	18.3
853.5559	14.4
1021.6690	6.44
1072.2620	6.97
1134.7114	15.2
1160.3358	19.4
1214.1559	1.57
1265.6707	4.09
1327.0379	3.53
1383.6575	1.24
3120.9026	0.743
3132.8326	0.351



$\Delta E = 0.70$ kcal mol^{-1}
Population = 0.086



$\Delta E = 1.03$ kcal mol^{-1}
Population = 0.049

Optimized Coordinates (Angstroms)

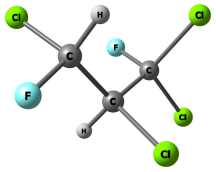
Atom	X	Y	Z
C	-1.431621426445	0.574383737808	0.205400772880
C	-0.287637541350	-0.278613286367	-0.381920735448
C	1.103772468924	0.392287785843	-0.233457970026
Cl	-3.019615022337	-0.061860399941	-0.350645044978
H	-1.438707582567	0.535976664790	1.294885696043
F	-1.320191809811	1.855573653038	-0.206477084905
H	-0.445940800826	-0.416740740374	-1.452929817901
Cl	-0.328525518365	-1.886019588471	0.391680156391
Cl	1.471285463738	0.818121531303	1.469576704417
Cl	2.394715254019	-0.664045721423	-0.890028383368
F	1.106917515020	1.517422363794	-0.958486293106

Atom	X	Y	Z
C	-1.449262254355	0.478780246992	-0.656471725816
C	-0.195114316953	-0.411050104064	-0.571457011267
C	1.014438501318	0.203105550186	0.166035474810
Cl	-2.188863019051	0.857448195557	0.929738465862
H	-1.203931342039	1.436380488830	-1.116109469351
F	-2.355269884161	-0.164407347862	-1.427104634378
H	0.113075738309	-0.596106576056	-1.601983541131
Cl	-0.605598734052	-2.001099126117	0.139454189212
Cl	2.472180170154	-0.816132648043	-0.065629038798
Cl	1.362166190626	1.846305748915	-0.505980583767
F	0.789788950202	0.326165571661	1.470376874624

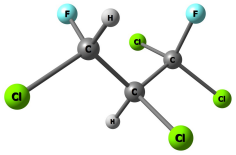
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
49.2016	0.0534
64.9028	0.0325
139.9524	0.101
176.6240	0.0319
192.5031	0.0835
218.8463	0.0185
272.4216	0.0266
318.8408	0.168
370.6422	0.345
383.0132	0.182
417.6120	1.60
456.7307	2.23
495.1641	0.430
606.6993	13.9
735.0887	21.9
846.7840	17.4
872.5814	8.58
1016.6156	8.11
1071.9486	13.4
1120.3465	2.22
1150.8141	32.0
1211.9476	1.06
1261.0331	3.97
1325.9432	2.95
1379.9869	1.78
3112.9945	0.593
3130.6916	0.489

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
45.5017	0.0479
80.0585	0.0399
145.4003	0.166
177.3696	0.0995
193.8204	0.0360
216.1706	0.0543
264.1651	0.217
301.0356	0.0956
321.3097	0.205
379.7471	0.193
407.6755	0.787
465.1475	0.468
595.3240	8.98
673.0369	8.09
753.8505	17.6
806.7409	24.5
826.6105	4.06
974.6935	6.33
1040.2433	16.2
1125.3444	14.1
1199.8788	14.2
1236.9178	2.64
1292.1018	7.96
1320.3783	2.40
1371.6485	2.05
3112.3102	0.332
3125.3823	0.801



$\Delta E = 1.39$ kcal mol^{-1}
Population = 0.027



$\Delta E = 1.73$ kcal mol^{-1}
Population = 0.015

Optimized Coordinates (Angstroms)

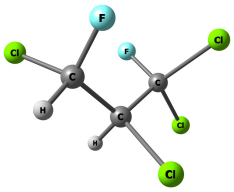
Atom	X	Y	Z
C	1.597316902918	0.296251992077	0.273048640596
C	0.239595447905	0.526858182538	-0.422299592046
C	-0.851319885106	-0.533178725776	-0.126228024939
Cl	2.396910935109	-1.216387329851	-0.282695288863
F	2.413154271058	1.325619548231	-0.040135483794
H	1.491832930373	0.223530135347	1.355704363185
H	0.389668620661	0.537493654442	-1.503439863117
Cl	-0.323161245203	2.161089458130	0.056965598621
Cl	-1.151357666744	-0.716916506191	1.633772311947
Cl	-2.381515153021	-0.117992874569	-0.963982145273
F	-0.454607157950	-1.717994534379	-0.604387516317

Atom	X	Y	Z
C	-1.406748034073	0.514296067680	0.391116262509
C	-0.284560554370	-0.289837521979	-0.308889747065
C	1.131702398522	0.133590584280	0.165680274734
Cl	-2.977595884443	0.218441853030	-0.433594324317
H	-1.523938186813	0.189235090991	1.425354017148
F	-1.161703354897	1.840340488488	0.361417312841
H	-0.340718677487	-0.179221946295	-1.390246430823
Cl	-0.587154108839	-2.016534346846	0.082613993497
Cl	2.390870254426	-1.036204134885	-0.336913474762
Cl	1.567036237679	1.731898523585	-0.531656646212
F	1.146155910293	0.228176341950	1.502634762453

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
31.0350	0.0321
76.7390	0.0389
147.2769	0.101
174.0032	0.0647
184.0931	0.0919
243.1285	0.0571
287.2227	0.148
308.7461	0.221
362.2912	0.616
382.6282	0.0610
413.8643	0.919
424.1899	2.99
498.1109	0.167
642.2211	9.59
751.9260	25.7
811.6913	25.3
836.7225	3.10
1030.0360	8.57
1073.8272	11.3
1127.6410	13.8
1144.5938	17.7
1212.1094	2.41
1268.0899	4.38
1308.4644	2.88
1386.5381	1.34
3113.2018	0.480
3130.5182	0.445

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
37.8275	0.0562
55.4729	0.0361
152.3091	0.0546
183.4131	0.0858
218.0517	0.207
234.1390	0.0720
244.7275	0.160
290.9552	0.170
351.4014	0.0180
378.1092	0.198
420.8501	1.75
454.3916	0.770
466.8468	2.35
681.9708	22.6
772.9890	29.1
817.8956	3.33
863.1166	4.62
952.0193	6.97
1049.2884	12.1
1135.7098	17.4
1163.3832	16.8
1205.1232	1.28
1270.0992	2.26
1325.2043	5.07
1383.9356	1.48
3123.0236	0.617
3149.4593	0.439



$\Delta E = 1.96$ kcal mol^{-1}
Population = 0.010

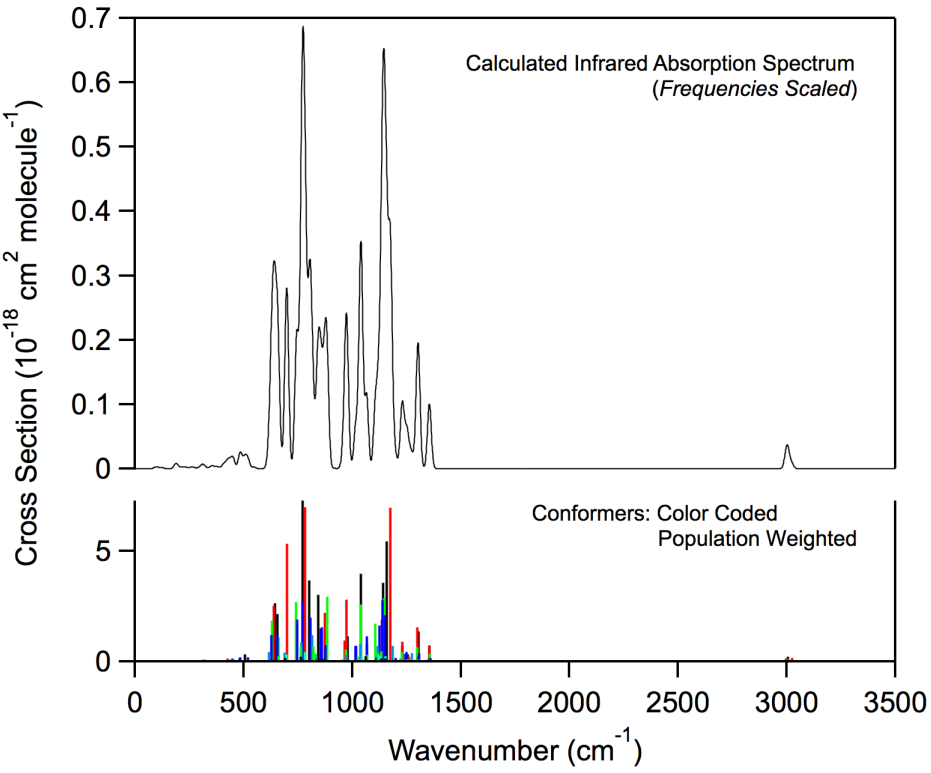
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.615929479689	-0.581038949947	-0.157938244937
C	-0.144667274252	-0.554525595206	-0.617752969904
C	0.741232344428	0.562597846121	-0.005470230930
Cl	-2.577784438693	0.717571282375	-0.964688212788
H	-2.069575791861	-1.519316018721	-0.479741112276
F	-1.735139466450	-0.458731600893	1.176235646980
H	-0.135789183115	-0.404321531282	-1.697015092903
Cl	0.562614912785	-2.177219499031	-0.322713405810
Cl	1.108340397156	0.334778284250	1.724926723700
Cl	2.281270905356	0.669231482051	-0.933688455355
F	0.103709074336	1.731918300282	-0.147063645776

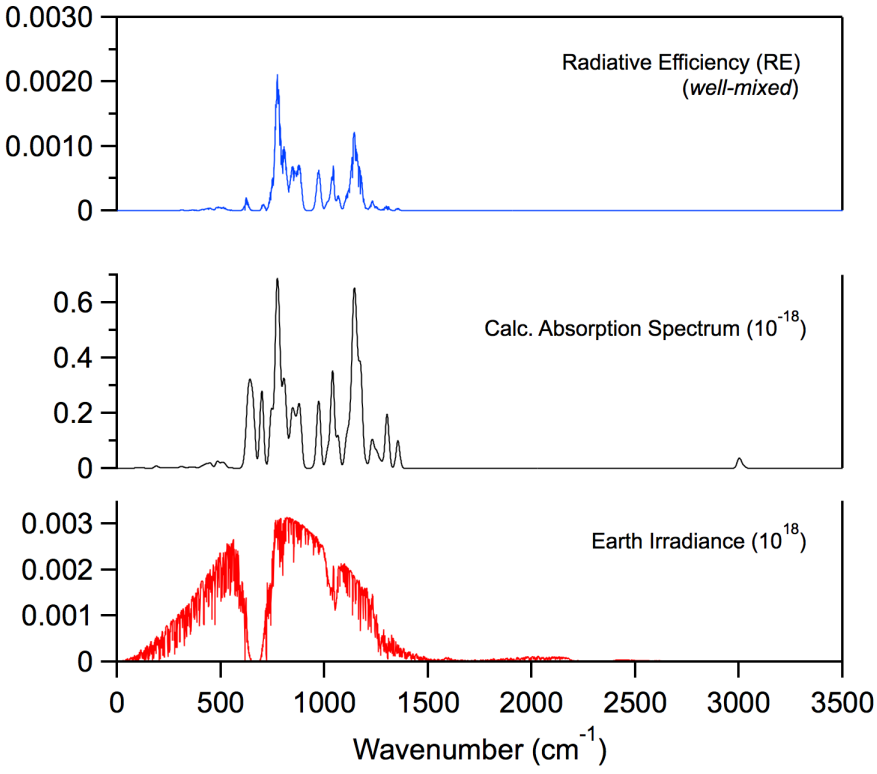
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
29.0256	0.0653
84.4701	0.0540
153.4608	0.0288
165.0241	0.102
175.6084	0.112
240.3029	0.0860
242.6122	0.0381
287.9752	0.0694
368.1678	0.189
377.6526	0.00423
397.5608	0.393
471.7500	3.17
523.9931	5.12
675.2925	15.5
751.9165	22.2
839.1159	9.33
858.2311	11.0
913.4818	1.33
1068.1105	24.6
1144.3625	12.5
1163.6718	13.8
1234.1122	3.56
1290.3582	5.30
1314.6694	2.68
1396.7162	0.860
3114.6890	0.836
3131.2425	0.395

Infrared Spectrum

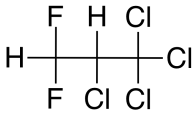


Radiative Efficiency



HCFC-232dc

Molecular Formula:	$CHF_2CHClCCl_3$
Name:	1,1,1,2-Tetrachloro-3,3-difluoropropane
CAS number:	–
Molecular Weight:	217.86



Global Atmospheric Lifetime (years):	2.83
Tropospheric Atmospheric Lifetime (years):	3.15
Stratospheric Atmospheric Lifetime (years):	27.8
Ozone Depletion Potential (ODP):	0.060

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.210	0.184
Global Warming Potential (GWP_H):		
GWP_{20}	613	539
GWP_{100}	166	146
Global Temperature Potentials (GTP_H)		
GTP_{20}		224
GTP_{50}		27
GTP_{100}		20

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 1.86 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 1.19 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 3.05$ years

$\tau^{OH}_{Trop} = 3.15$ years

$\tau^{OH}_{Strat} = 94.8$ years

Fractional Atmospheric Loss: 0.928

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: 0.015

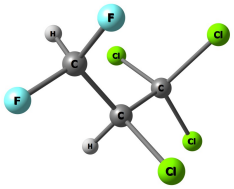
UV Photolysis

UV Spectrum: *No Recommendation*

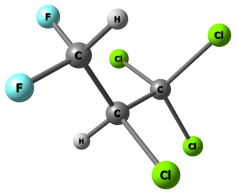
$\tau_{hv} = 50$ years

Fractional Atmospheric Loss: 0.057

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.705



$\Delta E = 0.61$ kcal mol^{-1}
Population = 0.249

Optimized Coordinates (Angstroms)

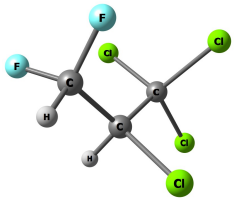
Atom	X	Y	Z
C	1.646998466901	-0.856750797121	-0.291066087410
C	0.591990705317	0.238439748719	-0.552133800080
C	-0.840045011400	-0.093921391463	-0.067420723006
F	2.747773533772	-0.541180481536	-1.009796818681
F	1.992751595232	-0.913530476706	1.007492506846
H	1.290351438008	-1.841572382600	-0.608621390134
H	0.528473692065	0.368856529836	-1.633581606548
Cl	1.178356090164	1.786572967423	0.125201602872
Cl	-1.966430901337	1.206896935995	-0.561644899730
Cl	-1.360546803199	-1.614582297971	-0.898909832276
Cl	-0.938616805522	-0.330384354577	1.693261048148

Atom	X	Y	Z
C	1.783420690063	-0.527597473468	0.239426220328
C	0.646558298761	0.263765191085	-0.449368955349
C	-0.796599056004	-0.118499461954	-0.032931551637
F	1.637361862215	-1.854809895834	0.050540690690
F	2.945045825398	-0.161236012233	-0.342480546421
H	1.831482442395	-0.317301511105	1.312030171820
H	0.726094406020	0.121864665852	-1.528215874204
Cl	0.980826751538	1.996174591855	-0.114206250151
Cl	-1.976655001684	1.002185170688	-0.782765687904
Cl	-1.171914187988	-1.768335055884	-0.628648777125
Cl	-0.988820030714	-0.073280209002	1.748745559954

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
49.8603	0.127
83.5311	0.0971
152.2410	0.135
166.5190	0.0808
201.2822	0.0832
224.8726	0.0534
243.5171	0.0865
270.2827	0.202
298.2410	0.0541
326.9407	0.465
399.3896	0.0804
542.0889	3.29
639.3445	8.03
662.8823	8.86
732.9211	16.2
762.0866	12.7
827.8505	5.93
980.8463	4.27
1049.9666	2.50
1136.0714	21.9
1178.8648	18.3
1252.2758	2.80
1298.9148	1.62
1389.7331	5.93
1411.6675	2.74
3085.6759	2.53
3116.2903	0.658

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
37.4822	0.0618
78.5481	0.0624
156.0722	0.0826
169.5221	0.0180
203.1496	0.105
226.3734	0.0279
267.8916	0.162
277.7225	0.136
301.3606	0.0696
380.7934	0.213
401.4145	0.0383
447.5480	4.97
564.6519	2.78
641.9339	4.95
749.9379	23.3
768.2374	17.0
841.9344	2.03
1022.2959	4.56
1077.5346	5.51
1130.9807	18.5
1147.4970	23.1
1233.3158	1.80
1285.6414	0.841
1397.3540	1.74
1407.3306	6.65
3091.0004	2.54
3122.0030	0.401



$\Delta E = 1.62$ kcal mol^{-1}
Population = 0.046

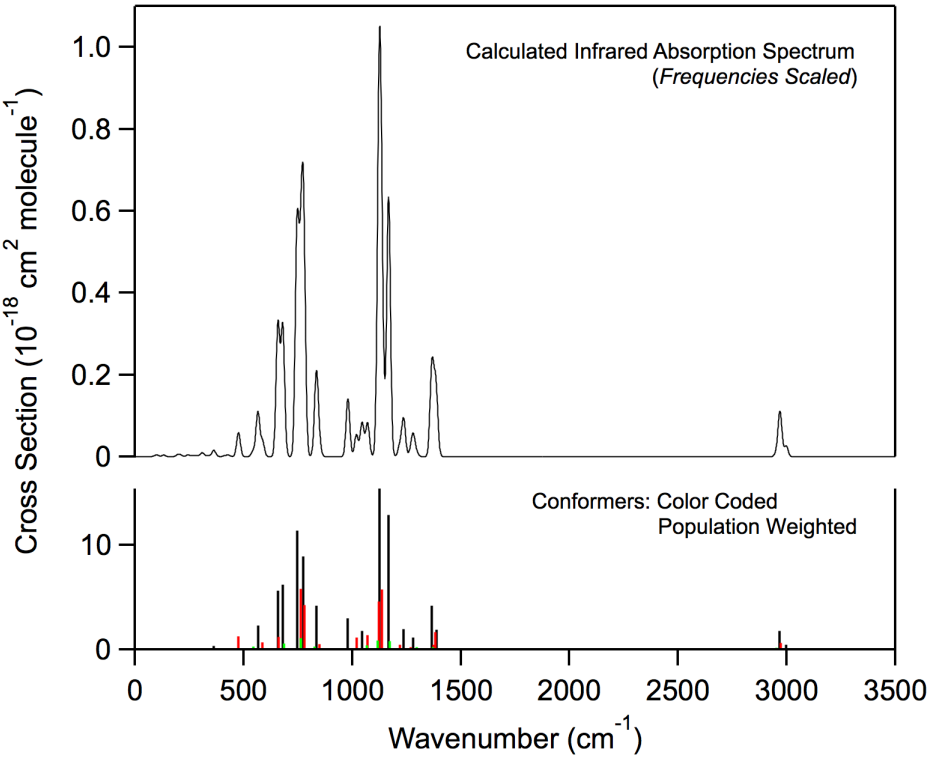
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.906186319659	-0.289923945560	-0.396721800009
C	0.546592773562	0.395831550953	-0.678105414135
C	-0.706275257856	-0.147620974176	0.056239653909
F	2.098281196568	-0.528100555860	0.912454770449
F	1.968384880318	-1.468388922370	-1.057020919352
H	2.711625983761	0.355755745635	-0.764115527930
H	0.354688327331	0.286507157379	-1.746269922061
Cl	0.757634110896	2.154593938457	-0.372644383239
Cl	-2.164128414070	0.652032610639	-0.634972778945
Cl	-0.848170583490	-1.909502596296	-0.253158568902
Cl	-0.669070336680	0.141211991198	1.813557890215

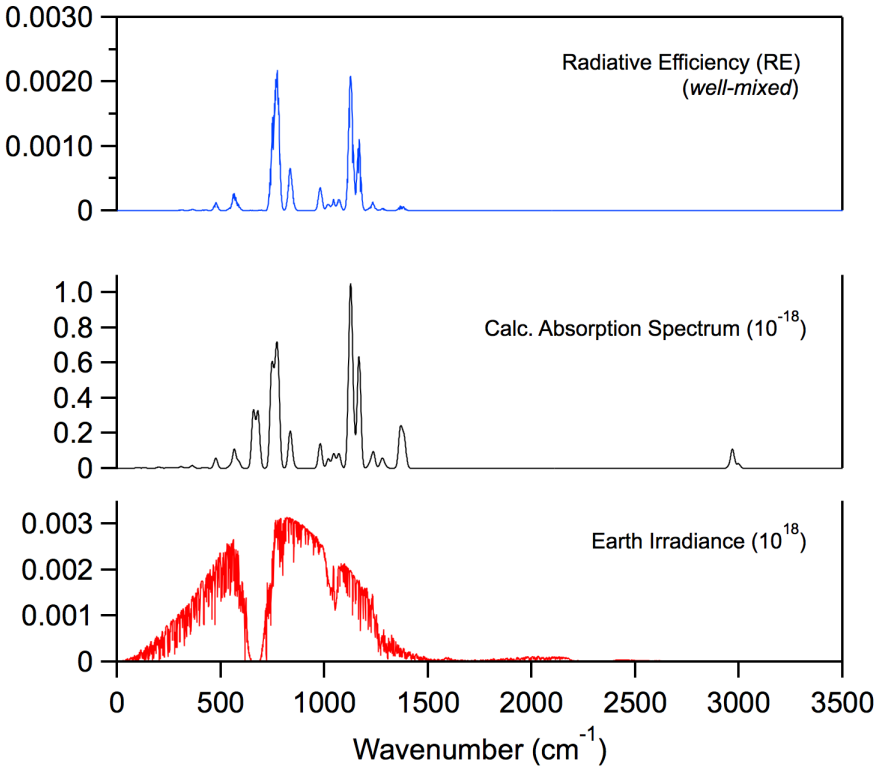
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
28.8847	0.111
88.7929	0.0795
157.0720	0.0422
175.5297	0.0841
196.1918	0.189
222.6107	0.0148
232.6327	0.0802
290.9090	0.0313
305.1050	0.171
341.9613	0.421
393.0162	0.309
518.6060	6.22
566.0148	2.26
668.9267	13.1
750.6236	24.3
818.2163	6.71
850.6389	0.623
899.0144	0.0273
1073.0053	9.28
1125.4339	18.7
1184.7095	17.0
1234.1516	2.38
1316.1911	4.42
1395.1092	4.42
1421.3317	2.68
3068.7829	3.83
3120.3642	0.306

Infrared Spectrum

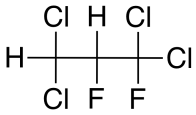


Radiative Efficiency



HCFC-232ea

Molecular Formula:	$CHCl_2CHFCCl_2F$
Name:	1,1,3,3-Tetrachloro-2,3-difluoropropane
CAS number:	–
Molecular Weight:	217.86



Global Atmospheric Lifetime (years):	0.829
Tropospheric Atmospheric Lifetime (years):	0.872
Stratospheric Atmospheric Lifetime (years):	20
Ozone Depletion Potential (ODP):	0.019

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.233	0.165
Global Warming Potential (GWP_H):		
GWP_{20}	200	142
GWP_{100}	54	38
Global Temperature Potentials (GTP_H)		
GTP_{20}		45
GTP_{50}		7
GTP_{100}		5

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 6.73 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 4.29 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 0.847$ years

$\tau^{OH}_{Trop} = 0.872$ years

$\tau^{OH}_{Strat} = 29.8$ years

Fractional Atmospheric Loss: 0.979

$O(^1D)$ 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: 0.004

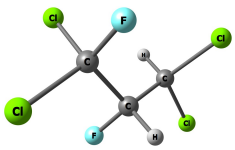
UV Photolysis

UV Spectrum: *No Recommendation*

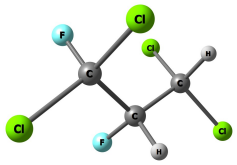
$\tau_{hv} = 50$ years

Fractional Atmospheric Loss: 0.017

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.555



$\Delta E = 0.17$ kcal mol^{-1}
Population = 0.420

Optimized Coordinates (Angstroms)

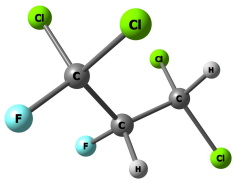
Atom	X	Y	Z
C	1.376438817041	-0.038281845061	0.306159597082
C	0.124293543134	0.570192695843	-0.353001567897
C	-1.190998318985	-0.225908849689	-0.141777176840
Cl	1.805738995326	-1.614016090817	-0.414518190088
Cl	2.732752900598	1.119657260694	0.135071269048
H	1.225337745833	-0.192499096868	1.371358024686
H	0.281803071879	0.656409872882	-1.433686319139
F	-0.067139998845	1.806258369775	0.188781867109
Cl	-1.521377382310	-0.485797887931	1.602754131869
Cl	-2.540937192260	0.699685413695	-0.876336670476
F	-1.127665181411	-1.412086842523	-0.748336965355

Atom	X	Y	Z
C	1.336258725584	-0.238934526187	-0.384832073088
C	0.102582729824	0.655979779997	-0.180172171591
C	-1.226209655922	-0.102812556984	0.062003266278
Cl	2.678782705300	0.785991436390	-0.998459367843
Cl	1.824144970802	-1.085838793627	1.106414254025
H	1.149225838248	-0.992861741642	-1.143766840353
H	-0.031851313668	1.251333360343	-1.088683070268
F	0.307560727435	1.481206803323	0.881695296752
Cl	-2.550693821560	1.091593555098	0.242910218086
Cl	-1.573300415831	-1.174768950970	-1.342812081834
F	-1.180879490212	-0.844589365740	1.165882569837

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
25.8996	0.0195
78.8269	0.0345
134.4081	0.114
180.1369	0.119
187.9824	0.0873
234.4594	0.148
282.4520	0.148
293.1143	0.0453
348.2159	0.224
367.2413	0.438
413.8107	2.67
438.8924	1.07
552.0460	0.0873
619.3865	15.3
723.6853	20.2
792.0738	13.7
851.7606	21.9
1025.5265	5.42
1091.7488	4.33
1134.3318	12.0
1174.9110	14.0
1228.6886	4.09
1238.1881	1.80
1343.6896	1.89
1368.1806	0.136
3074.4320	0.525
3161.3998	0.225

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
28.5453	0.0307
82.8168	0.0415
125.7895	0.206
185.9785	0.177
188.8142	0.00638
236.0809	0.0335
250.4318	0.0217
286.6805	0.133
321.2122	0.342
338.5208	0.352
392.4980	0.775
461.5117	0.753
624.5484	12.5
700.0248	22.1
731.4040	1.59
831.3716	27.0
851.8186	9.58
922.0859	6.08
1018.9234	11.4
1152.9062	6.15
1201.0170	10.8
1230.3619	10.4
1279.5753	0.629
1341.8378	0.500
1376.2700	0.772
3081.7862	0.446
3168.4122	0.244



$\Delta E = 1.83$ kcal mol^{-1}
Population = 0.025

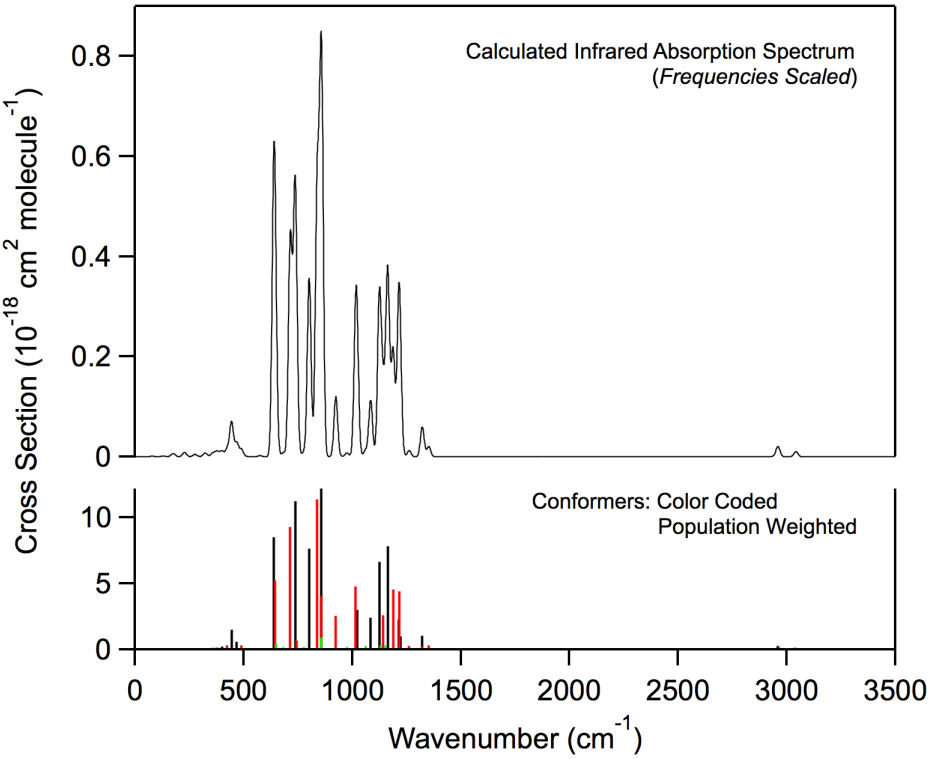
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.241969215938	-0.113762185571	0.503284813572
C	0.187837752662	-0.684910711581	-0.455887257196
C	-1.303874524389	-0.378025668172	-0.162283463215
Cl	2.765485150324	-1.046789059805	0.282115072683
Cl	1.545716737416	1.624311352630	0.261637628614
H	0.942016295924	-0.255057034813	1.537363927099
H	0.252238244941	-1.777930439978	-0.391446324377
F	0.443791349477	-0.300148969424	-1.733880130485
Cl	-1.701678665675	-0.862939516596	1.526549073412
Cl	-1.779077547708	1.308827683614	-0.456587376631
F	-2.019453008912	-1.155121450304	-0.989132963475

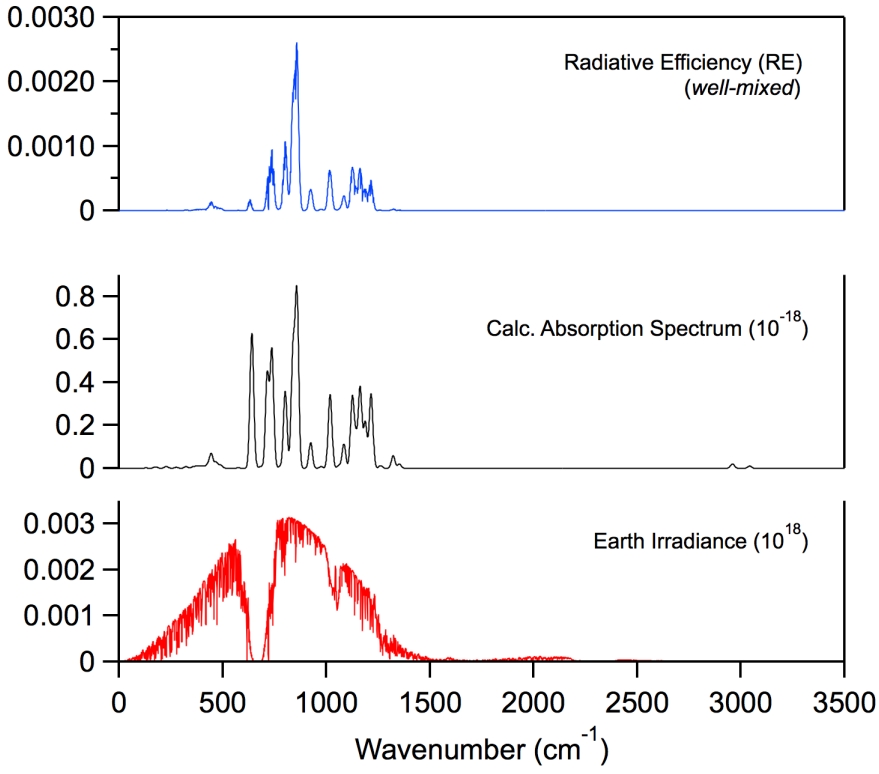
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
20.5987	0.0344
82.0597	0.0735
133.8175	0.170
177.8057	0.154
196.3205	0.0448
210.0140	0.0668
253.2392	0.0389
284.2720	0.309
321.5136	0.184
371.0418	0.133
392.8918	0.594
480.0430	0.900
632.6842	17.5
666.3896	6.87
736.0421	0.639
764.9815	6.93
850.1538	36.9
976.1562	6.47
1066.6441	11.2
1140.7332	12.0
1164.9252	12.4
1224.5271	4.94
1280.3774	0.0324
1343.9703	0.0992
1375.6805	2.13
3056.3514	0.533
3169.4185	0.298

Infrared Spectrum

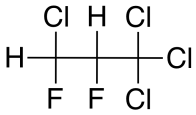


Radiative Efficiency



HCFC-232eb

Molecular Formula:	$CHClFCHFCCl_3$
Name:	1,1,1,3-Tetrachloro-2,3-difluoropropane
CAS number:	–
Molecular Weight:	217.86



Global Atmospheric Lifetime (years):	2.04
Tropospheric Atmospheric Lifetime (years):	2.22
Stratospheric Atmospheric Lifetime (years):	25.1
Ozone Depletion Potential (ODP):	0.045

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.217	0.183
Global Warming Potential (GWP_H):		
GWP_{20}	458	387
GWP_{100}	124	105
Global Temperature Potentials (GTP_H)		
GTP_{20}		144
GTP_{50}		19
GTP_{100}		15

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 2.64 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 1.68 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 2.15$ years

$\tau^{OH}_{Trop} = 2.22$ years

$\tau^{OH}_{Strat} = 69.3$ years

Fractional Atmospheric Loss: 0.948

$O(^1D)$ 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: 0.011

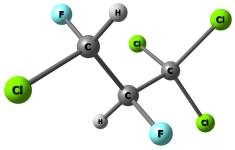
UV Photolysis

UV Spectrum: *No Recommendation*

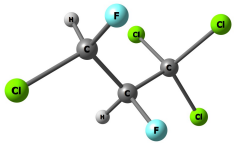
$\tau_{hv} = 50$ years

Fractional Atmospheric Loss: 0.041

Molecular Structure and Infrared Spectrum (2 conformers)



E = 0
Population = 0.580



$\Delta E = 0.19$ kcal mol^{-1}
Population = 0.420

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.569173343489	0.302317893726	0.349688903833
C	-0.441938852621	-0.433505651066	-0.397596456197
C	1.001762594395	0.020397315814	-0.043068873801
Cl	-3.146787281164	-0.360343795173	-0.207095165614
H	-1.516613668880	0.120232328243	1.423571486197
F	-1.540327909350	1.626377663615	0.101416302261
H	-0.567426837378	-0.309154205618	-1.478097421525
F	-0.553131276472	-1.751378907216	-0.064112221453
Cl	2.141085885956	-1.108366734385	-0.844258616155
Cl	1.306749243815	1.670345757588	-0.647728485708
Cl	1.266121445189	-0.044770665529	1.728445548161

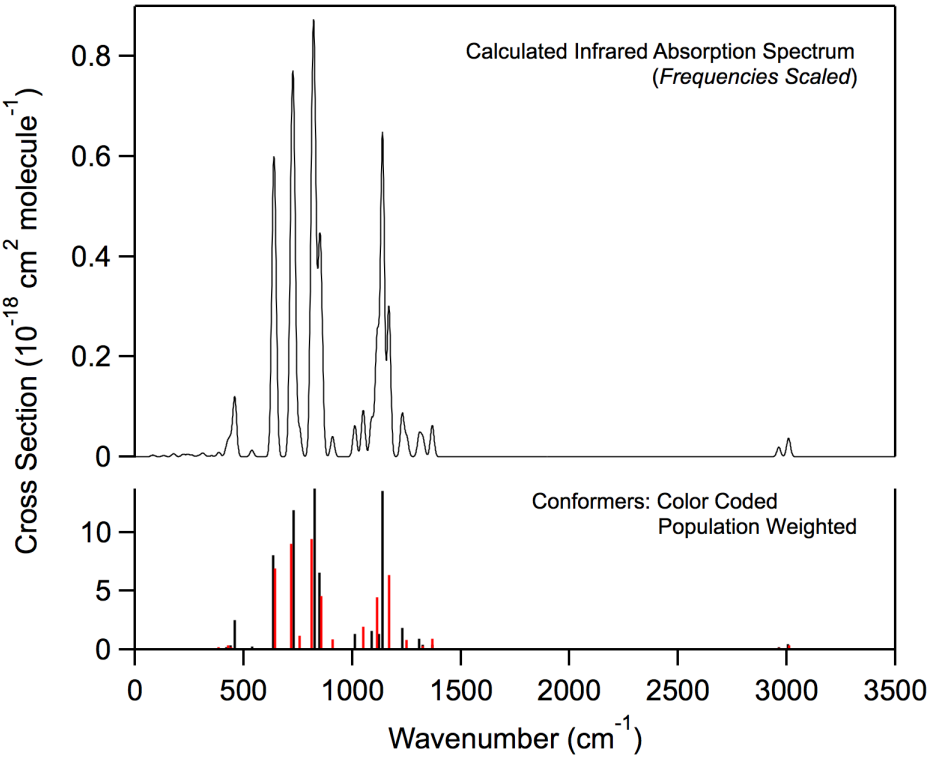
Atom	X	Y	Z
C	1.549614314766	-0.485826467826	-0.190452435800
C	0.430718663238	0.569112876813	-0.193216466186
C	-1.013797469376	0.004647755637	-0.117394905155
Cl	3.098600787802	0.324083654313	-0.636032888161
F	1.683119186030	-1.034188772034	1.031915030175
H	1.384862660672	-1.264364736359	-0.934986952433
H	0.489358060624	1.136799687677	-1.127118961748
F	0.620511752810	1.400104919596	0.866309642279
Cl	-2.145566145552	1.392630205246	-0.187267704410
Cl	-1.289964538972	-1.046039157619	-1.549675982005
Cl	-1.305706272043	-0.913023965445	1.378017623445

Infrared Absorption Spectrum (unscaled frequencies)

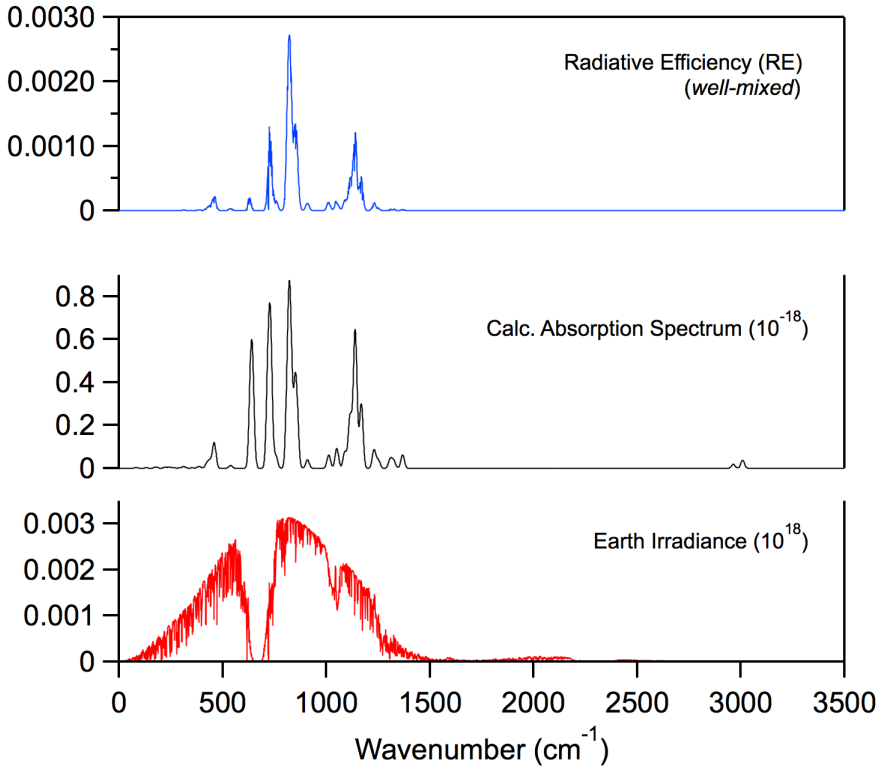
Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
26.3374	0.0627
80.5731	0.0385
134.0498	0.0823
178.0912	0.0958
199.1975	0.136
217.8982	0.0158
269.5784	0.0984
276.5659	0.180
316.1481	0.0756
389.3247	0.396
409.7313	0.646
429.4785	4.32
512.9716	0.486
616.0583	13.9
717.3704	20.5
817.5931	23.7
841.2808	11.3
1014.4317	2.29
1096.5910	2.76
1132.8830	2.34
1149.7470	23.3
1245.9094	3.16
1328.4196	1.57
1346.2527	0.706
1392.6661	0.704
3080.4796	0.404
3126.9395	0.818

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
35.0234	0.0869
84.8936	0.0675
129.8308	0.204
177.3441	0.104
210.2065	0.0445
221.2581	0.125
250.7640	0.0830
262.9481	0.0423
294.6022	0.0117
351.5355	0.448
397.0417	0.916
411.2207	0.502
626.1012	16.4
704.6321	21.4
744.8726	2.80
805.2098	22.4
851.9620	10.9
905.8746	2.04
1055.4969	4.70
1122.2092	10.6
1180.6483	15.2
1267.7377	1.92
1345.6322	0.757
1356.7625	0.0905
1391.7127	2.19
3081.7546	0.421
3131.1268	0.813

Infrared Spectrum

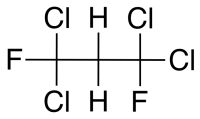


Radiative Efficiency



HCFC-232fa

Molecular Formula:	$CCl_2FCH_2CCl_2F$
Name:	1,1,3,3-Tetrachloro-1,3-difluoropropane
CAS number:	313696-57-0
Molecular Weight:	217.86



Global Atmospheric Lifetime (years):	9.23
Tropospheric Atmospheric Lifetime (years):	12.5
Stratospheric Atmospheric Lifetime (years):	35.2
Ozone Depletion Potential (ODP):	0.176

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.281	0.267
Global Warming Potential (GWP_H):		
GWP_{20}	2369	2254
GWP_{100}	725	689
Global Temperature Potentials (GTP_H)		
GTP_{20}		1644
GTP_{50}		242
GTP_{100}		99

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 4.69 \times 10^{-15}$; $k_{SAR}(272\ K) \approx 2.99 \times 10^{-15}$ cm^3 $molecule^{-1}$ s^{-1}

τ^{OH}_{Global} = 12.0 years
τ^{OH}_{Trop} = 12.5 years
τ^{OH}_{Strat} = 328.5 years

Fractional Atmospheric Loss: 0.766

O(^{1}D) Reactivity

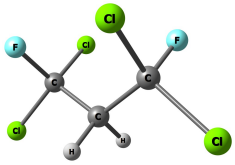
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 2.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)}$ = 185 years
Fractional Atmospheric Loss: 0.050

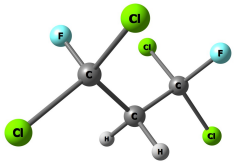
UV Photolysis

UV Spectrum: *No Recommendation*
τ_{hv} = 50 years
Fractional Atmospheric Loss: 0.184

Molecular Structure and Infrared Spectrum (4 conformers)



E = 0
Population = 0.425



E = 0
Population = 0.425

Optimized Coordinates (Angstroms)

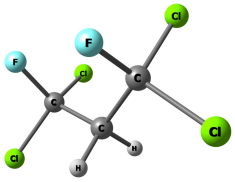
Atom	X	Y	Z
C	-1.303263087232	-0.008058471967	0.181538743456
C	0.000048866421	-0.798945473688	-0.000096499282
C	1.303265702943	-0.007919224774	-0.181807851975
Cl	-2.627832841014	-1.208973879170	0.461037918625
F	-1.256459790228	0.793917627362	1.248695557320
Cl	-1.725441000103	0.988819045194	-1.248082432198
H	-0.116962560011	-1.438120995074	-0.876778762051
H	0.117137151828	-1.438022571158	0.876647241269
Cl	1.725323717975	0.989146602948	1.247717399138
Cl	2.627979868388	-1.208702219197	-0.461191484897
F	1.256365970289	0.793948559523	-1.249041823415

Atom	X	Y	Z
C	-1.303263944252	-0.007687088815	-0.181951926926
C	-0.000120753315	-0.798885406796	-0.000462664068
C	1.303242869783	-0.008168312356	0.181540336495
Cl	-1.725332720028	0.988860641224	1.247931590837
F	-1.256234732228	0.794588278818	-1.248873373578
Cl	-2.628055362862	-1.208258034684	-0.461880200939
H	0.116890295843	-1.437743306154	-0.877376361069
H	-0.117309922989	-1.438280082436	0.876035928679
Cl	2.627699646183	-1.209289954047	0.460688694303
Cl	1.725589499062	0.989190258244	-1.247695654748
F	1.256437124805	0.793427007001	1.248982631014

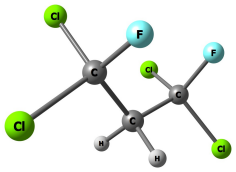
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
10.7826	0.00123
117.6259	0.175
129.9348	0.125
189.1352	0.00772
217.3471	0.0606
242.1124	0.0828
274.4334	0.0795
314.4306	0.0
369.9604	0.0445
377.4188	0.0928
404.0142	0.287
449.6712	0.578
456.6438	1.31
610.9472	15.1
655.9373	14.6
728.3885	29.3
876.4237	21.8
926.5034	4.27
949.5234	0.653
1074.8513	32.2
1171.6577	21.9
1202.6930	23.0
1300.9536	0.0343
1361.1391	3.98
1443.3418	0.845
3096.1774	0.0902
3153.7332	0.0426

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
10.7780	0.00123
117.6246	0.175
129.9350	0.125
189.1351	0.00772
217.3480	0.0606
242.1117	0.0828
274.4337	0.0795
314.4304	0.0
369.9598	0.0445
377.4187	0.0928
404.0144	0.287
449.6714	0.578
456.6436	1.31
610.9466	15.1
655.9384	14.6
728.3870	29.3
876.4230	21.8
926.5048	4.27
949.5233	0.653
1074.8510	32.2
1171.6588	21.9
1202.6935	23.0
1300.9541	0.0343
1361.1398	3.98
1443.3435	0.845
3096.1780	0.0902
3153.7337	0.0426



$\Delta E = 1.11$ kcal mol^{-1}
Population = 0.065



$\Delta E = 1.11$ kcal mol^{-1}
Population = 0.065

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.311959467956	-0.201903430248	-0.244630202464
C	-0.000452425054	-0.737775598966	0.345974510846
C	1.308581393045	-0.125556835136	-0.183330923948
Cl	-1.615051583101	1.533625912924	0.065579822059
F	-1.344832636535	-0.399223433537	-1.567588533057
Cl	-2.661545234424	-1.164195756318	0.483580579542
H	0.016357051201	-1.799026304266	0.086124702642
H	-0.022611070107	-0.652240626311	1.431194835694
Cl	1.738427102703	1.422651989259	0.614969529350
Cl	2.642247158469	-1.307263165593	0.129970949017
F	1.250791711759	0.084986248191	-1.501863269682

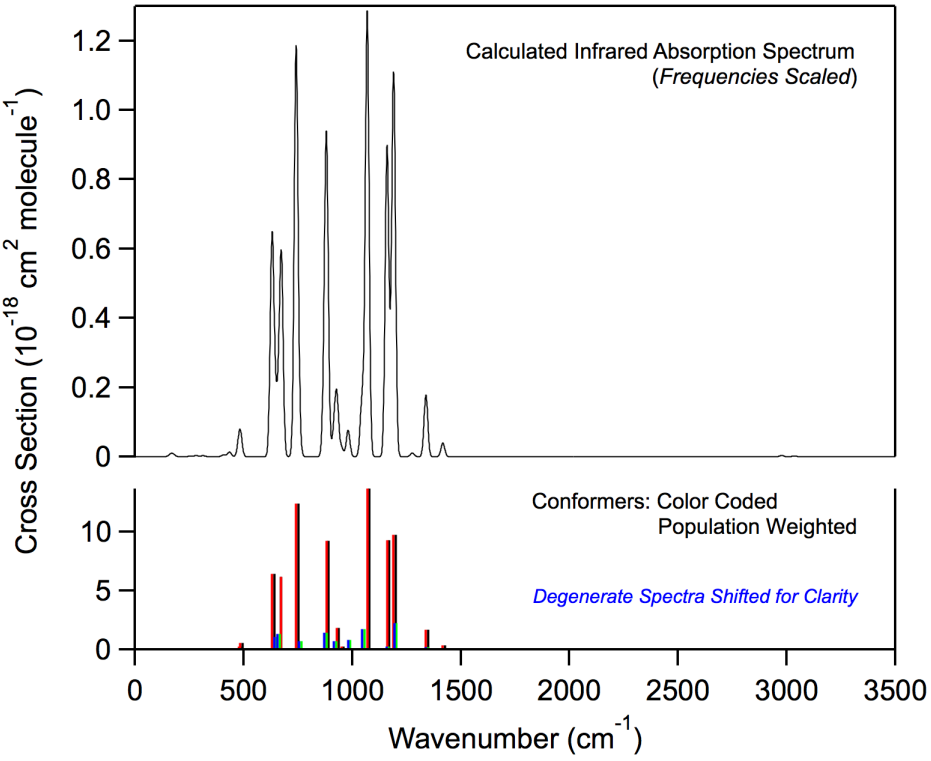
Atom	X	Y	Z
C	-1.311997114147	-0.202951041957	0.256933588632
C	-0.000510879759	-0.739622396680	-0.332982653054
C	1.308589080940	-0.127664907768	0.196467038949
Cl	-2.661723781032	-1.165041431281	-0.471283950677
F	-1.345391731132	-0.399653087518	1.579971334675
Cl	-1.614287976285	1.532554866625	-0.054176467571
H	-0.022276871252	-0.654589435675	-1.418250591389
H	0.015789596356	-1.800756425297	-0.072626086511
Cl	2.641890826286	-1.310056675499	-0.115780653698
Cl	1.739325310330	1.419977587338	-0.602454625501
F	1.250427539696	0.083563947710	1.514874066145

Infrared Absorption Spectrum (unscaled frequencies)

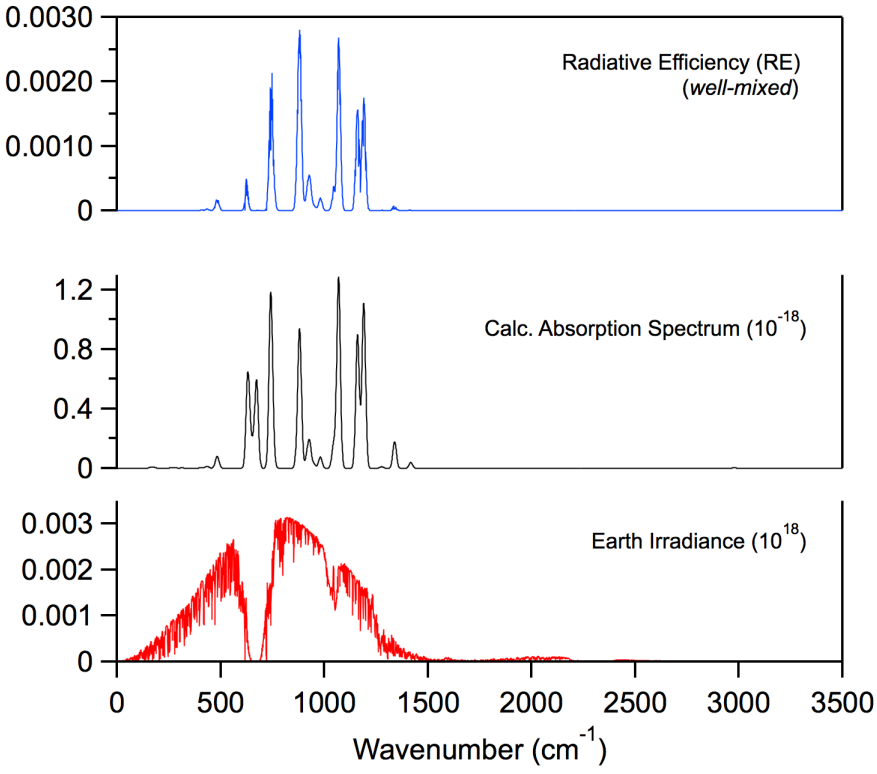
Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
14.8249	0.00289
104.3621	0.120
136.9855	0.168
189.6841	0.0138
204.0154	0.0382
239.1896	0.00289
297.6271	0.0803
329.0566	0.0101
347.9099	0.0418
376.2292	0.0325
398.3805	0.347
448.5540	0.422
455.9962	1.10
623.0424	16.7
637.4102	20.4
742.3691	10.7
865.9246	22.3
912.8844	10.9
981.8010	12.5
1049.6738	26.6
1169.0351	4.22
1207.0651	35.0
1294.0278	1.55
1360.2862	3.15
1445.2613	0.944
3091.2247	0.0944
3166.0294	0.103

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
14.8266	0.00289
104.3595	0.120
136.9854	0.168
189.6855	0.0138
204.0154	0.0382
239.1901	0.00289
297.6271	0.0803
329.0564	0.0101
347.9100	0.0418
376.2300	0.0325
398.3804	0.347
448.5544	0.422
455.9966	1.10
623.0435	16.7
637.4114	20.4
742.3699	10.7
865.9241	22.3
912.8868	10.9
981.8012	12.5
1049.6759	26.6
1169.0349	4.22
1207.0628	35.0
1294.0274	1.55
1360.2865	3.15
1445.2621	0.944
3091.2273	0.0944
3166.0282	0.103

Infrared Spectrum

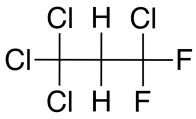


Radiative Efficiency



HCFC-232fb

Molecular Formula: $CCl_3CH_2CClF_2$
Name: 1,1,1,3-Tetrachloro-3,3-difluoropropane
CAS number: 460-89-9
Molecular Weight: 217.86



Global Atmospheric Lifetime (years): 10.2
  Tropospheric Atmospheric Lifetime (years): 14.4
  Stratospheric Atmospheric Lifetime (years): 35.6
Ozone Depletion Potential (ODP): 0.194

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.261	0.249
Global Warming Potential (GWP_H):		
GWP_{20}	2366	2260
GWP_{100}	747	713
Global Temperature Potentials (GTP_H)		
GTP_{20}		1712
GTP_{50}		282
GTP_{100}		103

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 4.08 \times 10^{-15}$; $k_{SAR}(272\ K) \approx 2.61 \times 10^{-15}$ cm^3 $molecule^{-1}$ s^{-1}

τ^{OH}_{Global} = 13.8 years
τ^{OH}_{Trop} = 14.4 years
τ^{OH}_{Strat} = 372.1 years

Fractional Atmospheric Loss: 0.740

O(^{1}D) Reactivity

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

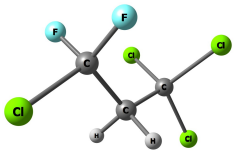
$k_{Est}(T) = 2.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)}$ = 185 years
Fractional Atmospheric Loss: 0.055

UV Photolysis

UV Spectrum: *No Recommendation*
τ_{hv} = 50 years
Fractional Atmospheric Loss: 0.205

Papanastasiou et al. (2018)

Molecular Structure and Infrared Spectrum (1 conformer)



E = 0
Population = 0.943

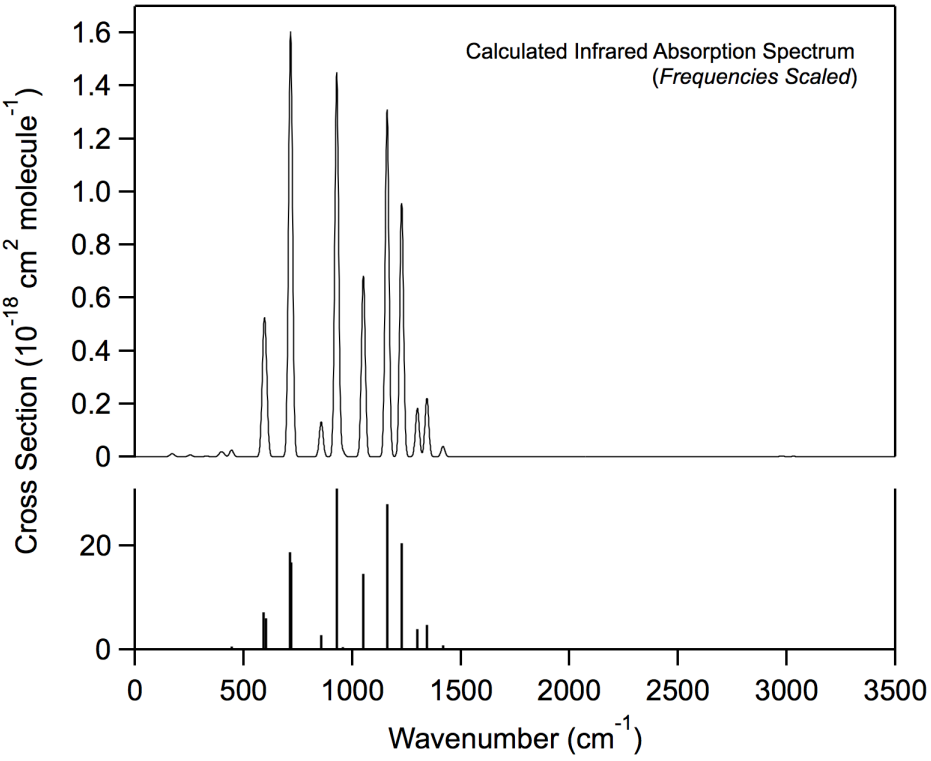
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	0.089749990767	-1.088980306239	0.000000000000
C	0.764371116126	0.294651531598	0.000000000000
C	-0.130615033765	1.538551770906	0.000000000000
Cl	1.423288165979	-2.307580052741	0.000000000000
Cl	-0.911133116565	-1.352881420865	1.460038260107
Cl	-0.911133116565	-1.352881420865	-1.460038260107
H	1.401623023519	0.349406783897	-0.884152663394
H	1.401623023519	0.349406783897	0.884152663394
Cl	0.944290872716	3.003382499703	0.000000000000
F	-0.911019462769	1.611312915332	-1.078331532058
F	-0.911019462769	1.611312915332	1.078331532058

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
18.1146	0.000
118.4845	0.148
129.5990	0.154
200.2680	0.0124
211.9463	0.0833
214.4901	0.0638
292.0516	0.0547
294.8945	0.00621
359.6895	0.298
372.5107	0.257
413.6345	0.576
426.9333	0.000
569.9338	7.61
580.3913	6.39
699.1571	19.8
703.8509	17.7
850.7620	2.97
926.3645	32.8
955.1322	0.476
1056.1462	15.4
1171.9209	29.6
1242.8237	21.6
1319.6381	4.14
1365.9052	4.98
1444.5898	0.876
3095.8881	0.0766
3153.1227	0.0383

Infrared Spectrum



Radiative Efficiency