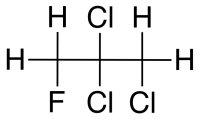
HCFC-251aa

Molecular Formula:	$CH_2FCCl_2CH_2Cl$
Name:	1,2,2-Trichloro-3-fluoropropane
CAS number:	70192-89-1
Molecular Weight:	165.42



Global Atmospheric Lifetime (years):	1.26
Tropospheric Atmospheric Lifetime (years):	1.34
Stratospheric Atmospheric Lifetime (years):	23.3
Ozone Depletion Potential (ODP):	0.028

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.096	0.075
Global Warming Potential (GWP_H):		
GWP_{20}	166	129
GWP_{100}	45	35
Global Temperature Potentials (GTP_H)		
GTP_{20}		43
GTP_{50}		6
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*

$k_{SAR}(298\ K) = 4.39 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 2.80 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 1.30$ years

$\tau^{OH}_{Trop} = 1.34$ years

$\tau^{OH}_{Strat} = 43.8$ 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: 0.007

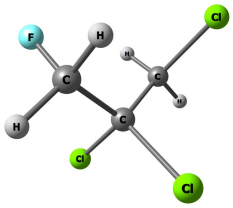
UV Photolysis

UV Spectrum: *No Recommendation*

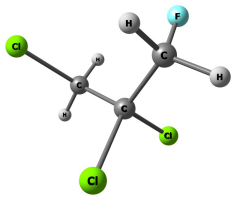
$\tau_{hv} = 68$ years

Fractional Atmospheric Loss: 0.018

Molecular Structure and Infrared Spectrum (6 conformers)



E = 0
Population = 0.463



E = 0
Population = 0.463

Optimized Coordinates (Angstroms)

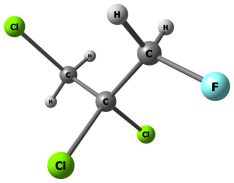
Atom	X	Y	Z
C	0.721414500053	-0.237772432561	1.002247341382
C	-0.353073034840	0.118227952911	-0.025462028697
C	-0.409362637713	-0.832453142062	-1.222323269184
Cl	2.384029121365	-0.230206764037	0.311604596478
H	0.705452766844	0.470545865408	1.827639591397
H	0.530362413783	-1.248149756228	1.360801096156
Cl	-0.133677664264	1.779822954965	-0.669695825984
Cl	-1.922469999932	0.023437572894	0.874244756302
H	-1.260812997279	-0.575631918256	-1.857794573488
H	0.523450155532	-0.747197841483	-1.787634917256
F	-0.543722623549	-2.118295491550	-0.762280767105

Atom	X	Y	Z
C	0.721353346343	0.237648679434	1.001692725757
C	-0.355163231926	-0.115162022660	-0.024992660712
C	-0.407885928432	0.834015423213	-1.223209214928
Cl	2.383589374196	0.221847489679	0.310278404709
H	0.534870402878	1.249366232466	1.358870049244
H	0.702703988097	-0.469396684377	1.828119365680
Cl	-1.923703773676	-0.012236783112	0.875312971128
Cl	-0.143306598850	-1.778629793758	-0.666913467249
H	0.524277946214	0.743881428781	-1.788834352264
H	-1.260747594765	0.579976598431	-1.857905992319
F	-0.536433930081	2.121097431903	-0.764976829048

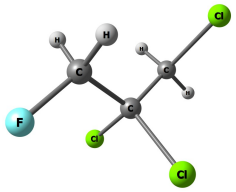
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
82.7669	0.164
139.8818	0.267
153.1049	0.279
226.5946	1.13
249.4061	0.705
293.8954	0.364
318.2171	0.322
385.6315	0.335
431.4930	1.97
648.1967	7.36
707.3875	15.1
758.1611	4.32
895.1933	0.488
969.8537	9.57
1064.8927	2.38
1104.3645	10.2
1167.1435	2.11
1242.3794	0.126
1275.3759	2.04
1306.7726	0.916
1413.7381	0.794
1456.1185	1.26
1494.1188	1.40
3064.5639	1.45
3114.3243	0.514
3125.5191	1.40
3186.3478	0.0410

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
82.7665	0.164
139.8812	0.267
153.1048	0.279
226.5938	1.13
249.4057	0.705
293.8951	0.364
318.2170	0.322
385.6314	0.335
431.4930	1.97
648.1968	7.36
707.3875	15.1
758.1609	4.32
895.1932	0.488
969.8533	9.57
1064.8926	2.38
1104.3650	10.2
1167.1436	2.11
1242.3793	0.126
1275.3766	2.04
1306.7727	0.916
1413.7385	0.794
1456.1186	1.26
1494.1188	1.40
3064.5637	1.45
3114.3245	0.514
3125.5187	1.40
3186.3479	0.0410



$\Delta E = 1.94$ kcal mol^{-1}
Population = 0.017



$\Delta E = 1.94$ kcal mol^{-1}
Population = 0.017

Optimized Coordinates (Angstroms)

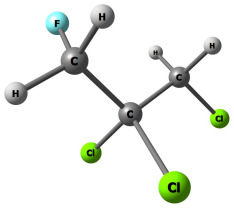
Atom	X	Y	Z
C	1.005098488821	0.993072406605	-0.238466832161
C	-0.254580916984	0.149810557221	-0.036997783186
C	-0.471838975059	-0.895910524293	-1.132259615465
Cl	2.512394873214	0.009047869042	-0.331378447038
H	0.926104779719	1.542855816113	-1.176558356678
H	1.120078377936	1.689280715382	0.589736001400
Cl	-1.631744754083	1.328271780259	-0.080499544725
Cl	-0.231603380002	-0.659463925210	1.567013113107
H	-0.478338316961	-0.389085251682	-2.105096828492
H	0.346142103964	-1.621302145216	-1.098287673020
F	-1.659744280567	-1.539453298220	-0.949287033742

Atom	X	Y	Z
C	1.006044736351	-0.991459284752	-0.244542432472
C	-0.253717733518	-0.149436985419	-0.038462231427
C	-0.469470524964	0.904250793460	-1.126361600026
Cl	2.513634344449	-0.007079705402	-0.328504106965
H	1.119903316894	-1.693684806116	0.578720490310
H	0.928071826091	-1.534401814102	-1.186694817042
Cl	-0.232508580390	0.648165612118	1.571408667961
Cl	-1.631047651455	-1.327283179339	-0.092165394194
H	0.348603443789	1.629218229628	-1.086146001912
H	-0.474899142695	0.404502838762	-2.102859872289
F	-1.657475034552	1.546678301164	-0.940142701944

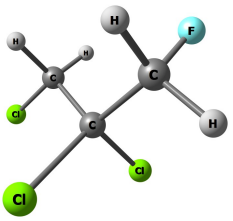
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
97.0624	0.603
115.5548	0.178
149.3687	0.256
203.2059	0.128
249.0214	0.158
293.3472	0.225
338.5313	0.0273
345.3735	0.479
546.0101	3.49
578.8690	4.80
688.9034	18.2
747.4743	5.16
884.0687	1.21
1027.0760	1.76
1066.1415	2.81
1109.6249	4.48
1145.5929	9.22
1242.3543	1.25
1285.0977	1.99
1301.0339	1.98
1420.4869	0.619
1464.8295	1.35
1495.6210	0.480
3038.1662	2.83
3103.2254	0.145
3107.3294	1.99
3176.1378	0.0192

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
97.0623	0.603
115.5547	0.178
149.3686	0.256
203.2058	0.128
249.0214	0.158
293.3472	0.225
338.5313	0.0273
345.3735	0.479
546.0101	3.49
578.8690	4.80
688.9036	18.2
747.4743	5.16
884.0687	1.21
1027.0760	1.76
1066.1414	2.81
1109.6250	4.48
1145.5930	9.22
1242.3544	1.25
1285.0978	1.99
1301.0340	1.98
1420.4868	0.619
1464.8296	1.35
1495.6209	0.480
3038.1661	2.83
3103.2255	0.145
3107.3296	1.99
3176.1378	0.0192



$\Delta E = 1.95$ kcal mol^{-1}
Population = 0.017



$\Delta E = 1.95$ kcal mol^{-1}
Population = 0.017

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	0.655442405404	-0.659690671346	-0.858713265049
C	-0.380666851453	0.160660816435	-0.091205766249
C	-1.760374584171	0.017760055955	-0.750276838536
Cl	2.313423276940	-0.583883377088	-0.196216876931
H	0.338829373025	-1.702169574047	-0.851476385008
H	0.701702997894	-0.294540950184	-1.885952276930
Cl	0.018309259239	1.916620113455	-0.139215590394
Cl	-0.493261314643	-0.398921712030	1.613067645848
H	-2.501954740198	0.574564467206	-0.171928986467
H	-1.712866288538	0.413292739079	-1.771384532395
F	-2.109463533499	-1.308395907436	-0.798329127890

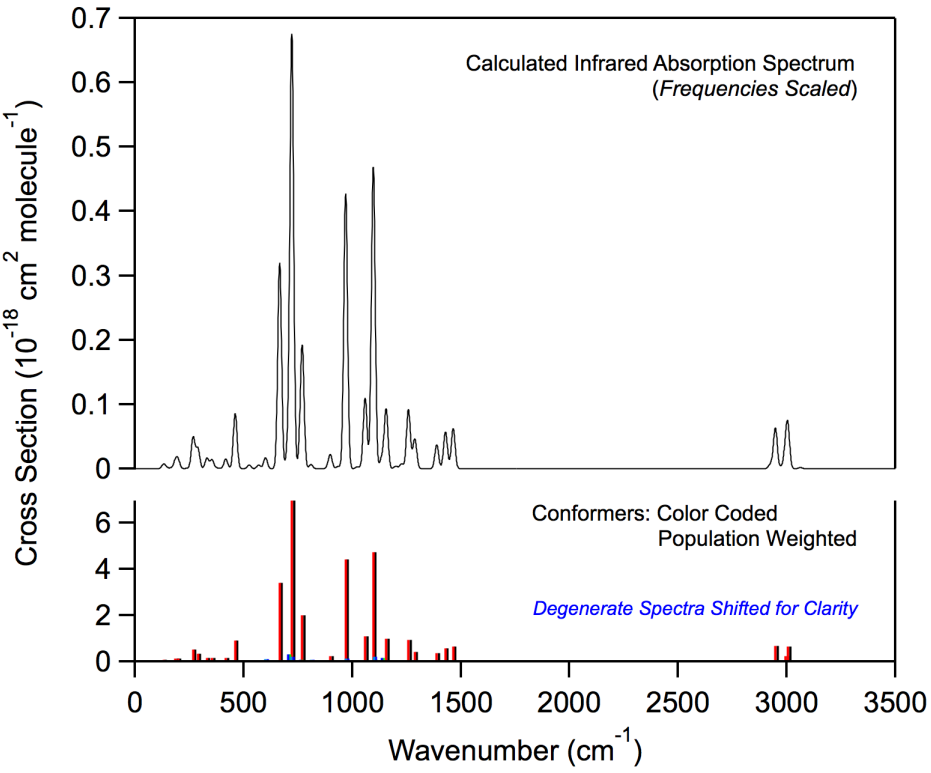
Atom	X	Y	Z
C	0.655254302393	0.662252465792	-0.857054787630
C	-0.381082991862	-0.159544601209	-0.091403897500
C	-1.760869367606	-0.014285694113	-0.749794882035
Cl	2.313348309298	0.583945406169	-0.195132554417
H	0.701102284086	0.299699536028	-1.885231565349
H	0.339153529363	1.704864351748	-0.847088582639
Cl	-0.493015547457	0.395747469864	1.614316011073
Cl	0.017020113006	-1.915571009317	-0.143979589722
H	-1.713787856456	-0.407243661970	-1.771915953162
H	-2.502593817397	-0.572194854149	-0.172697852274
F	-2.109311957367	1.312160591157	-0.794393346345

Infrared Absorption Spectrum (unscaled frequencies)

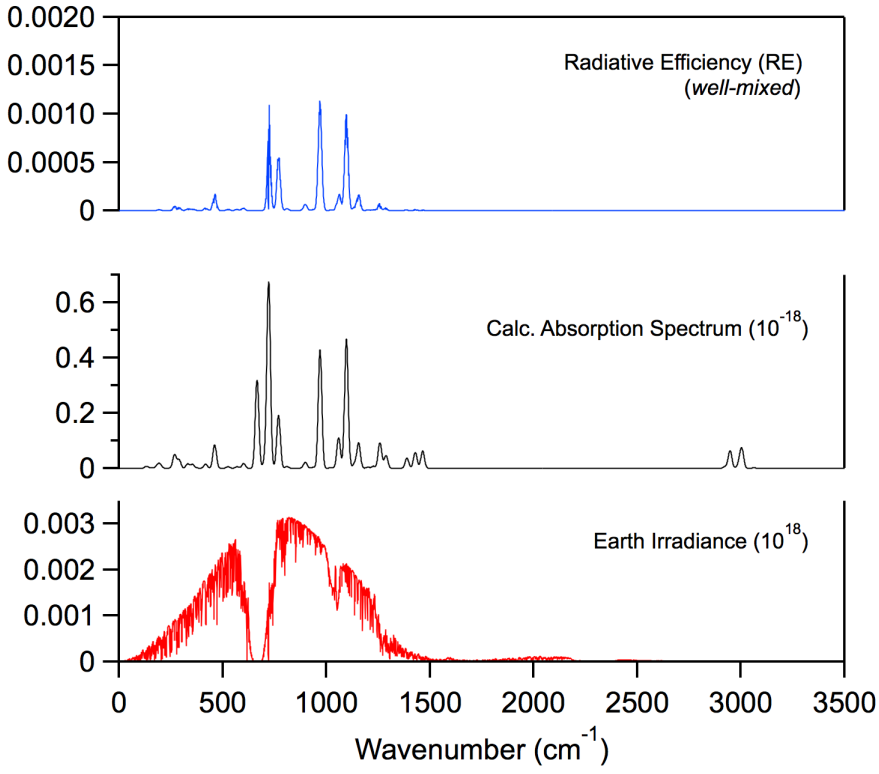
Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
93.9791	0.139
116.6393	0.500
152.7844	0.116
195.6810	0.349
258.3790	0.298
296.0013	0.0898
337.1383	0.277
380.5928	0.259
499.6455	3.56
579.7229	5.82
704.3447	11.5
800.8429	4.02
932.2695	2.04
971.8908	7.92
1055.4907	1.95
1107.5809	11.4
1152.3708	1.24
1214.2151	2.37
1281.8349	1.45
1312.5140	2.80
1410.0406	1.26
1461.2303	0.770
1496.9993	0.729
3047.6852	2.31
3091.0398	1.17
3117.5709	1.59
3160.9417	0.0586

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
93.9791	0.139
116.6395	0.500
152.7844	0.116
195.6812	0.349
258.3792	0.298
296.0013	0.0898
337.1385	0.277
380.5929	0.259
499.6455	3.56
579.7229	5.82
704.3445	11.5
800.8432	4.02
932.2694	2.04
971.8913	7.92
1055.4905	1.95
1107.5813	11.4
1152.3703	1.24
1214.2154	2.37
1281.8341	1.45
1312.5141	2.80
1410.0405	1.26
1461.2301	0.770
1496.9999	0.729
3047.6851	2.31
3091.0402	1.17
3117.5697	1.59
3160.9417	0.0586

Infrared Spectrum

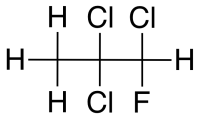


Radiative Efficiency



HCFC-251ab

Molecular Formula:	CH_3CCl_2CHFCl
Name:	1,2,2-Trichloro-1-fluoropropane
CAS number:	–
Molecular Weight:	165.42



Global Atmospheric Lifetime (years):	1.73
Tropospheric Atmospheric Lifetime (years):	1.85
Stratospheric Atmospheric Lifetime (years):	26.9
Ozone Depletion Potential (ODP):	0.037

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.134	0.110
Global Warming Potential (GWP_H):		
GWP_{20}	315	260
GWP_{100}	85	70
Global Temperature Potentials (GTP_H)		
GTP_{20}		93
GTP_{50}		12
GTP_{100}		10

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 3.17 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 2.02 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

τ^{OH}_{Global} = 1.80 years
τ^{OH}_{Trop} = 1.85 years
τ^{OH}_{Strat} = 58.8 years

Fractional Atmospheric Loss: 0.965

O(^{1}D) Reactivity

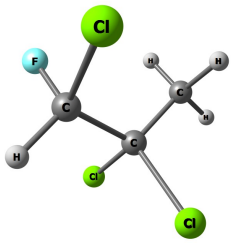
k_{Rec}(T), *No recommendation*

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

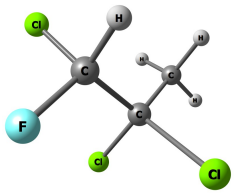
UV Photolysis

UV Spectrum: *No Recommendation*
τ_{hv} = 68 years
Fractional Atmospheric Loss: 0.026

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.704



$\Delta E = 0.70$ kcal mol^{-1}
Population = 0.216

Optimized Coordinates (Angstroms)

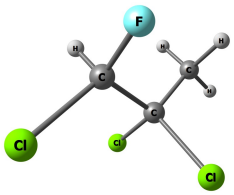
Atom	X	Y	Z
C	-0.403284453277	0.010905033640	1.748715658892
C	-0.484608732653	0.095162368623	0.234927860305
C	0.696736071595	-0.577696297348	-0.500272733965
H	-1.309273670606	0.424939230955	2.191532679438
H	-0.300991598150	-1.035864729660	2.043320111756
H	0.462595680270	0.572801229993	2.103844627571
Cl	-0.598473059025	1.805277044149	-0.310746128806
Cl	-1.964960190952	-0.786037568958	-0.338486836635
H	0.585767355110	-0.489798311669	-1.581281637640
Cl	2.276460063015	0.176727075912	-0.076627688840
F	0.745922534673	-1.879588075638	-0.142232912077

Atom	X	Y	Z
C	-0.472367205483	-0.856734845652	1.665996798823
C	-0.481704654686	-0.180191508014	0.305238470736
C	0.678217424369	0.815060165085	0.095837226090
H	-0.445277527707	-0.101676774329	2.457033467498
H	-1.377717946723	-1.453529907741	1.780950500265
H	0.401188984530	-1.504145349149	1.754653971161
Cl	-1.990972872954	0.824870907371	0.160212760521
Cl	-0.474896761508	-1.407397574769	-1.005662020674
H	0.614623802539	1.606311053826	0.846323729936
Cl	2.286224573565	0.032619110550	0.327470674902
F	0.634005184059	1.349861722821	-1.134770579259

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
83.6632	0.0956
161.8430	0.0776
225.2392	0.447
248.1044	0.279
267.9216	0.218
298.7755	0.255
316.6909	0.309
356.6280	0.274
399.6956	0.633
454.6971	1.02
659.4438	11.7
726.1338	16.3
770.9991	8.67
906.3728	2.95
1078.2702	7.13
1096.3613	8.54
1115.1557	14.6
1196.2498	1.30
1281.1504	2.53
1361.2165	0.461
1410.8417	2.00
1479.4839	0.376
1483.2957	1.31
3066.8437	0.324
3126.9732	0.571
3149.3146	0.350
3161.3231	0.374

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
82.1059	0.0704
171.8285	0.246
198.7071	0.0617
244.0012	0.0494
270.4723	0.0988
289.3442	0.175
328.1370	0.0953
364.1221	0.127
398.6464	0.353
547.7290	1.13
598.8007	7.78
687.2064	22.9
784.7186	6.71
920.7641	4.47
1082.5308	5.97
1093.5932	6.84
1150.5863	11.5
1191.4624	4.02
1269.8327	2.87
1371.9224	1.73
1414.2824	1.74
1477.8489	0.953
1483.7980	0.781
3059.0811	0.617
3099.7472	1.04
3140.1014	0.734
3161.2907	0.367



$\Delta E = 1.29$ kcal mol^{-1}
Population = 0.080

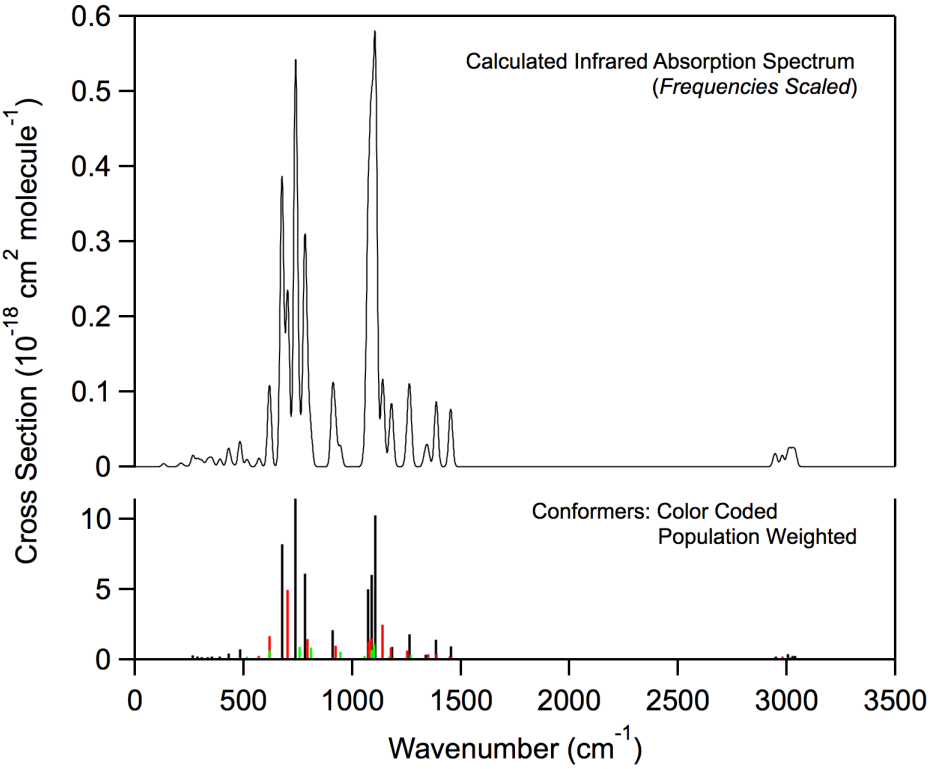
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.554293192472	0.912170840039	1.163156350903
C	-0.636130858196	0.134441799378	0.225091022613
C	0.819614934845	0.188708535633	0.739306364633
H	-2.582364714505	0.851155991502	0.805682679744
H	-1.504090248467	0.487221333778	2.169755967638
H	-1.241211092806	1.957036428483	1.194902743619
Cl	-0.737274457861	0.843119899607	-1.423386522601
Cl	-1.149354826289	-1.593694746760	0.187429014384
H	0.870767564939	-0.303417720478	1.713748223457
Cl	2.006989563626	-0.636453465122	-0.310018326257
F	1.178515327186	1.487800103942	0.872297481866

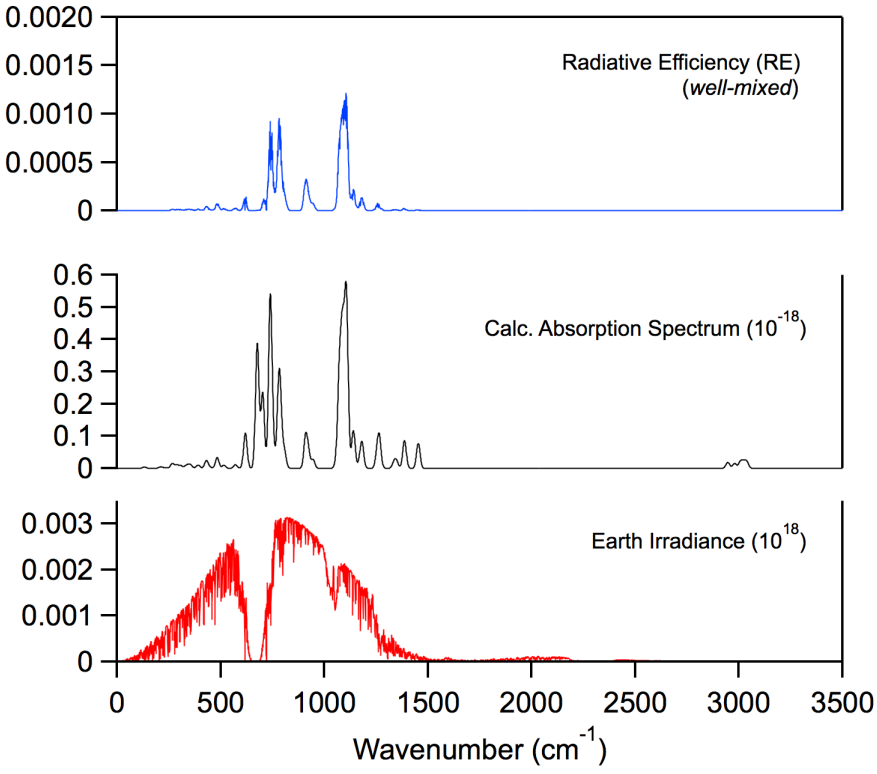
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
80.5338	0.0794
166.6159	0.0686
184.7244	0.147
252.9232	0.145
268.9154	0.00576
307.7701	0.275
329.8312	0.120
372.0663	0.0823
419.8637	0.768
488.8494	2.63
597.8775	8.01
744.5627	11.3
799.9538	10.5
944.3415	7.07
1061.6980	3.45
1095.3886	8.77
1109.6191	14.1
1180.4496	2.74
1287.6997	4.53
1353.6375	1.64
1409.1185	0.994
1480.9859	0.804
1483.0517	0.646
3058.2790	0.730
3094.3152	1.32
3139.3389	0.897
3162.3333	0.270

Infrared Spectrum

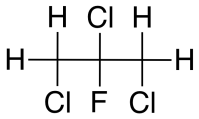


Radiative Efficiency



HCFC-251ba

Molecular Formula:	$CH_2ClCClFCH_2Cl$
Name:	1,2,3-Trichloro-2-fluoropropane
CAS number:	7126-16-1
Molecular Weight:	165.42



Global Atmospheric Lifetime (years):	1.34
Tropospheric Atmospheric Lifetime (years):	1.40
Stratospheric Atmospheric Lifetime (years):	29.4
Ozone Depletion Potential (ODP):	0.027

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.121	0.095
Global Warming Potential (GWP_H):		
GWP_{20}	219	173
GWP_{100}	59	47
Global Temperature Potentials (GTP_H)		
GTP_{20}		59
GTP_{50}		8
GTP_{100}		7

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 4.19 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 2.67 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 1.36$ years

$\tau^{OH}_{Trop} = 1.40$ years

$\tau^{OH}_{Strat} = 45.7$ years

Fractional Atmospheric Loss: 0.984

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: 0.007

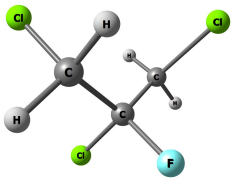
UV Photolysis

UV Spectrum: *No Recommendation*

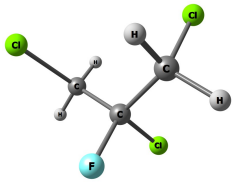
$\tau_{hv} = 150$ years

Fractional Atmospheric Loss: 0.009

Molecular Structure and Infrared Spectrum (4 conformers)



E = 0
Population = 0.405



E = 0
Population = 0.405

Optimized Coordinates (Angstroms)

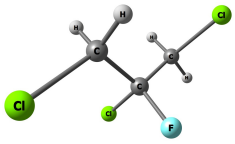
Atom	X	Y	Z
C	0.950266833835	-0.380795656906	-0.833433699332
C	-0.081106620541	-0.580021289983	0.271004257895
C	-0.592248300543	0.677751815002	0.973518537897
Cl	2.431715479697	0.430727025952	-0.204220195343
H	1.252257370194	-1.351484381370	-1.222401971612
H	0.542320815914	0.240323530431	-1.627494395629
F	0.440335131812	-1.366268274387	1.248567645938
Cl	-1.461697020919	-1.490173909361	-0.482445680402
H	-1.357611218948	0.396414885523	1.694966773303
H	0.247933083007	1.151652511162	1.480912932989
Cl	-1.296889553508	1.884684743937	-0.146531205705

Atom	X	Y	Z
C	0.593804326826	0.675667840731	0.971504067576
C	0.070638345628	-0.578578399711	0.271540660410
C	-0.956588890877	-0.371528036198	-0.835319734326
Cl	1.313184820324	1.871955255051	-0.150594827524
H	-0.242221645320	1.159841041447	1.476055919385
H	1.354853560626	0.388259857484	1.695119337358
F	-0.460845147562	-1.356541577862	1.250322717049
Cl	1.442866349740	-1.505377945569	-0.476876499862
H	-0.540670697375	0.243029992044	-1.630349308535
H	-1.268137435022	-1.340046479579	-1.222154084030
Cl	-2.430491586986	0.457366452162	-0.211049247501

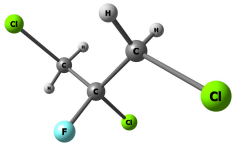
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
63.9815	0.132
129.0983	0.387
156.4585	0.147
210.9318	1.45
276.2816	0.0210
306.2318	0.614
362.0797	0.275
426.9821	1.14
459.9734	1.13
662.5537	11.9
738.8503	7.62
786.9335	5.65
849.0992	3.30
902.9592	0.905
980.8518	10.3
1093.3879	8.16
1157.7421	6.66
1232.9712	3.96
1259.8833	3.68
1303.3325	0.766
1323.5205	0.432
1456.9757	2.29
1463.9464	2.10
3105.5472	0.777
3119.8159	0.605
3173.9282	0.0284
3191.9465	0.0156

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
63.9812	0.132
129.0981	0.387
156.4585	0.147
210.9316	1.45
276.2817	0.0210
306.2317	0.614
362.0796	0.275
426.9820	1.14
459.9734	1.13
662.5534	11.9
738.8502	7.62
786.9333	5.65
849.0991	3.30
902.9597	0.905
980.8521	10.3
1093.3884	8.16
1157.7422	6.66
1232.9720	3.96
1259.8841	3.68
1303.3334	0.766
1323.5212	0.432
1456.9771	2.29
1463.9476	2.10
3105.5473	0.777
3119.8155	0.605
3173.9283	0.0284
3191.9459	0.0156



$\Delta E = 0.91$ kcal mol^{-1}
Population = 0.087



$\Delta E = 0.91$ kcal mol^{-1}
Population = 0.087

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.473784429544	-0.662221123089	-0.327399077418
C	0.049559958668	-0.333858800513	0.127116802134
C	-0.571473493130	0.844923185238	-0.617167048774
Cl	2.608433956507	0.707335799036	-0.028687377082
H	1.840006422844	-1.513874812350	0.243097194858
H	1.496657787612	-0.887690890956	-1.392208689252
F	0.042558521869	-0.100611115838	1.455839346331
Cl	-0.909818975839	-1.851104586656	-0.183441019187
H	0.061933592720	1.719918066040	-0.471443909275
H	-0.651908818213	0.616205441340	-1.679217559602
Cl	-2.201848382582	1.264521837749	-0.012341662732

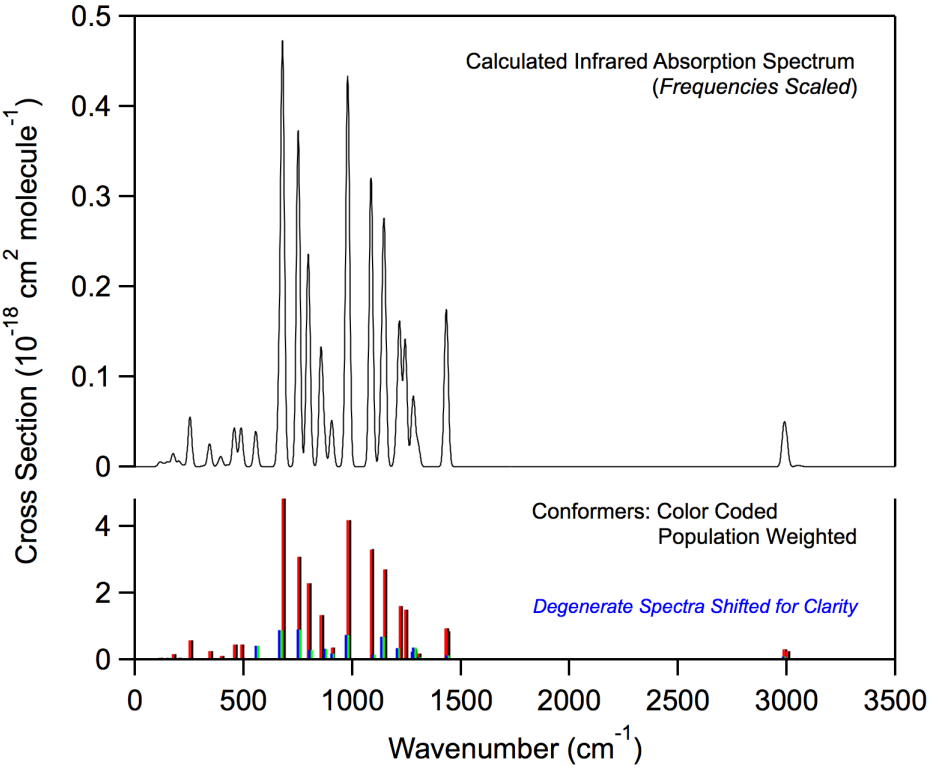
Atom	X	Y	Z
C	0.572317054588	0.853240805231	-0.606616688563
C	-0.050531070577	-0.332236565084	0.125417060598
C	-1.473436904511	-0.656770965405	-0.335926383111
Cl	2.200929206314	1.267727258430	0.006426603026
H	0.655732875685	0.634007495631	-1.670435910003
H	-0.061667391138	1.726789925507	-0.454855489807
F	-0.047230528256	-0.110844281598	1.456180671399
Cl	0.909991633210	-1.846490699593	-0.196014630209
H	-1.493342769258	-0.872722289249	-1.402766654411
H	-1.841058980095	-1.513549264353	0.225930947385
Cl	-2.609165125961	0.709872580485	-0.028109526304

Infrared Absorption Spectrum (unscaled frequencies)

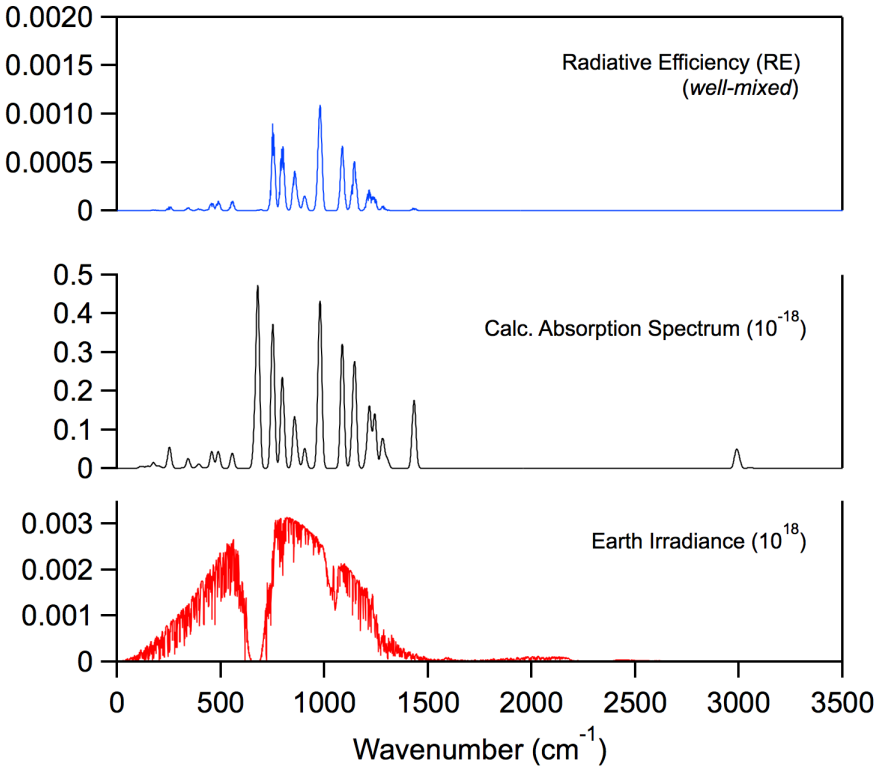
Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
82.2389	0.337
101.9420	0.636
157.2304	0.0739
178.3568	0.181
274.2017	0.0230
306.8169	0.259
349.0516	0.283
394.1910	0.238
531.8386	4.80
647.1443	10.1
737.8649	10.3
793.6185	3.40
864.4400	3.65
900.0106	2.18
971.1728	8.57
1099.9935	1.69
1144.1740	7.84
1218.9868	3.88
1292.7061	2.64
1299.7333	4.25
1322.6033	0.897
1460.1660	1.51
1461.6521	0.962
3101.1302	1.09
3112.6501	0.691
3167.2903	0.0495
3182.1482	0.0181

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
82.2370	0.337
101.9431	0.636
157.2325	0.0739
178.3559	0.181
274.2023	0.0230
306.8175	0.259
349.0514	0.283
394.1909	0.238
531.8396	4.80
647.1446	10.1
737.8651	10.3
793.6185	3.40
864.4396	3.65
900.0117	2.18
971.1741	8.57
1099.9919	1.69
1144.1754	7.84
1218.9876	3.88
1292.7060	2.64
1299.7330	4.25
1322.6039	0.897
1460.1674	1.51
1461.6527	0.962
3101.1302	1.09
3112.6496	0.691
3167.2908	0.0495
3182.1477	0.0181

Infrared Spectrum

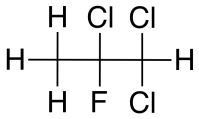


Radiative Efficiency



HCFC-251bb

Molecular Formula:	$CH_3CClFCHCl_2$
Name:	1,1,2-Trichloro-2-fluoropropane
CAS number:	3175-24-4
Molecular Weight:	165.42



Global Atmospheric Lifetime (years): 1.02
- Tropospheric Atmospheric Lifetime (years): 1.07
- Stratospheric Atmospheric Lifetime (years): 20.9

Ozone Depletion Potential (ODP): 0.023

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.147	0.109
Global Warming Potential (GWP_H):		
GWP_{20}	204	152
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: 0.979

$O(^1D)$ 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: 0.006

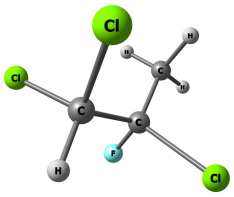
UV Photolysis

UV Spectrum: *No Recommendation*

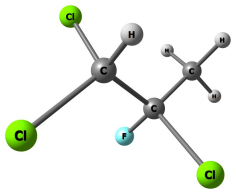
τ_{hv} = 68 years

Fractional Atmospheric Loss: 0.015

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.777



$\Delta E = 0.97$ kcal mol^{-1}
Population = 0.151

Optimized Coordinates (Angstroms)

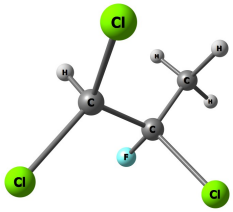
Atom	X	Y	Z
C	-0.586520006712	0.167989203020	0.477176921018
C	0.659534805283	-0.527596506227	-0.123237880844
C	0.685078239613	-0.697917015516	-1.626919414350
Cl	-0.858234155066	1.793203573194	-0.206203600849
Cl	-2.035331018423	-0.866873630448	0.243864851661
H	-0.454377247622	0.281179326545	1.550120420320
F	0.741487312624	-1.741872296310	0.480855117117
Cl	2.113349379300	0.422395789762	0.425567501296
H	1.587893883075	-1.245611332990	-1.901411782153
H	-0.192050773610	-1.270574348566	-1.938466075069
H	0.682839581540	0.270188237535	-2.126878058146

Atom	X	Y	Z
C	-0.576147608246	0.142971366841	-0.509279994004
C	0.669094400264	-0.509401438592	0.133718771686
C	0.939771823779	-1.933289162087	-0.323163387030
Cl	-2.023206393183	-0.900227706364	-0.269674215281
Cl	-0.893069605985	1.769716975608	0.145561586153
H	-0.432529040271	0.240486905812	-1.582112221860
F	0.548232112321	-0.474116960963	1.477908133887
Cl	2.102570891685	0.522475385551	-0.329304578180
H	1.884694395981	-2.264383949884	0.110197649072
H	0.135690565650	-2.586628614611	0.018931366761
H	1.011772458005	-1.984529801312	-1.411203111204

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
75.4610	0.123
166.3624	0.0590
221.8204	0.257
229.8481	0.293
241.4224	0.345
290.6811	0.108
334.4623	0.210
380.8163	0.127
411.0127	1.11
480.2430	1.14
669.6984	14.0
724.5824	9.87
793.3203	13.2
865.3890	5.10
971.9125	3.90
1089.3807	10.0
1165.6354	12.1
1214.7839	4.74
1228.2051	1.39
1297.5853	0.768
1413.3551	3.62
1478.8143	0.379
1483.4792	0.567
3068.6941	0.287
3148.3043	0.510
3158.0455	0.345
3169.6684	0.326

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
63.2448	0.131
174.4960	0.180
209.6769	0.0495
224.6818	0.0266
264.5594	0.0357
294.0337	0.245
324.1841	0.0822
366.6655	0.172
397.6910	0.361
529.7503	3.94
687.2471	20.4
739.6707	0.566
771.8811	14.2
860.2800	5.02
973.4881	3.45
1095.5765	9.04
1146.7011	6.34
1224.0184	2.43
1226.6373	8.62
1297.6751	1.23
1411.6163	2.11
1476.3398	0.291
1485.1722	0.734
3068.7562	0.310
3153.0369	0.743
3157.3984	0.358
3159.5323	0.489



$\Delta E = 1.41$ kcal mol^{-1}
Population = 0.071

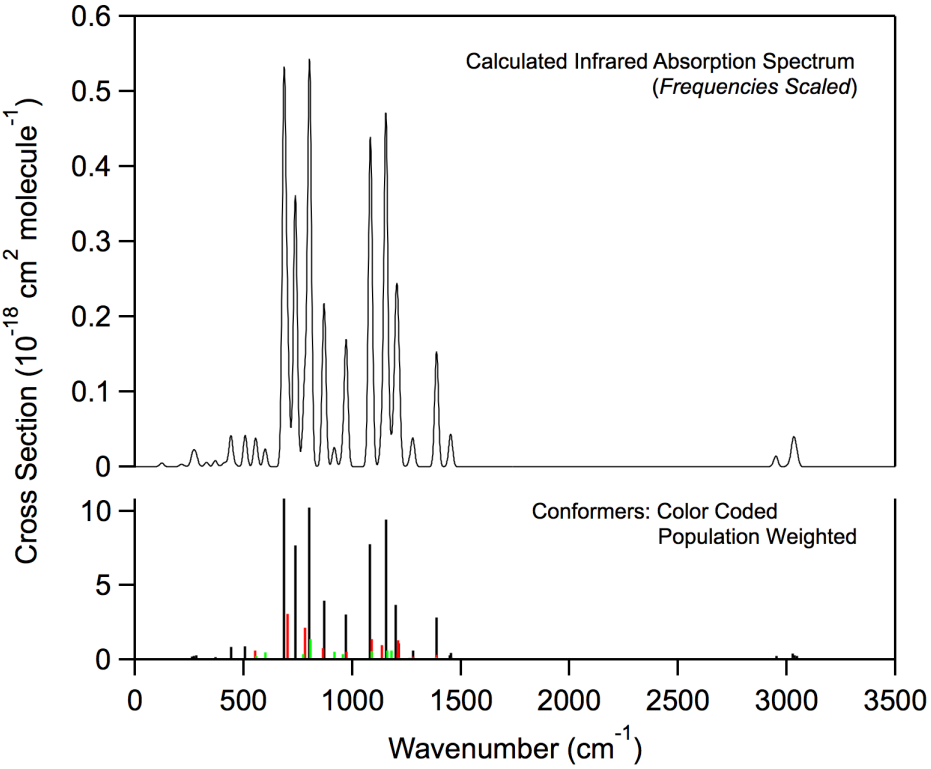
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-0.670668929511	0.105092277038	-0.566997346920
C	0.861609296880	0.039006208457	-0.364083179637
C	1.584107584149	1.293437740198	-0.826580556257
Cl	-1.468236499583	-1.438543082913	-0.170618702784
Cl	-1.412931425577	1.469343284698	0.315496516547
H	-0.852977387182	0.281191735368	-1.626414065301
F	1.288322264950	-1.012939322254	-1.116430449324
Cl	1.278813939040	-0.311058054489	1.357536810278
H	2.658993003766	1.117443555644	-0.759750074719
H	1.323428454333	1.499689518394	-1.869534068947
H	1.318401698736	2.151155139860	-0.210444882936

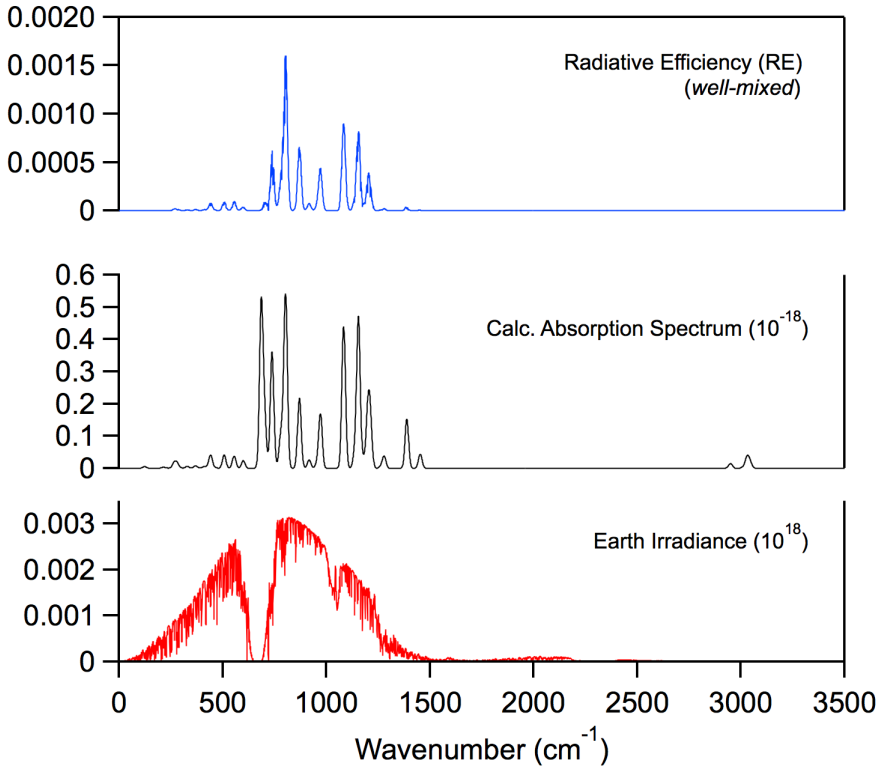
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
72.6966	0.0663
168.0493	0.0226
190.4451	0.191
232.1124	0.00251
260.0950	0.129
291.7073	0.118
352.4722	0.0611
378.0076	0.0737
432.4558	0.755
534.8898	3.41
577.6333	7.06
762.4023	4.91
798.0067	19.2
914.1802	7.64
955.6925	5.03
1095.9306	7.85
1172.1059	8.77
1192.8590	8.29
1232.8473	1.62
1282.3421	1.92
1410.4558	2.04
1479.8846	0.461
1482.4691	0.494
3056.4088	1.05
3126.8213	0.555
3137.6009	0.857
3173.7526	0.318

Infrared Spectrum

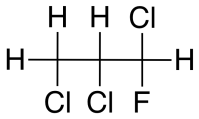


Radiative Efficiency



HCFC-251da

Molecular Formula:	$CH_2ClCHClCHFCl$
Name:	1,2,3-Trichloro-1-fluoropropane
CAS number:	339202-89-0
Molecular Weight:	165.42



Global Atmospheric Lifetime (years):	0.693
Tropospheric Atmospheric Lifetime (years):	0.719
Stratospheric Atmospheric Lifetime (years):	20
Ozone Depletion Potential (ODP):	0.016

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.122	0.082
Global Warming Potential (GWP_H):		
GWP_{20}	115	77
GWP_{100}	31	21
Global Temperature Potentials (GTP_H)		
GTP_{20}		24
GTP_{50}		4
GTP_{100}		3

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 8.15 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 5.20 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 0.699$ years

$\tau^{OH}_{Trop} = 0.719$ years

$\tau^{OH}_{Strat} = 25.1$ years

Fractional Atmospheric Loss: 0.992

$O(^1D)$ Reactivity

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

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

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

Fractional Atmospheric Loss: 0.003

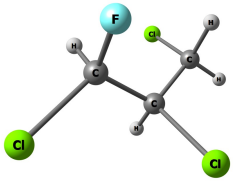
UV Photolysis

UV Spectrum: *No Recommendation*

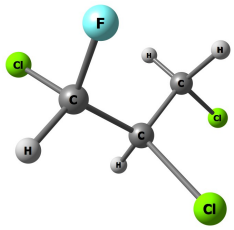
$\tau_{hv} = 150$ years

Fractional Atmospheric Loss: 0.005

Molecular Structure and Infrared Spectrum (9 conformers)



E = 0
Population = 0.303



$\Delta E = 0.18$ kcal mol^{-1}
Population = 0.222

Optimized Coordinates (Angstroms)

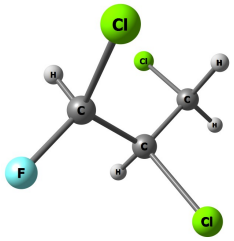
Atom	X	Y	Z
C	-1.542601858971	0.701147668375	0.130490772566
C	-0.138430391316	0.450031952640	-0.416440539757
C	0.512303583936	-0.773885237065	0.225868371445
Cl	-2.671844995348	-0.626798143235	-0.358103928292
H	-1.535125069969	0.740268271821	1.218786308181
H	-1.948298502178	1.625077727699	-0.275508851742
Cl	0.826822060778	1.938544026299	-0.082997970994
H	-0.159625708242	0.318724025974	-1.498033101422
H	-0.102458513164	-1.658216760297	0.045641979439
Cl	2.120202278389	-1.135672616990	-0.488579352265
F	0.641681116084	-0.587608915220	1.559917312841

Atom	X	Y	Z
C	-0.741583276021	-0.790635647470	0.507803515581
C	-0.093812973381	0.224215857181	-0.424824001368
C	1.379692317965	0.460168496403	-0.087613459992
Cl	-2.381318137434	-1.264384301585	-0.053117711871
H	-0.140314116077	-1.700100872016	0.529656812518
H	-0.838503122153	-0.388922621328	1.514670557850
Cl	-0.926883370355	1.829202766261	-0.316101040436
H	-0.175112186308	-0.090090280909	-1.464676010566
H	1.796404010716	1.293890001528	-0.653085819151
F	1.534146443241	0.685037539274	1.235212675927
Cl	2.358589409807	-0.994560937339	-0.549054518491

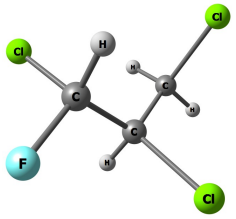
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
63.9274	0.281
103.0519	0.580
165.9828	0.285
175.9205	0.153
223.9579	0.101
300.2463	0.146
370.1028	1.40
418.6791	2.32
607.9062	4.37
695.1851	8.44
729.4532	5.54
814.9656	10.1
908.8833	6.19
979.5430	3.65
1057.2557	2.02
1131.7292	8.47
1180.6941	6.14
1227.4301	2.60
1282.6337	2.18
1303.8698	1.11
1354.1116	0.961
1378.5329	2.86
1475.6552	0.910
3105.9068	0.727
3114.2526	0.331
3130.3703	0.454
3185.3251	0.00609

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
71.7517	0.0256
78.9438	0.519
161.8139	0.363
180.8035	0.763
253.5567	0.0552
269.9634	0.198
388.0932	0.324
391.0535	1.46
614.8359	5.67
675.8488	10.0
758.8919	15.9
806.4125	2.53
919.1800	3.01
939.2042	1.60
1071.4403	4.29
1141.4346	12.5
1182.8070	1.74
1257.8711	4.30
1265.6609	1.11
1288.5190	1.43
1344.2744	4.11
1392.6584	1.30
1468.6914	1.08
3101.9888	0.805
3123.9785	0.875
3133.9444	0.231
3172.1994	0.0159



$\Delta E = 0.33$ kcal mol^{-1}
Population = 0.174



$\Delta E = 0.55$ kcal mol^{-1}
Population = 0.119

Optimized Coordinates (Angstroms)

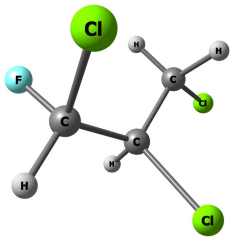
Atom	X	Y	Z
C	-1.257540210173	0.724686061071	0.515913849533
C	-0.040711003734	0.679139214438	-0.397091763408
C	0.533670715266	-0.716210604507	-0.641082481350
Cl	-2.644257561277	-0.176047566907	-0.221724829007
H	-1.048379947754	0.267487362226	1.481668029861
H	-1.586216116048	1.753096824993	0.650887333361
Cl	1.212240837403	1.782462214480	0.287587739766
H	-0.290493590141	1.084858666190	-1.380322566943
H	-0.230564893281	-1.360860492095	-1.079861361701
F	1.585983546814	-0.629336901106	-1.482444129965
Cl	1.056347222925	-1.537704778781	0.874385179853

Atom	X	Y	Z
C	-0.948943668107	-0.772558999800	-0.928725911463
C	-0.106107561332	0.458140799596	-0.629193996359
C	0.989736362711	0.266851987041	0.419663615829
Cl	-1.730154928895	-1.484752042431	0.531434823203
H	-1.748084251484	-0.512749489846	-1.621172169034
H	-0.321735734854	-1.551947559758	-1.360833343939
Cl	-1.148215594109	1.837538358780	-0.094437911094
H	0.365847592969	0.784108683591	-1.559694923336
H	0.596077660759	-0.055605439806	1.383397828160
Cl	2.131863964743	-1.029233260359	-0.130812449104
F	1.691433157601	1.408091962992	0.564307437135

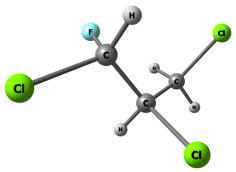
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
58.2931	0.252
109.9743	0.380
167.1855	0.445
186.3852	0.287
217.0280	0.388
300.9467	0.0422
377.5595	0.623
489.9925	1.15
555.0787	4.75
651.7598	7.18
725.9247	8.95
798.8588	10.6
889.0657	1.53
1029.6377	2.20
1094.9390	1.37
1129.0242	14.6
1178.3497	3.67
1226.6375	3.08
1291.2487	3.51
1307.9539	2.40
1339.6326	2.23
1384.0354	2.00
1476.8956	1.64
3095.5595	0.120
3108.7889	0.847
3115.3402	0.650
3183.6838	0.0112

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
59.4944	0.192
90.9345	0.115
153.0612	0.0333
205.0565	0.898
270.9418	0.297
341.1468	0.0300
376.8894	1.31
412.1021	1.26
573.1843	2.34
668.5233	7.30
710.5105	12.4
776.8881	7.33
912.3539	4.77
999.1438	1.33
1089.9862	1.42
1140.2106	18.1
1200.4891	1.42
1234.6235	4.29
1252.3533	0.0308
1302.0226	3.60
1330.9629	2.74
1399.5505	1.02
1463.4640	2.28
3091.0738	0.238
3106.5869	0.844
3135.9735	0.548
3168.7383	0.0840



ΔE = 1.10 kcal mol^{-1}
Population = 0.047



ΔE = 1.11 kcal mol^{-1}
Population = 0.047

Optimized Coordinates (Angstroms)

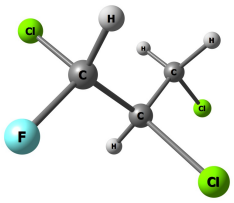
Atom	X	Y	Z
C	-0.872465634686	-0.827700777234	0.352332854019
C	-0.140479010561	0.095519753672	-0.610526403359
C	1.362446727244	-0.196615841528	-0.680503234244
Cl	-2.649294581310	-0.801989406907	0.078361774912
H	-0.536712673120	-1.851840987037	0.183908953564
H	-0.695799864410	-0.546164434116	1.388334767782
Cl	-0.399113037021	1.832692185810	-0.224317054456
H	-0.522505357344	-0.048904380865	-1.623819122874
H	1.880335491251	0.527101767726	-1.311017578818
Cl	2.172887744733	-0.136299389562	0.926284471606
F	1.518506195224	-1.443683489959	-1.196896428131

Atom	X	Y	Z
C	-1.457711533202	-0.310006533912	-0.941556884496
C	-0.067404865606	0.261138579963	-0.684746802120
C	0.789466670145	-0.654134637124	0.196525352222
Cl	-2.400754407236	-0.623612415182	0.561696530343
H	-2.041075720809	0.382716463762	-1.546082370328
H	-1.360376679807	-1.265905348496	-1.455975293125
Cl	-0.152338722759	1.904396210826	0.040426748314
H	0.425934630861	0.376307988739	-1.653383012630
H	0.466698781967	-0.645823482806	1.237406062104
F	0.699671911769	-1.916963897464	-0.298466876567
Cl	2.516359934678	-0.159395928304	0.177306546283

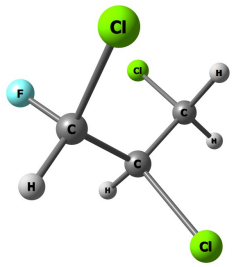
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
73.3414	0.0261
81.9148	0.406
143.5333	0.298
193.5561	0.724
222.7838	0.253
320.5298	0.301
388.8340	0.921
433.4739	0.506
560.1242	7.14
687.6037	4.65
724.5305	5.49
809.9939	6.79
945.6085	4.13
977.9610	5.47
1087.5444	11.5
1109.4008	9.02
1179.5225	0.390
1243.2008	0.314
1277.6377	2.32
1300.0820	9.44
1354.7146	2.54
1368.4121	0.381
1466.7523	0.937
3095.6408	0.704
3100.9309	0.645
3119.3840	1.02
3174.4014	0.0522

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
61.3799	0.152
83.7941	0.208
146.6137	0.0418
186.5817	0.292
300.1798	0.998
323.7867	0.852
371.7024	0.928
444.1934	0.491
529.6890	5.22
680.4400	2.41
730.9334	3.46
822.0030	15.8
921.5177	4.16
986.2056	3.63
1085.2552	9.86
1109.8481	10.0
1194.4960	0.672
1239.3331	1.20
1246.2932	1.83
1307.6022	8.14
1337.7321	0.696
1383.3165	1.20
1461.1114	1.33
3088.1803	0.348
3104.8193	1.05
3134.7358	0.624
3168.8142	0.0384



ΔE = 1.30 kcal mol^{-1}
Population = 0.034



ΔE = 1.67 kcal mol^{-1}
Population = 0.018

Optimized Coordinates (Angstroms)

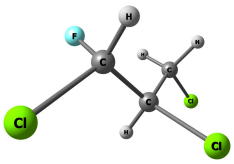
Atom	X	Y	Z
C	-0.909438368134	-0.873867267120	0.447952545003
C	-0.090369296373	0.226951152496	-0.213238774627
C	1.361777270677	0.269327243581	0.273736490222
Cl	-2.545016533959	-1.022962529127	-0.281724974148
H	-0.417976855497	-1.835864872766	0.309358359778
H	-1.046012794868	-0.677790541615	1.512027974334
Cl	-0.806053768318	1.849669941414	0.145463709814
H	-0.094061302390	0.120178739793	-1.298739520482
H	1.437158150870	0.400644371492	1.355240832042
Cl	2.197325608583	-1.293716274935	-0.110331338364
F	2.028443889409	1.258344036788	-0.350723303572

Atom	X	Y	Z
C	-0.870884304506	0.980787072663	0.587210492174
C	0.127389500191	0.687622321161	-0.525811498780
C	0.571533679947	-0.770239888406	-0.716599831146
Cl	-2.492220107945	0.274211281457	0.231150112762
H	-0.534093686087	0.570043741643	1.537450672027
H	-1.009734619088	2.056484213108	0.676919976540
Cl	1.602032804442	1.692930665937	-0.220463251801
H	-0.270824955284	1.016426693114	-1.488151550382
H	1.449558163104	-0.818332101362	-1.362646646647
Cl	1.055136594193	-1.566344948322	0.825842026994
F	-0.435663068967	-1.476469050995	-1.277335501741

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
64.6249	0.0765
77.8364	0.430
164.1662	0.632
181.1093	0.226
267.5386	0.245
332.7864	0.0217
350.8358	1.02
405.6610	0.937
507.0191	2.38
679.5070	11.9
753.2713	13.1
767.4017	7.19
936.1224	1.91
1055.2777	2.02
1064.5614	1.26
1140.1170	15.6
1178.5540	0.572
1211.0218	5.26
1277.7348	2.10
1297.1863	1.17
1343.7708	2.45
1398.8188	2.54
1469.3656	0.790
3096.0247	1.03
3102.0964	1.18
3123.9064	0.420
3164.9359	0.0983

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
43.9186	0.0547
114.1386	0.368
163.6058	0.134
200.2166	0.390
257.8969	0.885
294.0752	1.91
351.7589	0.301
430.0477	0.358
523.9243	2.84
718.2618	9.23
744.8834	12.1
814.7986	3.77
874.5690	4.81
988.0973	1.75
1112.0668	15.0
1125.4695	3.77
1173.7224	2.32
1215.7520	0.533
1291.4061	4.81
1304.8477	2.23
1374.1145	1.62
1377.6260	1.30
1475.3412	1.70
3100.7128	0.226
3111.9911	1.08
3113.9538	0.816
3180.0075	0.0158



$\Delta E = 1.67$ kcal mol^{-1}
Population = 0.018

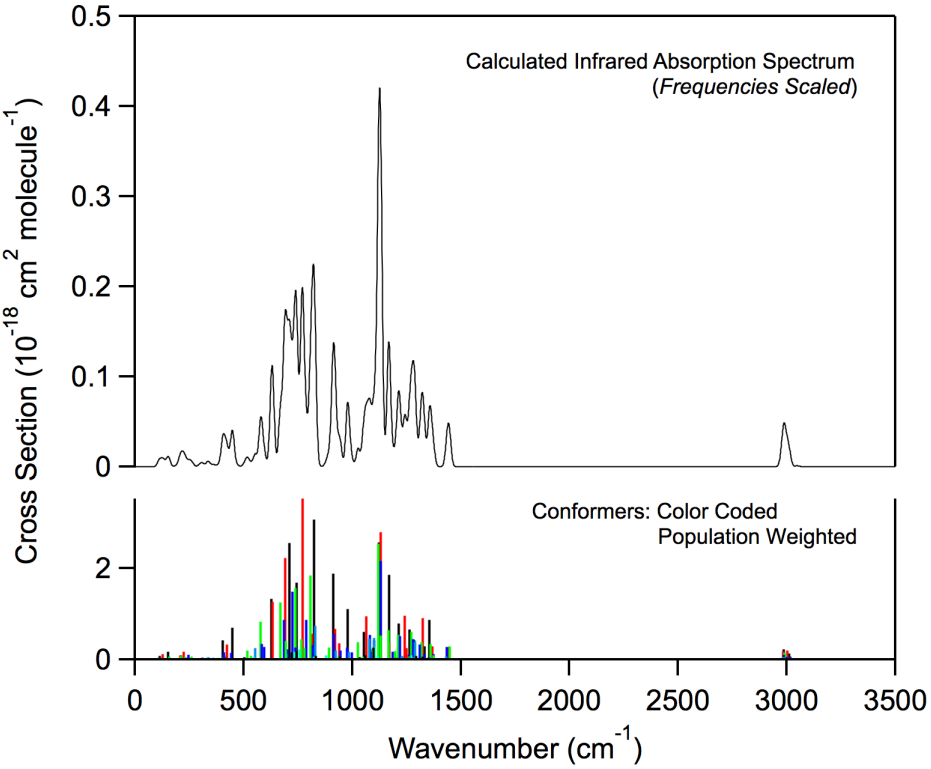
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.301889664919	-0.824811849758	0.364797252063
C	-0.123997382682	-0.004165682082	-0.154506239865
C	1.198428092835	-0.575478408679	0.378144660290
Cl	-2.845985465746	-0.357822743932	-0.425374618352
H	-1.134431576566	-1.876839828296	0.137905286494
H	-1.433485381872	-0.693993657774	1.439461450255
Cl	-0.258700648645	1.714880716108	0.359736405015
H	-0.108155746715	-0.009170053601	-1.244900107549
H	1.326372518222	-0.387495517639	1.446104925036
F	1.217007103613	-1.916977176711	0.152331575615
Cl	2.614578152476	0.154621202363	-0.447451589001

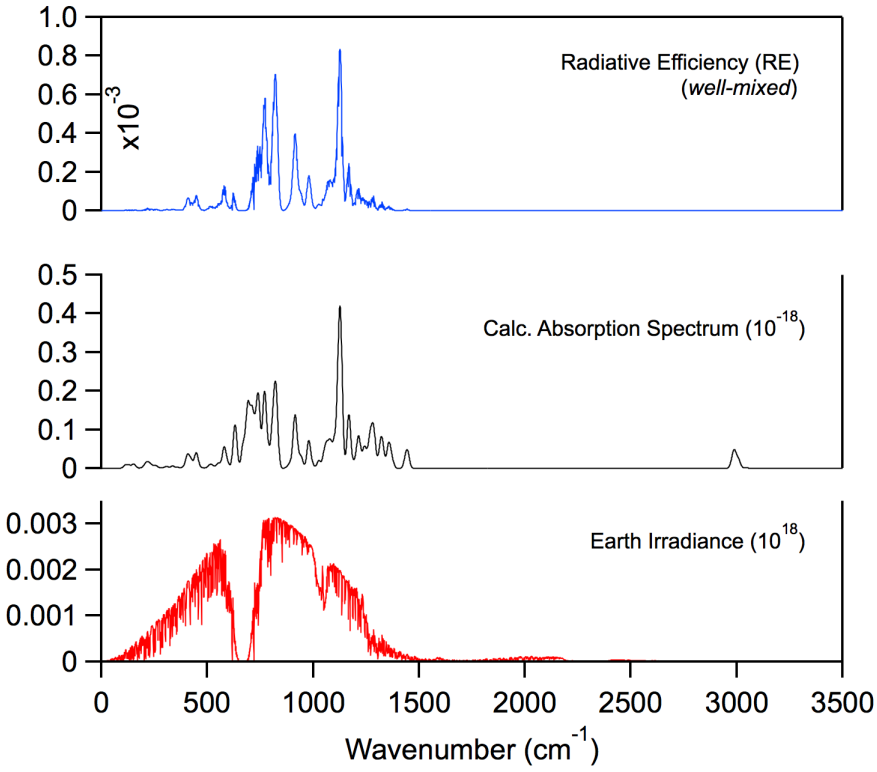
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
57.8058	0.0352
86.2615	0.467
145.8922	0.434
185.1392	0.272
261.7166	0.285
337.6190	0.280
379.8985	1.05
417.4228	0.986
475.7274	3.15
708.2217	9.09
731.7538	10.0
824.9674	4.03
941.8470	3.96
1036.7668	3.21
1063.0988	4.95
1105.1006	14.6
1174.3833	0.486
1215.5568	2.16
1281.9963	2.33
1312.5485	4.05
1346.5846	3.40
1371.8513	1.85
1469.9118	0.670
3095.7349	0.962
3103.5523	1.06
3123.6188	0.500
3164.9974	0.0861

Infrared Spectrum

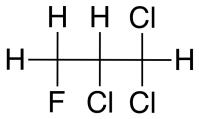


Radiative Efficiency



HCFC-251db

Molecular Formula:	$CH_2FCHClCHCl_2$
Name:	1,1,2-Trichloro-3-fluoropropane
CAS number:	–
Molecular Weight:	165.42



Global Atmospheric Lifetime (years):	0.404
Tropospheric Atmospheric Lifetime (years):	0.416
Stratospheric Atmospheric Lifetime (years):	20
Ozone Depletion Potential (ODP):	0.009

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.113	0.063
Global Warming Potential (GWP_H):		
GWP_{20}	62	35
GWP_{100}	17	9
Global Temperature Potentials (GTP_H)		
GTP_{20}		11
GTP_{50}		2
GTP_{100}		1

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 1.41 \times 10^{-13}$; $k_{SAR}(272\ K) \approx 0.899 \times 10^{-13}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 0.408$ years

$\tau^{OH}_{Trop} = 0.416$ years

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

Fractional Atmospheric Loss: 0.992

$O(^1D)$ Reactivity

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

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

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

Fractional Atmospheric Loss: 0.002

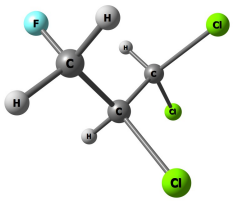
UV Photolysis

UV Spectrum: *No Recommendation*

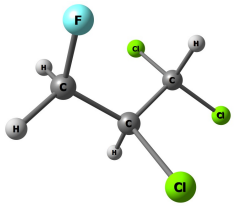
$\tau_{hv} = 68$ years

Fractional Atmospheric Loss: 0.006

Molecular Structure and Infrared Spectrum (7 conformers)



E = 0
Population = 0.395



$\Delta E = 0.31$ kcal mol^{-1}
Population = 0.234

Optimized Coordinates (Angstroms)

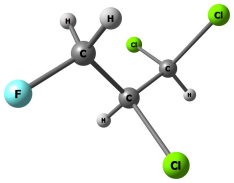
Atom	X	Y	Z
C	-2.009968398612	0.197848634991	-0.127534479355
C	-0.661567410464	-0.457683777995	-0.425573341470
C	0.491781404719	0.544375276450	-0.366248288802
F	-2.186502032321	1.239874642792	-1.016221520700
H	-2.812780654495	-0.532343906890	-0.265043501372
H	-2.037107931162	0.586684347222	0.894217268104
H	-0.672291091340	-0.866286551371	-1.438337289614
Cl	-0.454149170522	-1.853706828239	0.684061363353
H	0.243469760269	1.378565807551	-1.019333711400
Cl	0.732803725401	1.241847828761	1.266029026331
Cl	2.010863798527	-0.166038473273	-0.992010525072

Atom	X	Y	Z
C	-1.430451689319	1.283139558347	-0.462234008992
C	-0.602370602317	0.007218335922	-0.581567676547
C	0.638525091170	0.017961671125	0.319155376073
F	-1.723460288486	1.526315266269	0.858431700995
H	-0.865963802597	2.131340898161	-0.861875407143
H	-2.362666879470	1.165388738702	-1.023073412395
H	-0.306358711263	-0.147239474530	-1.620564816560
Cl	-1.644365593220	-1.400707308154	-0.120546357055
H	0.359848194596	0.115217622246	1.364635873947
Cl	1.609383998718	-1.472659528106	0.151104457966
Cl	1.665049282188	1.447870220017	-0.077306730289

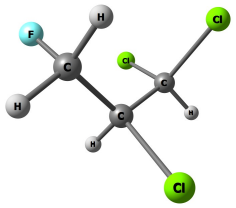
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
61.8915	0.124
116.7694	0.514
164.0667	0.0302
184.9408	0.373
209.5456	0.308
285.2658	0.552
363.9203	0.109
455.4113	3.57
530.9339	2.59
640.5019	2.67
762.5535	17.6
808.8429	5.01
937.1844	1.89
1065.5589	12.2
1087.2813	0.360
1096.8191	5.52
1219.8568	0.538
1234.6283	2.32
1257.3261	1.48
1289.6343	2.21
1348.6490	1.19
1414.7998	1.34
1508.4393	0.782
3061.9966	2.28
3097.6221	0.701
3123.5627	1.93
3145.5662	0.270

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
53.1769	0.171
91.4919	0.297
170.1446	0.0705
205.6596	0.489
258.8245	0.501
314.6535	1.13
336.3147	0.482
370.9349	0.387
582.4868	5.94
683.9843	12.3
749.3782	7.45
797.4024	5.77
913.1932	1.24
1002.2120	1.72
1102.4075	4.49
1122.4549	7.48
1203.4446	1.53
1226.2723	3.07
1258.0777	0.350
1277.4384	1.75
1349.0698	1.26
1422.9620	1.43
1501.4230	1.50
3055.5066	2.90
3108.2075	2.20
3113.4908	0.539
3169.7062	0.216



$\Delta E = 0.36$ kcal mol^{-1}
Population = 0.215



$\Delta E = 1.07$ kcal mol^{-1}
Population = 0.065

Optimized Coordinates (Angstroms)

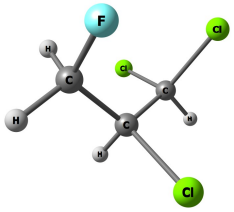
Atom	X	Y	Z
C	-0.963981521269	1.032833943319	0.832173461457
C	-0.581504550768	0.292010088630	-0.443044801881
C	0.850648573539	-0.241600888617	-0.485817419212
F	-2.175950246165	1.645810199767	0.638866083473
H	-1.037495432740	0.342694958787	1.676703481034
H	-0.207071604543	1.796063277228	1.047536915726
H	-0.707692743358	0.963095459025	-1.294656917219
Cl	-1.725741307746	-1.078424926041	-0.737885669286
H	0.998211116920	-0.875564624155	-1.355434890788
Cl	1.999021927543	1.137674138776	-0.664849715195
Cl	1.275301788586	-1.232744626718	0.945583471890

Atom	X	Y	Z
C	-0.649323684810	1.441898984712	0.759394093618
C	-0.630113344674	0.533664486123	-0.470332242211
C	0.419553944834	-0.584335218835	-0.502257436498
F	0.515702027164	2.165672906495	0.823401605591
H	-1.495502555465	2.130702322533	0.672674990595
H	-0.759236002221	0.847499737917	1.671040921579
H	-0.491698330440	1.132015626237	-1.372536128943
Cl	-2.272683135702	-0.215221711331	-0.610812943580
H	0.200496105147	-1.277148948933	-1.310047928910
Cl	2.045090370670	0.095664417326	-0.853568472223
Cl	0.448847605498	-1.563520602244	0.998823540982

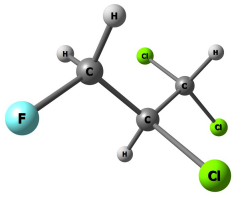
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
71.5894	0.118
93.2546	0.494
157.7297	0.142
188.8055	0.834
243.6865	0.146
254.0811	0.332
336.8786	0.0336
422.6142	1.78
589.1311	3.76
677.1182	11.1
693.8482	5.62
750.3250	12.4
982.0573	2.60
1011.4464	2.98
1109.7538	12.4
1124.2505	2.00
1221.1811	2.44
1245.1024	1.99
1258.7331	0.357
1294.3061	1.81
1331.6590	1.47
1431.1560	0.989
1503.6700	0.626
3047.3361	2.52
3103.3557	0.356
3117.6965	1.58
3162.3474	0.182

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
44.0040	0.0538
119.5696	0.452
164.5894	0.108
202.7118	0.431
239.7540	0.0623
278.9307	2.11
327.3935	0.830
386.7137	0.457
527.6120	2.07
698.6055	3.90
739.7187	22.5
816.8708	4.63
892.7006	1.45
1050.5301	3.55
1101.4895	11.5
1121.1126	0.889
1211.7778	1.43
1239.9860	2.63
1256.6674	0.483
1298.6697	0.485
1361.2826	0.798
1431.1644	1.08
1507.8881	0.756
3057.0490	2.55
3103.7178	1.20
3119.6196	1.36
3156.2854	0.223



ΔE = 1.47 kcal mol^{-1}
Population = 0.033



ΔE = 1.52 kcal mol^{-1}
Population = 0.030

Optimized Coordinates (Angstroms)

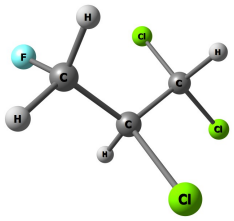
Atom	X	Y	Z
C	-0.794710944370	1.416009447284	0.738237185121
C	-0.571074303335	0.604199117512	-0.533927238029
C	0.671360122616	-0.292842557869	-0.587866234723
F	-1.147220928266	0.625391893601	1.797082766829
H	0.127567960299	1.956929483670	0.982107482713
H	-1.597606938333	2.138331483412	0.554694825198
H	-0.475730547042	1.307609486223	-1.364669774453
Cl	-2.029455563034	-0.396702160114	-0.904913746835
H	0.684153472375	-0.857167183683	-1.516361018929
Cl	2.141806190236	0.758978287296	-0.628202135867
Cl	0.786195478856	-1.482058297333	0.735395888974

Atom	X	Y	Z
C	-1.482532234119	1.188486491841	0.210354297240
C	-0.597396459161	0.025218761179	-0.242738315102
C	0.799198857802	0.037360892880	0.384038693665
F	-2.710606755944	1.071058555259	-0.385438256796
H	-1.606289989985	1.175459330673	1.299779519296
H	-1.032664648340	2.137472057832	-0.094568217389
H	-0.516989152883	0.019573851532	-1.330698593178
Cl	-1.414051926853	-1.521854792014	0.216583755382
H	0.755001980353	-0.103676596749	1.461770029322
Cl	1.832230291480	-1.267151996761	-0.270704433092
Cl	1.601455037650	1.631079444327	0.108921520651

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
58.2663	0.246
117.8976	0.258
170.0830	0.294
184.2205	0.144
230.2093	0.707
279.9448	0.350
321.3722	0.477
416.7282	1.54
637.6976	5.87
680.4943	10.5
723.6977	11.5
808.5594	3.39
877.9735	0.115
1012.3203	3.42
1078.8428	6.96
1147.2069	5.75
1213.1137	1.86
1249.4817	2.18
1262.4889	1.36
1306.8219	1.19
1361.2837	1.27
1430.0873	1.21
1500.2615	1.10
3038.1784	3.04
3088.0501	2.95
3094.8310	0.524
3156.2242	0.212

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
54.6497	0.0524
104.9325	0.912
160.3228	0.265
209.3094	0.370
245.3032	0.216
300.5674	0.317
322.6887	0.404
376.9066	0.539
500.1096	3.02
686.8755	12.9
735.4549	4.13
758.0828	14.7
994.2503	1.86
1065.1461	0.168
1078.1702	0.871
1118.4181	12.9
1203.5312	2.39
1228.7262	3.01
1250.5254	0.100
1312.6303	1.93
1338.5530	1.25
1427.7374	1.61
1504.2487	0.258
3041.0470	3.33
3103.3453	1.37
3120.0862	0.984
3148.5005	0.271



$\Delta E = 1.91$ kcal mol^{-1}
Population = 0.016

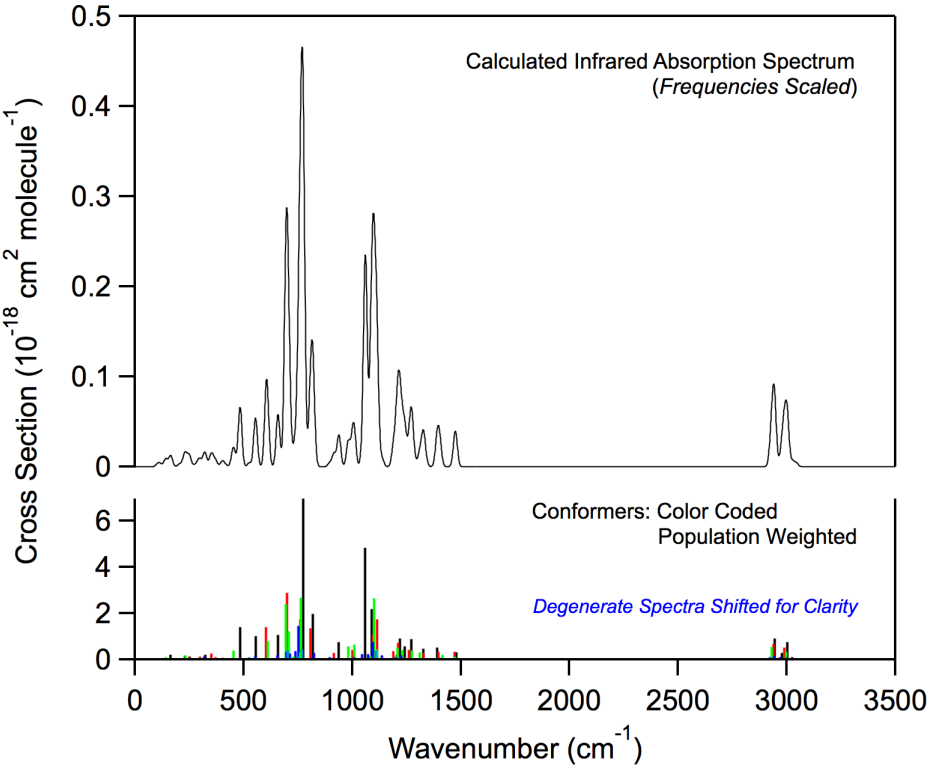
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.469073689374	1.341434677823	0.069508558522
C	-0.738110318960	0.052717820929	-0.335857489792
C	0.570831876096	-0.216865340192	0.413645983526
F	-0.896436098558	2.424939516763	-0.546284994653
H	-2.511350353036	1.266334646832	-0.253229600019
H	-1.440896977187	1.480717976498	1.156623982059
H	-0.560154084808	0.055129638285	-1.411888677494
Cl	-1.869931461685	-1.318253010778	0.015841173000
H	0.384248616367	-0.405357649536	1.468889318080
Cl	1.402409793365	-1.668853630021	-0.231609430572
Cl	1.672813697780	1.197601353397	0.328823177343

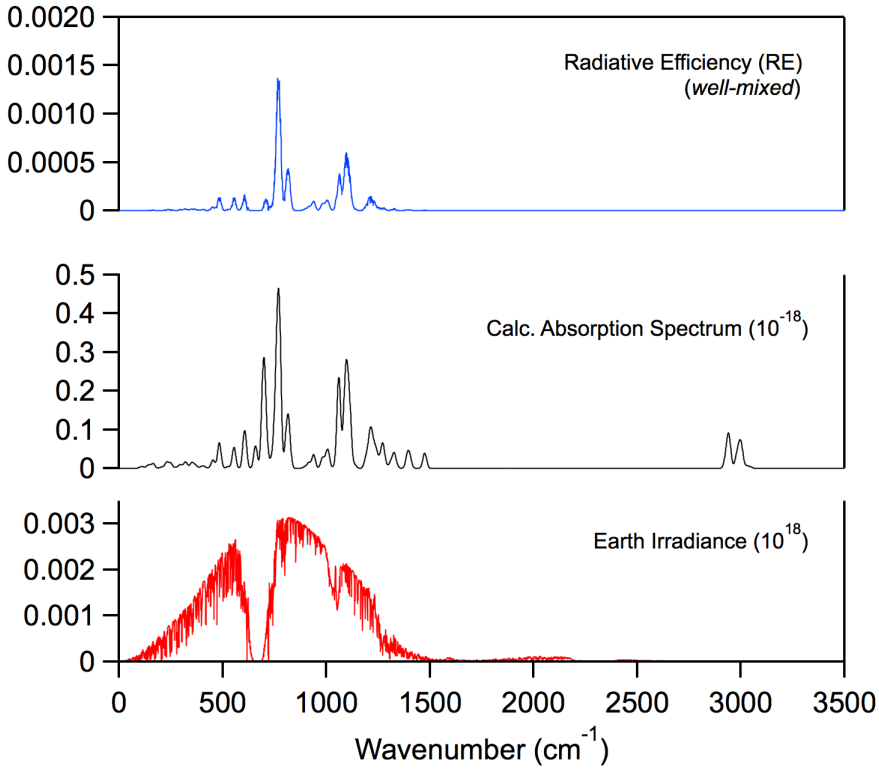
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
46.2134	0.0173
122.7113	1.09
164.3095	0.0736
205.0348	0.293
245.1172	0.168
304.8437	0.488
323.9231	0.733
378.1507	0.0813
432.7261	3.95
716.7390	8.75
749.3963	20.3
803.7585	0.558
912.2001	0.941
1073.0792	2.09
1092.0757	9.01
1119.6005	4.41
1197.5046	1.56
1228.7585	3.74
1237.3536	0.500
1297.6634	0.797
1364.8101	0.888
1424.7889	1.85
1505.7499	0.528
3043.0776	2.91
3101.5911	2.55
3122.9108	0.358
3144.7076	0.259

Infrared Spectrum

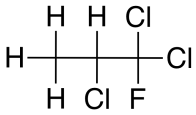


Radiative Efficiency



HCFC-251dc

Molecular Formula:	$CH_3CHClCFCl_2$
Name:	1,1,2-Trichloro-1-fluoropropane
CAS number:	421-41-0
Molecular Weight:	165.42



Global Atmospheric Lifetime (years):	0.515
Tropospheric Atmospheric Lifetime (years):	0.535
Stratospheric Atmospheric Lifetime (years):	20
Ozone Depletion Potential (ODP):	0.012

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.199	0.122
Global Warming Potential (GWP_H):		
GWP_{20}	140	85
GWP_{100}	38	23
Global Temperature Potentials (GTP_H)		
GTP_{20}		26
GTP_{50}		4
GTP_{100}		3

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 1.10 \times 10^{-13}$; $k_{SAR}(272\ K) \approx 0.700 \times 10^{-13}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 0.521$ years
$\tau^{OH}_{Trop} = 0.535$ years
$\tau^{OH}_{Strat} = 20$ years

Fractional Atmospheric Loss: 0.990

O(^{1}D) Reactivity

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

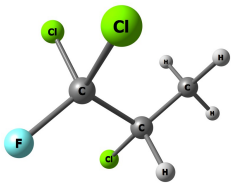
$k_{Est}(T) = 2.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)} = 185$ years
Fractional Atmospheric Loss: 0.002

UV Photolysis

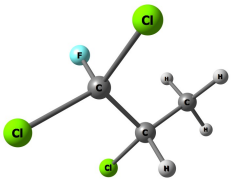
UV Spectrum: *No Recommendation*
$\tau_{hv} = 68$ years
Fractional Atmospheric Loss: 0.008

Papanastasiou et al. (2018)

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.582



$\Delta E = 0.49$ kcal mol^{-1}
Population = 0.255

Optimized Coordinates (Angstroms)

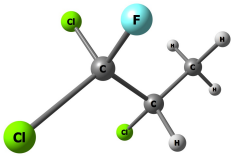
Atom	X	Y	Z
C	-0.756335974046	1.608157775944	1.117717283252
C	-0.706674663212	0.804704237373	-0.171264935957
C	0.478785075374	-0.170522226553	-0.301834385824
H	0.161555615004	2.189021700769	1.236868345314
H	-1.602986980250	2.295916106731	1.078488099645
H	-0.878051794911	0.951776674658	1.981006249045
H	-0.640414929321	1.456774377200	-1.044428065701
Cl	-2.246737204328	-0.123348610645	-0.389877066156
Cl	2.010645418611	0.791973038080	-0.377543715171
Cl	0.582472052232	-1.341981182332	1.048876852990
F	0.388744384846	-0.855578891224	-1.444038661438

Atom	X	Y	Z
C	-0.978337187551	2.012052374531	-0.115027711628
C	-0.741400283052	0.555767632168	-0.503271089168
C	0.474705780236	-0.066656553831	0.210483467457
H	-1.884783715383	2.370014178407	-0.605633336706
H	-1.104814973622	2.103330868845	0.965518690731
H	-0.138339635114	2.634027948270	-0.430648065599
H	-0.594314745978	0.437335343428	-1.576171004612
Cl	-2.219665897636	-0.407825144302	-0.089876914970
Cl	0.725240507550	-1.784285230272	-0.232434038640
Cl	1.964914573818	0.852594109754	-0.252578704845
F	0.336741576731	0.016068473005	1.536539707978

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
79.3822	0.159
172.3851	0.0938
209.3404	0.111
232.7035	0.0372
246.5457	0.0560
288.8339	0.173
344.7148	0.0287
380.9600	0.133
421.9686	0.822
514.1836	0.894
581.7430	4.81
688.9461	14.4
799.6605	30.0
934.0979	7.54
1018.1008	6.13
1105.2276	3.28
1132.2294	5.22
1176.4809	11.3
1261.9105	3.18
1338.0359	1.93
1414.5900	1.59
1487.8349	1.22
1491.9222	0.611
3063.9043	0.783
3102.9861	0.472
3141.1094	1.07
3153.1414	0.739

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
68.2807	0.168
170.7007	0.104
223.1392	0.0205
227.8474	0.00641
260.7599	0.0328
299.5790	0.193
323.6826	0.408
376.9411	0.0921
409.6431	1.85
450.0255	0.532
680.0030	12.0
694.1826	3.85
811.1502	29.7
938.4140	12.1
992.4618	6.36
1065.3156	4.50
1105.7964	2.07
1201.2144	12.4
1260.1696	1.86
1338.6225	0.545
1410.4813	0.937
1488.9450	1.08
1492.3757	0.819
3066.3025	0.954
3128.3714	0.240
3147.4462	1.08
3153.7296	0.742



$\Delta E = 0.75$ kcal mol^{-1}
Population = 0.163

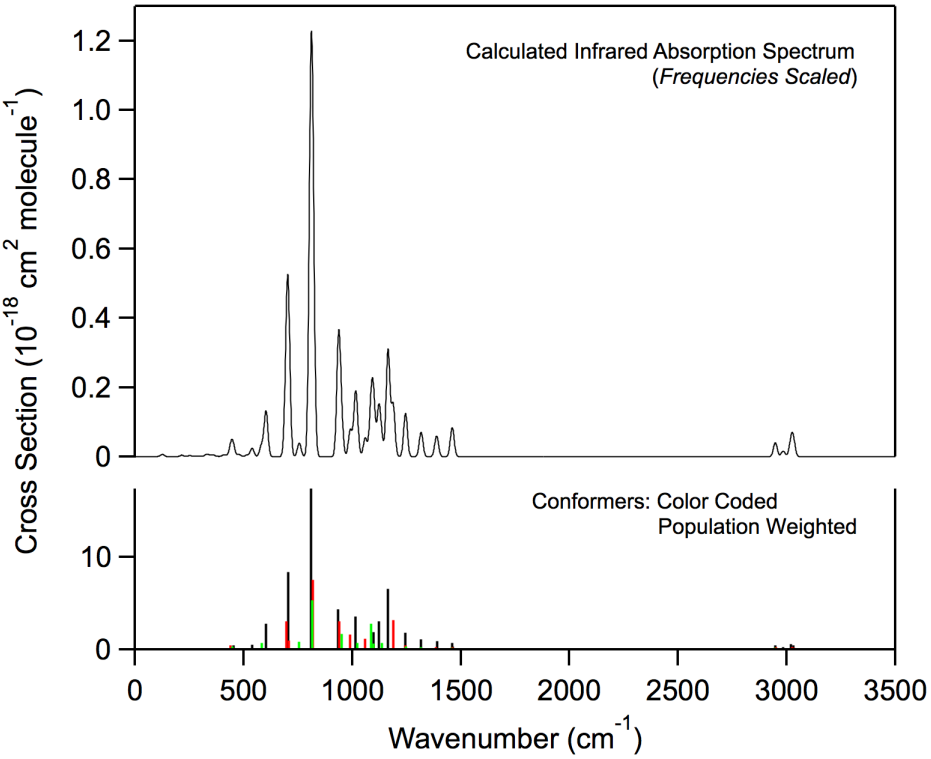
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.619881742711	1.412941473425	-0.771173917994
C	-0.916200608146	0.066943776898	-0.649227271935
C	0.576357598270	0.208574244888	-0.282451159610
H	-2.640672076562	1.255586174178	-1.124103262003
H	-1.656262552540	1.924948396248	0.191996070745
H	-1.090026154228	2.042021356586	-1.490868684694
H	-0.928445117923	-0.464270148994	-1.603210094602
Cl	-1.779386844868	-0.999020797957	0.514940204976
Cl	0.836425224075	0.970440124226	1.318458102095
Cl	1.424924381609	-1.370146536558	-0.345160371043
F	1.138486893025	1.004364937060	-1.212723615935

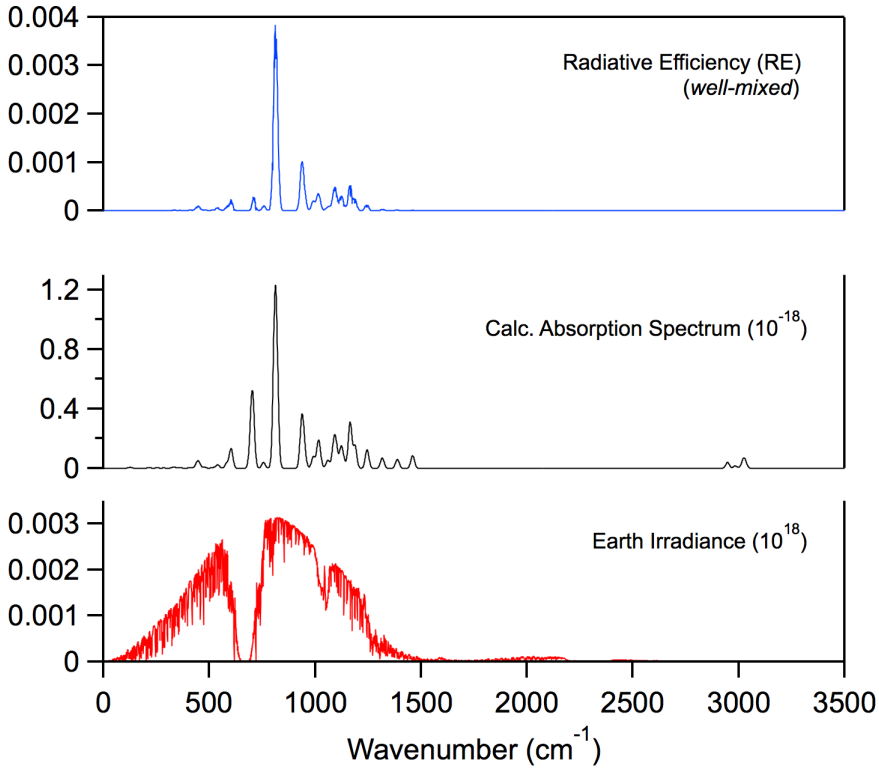
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
78.0211	0.122
167.4344	0.0946
191.8143	0.0131
234.8871	0.00865
261.0058	0.0720
302.3507	0.276
369.0236	0.137
377.3745	0.0567
416.2639	2.03
488.8660	0.635
559.6302	4.23
743.7126	5.13
807.0369	32.9
949.7379	10.2
1027.2392	4.57
1094.2159	17.1
1106.0229	4.15
1147.3763	4.46
1263.1469	2.20
1335.6662	1.51
1408.8480	0.904
1486.9187	1.07
1492.2537	0.718
3061.8540	1.05
3099.3118	0.466
3140.6087	0.900
3151.8950	0.834

Infrared Spectrum

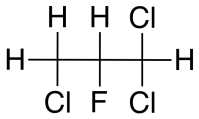


Radiative Efficiency



HCFC-251ea

Molecular Formula:	$CH_2ClCHFCHCl_2$
Name:	1,1,3-Trichloro-2-fluoropropane
CAS number:	76937-36-5
Molecular Weight:	165.42



Global Atmospheric Lifetime (years):	0.473
Tropospheric Atmospheric Lifetime (years):	0.489
Stratospheric Atmospheric Lifetime (years):	20
Ozone Depletion Potential (ODP):	0.011

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.131	0.078
Global Warming Potential (GWP_H):		
GWP_{20}	84	50
GWP_{100}	23	14
Global Temperature Potentials (GTP_H)		
GTP_{20}		15
GTP_{50}		2
GTP_{100}		2

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 1.20 \times 10^{-13}$; $k_{SAR}(272\ K) \approx 0.765 \times 10^{-13}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 0.478$ years
$\tau^{OH}_{Trop} = 0.489$ years
$\tau^{OH}_{Strat} = 20$ years

Fractional Atmospheric Loss: 0.991

O(^{1}D) Reactivity

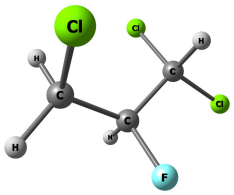
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 2.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)} = 185$ years
Fractional Atmospheric Loss: 0.002

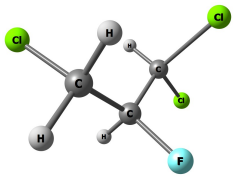
UV Photolysis

UV Spectrum: *No Recommendation*
$\tau_{hv} = 68$ years
Fractional Atmospheric Loss: 0.007

Molecular Structure and Infrared Spectrum (5 conformers)



E = 0
Population = 0.320



$\Delta E = 0.05$ kcal mol^{-1}
Population = 0.293

Optimized Coordinates (Angstroms)

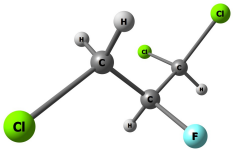
Atom	X	Y	Z
C	1.581769541262	0.123602189013	0.879154278090
C	0.219574330335	-0.547124907179	0.757137551454
C	-0.718215601812	0.085681420269	-0.279129060508
Cl	2.486161035187	0.136579368130	-0.681136188964
H	1.484519675156	1.155406993164	1.211439596984
H	2.187639140309	-0.441206222360	1.587642424848
H	-0.268774309892	-0.507989286624	1.739962837182
F	0.402719193329	-1.861754747787	0.408865752277
H	-0.269857017810	0.097133633660	-1.269097264160
Cl	-2.233119602009	-0.856231989473	-0.396115875263
Cl	-1.059830384055	1.789636549186	0.169586948059

Atom	X	Y	Z
C	1.639529476312	-0.274613280982	-0.725700742916
C	0.254032600961	-0.828785901375	-0.399799172854
C	-0.628107523668	0.119904445905	0.414128738714
Cl	2.623917179437	-0.081397499870	0.770992307764
H	2.160031895312	-0.981253680795	-1.371284549148
H	1.577211189429	0.697972661234	-1.211647704790
H	0.352275605444	-1.756591740912	0.176102997294
F	-0.355224068349	-1.114114087162	-1.595788448386
H	-0.135625882654	0.397321934426	1.342693889344
Cl	-0.958531543055	1.639269462268	-0.479161719706
Cl	-2.158965929170	-0.700389312738	0.854905404684

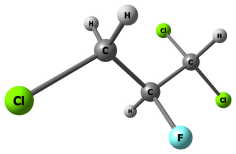
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
49.2194	0.208
89.6982	0.201
173.9521	0.111
193.0142	0.459
254.6661	0.499
336.5437	0.422
370.2384	0.318
391.5306	2.07
566.6933	5.40
684.1595	2.48
775.2706	18.0
793.7389	4.70
894.1593	4.65
942.4522	0.829
1077.0174	4.82
1121.6226	4.91
1219.0437	2.26
1225.7398	1.62
1239.2152	1.98
1305.9230	2.88
1358.2345	2.52
1385.6715	1.25
1460.2692	1.95
3038.4942	1.31
3106.3177	1.27
3163.5417	0.213
3174.1340	0.116

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
49.7554	0.180
94.9961	0.463
179.3300	0.455
204.8402	0.109
208.7828	0.149
292.0431	0.470
369.3335	0.188
436.4069	3.26
580.2089	4.23
722.1387	0.900
756.0890	16.8
776.9823	8.50
863.7634	3.01
995.7382	1.24
1074.8716	4.85
1129.9357	7.20
1167.4253	1.12
1236.3136	3.72
1270.6979	0.685
1285.8298	1.16
1372.1649	0.810
1378.0559	1.71
1479.9822	1.59
3056.3065	1.23
3106.0416	0.988
3158.0424	0.275
3173.9824	0.0810



$\Delta E = 0.16$ kcal mol^{-1}
Population = 0.243



$\Delta E = 0.75$ kcal mol^{-1}
Population = 0.091

Optimized Coordinates (Angstroms)

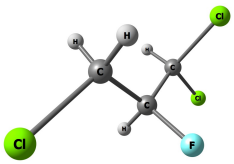
Atom	X	Y	Z
C	1.134663785687	0.237308953776	-0.608446644153
C	0.371698747793	-0.038530126040	0.676359598481
C	-1.157046582132	-0.036872892144	0.525015835261
Cl	2.892639775235	0.417993741934	-0.265338582768
H	1.024691632454	-0.591430052751	-1.305885893002
H	0.794386350377	1.163146093858	-1.070151799922
H	0.620211594900	0.716111561885	1.432043288596
F	0.719027174953	-1.273856938440	1.166646458146
H	-1.610951145538	-0.347068766836	1.463385259999
Cl	-1.748462267286	1.621584793009	0.182943198387
Cl	-1.719126066445	-1.203314368251	-0.713210719025

Atom	X	Y	Z
C	1.447416003166	0.549478005598	-0.418765159650
C	0.343039037570	-0.346511228689	0.129901810736
C	-1.044976551181	0.051640467150	-0.398582197271
Cl	3.043431650848	0.055904339996	0.248301203245
H	1.510376132988	0.455571514028	-1.504305109328
H	1.287934163835	1.589456411180	-0.142785883097
H	0.332567659005	-0.325222494822	1.224558310968
F	0.574669701095	-1.633336268471	-0.288848872734
H	-1.074652876596	0.039304735904	-1.486724332032
Cl	-2.276709567562	-1.116085728233	0.162134000518
Cl	-1.464732353167	1.717021246361	0.122721228644

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
66.4840	0.273
79.8124	0.320
152.5500	0.592
193.4462	0.277
219.7997	0.213
271.7444	0.0850
373.2954	0.743
456.9892	1.72
559.7728	5.42
678.0283	5.19
773.4130	15.7
801.7950	7.04
863.3556	1.51
977.3772	1.61
1075.2224	6.74
1118.7028	4.97
1217.7695	1.16
1226.3797	2.24
1250.6758	0.158
1292.7341	5.27
1361.9024	0.695
1396.5608	0.932
1465.3726	1.35
3055.9965	1.26
3110.5167	1.02
3148.2383	0.252
3178.2999	0.0360

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
63.3123	0.163
74.2319	0.433
139.0206	0.531
205.7683	0.241
242.8011	0.162
320.4164	0.0344
347.1217	0.770
404.4317	1.54
499.3585	3.52
709.8862	12.1
770.4411	12.1
811.3746	6.70
870.2872	2.42
1026.7986	1.51
1066.2986	1.45
1117.8547	7.78
1184.1448	2.04
1226.3538	2.51
1251.2523	0.482
1300.3261	1.68
1367.4915	0.514
1385.5153	0.930
1465.9013	0.917
3074.5645	0.691
3095.6486	1.59
3137.6444	0.454
3174.6361	0.189



$\Delta E = 1.06$ kcal mol^{-1}
Population = 0.054

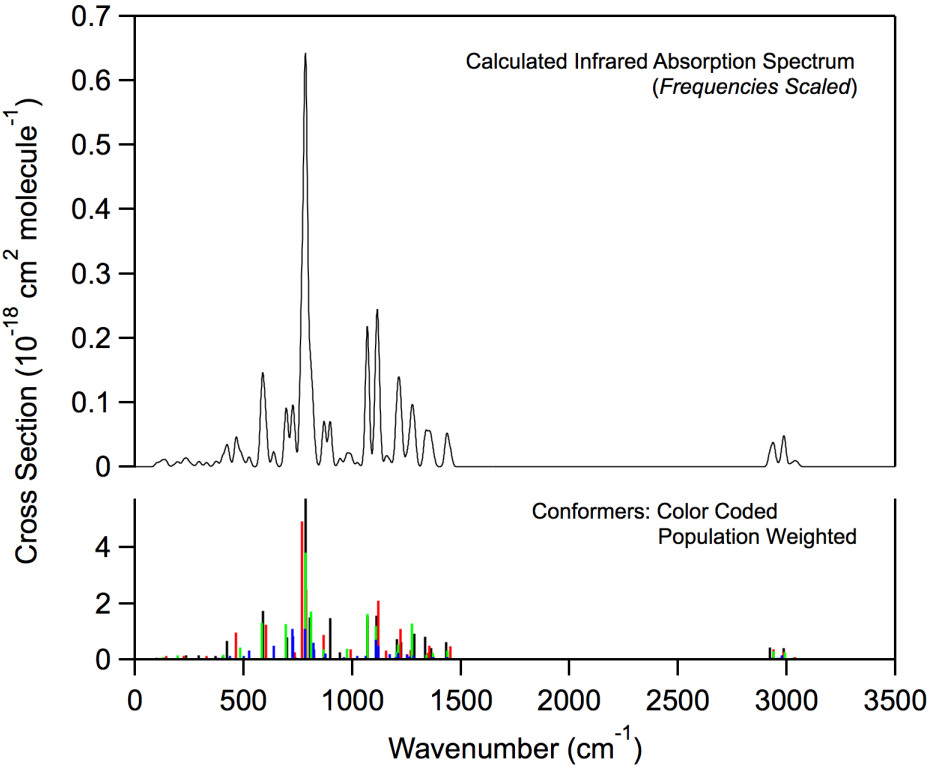
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.469043815396	0.497125709677	0.507200680803
C	0.352239171700	-0.460801643205	0.110900568751
C	-1.023053971210	0.035272215769	0.574250665520
Cl	3.078544968662	-0.251723974419	0.211710234404
H	1.420653632995	1.409546337300	-0.084901453589
H	1.416986480030	0.741463719488	1.569215464878
H	0.515470532803	-1.437840807134	0.582529128633
F	0.348518019884	-0.627268627172	-1.244993050205
H	-1.040956419223	0.162105116952	1.655147309241
Cl	-1.432868130885	1.628701233601	-0.140830471993
Cl	-2.278407100153	-1.178701280858	0.178418923556

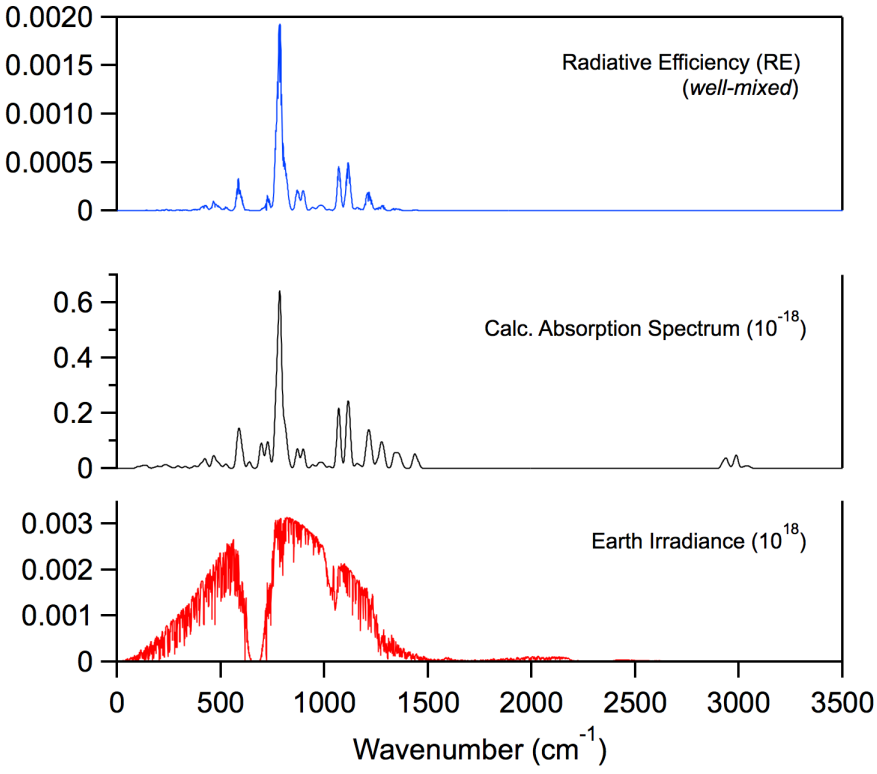
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
70.9359	0.0363
75.9102	0.607
128.9075	0.402
198.7538	0.00943
236.0743	0.102
264.6675	0.120
324.1343	0.161
472.7822	2.60
618.9749	9.18
713.8879	15.6
726.5472	1.04
816.8135	6.68
866.6034	1.59
962.4610	1.45
1058.5979	0.187
1129.1899	9.26
1214.3036	1.51
1229.9457	1.78
1270.5963	3.27
1282.5694	1.92
1353.6410	0.638
1397.2627	1.55
1463.6230	0.802
3048.9392	1.29
3094.4342	1.59
3135.8699	0.419
3168.4609	0.168

Infrared Spectrum

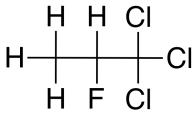


Radiative Efficiency



HCFC-251eb

Molecular Formula:	$CH_3CHFCCl_3$
Name:	1,1,1-Trichloro-2-fluoropropane
CAS number:	1448144-70-4
Molecular Weight:	165.42



Global Atmospheric Lifetime (years):	0.678
Tropospheric Atmospheric Lifetime (years):	0.709
Stratospheric Atmospheric Lifetime (years):	20
Ozone Depletion Potential (ODP):	0.016

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.201	0.134
Global Warming Potential (GWP_H):		
GWP_{20}	185	124
GWP_{100}	50	34
Global Temperature Potentials (GTP_H)		
GTP_{20}		39
GTP_{50}		6
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) = 8.27×10^{-14}; k_{SAR}(272 K) ≈ 5.28×10^{-14} cm^3 $molecule^{-1}$ s^{-1}

τ^{OH}_{Global} = 0.690 years
τ^{OH}_{Trop} = 0.709 years
τ^{OH}_{Strat} = 24.8 years

Fractional Atmospheric Loss: 0.983

O(^{1}D) Reactivity

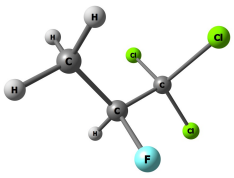
k_{Rec}(T), *No recommendation*

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

UV Photolysis

UV Spectrum: *No Recommendation*
τ_{hv} = 50 years
Fractional Atmospheric Loss: 0.013

Molecular Structure and Infrared Spectrum (1 conformer)



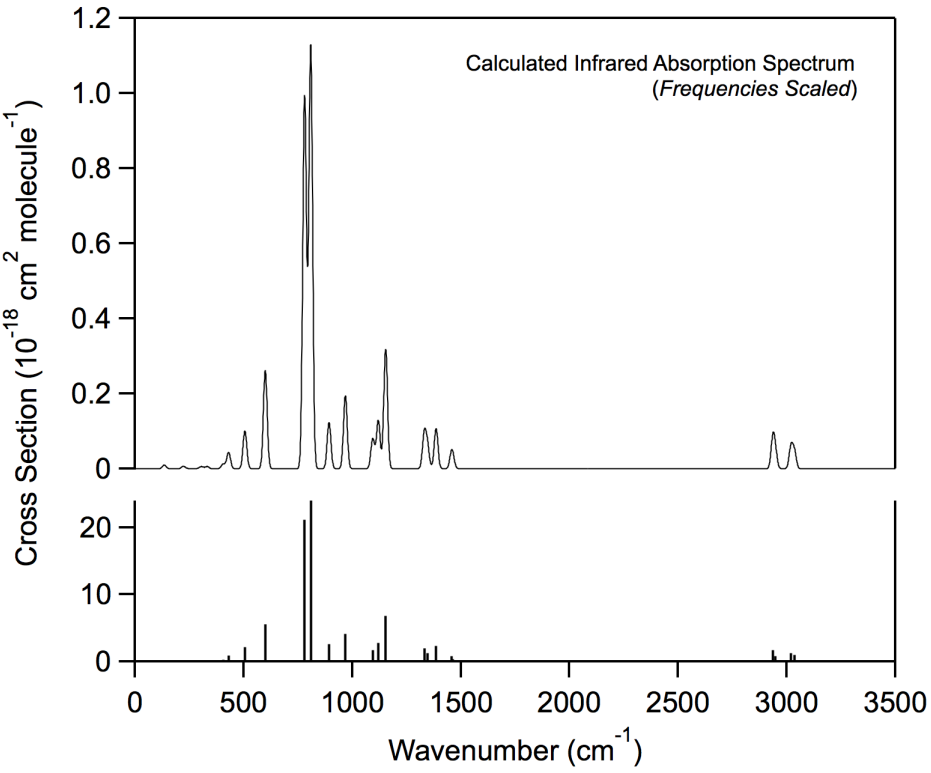
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-2.219219019590	0.774897015215	-0.321580092467
C	-1.115455201015	-0.195327393521	-0.705954097332
C	0.250596130692	0.040355179796	-0.012273211018
H	-3.128277974871	0.478522571120	-0.850774389659
H	-2.411606733468	0.737218418299	0.752316098149
H	-1.965732214836	1.796729348283	-0.607141011495
H	-0.911941081291	-0.155099997593	-1.782709727282
F	-1.512559843585	-1.472491220121	-0.390873393792
Cl	1.408619644874	-1.210877968163	-0.565168499039
Cl	0.875511844334	1.656791478954	-0.478821138539
Cl	0.097277448758	-0.059697432270	1.767256462473

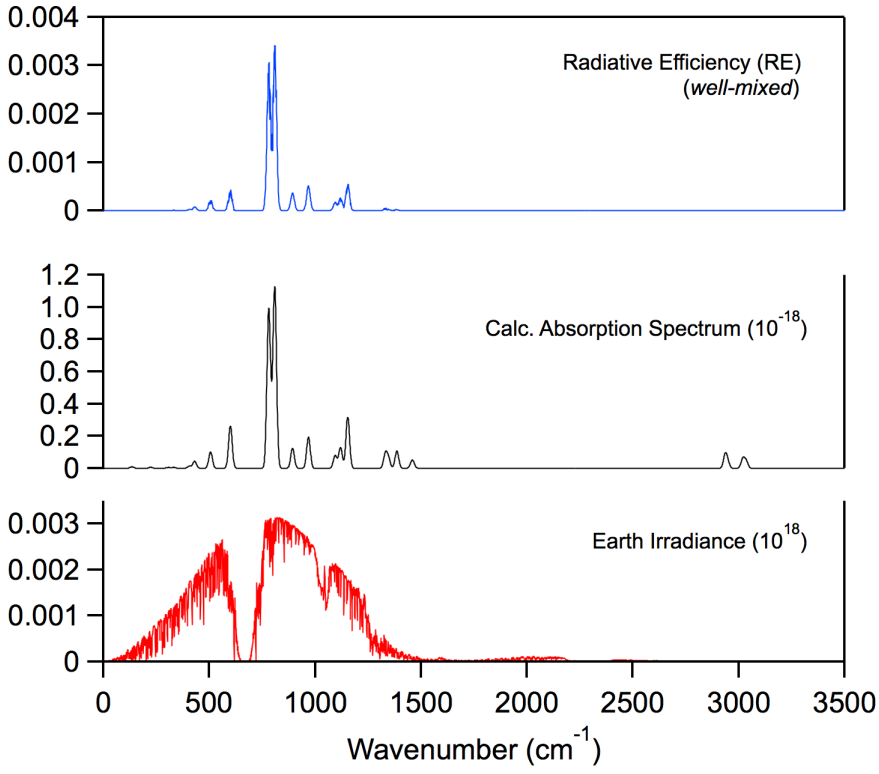
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
85.7167	0.206
179.0220	0.140
192.2844	0.00159
209.6979	0.0132
261.3782	0.0510
270.2837	0.0834
294.8639	0.122
372.6884	0.270
399.3254	0.933
478.8411	2.15
578.1290	5.58
769.8864	21.1
799.6532	24.0
888.9416	2.64
968.4447	4.13
1101.8805	1.69
1128.9064	2.73
1164.9422	6.79
1353.2137	1.94
1368.7721	1.23
1410.6912	2.29
1486.0896	0.829
1493.2966	0.341
3052.4703	1.72
3065.0383	0.807
3140.6624	1.26
3157.4520	0.969

Infrared Spectrum

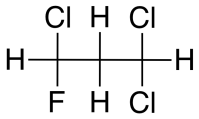


Radiative Efficiency



HCFC-251fa

Molecular Formula:	$CHClFCH_2CCl_2H$
Name:	1,1,3-Trichloro-3-fluoropropane
CAS number:	2106760-90-9
Molecular Weight:	165.42



Global Atmospheric Lifetime (years):	0.331
Tropospheric Atmospheric Lifetime (years):	0.339
Stratospheric Atmospheric Lifetime (years):	20
Ozone Depletion Potential (ODP):	0.008

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.145	0.074
Global Warming Potential (GWP_H):		
GWP_{20}	65	33
GWP_{100}	18	9
Global Temperature Potentials (GTP_H)		
GTP_{20}		10
GTP_{50}		2
GTP_{100}		1

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 1.73 \times 10^{-13}$; $k_{SAR}(272\ K) \approx 1.11 \times 10^{-13}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 0.333$ years

$\tau^{OH}_{Trop} = 0.339$ years

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

Fractional Atmospheric Loss: 0.993

$O(^1D)$ Reactivity

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

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

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

Fractional Atmospheric Loss: 0.002

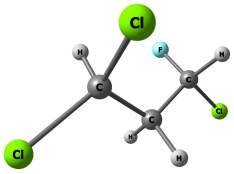
UV Photolysis

UV Spectrum: *No Recommendation*

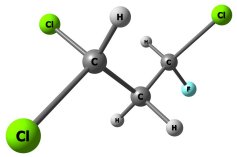
$\tau_{hv} = 68$ years

Fractional Atmospheric Loss: 0.005

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.659



$\Delta E = 0.49$ kcal mol^{-1}
Population = 0.287

Optimized Coordinates (Angstroms)

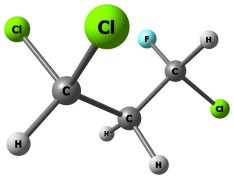
Atom	X	Y	Z
C	-1.384234919895	0.304445127731	0.122793581681
C	-0.204880360980	-0.607735038928	-0.181849329573
C	1.105832268484	-0.039002147336	0.352567691221
Cl	-2.917775434810	-0.465301251594	-0.438156068883
F	-1.463988066422	0.515227586036	1.463621441477
H	-1.329000616259	1.269144520594	-0.382394671441
H	-0.131560711909	-0.771482738331	-1.258728126457
H	-0.379342381343	-1.572992017080	0.302124270813
Cl	2.423213095165	-1.241676387929	0.160974778463
Cl	1.538605292491	1.503006010201	-0.473545897803
H	1.046769835476	0.194146336635	1.412232330503

Atom	X	Y	Z
C	-1.486388783449	0.002060426288	-0.550660319503
C	-0.149764645870	0.730834583461	-0.524815947206
C	0.937091429692	0.033401833476	0.278289895868
Cl	-2.194769321536	-0.126162380587	1.114481323719
F	-2.344967809650	0.702657841739	-1.328072906839
H	-1.417758406004	-1.022065655173	-0.918643456812
H	-0.308830103187	1.727527998015	-0.103406798028
H	0.181544454034	0.847782717252	-1.561423487282
Cl	1.322225553155	-1.587615193657	-0.408966461221
Cl	2.412293710809	1.056049652887	0.326212924127
H	0.646411922006	-0.139380823702	1.310975233175

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
53.5861	0.0898
96.1833	0.630
123.3141	0.365
205.7048	0.0188
294.1647	0.471
310.8039	0.239
385.8903	0.302
422.6466	2.21
497.3780	2.75
653.3286	7.91
708.6879	20.7
828.9055	8.32
895.6142	7.08
1008.6290	3.99
1082.5888	5.13
1123.4139	14.2
1207.1425	2.03
1231.9396	1.19
1262.4718	6.54
1316.3803	0.358
1363.4106	4.41
1393.8008	2.65
1458.6932	0.829
3076.0034	0.0360
3120.3573	0.835
3137.4424	0.353
3162.8020	0.0772

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
47.5488	0.0901
100.6128	0.613
129.1000	0.204
226.6414	0.227
288.6000	0.303
331.1744	0.305
389.4269	0.978
416.3668	1.80
504.4936	1.83
646.6946	10.1
678.6718	9.22
759.0231	15.0
954.0735	7.59
1045.9344	4.76
1091.1062	3.70
1120.6643	19.2
1186.6130	1.37
1236.7294	3.60
1274.3884	6.46
1321.8962	4.78
1342.5067	0.497
1403.5087	3.05
1462.5663	0.755
3063.9180	0.208
3112.5927	0.151
3127.7782	1.08
3161.9395	0.109



$\Delta E = 1.99$ kcal mol^{-1}
Population = 0.023

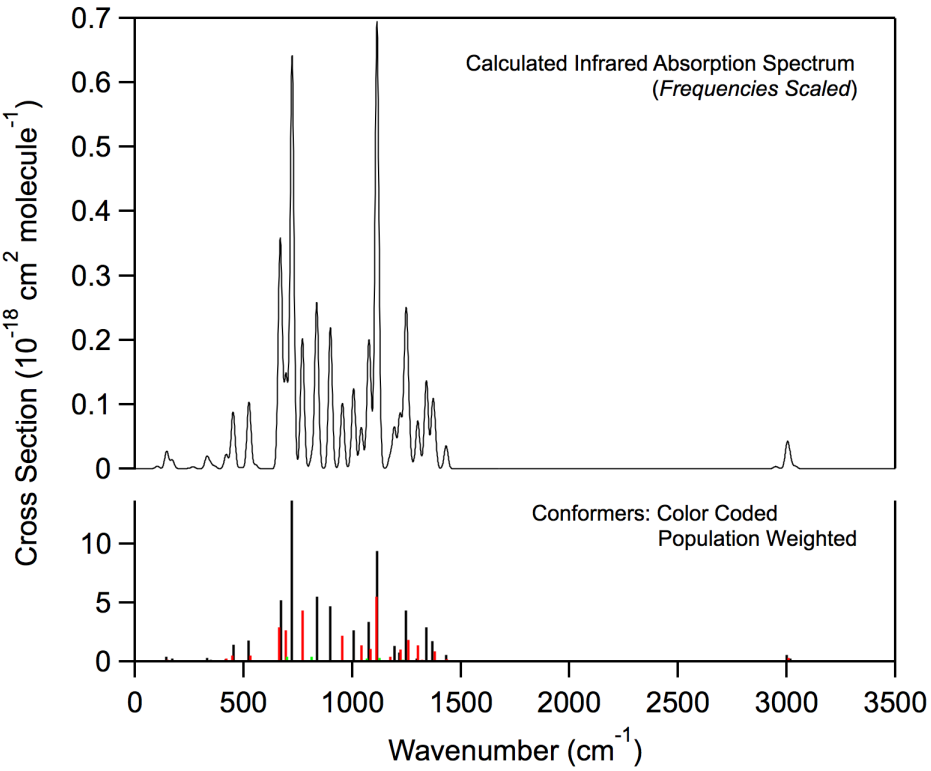
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.168698529803	0.087170449517	0.335973819801
C	-0.306567060757	0.181418052344	-0.915300582820
C	1.204928532358	0.181644464536	-0.689453138397
Cl	-2.899860562522	0.390212776461	-0.113280252028
F	-1.084273663899	-1.139552652360	0.896599856741
H	-0.921426700322	0.841555521700	1.083821668946
H	-0.555139461584	1.111306264640	-1.433720652233
H	-0.558489923411	-0.654112779687	-1.575497949145
Cl	1.713180266860	1.567202305051	0.350476255635
Cl	1.826592013690	-1.365263824911	-0.028133920765
H	1.721178089389	0.326821422708	-1.635104105734

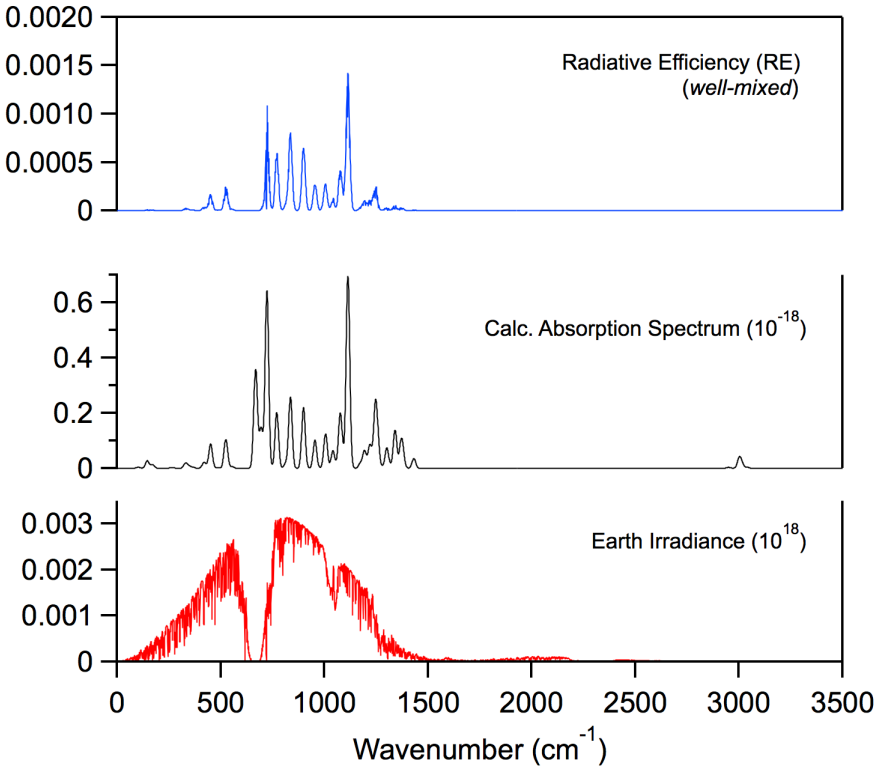
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
34.4704	0.135
99.3853	0.160
147.5666	0.193
214.0877	0.116
287.7965	0.196
304.4471	0.738
375.0480	0.511
459.1578	1.84
531.2398	5.58
655.1395	0.232
682.5096	18.1
805.3307	17.3
890.8210	0.263
995.2305	2.85
1074.4348	12.2
1134.9935	13.5
1219.0354	1.24
1248.3281	5.63
1263.1779	4.01
1295.4579	4.35
1372.3325	0.777
1410.5229	2.08
1449.5551	1.20
3067.3303	0.0737
3114.6754	0.304
3127.6820	0.862
3146.1016	0.268

Infrared Spectrum

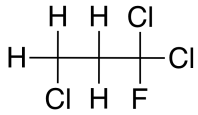


Radiative Efficiency



HCFC-251fb

Molecular Formula: $CH_2ClCH_2CCl_2F$
Name: 1,1,3-Trichloro-1-fluoropropane
CAS number: 818-99-5
Molecular Weight: 165.42



Global Atmospheric Lifetime (years): 0.452
  Tropospheric Atmospheric Lifetime (years): 0.467
  Stratospheric Atmospheric Lifetime (years): 20
Ozone Depletion Potential (ODP): 0.011

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.184	0.107
Global Warming Potential (GWP_H):		
GWP_{20}	113	66
GWP_{100}	31	18
Global Temperature Potentials (GTP_H)		
GTP_{20}		20
GTP_{50}		3
GTP_{100}		2

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 1.26 \times 10^{-13}$; $k_{SAR}(272\ K) \approx 0.801 \times 10^{-13}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 0.457$ years
$\tau^{OH}_{Trop} = 0.467$ years
$\tau^{OH}_{Strat} = 20$ years

Fractional Atmospheric Loss: 0.991

O(^{1}D) Reactivity

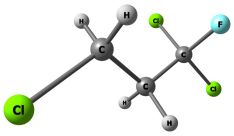
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 2.0 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)} = 185$ years
Fractional Atmospheric Loss: 0.002

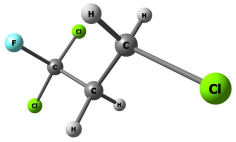
UV Photolysis

UV Spectrum: *No Recommendation*
$\tau_{hv} = 68$ years
Fractional Atmospheric Loss: 0.007

Molecular Structure and Infrared Spectrum (5 conformers)



E = 0
Population = 0.339



E = 0
Population = 0.339

Optimized Coordinates (Angstroms)

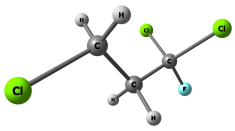
Atom	X	Y	Z
C	-1.613324554237	0.369714492379	0.329734620910
C	-0.502490314732	-0.528500028795	-0.210669540200
C	0.881713119579	-0.068068660761	0.235099660020
Cl	-3.223264345304	-0.299481404747	-0.136498586870
H	-1.593282925159	0.418603258663	1.417704184208
H	-1.560523494863	1.376899181531	-0.080641952409
H	-0.527546149078	-0.566391397753	-1.300832655762
H	-0.634069123076	-1.546812336499	0.166249568471
Cl	2.133162483017	-1.244748852815	-0.300417933611
Cl	1.290939982556	1.561520536752	-0.426206280475
F	0.939837321296	0.014191212045	1.574680915719

Atom	X	Y	Z
C	-1.613861392383	-0.365604590669	0.332103106346
C	-0.502409055127	0.525193858218	-0.219196096064
C	0.881523419280	0.068922590613	0.231663426356
Cl	-3.223355546807	0.299370095118	-0.141648865336
H	-1.562013542162	-1.377634011335	-0.066300742437
H	-1.593585721136	-0.401591594731	1.420571532134
H	-0.633035662807	1.548018356756	0.145643285337
H	-0.527712748724	0.550167243040	-1.309726003118
Cl	1.289220456273	-1.568743968401	-0.410351806257
Cl	2.133818361136	1.238110494399	-0.318099004584
F	0.939926432457	0.002523526991	1.572112167622

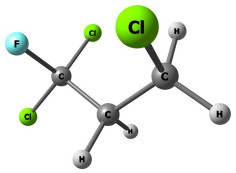
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
67.8380	0.664
108.2520	0.0182
125.0006	0.421
221.4815	0.0480
270.9199	0.0444
302.3360	0.752
374.4829	0.654
389.1034	0.913
445.8897	0.429
623.0332	10.6
721.1778	18.8
784.3291	0.783
839.5809	18.5
955.1440	12.4
1043.4760	4.05
1061.6004	6.20
1157.7239	8.49
1204.6099	10.4
1272.3786	1.71
1312.6378	1.21
1365.9971	3.78
1469.1820	0.598
1491.8226	0.417
3076.8609	0.254
3106.8167	1.11
3135.8921	0.0659
3172.8351	0.272

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
67.8377	0.664
108.2497	0.0182
124.9994	0.421
221.4810	0.0480
270.9202	0.0444
302.3354	0.752
374.4825	0.654
389.1031	0.913
445.8899	0.429
623.0330	10.6
721.1771	18.8
784.3287	0.783
839.5802	18.5
955.1434	12.4
1043.4755	4.05
1061.6006	6.20
1157.7241	8.49
1204.6101	10.4
1272.3786	1.71
1312.6391	1.21
1365.9981	3.78
1469.1827	0.598
1491.8230	0.417
3076.8604	0.254
3106.8173	1.11
3135.8911	0.0659
3172.8357	0.272



$\Delta E = 0.27$ kcal mol^{-1}
Population = 0.213



$\Delta E = 1.08$ kcal mol^{-1}
Population = 0.054

Optimized Coordinates (Angstroms)

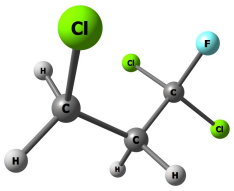
Atom	X	Y	Z
C	-1.448294634250	0.007034205902	0.505920762970
C	-0.530105406787	-0.009276377970	-0.708810843672
C	0.961334883532	-0.001394484645	-0.388918294539
Cl	-3.172430461680	-0.004607520137	-0.032603607775
H	-1.309736413096	-0.873003270805	1.132229029260
H	-1.313418065171	0.906016795826	1.105558213052
H	-0.718766807294	0.865652505001	-1.337841459379
H	-0.715106360703	-0.903440689549	-1.311320600279
Cl	1.443310222872	1.483001264428	0.516853577679
Cl	1.449395438487	-1.455971620578	0.560900673194
F	1.655784604088	-0.017128807473	-1.534693450510

Atom	X	Y	Z
C	-1.646897309574	-0.073615758183	-1.038273491715
C	-0.271200748731	0.586285968461	-1.005363318599
C	0.683145303636	0.075688383014	0.071985894783
Cl	-2.730002861701	0.464673455345	0.304078926180
H	-2.155307454049	0.200551935340	-1.962440618249
H	-1.580860112509	-1.159298855082	-0.976320913656
H	-0.373409966658	1.665609678940	-0.861236640980
H	0.214710988952	0.423081402453	-1.971480070491
Cl	1.023055671059	-1.688802096401	-0.129751391493
Cl	2.244061318567	0.978004551443	-0.032832206791
F	0.191098171008	0.254778334670	1.299741831011

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
64.3157	0.580
108.7220	0.0403
138.1432	0.428
229.2718	0.274
264.5810	0.0174
291.1486	0.161
387.9683	0.452
398.7825	0.803
484.9476	0.507
588.1946	7.24
699.5996	21.2
758.6133	6.61
803.9770	11.8
1042.1427	4.58
1056.8823	17.9
1066.1047	1.32
1154.8509	15.6
1179.5997	5.94
1276.6764	3.91
1305.7955	0.746
1372.2105	2.69
1470.3134	0.509
1492.0162	0.503
3065.0334	0.387
3108.0011	1.12
3115.9569	0.192
3172.9993	0.209

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
37.5823	0.264
114.2497	0.147
192.8162	0.163
213.4368	0.101
289.3602	0.0654
330.2836	0.472
387.4903	0.634
406.9507	1.71
453.3683	2.29
580.4897	4.74
671.6884	4.70
776.2650	29.7
898.6064	5.62
924.0455	3.77
1024.6246	20.1
1050.0518	3.68
1181.7951	7.80
1191.1658	4.26
1278.5291	9.40
1331.3523	3.19
1376.3512	0.821
1452.7770	1.04
1477.8551	1.27
3068.6326	0.230
3098.4708	1.21
3120.3352	0.398
3160.4769	0.250



$\Delta E = 1.08$ kcal mol^{-1}
Population = 0.054

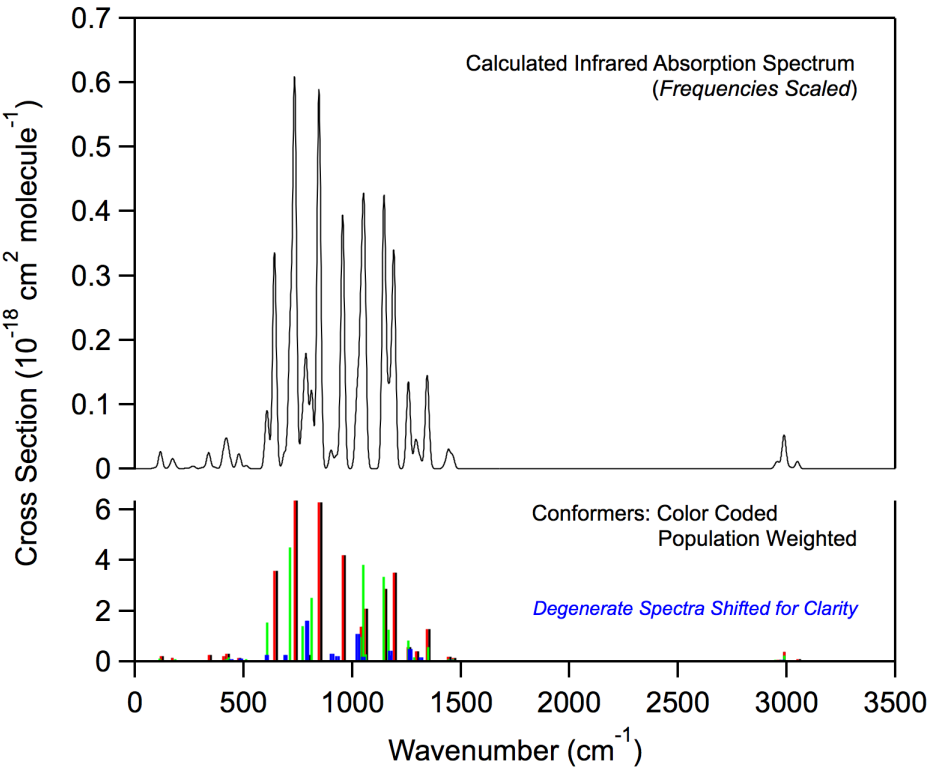
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.647598280922	0.070250346351	-1.038574255499
C	-0.270894272629	-0.587557139271	-1.005867050894
C	0.683615414552	-0.073941056904	0.069901237946
Cl	-2.728750237862	-0.467650895201	0.305507437658
H	-1.583122369180	1.156121270842	-0.978291452297
H	-2.156392829123	-0.206046189224	-1.961895442829
H	0.213945245901	-0.425067462216	-1.972642764899
H	-0.371374766490	-1.666816035725	-0.860049296845
Cl	2.245780923576	-0.974092056260	-0.034918909548
Cl	1.020728532072	1.690750564689	-0.134749148348
F	0.192888640104	-0.251936347079	1.298344645555

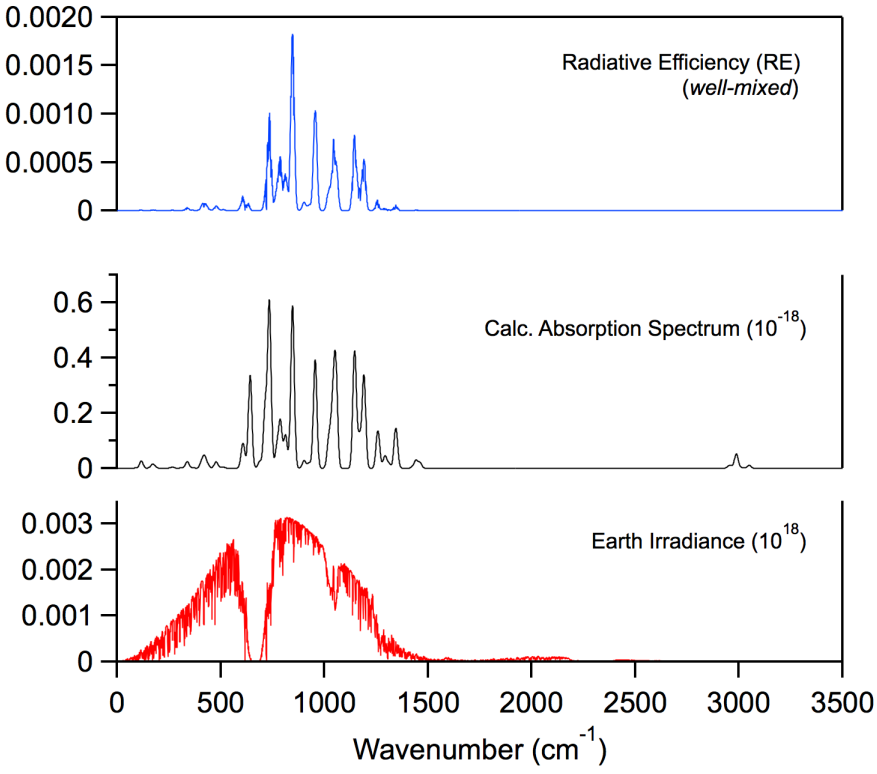
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
37.5802	0.264
114.2490	0.147
192.8156	0.163
213.4367	0.101
289.3601	0.0654
330.2831	0.472
387.4901	0.634
406.9504	1.71
453.3683	2.29
580.4894	4.74
671.6882	4.70
776.2644	29.7
898.6062	5.62
924.0462	3.77
1024.6243	20.1
1050.0521	3.68
1181.7946	7.80
1191.1667	4.26
1278.5297	9.40
1331.3537	3.19
1376.3522	0.821
1452.7785	1.04
1477.8569	1.27
3068.6324	0.230
3098.4706	1.21
3120.3350	0.398
3160.4768	0.250

Infrared Spectrum

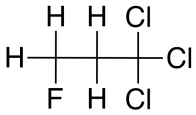


Radiative Efficiency



HCFC-251fc

Molecular Formula:	$CH_2FCH_2CCl_3$
Name:	1,1,1-Trichloro-3-fluoropropane
CAS number:	2035078-31-8
Molecular Weight:	165.42



Global Atmospheric Lifetime (years):	0.646
Tropospheric Atmospheric Lifetime (years):	0.676
Stratospheric Atmospheric Lifetime (years):	20
Ozone Depletion Potential (ODP):	0.015

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.157	0.103
Global Warming Potential (GWP_H):		
GWP_{20}	138	91
GWP_{100}	37	25
Global Temperature Potentials (GTP_H)		
GTP_{20}		28
GTP_{50}		4
GTP_{100}		3

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 8.68 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 5.54 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 0.657$ years

$\tau^{OH}_{Trop} = 0.676$ years

$\tau^{OH}_{Strat} = 23.7$ years

Fractional Atmospheric Loss: 0.984

O(^{1}D) Reactivity

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

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

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

Fractional Atmospheric Loss: 0.003

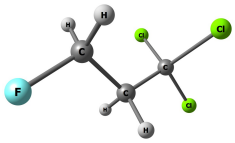
UV Photolysis

UV Spectrum: *No Recommendation*

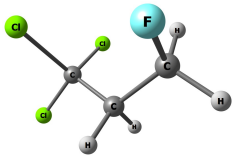
$\tau_{hv} = 50$ years

Fractional Atmospheric Loss: 0.013

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.373



$\Delta E = 0.10$ kcal mol^{-1}
Population = 0.314

Optimized Coordinates (Angstroms)

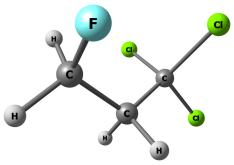
Atom	X	Y	Z
C	1.846128611705	-1.084760951405	0.000000000000
C	1.156753226402	0.280089423503	0.000000000000
C	-0.368082490414	0.247941129871	0.000000000000
F	3.205608976589	-0.856050392168	0.000000000000
H	1.586166494001	-1.664517008520	0.891169704446
H	1.586166494001	-1.664517008520	-0.891169704446
H	1.474393351556	0.840182062203	-0.884123475901
H	1.474393351556	0.840182062203	0.884123475901
Cl	-0.996263519505	1.932455742486	0.000000000000
Cl	-0.995778247911	-0.593040529850	-1.462786235659
Cl	-0.995778247911	-0.593040529850	1.462786235659

Atom	X	Y	Z
C	2.058493282340	0.605235509901	-0.722614608781
C	0.644798049531	0.261478171666	-1.182538988077
C	-0.403295817347	0.043188858679	-0.086716976329
F	2.707429391307	-0.505667028421	-0.235277892681
H	2.619949253020	0.978948727670	-1.587625411034
H	2.052621110325	1.380266968658	0.050967817657
H	0.678721921549	-0.645956462325	-1.792526433662
H	0.274035036373	1.075319164625	-1.813094549500
Cl	-1.983577852221	-0.327101928898	-0.872196720961
Cl	0.027990891782	-1.313729114081	0.995958844868
Cl	-0.603629266660	1.537096132526	0.902287918502

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
72.8148	0.761
115.4198	0.00191
138.7145	0.263
238.3814	0.0462
249.7377	0.178
274.3551	0.0955
337.5365	0.391
367.2173	2.42
395.1520	0.0107
597.5259	4.56
678.4714	17.0
764.8846	21.6
822.5235	4.86
1044.7243	3.79
1075.2166	13.1
1099.7588	7.85
1117.6606	6.27
1246.6440	0.130
1313.2086	0.172
1320.9466	0.775
1434.6336	2.03
1469.8564	0.564
1525.0438	0.190
3051.1083	2.85
3067.6978	0.872
3098.9868	1.76
3124.5352	1.65

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
51.3615	0.387
137.1910	0.348
184.4758	0.189
217.9842	0.0886
257.3659	0.128
294.3441	0.0142
331.6773	0.650
368.2553	0.242
475.2035	3.57
528.8907	2.82
692.4744	18.8
755.3558	20.1
887.9079	0.789
939.8111	1.49
1077.5051	3.65
1097.6170	7.03
1111.8929	16.9
1253.1235	0.352
1301.4093	0.595
1370.1877	0.779
1430.0457	2.30
1449.0263	0.689
1510.8700	0.814
3034.1046	5.07
3063.1414	0.255
3088.8604	3.36
3116.8600	0.610



$\Delta E = 0.10$ kcal mol^{-1}
Population = 0.314

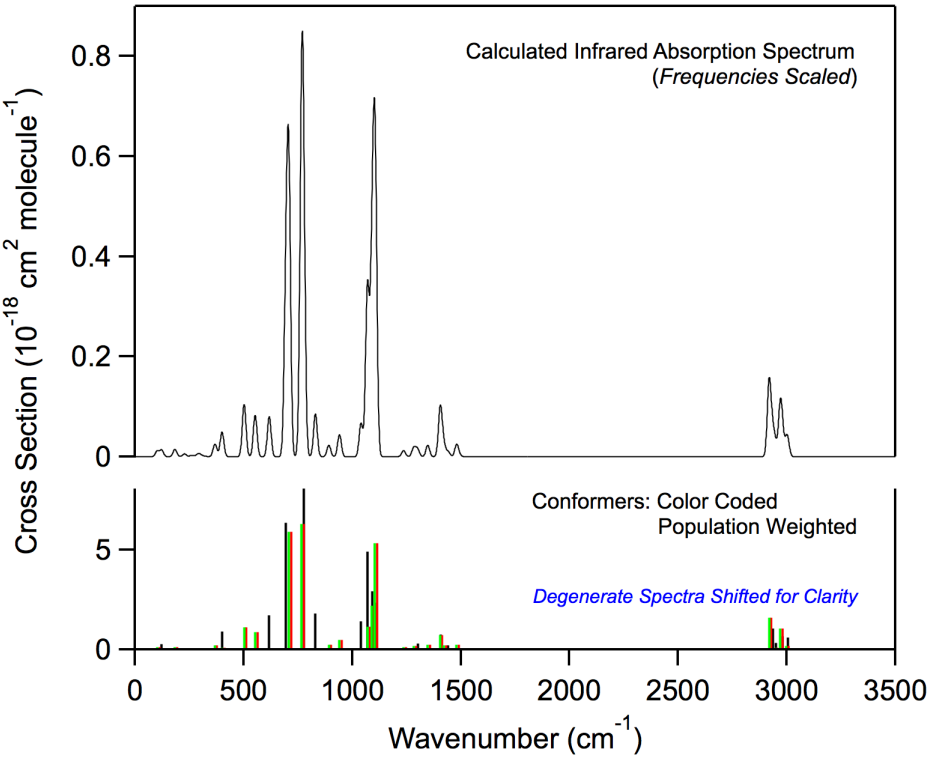
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	2.059093876836	-0.603787373960	-0.722557171412
C	0.645248457031	-0.260767251778	-1.182570269390
C	-0.403117062074	-0.043405244931	-0.086823781972
F	2.707292860731	0.507380095099	-0.234843579699
H	2.053594414416	-1.379027263626	0.050819120456
H	2.620886721939	-0.976930062323	-1.587595552875
H	0.275060198930	-1.074666268392	-1.813388575577
H	0.678698395053	0.646849443476	-1.792312973439
Cl	-1.983524033029	0.326133384830	-0.872406379332
Cl	-0.602668301096	-1.537696021600	0.901759804759
Cl	0.027207471263	1.313487563206	0.996266358481

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
51.3615	0.387
137.1911	0.348
184.4758	0.189
217.9842	0.0886
257.3659	0.128
294.3441	0.0142
331.6773	0.650
368.2553	0.242
475.2035	3.57
528.8907	2.82
692.4744	18.8
755.3558	20.1
887.9079	0.789
939.8111	1.49
1077.5051	3.65
1097.6170	7.03
1111.8929	16.9
1253.1235	0.352
1301.4093	0.595
1370.1877	0.779
1430.0457	2.30
1449.0263	0.689
1510.8700	0.814
3034.1046	5.07
3063.1414	0.255
3088.8604	3.36
3116.8600	0.610

Infrared Spectrum



Radiative Efficiency