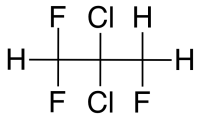
HCFC-243aa

Molecular Formula:	$CHF_2CCl_2CH_2F$
Name:	2,2-Dichloro-1,1,3-trifluoropropane
CAS number:	155329-34-3
Molecular Weight:	166.96



Global Atmospheric Lifetime (years):	2.99
Tropospheric Atmospheric Lifetime (years):	3.25
Stratospheric Atmospheric Lifetime (years):	37.3
Ozone Depletion Potential (ODP):	0.036

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.174	0.154
Global Warming Potential (GWP_H):		
GWP_{20}	701	619
GWP_{100}	190	168
Global Temperature Potentials (GTP_H)		
GTP_{20}		264
GTP_{50}		31
GTP_{100}		23

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 1.80 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 1.15 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

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

$\tau^{OH}_{Trop} = 3.25$ years

$\tau^{OH}_{Strat} = 97.5$ years

Fractional Atmospheric Loss: 0.951

O(^{1}D) Reactivity

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

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

$\tau_{O(^1D)} = 250$ years

Fractional Atmospheric Loss: 0.012

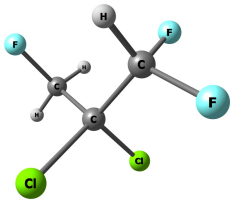
UV Photolysis

UV Spectrum: *No Recommendation*

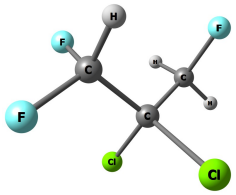
$\tau_{hv} = 80$ years

Fractional Atmospheric Loss: 0.037

Molecular Structure and Infrared Spectrum (7 conformers)



E = 0
Population = 0.351



E = 0
Population = 0.351

Optimized Coordinates (Angstroms)

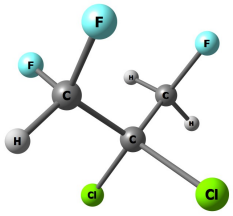
Atom	X	Y	Z
C	-0.744859656608	-0.762659154808	0.706257996946
C	0.178016232990	0.122854783011	-0.157184004450
C	1.114674245728	-0.726528085699	-1.018362370187
F	-1.622835040742	-0.014361616079	1.390813050806
F	-1.433831927942	-1.591928299343	-0.111839549784
H	-0.145429288989	-1.359638811589	1.401243472786
Cl	1.136517622501	1.150630361096	0.959291735856
Cl	-0.806281199052	1.130884446439	-1.261882632452
H	0.511836148321	-1.329729097088	-1.703660149756
H	1.791337801034	-0.076870485238	-1.579250437447
F	1.839289062759	-1.559518040703	-0.201140112318

Atom	X	Y	Z
C	-0.746198758481	0.756571572287	0.712862508638
C	0.175348361070	-0.122502258472	-0.158543530338
C	1.116142922553	0.733143374887	-1.008945603083
F	-1.431161930922	1.596794116033	-0.097387473863
F	-1.627690997819	0.003723754793	1.387841908440
H	-0.146071728170	1.344119298999	1.415245198762
Cl	-0.810240160661	-1.115435429325	-1.275692947298
Cl	1.128705222462	-1.165290438665	0.948375312509
H	1.791707758078	0.087429690773	-1.575681763331
H	0.516375690563	1.345607874002	-1.688699167253
F	1.841989621327	1.554970444688	-0.181577443183

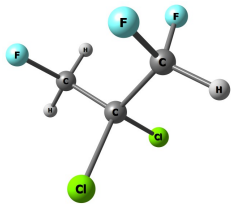
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
81.3905	0.209
116.6165	0.401
161.9604	0.0760
195.7326	0.151
229.9092	0.747
259.8183	0.165
304.8359	0.383
382.9131	0.293
408.8272	0.234
522.2226	3.19
611.0971	4.72
677.9384	8.67
782.8275	11.2
985.7900	7.73
1068.9639	4.47
1105.7095	11.1
1125.3736	7.85
1159.4784	10.9
1191.5355	17.7
1280.1108	0.648
1378.3705	4.72
1394.5499	2.28
1413.3307	2.11
1494.5747	0.959
3064.6994	1.48
3085.5233	2.15
3127.4480	1.19

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
81.3894	0.209
116.6166	0.401
161.9604	0.0760
195.7322	0.151
229.9091	0.747
259.8184	0.165
304.8357	0.383
382.9134	0.293
408.8272	0.234
522.2228	3.19
611.0972	4.72
677.9382	8.67
782.8270	11.2
985.7899	7.73
1068.9641	4.47
1105.7099	11.1
1125.3739	7.85
1159.4786	10.9
1191.5355	17.7
1280.1116	0.648
1378.3716	4.72
1394.5509	2.28
1413.3315	2.11
1494.5755	0.959
3064.6993	1.48
3085.5236	2.15
3127.4481	1.19



$\Delta E = 0.74$ kcal mol^{-1}
Population = 0.100



$\Delta E = 0.74$ kcal mol^{-1}
Population = 0.100

Optimized Coordinates (Angstroms)

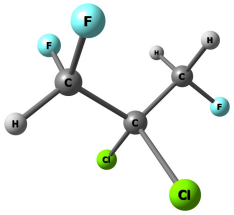
Atom	X	Y	Z
C	0.576366822434	0.886741159318	0.761544441539
C	-0.278873283799	-0.111859350155	-0.053605557221
C	0.253225939010	-0.358570838144	-1.469465993672
F	1.803906151395	0.379554138029	0.968829483209
F	0.710082310666	2.023489519627	0.040285669800
H	0.104599241815	1.118012266924	1.722304530638
Cl	-1.919573165023	0.606098276138	-0.226670453502
Cl	-0.363254126224	-1.646171147463	0.863040314885
H	-0.445572057135	-1.006249842858	-2.006362806896
H	0.335656306959	0.607212338602	-1.978316287224
F	1.483455859901	-0.951155520017	-1.412585341556

Atom	X	Y	Z
C	0.552025971447	-0.911645821526	0.748683629010
C	-0.273591876885	0.123982358237	-0.050653959852
C	0.262600030611	0.373044334417	-1.464557400267
F	0.648540671870	-2.042196102066	0.011912932079
F	1.795264246826	-0.445762346684	0.959325115299
H	0.075547227671	-1.141025676120	1.707570323847
Cl	-0.307944812611	1.647700234890	0.886670232405
Cl	-1.936277602627	-0.540145442374	-0.228757062008
H	0.313688488435	-0.587899434930	-1.986512903726
H	-0.416934383174	1.049334906211	-1.990797804193
F	1.510833038437	0.926219989945	-1.403166102594

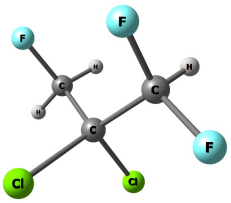
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
71.3851	0.106
130.5629	0.326
165.2287	0.0294
199.5008	0.245
241.7668	0.316
280.4729	1.22
297.6333	0.265
388.8765	0.482
406.7086	0.296
445.9054	3.82
573.2526	1.93
724.4101	8.77
865.5911	18.3
902.0520	1.91
1072.9691	8.63
1108.5436	3.56
1133.6620	12.4
1160.9110	21.7
1197.8611	8.24
1290.1022	0.561
1377.4352	2.83
1389.7639	1.54
1426.7897	3.37
1494.1642	0.917
3057.7038	1.77
3080.9117	3.02
3117.5255	1.33

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
71.3846	0.106
130.5634	0.326
165.2286	0.0294
199.5009	0.245
241.7668	0.316
280.4723	1.22
297.6332	0.265
388.8760	0.482
406.7086	0.296
445.9055	3.82
573.2528	1.93
724.4102	8.77
865.5912	18.3
902.0512	1.91
1072.9690	8.63
1108.5436	3.56
1133.6630	12.4
1160.9110	21.7
1197.8601	8.24
1290.1018	0.561
1377.4349	2.83
1389.7637	1.54
1426.7893	3.37
1494.1641	0.917
3057.7038	1.77
3080.9121	3.02
3117.5255	1.33



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



$\Delta E = 1.83$ kcal mol^{-1}
Population = 0.016

Optimized Coordinates (Angstroms)

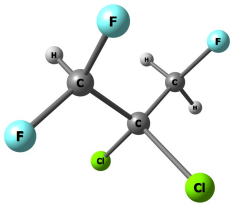
Atom	X	Y	Z
C	-1.434104583938	0.010118462779	-0.255447000904
C	0.097635578025	0.003617160831	-0.065726506254
C	0.471773609329	0.012333353897	1.418145120553
F	-1.958703251516	-1.073791839286	0.358104095478
F	-1.947506127271	1.108034785714	0.342473566716
H	-1.708482943073	0.003938493485	-1.314650218937
Cl	0.758826370678	1.461933320176	-0.876691876680
Cl	0.743763947946	-1.472884048432	-0.855655147408
H	0.053002885735	0.913866602956	1.876424652074
H	0.043808890142	-0.878194081271	1.889269619314
F	1.826408623942	0.006461789150	1.568574696049

Atom	X	Y	Z
C	0.153733006571	-1.135528741125	-0.633592490780
C	-0.156552493869	0.267173078554	-0.066278426237
C	0.681406183827	1.374399501425	-0.718811542089
F	1.444078939036	-1.440271972365	-0.400400654146
F	-0.616968485032	-2.063521240967	-0.043102130282
H	-0.031389835699	-1.148295144097	-1.715841969940
Cl	0.100461507087	0.263045088419	1.700431397070
Cl	-1.875217306322	0.632577018381	-0.465228992867
H	0.538393635497	1.332536914566	-1.805880220834
H	0.336455472472	2.342608144427	-0.344951122724
F	2.005315376433	1.211199352782	-0.428656847171

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
84.5244	0.306
102.9808	0.168
161.3930	0.322
177.4959	0.202
241.5154	0.158
266.8171	0.544
313.5079	0.0878
361.7978	0.183
398.3329	0.745
561.8927	3.04
567.9432	3.36
709.1817	5.18
747.8183	16.8
998.4409	5.02
1078.6474	5.67
1129.6559	18.8
1131.7392	2.11
1139.2784	5.51
1172.2812	22.6
1278.9352	2.76
1383.8718	1.18
1385.6599	4.56
1419.6154	0.702
1502.7523	0.610
3053.3622	1.77
3091.7866	2.68
3110.9547	1.29

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
70.7673	0.132
127.2594	0.333
173.0748	0.0750
196.3127	0.407
224.0296	0.222
264.8806	0.346
304.3885	0.0783
358.0464	0.119
408.3916	0.364
525.7673	3.26
606.3506	7.30
653.9668	5.59
861.6967	19.2
920.9428	0.995
1073.8162	1.98
1120.2548	0.633
1140.9741	8.21
1169.1953	26.0
1191.6176	12.0
1293.3145	1.53
1376.5113	4.50
1396.5460	3.60
1421.7473	2.56
1496.6118	0.781
3036.5622	0.811
3046.8658	5.74
3105.9122	1.79



$\Delta E = 1.83$ kcal mol^{-1}
Population = 0.016

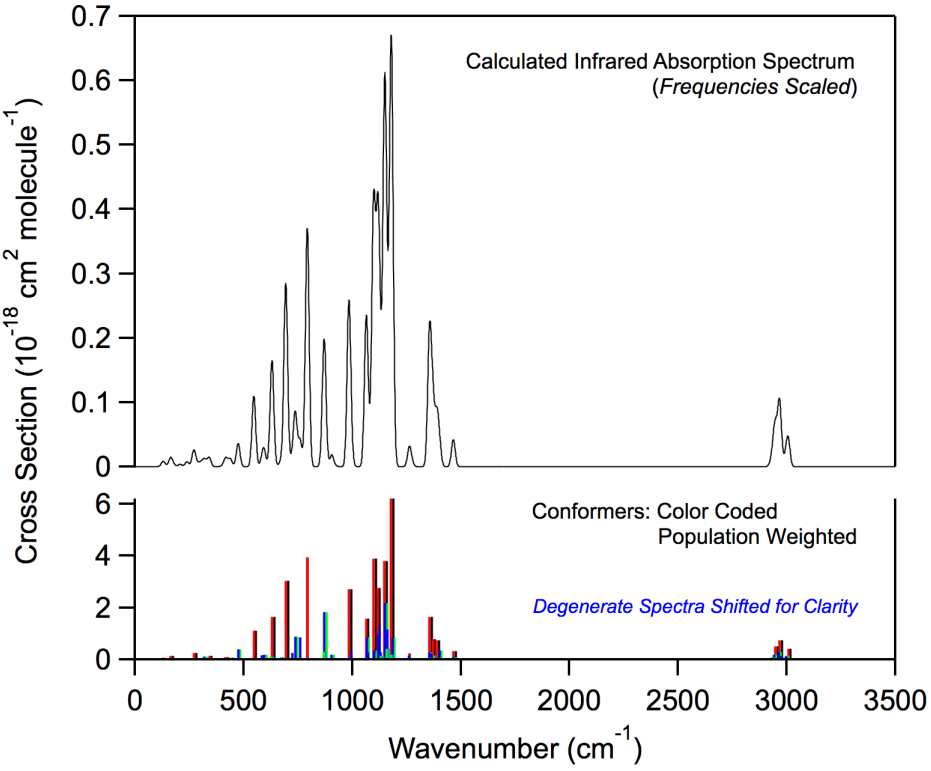
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	0.161985310722	1.130707380467	-0.637518632058
C	-0.156418663527	-0.267566777060	-0.063807829378
C	0.674986333455	-1.382619656228	-0.711379009182
F	-0.603223948862	2.065856251269	-0.051189937281
F	1.454112790773	1.428972640206	-0.405820387874
H	-0.023177227647	1.139634216833	-1.719799771839
Cl	-1.877234058899	-0.624738540647	-0.460939809297
Cl	0.100819015621	-0.256911815854	1.702842024544
H	0.324438224935	-2.347089790468	-0.333088358744
H	0.532087630432	-1.344865609387	-1.798613107335
F	1.999860592994	-1.225829299131	-0.422096181556

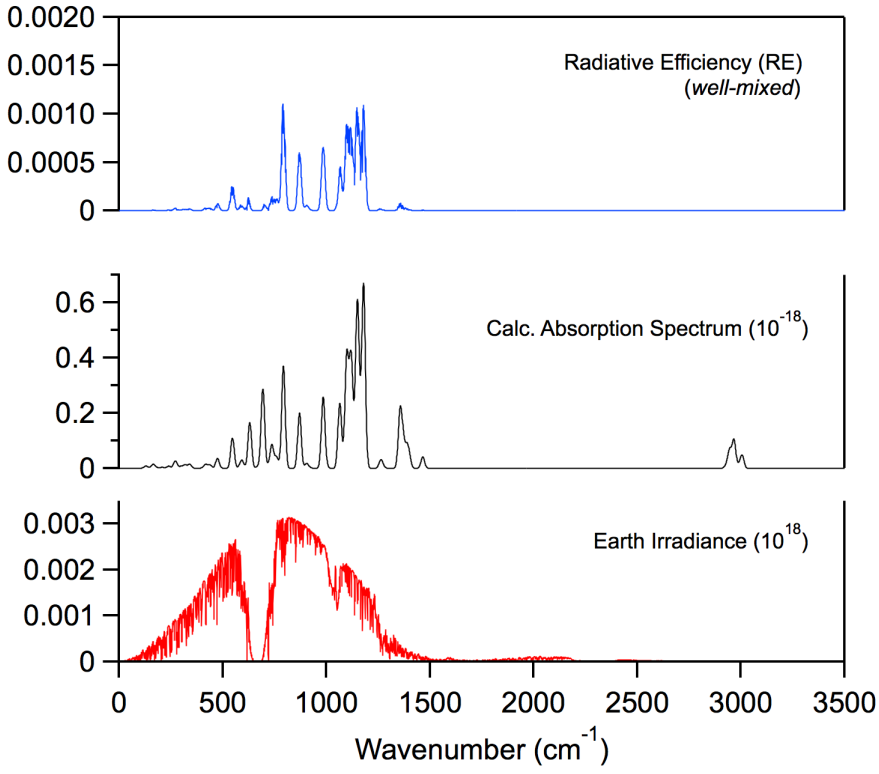
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
70.7667	0.132
127.2585	0.333
173.0745	0.0750
196.3127	0.407
224.0295	0.222
264.8807	0.346
304.3888	0.0783
358.0459	0.119
408.3914	0.364
525.7671	3.26
606.3506	7.30
653.9670	5.59
861.6965	19.2
920.9424	0.995
1073.8158	1.98
1120.2547	0.633
1140.9738	8.21
1169.1949	26.0
1191.6172	12.0
1293.3145	1.53
1376.5113	4.50
1396.5461	3.60
1421.7474	2.56
1496.6125	0.781
3036.5623	0.811
3046.8661	5.74
3105.9126	1.79

Infrared Spectrum

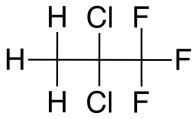


Radiative Efficiency



HCFC-243ab

Molecular Formula:	$CH_3CCl_2CF_3$
Name:	2,2-Dichloro-1,1,1-trifluoropropane
CAS number:	7126-01-4
Molecular Weight:	166.96



Global Atmospheric Lifetime (years):	8.33
Tropospheric Atmospheric Lifetime (years):	10.0
Stratospheric Atmospheric Lifetime (years):	49.3
Ozone Depletion Potential (ODP):	0.085

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.216	0.205
Global Warming Potential (GWP_H):		
GWP_{20}	2207	2091
GWP_{100}	657	623
Global Temperature Potentials (GTP_H)		
GTP_{20}		1465
GTP_{50}		195
GTP_{100}		89

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

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

OH Reactivity

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

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

$\tau^{OH}_{Global} = 9.67$ years

$\tau^{OH}_{Trop} = 10.0$ years

$\tau^{OH}_{Strat} = 269.2$ years

Fractional Atmospheric Loss: 0.862

O(^{1}D) Reactivity

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

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

$\tau_{O(^1D)} = 250$ years

Fractional Atmospheric Loss: 0.034

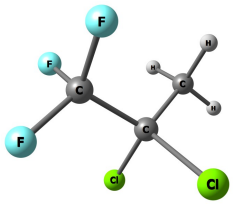
UV Photolysis

UV Spectrum: *No Recommendation*

$\tau_{hv} = 80$ years

Fractional Atmospheric Loss: 0.104

Molecular Structure and Infrared Spectrum (1 conformer)



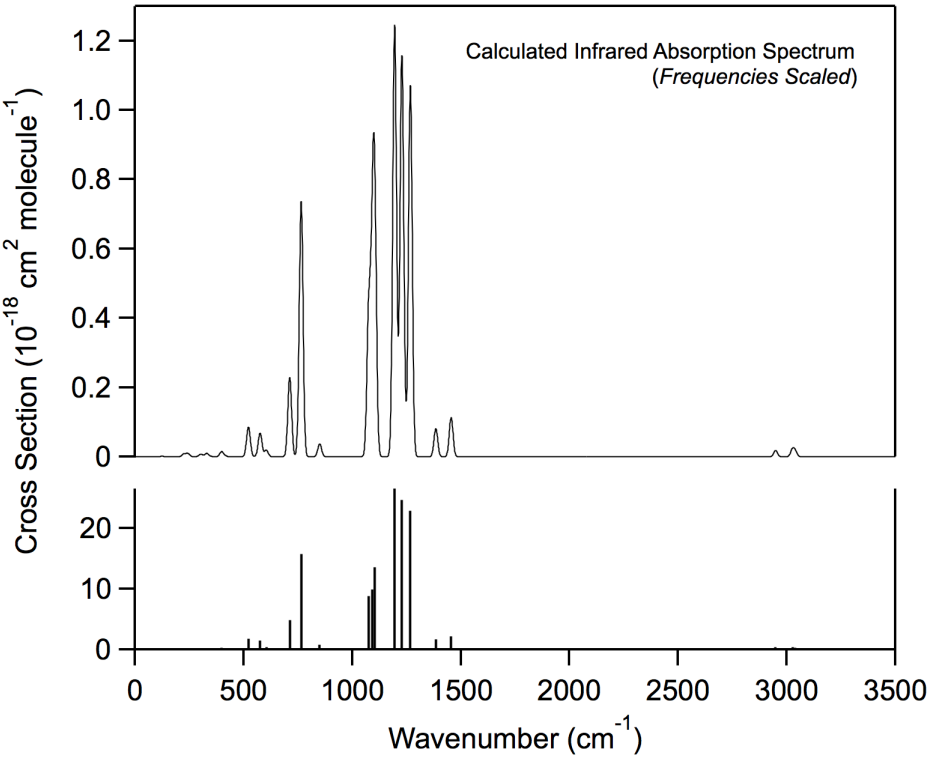
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-0.384035861095	1.011666982770	0.000000000000
C	0.413732891206	-0.318648904839	0.000000000000
C	1.913740433042	-0.068037653365	0.000000000000
F	-1.695191038678	0.813767730844	0.000000000000
F	-0.062067488812	1.730093303806	1.080261112151
F	-0.062067488812	1.730093303806	-1.080261112151
Cl	-0.062150910160	-1.241090205201	-1.469507401450
Cl	-0.062150910160	-1.241090205201	1.469507401450
H	2.444534561771	-1.020122780032	0.000000000000
H	2.188385905867	0.499856713722	-0.891389885797
H	2.188385905867	0.499856713722	0.891389885797

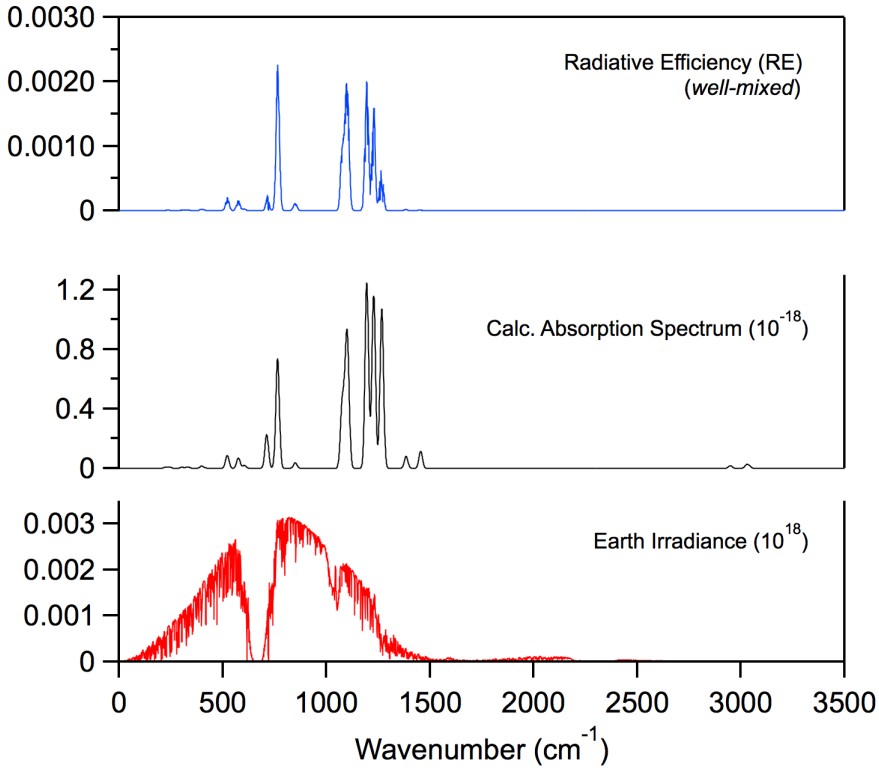
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
75.1998	0.0256
181.3772	0.171
200.8776	0.190
264.0027	0.154
264.3590	0.00262
292.2179	0.200
309.4478	0.0228
365.2023	0.314
383.1160	0.0430
495.9763	1.82
552.7547	1.46
583.0450	0.404
697.3049	4.85
753.0620	15.7
843.3528	0.792
1082.4107	8.76
1100.7392	9.93
1111.5203	13.5
1208.6595	26.5
1244.0361	24.7
1285.3792	22.8
1409.5276	1.73
1479.6325	0.228
1484.5799	2.21
3065.6281	0.386
3147.9669	0.447
3161.8777	0.301

Infrared Spectrum

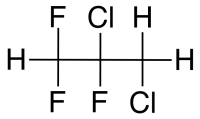


Radiative Efficiency



HCFC-243ba

Molecular Formula: $CHF_2CClFCH_2Cl$
Name: 1,2-Dichloro-2,3,3-trifluoropropane
CAS number: –
Molecular Weight: 166.96



Global Atmospheric Lifetime (years): 3.63
  Tropospheric Atmospheric Lifetime (years): 3.88
  Stratospheric Atmospheric Lifetime (years): 58.0
Ozone Depletion Potential (ODP): 0.033

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.162	0.146
Global Warming Potential (GWP_H):		
GWP_{20}	792	713
GWP_{100}	215	194
Global Temperature Potentials (GTP_H)		
GTP_{20}		332
GTP_{50}		37
GTP_{100}		27

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 1.51 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 0.966 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 3.75$ years
$\tau^{OH}_{Trop} = 3.88$ years
$\tau^{OH}_{Strat} = 114.3$ years

Fractional Atmospheric Loss: 0.969

O(^{1}D) Reactivity

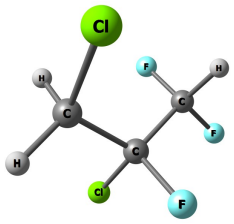
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 1.5 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)} = 250$ years
Fractional Atmospheric Loss: 0.015

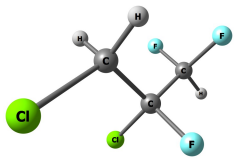
UV Photolysis

UV Spectrum: *No Recommendation*
$\tau_{hv} = 225$ years
Fractional Atmospheric Loss: 0.016

Molecular Structure and Infrared Spectrum (4 conformers)



E = 0
Population = 0.630



$\Delta E = 0.81$ kcal mol^{-1}
Population = 0.161

Optimized Coordinates (Angstroms)

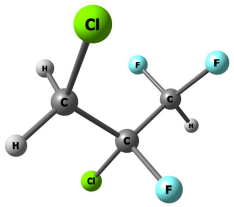
Atom	X	Y	Z
C	0.527982499280	1.155980652240	0.079120352313
C	0.160683618647	-0.332179618533	0.238604725879
C	-1.058516325359	-0.762115529050	-0.567528059233
F	1.684587690595	1.410903219413	0.712473473255
F	0.671412192695	1.438060153929	-1.233912894351
H	-0.262359185499	1.785315514581	0.502664128983
F	-0.033149197196	-0.560134177768	1.556726893504
Cl	1.542340937871	-1.347770352953	-0.329109951267
H	-0.898867793703	-0.555707876799	-1.623516235997
H	-1.243873767448	-1.822634781069	-0.407153086816
Cl	-2.538604669882	0.128463796007	-0.047514346270

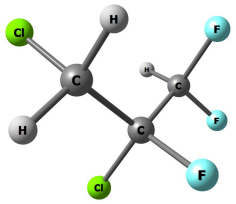
Atom	X	Y	Z
C	1.684198416827	0.177681201874	0.082341533062
C	0.182157448992	-0.095087607287	0.313694077932
C	-0.683277673333	0.795258462009	-0.570471589948
F	1.990033054569	-0.015406892275	-1.216303520329
F	1.929129988053	1.473059880768	0.386956698757
H	2.303575731939	-0.467653264792	0.713824895212
F	-0.060208308119	0.150889835997	1.621409070530
Cl	-0.108320384668	-1.843015025836	-0.004814337936
H	-0.401829215943	1.832126906573	-0.383474988507
H	-0.519378126531	0.549397990116	-1.617741114858
Cl	-2.426555931787	0.634723512851	-0.210761723916

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
65.1898	0.282
105.2460	0.410
154.8338	0.161
194.7384	0.177
226.3648	0.644
283.9923	0.0971
327.9937	0.301
377.1278	0.123
484.7000	0.114
535.3039	3.58
638.7101	7.47
672.9442	9.90
741.0946	7.35
890.1357	0.972
990.7754	9.61
1093.8137	4.43
1152.9660	11.2
1174.3394	26.8
1205.3294	10.2
1271.5492	2.65
1302.1752	1.32
1389.3785	2.68
1402.9218	3.24
1456.2644	1.85
3079.2977	2.67
3118.4949	0.624
3191.1958	0.0319

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
79.9591	0.00113
82.1140	0.508
144.4718	0.261
185.8133	0.170
225.9705	0.387
311.8377	0.169
316.9456	0.0781
400.8559	0.414
458.2716	1.32
551.4582	4.91
608.6884	4.31
673.4429	6.61
825.7942	3.45
875.1036	3.15
986.4753	14.5
1107.8756	6.80
1142.4592	24.1
1170.2580	1.55
1188.5181	10.3
1241.1258	12.1
1320.0546	2.07
1383.8946	1.52
1390.9143	6.47
1464.6244	1.11
3084.8819	3.21
3104.2151	0.625
3175.1029	0.0359





$\Delta E = 0.98$ kcal mol^{-1}
Population = 0.120

$\Delta E = 1.62$ kcal mol^{-1}
Population = 0.041

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	0.487954524032	1.254559983787	0.221032845449
C	0.390475342503	-0.284573624941	0.309995227610
C	-0.582140752493	-0.953040643770	-0.656500890062
F	0.630614268198	1.611578824613	-1.073348216128
F	-0.641637508388	1.807962451662	0.698289658429
H	1.342526999673	1.621071615264	0.800381616924
F	0.114023933650	-0.605887911914	1.589088299913
Cl	2.041024555656	-0.927061988268	-0.099427744195
H	-0.385170070308	-0.604541458234	-1.668369741059
H	-0.455408281519	-2.032564871815	-0.598294833242
Cl	-2.299485011004	-0.595600376384	-0.265505223641

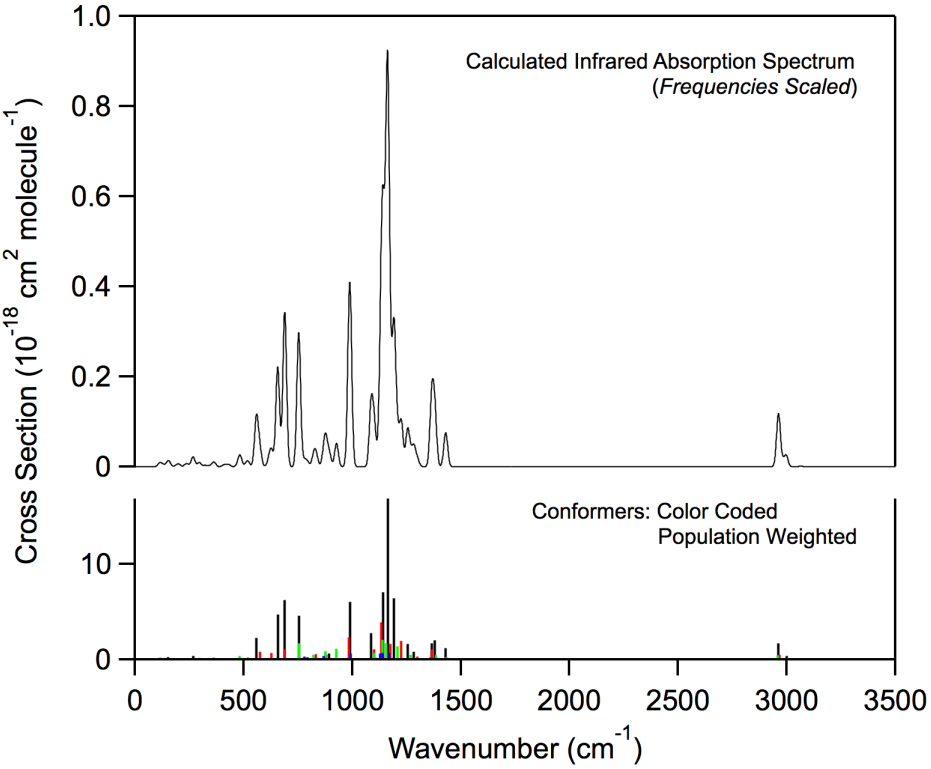
Atom	X	Y	Z
C	0.920845487121	0.743504529211	-0.571391542636
C	0.247698208276	-0.233449710421	0.413665917353
C	-1.109360922638	0.238489655072	0.930864557229
F	0.949847736096	1.963341981093	0.019511197768
F	2.186001717557	0.349295682326	-0.790176607184
H	0.379487744367	0.810154206962	-1.518755803272
F	1.051858330183	-0.340429187049	1.502760957340
Cl	0.134119295798	-1.846471771062	-0.372771784036
H	-1.516149203167	-0.512219307581	1.606592270243
H	-0.959004381550	1.181515315689	1.456042019443
Cl	-2.306111012044	0.527430605760	-0.371775182248

Infrared Absorption Spectrum (unscaled frequencies)

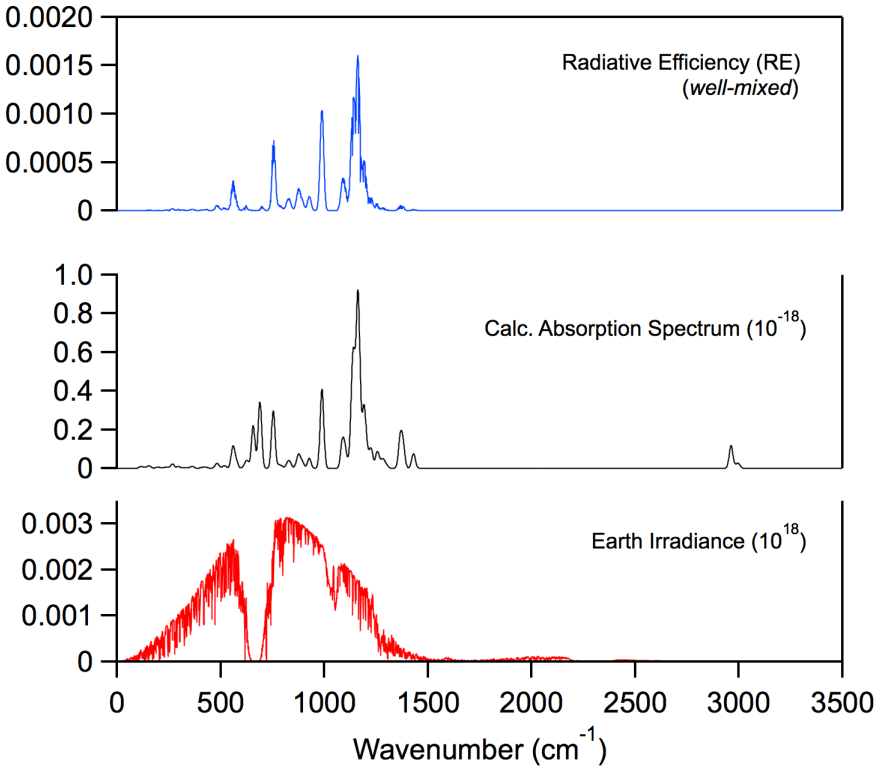
Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
53.7826	0.0885
114.3923	0.347
160.1169	0.132
191.8373	0.0975
256.2236	1.58
271.9239	0.0607
314.6065	0.177
393.8503	0.493
452.2353	3.02
493.1592	1.94
595.6517	1.77
741.3638	14.2
813.9695	4.26
870.4938	7.33
925.1961	9.29
1109.1380	5.88
1149.0063	17.4
1165.8055	14.5
1222.3974	11.7
1285.7127	4.44
1303.1200	0.583
1389.9963	1.06
1409.2369	3.83
1458.5489	2.17
3075.7501	3.62
3115.5475	0.749
3184.9225	0.0201

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
64.9586	0.204
93.9069	0.267
145.5894	0.0594
206.3322	0.603
252.7563	0.208
295.5009	0.344
336.2700	0.479
376.2530	0.319
442.0309	0.867
526.5101	2.46
599.3657	3.50
767.5252	7.08
782.8996	5.80
861.3020	8.82
994.9197	14.8
1117.5046	4.64
1137.1902	15.6
1148.5181	16.4
1182.6647	17.7
1243.3861	3.21
1311.6479	0.752
1392.7206	1.60
1407.8272	2.48
1462.7679	1.78
3102.8521	2.11
3104.8071	1.16
3174.7628	0.0111

Infrared Spectrum

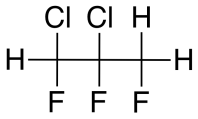


Radiative Efficiency



HCFC-243bb

Molecular Formula:	$CHFClCClFCH_2F$
Name:	1,2-Dichloro-1,2,3-trifluoropropane
CAS number:	1379241-46-9
Molecular Weight:	166.96



Global Atmospheric Lifetime (years):	2.67
Tropospheric Atmospheric Lifetime (years):	2.82
Stratospheric Atmospheric Lifetime (years):	49.7
Ozone Depletion Potential (ODP):	0.027

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.184	0.161
Global Warming Potential (GWP_H):		
GWP_{20}	662	578
GWP_{100}	179	157
Global Temperature Potentials (GTP_H)		
GTP_{20}		235
GTP_{50}		29
GTP_{100}		22

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 2.08 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 1.33 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 2.73$ years

$\tau^{OH}_{Trop} = 2.82$ years

$\tau^{OH}_{Strat} = 85.9$ years

Fractional Atmospheric Loss: 0.977

O(^{1}D) Reactivity

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

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

$\tau_{O(^1D)} = 250$ years

Fractional Atmospheric Loss: 0.011

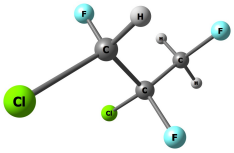
UV Photolysis

UV Spectrum: *No Recommendation*

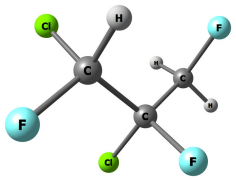
$\tau_{hv} = 225$ years

Fractional Atmospheric Loss: 0.012

Molecular Structure and Infrared Spectrum (8 conformers)



E = 0
Population = 0.399



$\Delta E = 0.73$ kcal mol^{-1}
Population = 0.115

Optimized Coordinates (Angstroms)

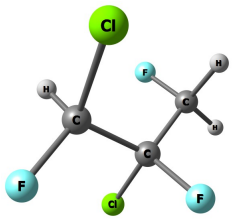
Atom	X	Y	Z
C	0.552398836285	-0.812274954372	-0.210494541497
C	-0.501935406470	0.219643675368	0.229172785438
C	-1.893651385052	-0.164088594297	-0.274660576785
Cl	2.172996145334	-0.451023030182	0.442743192507
H	0.262096180617	-1.790405751282	0.177677351321
F	0.591408001121	-0.852957411699	-1.561165214055
Cl	-0.129486148951	1.854942511164	-0.414875990876
F	-0.509411010591	0.256623572559	1.580557083756
H	-2.625131910636	0.538852984601	0.134180214904
H	-1.914487882233	-0.143411666650	-1.366872913841
F	-2.178497419425	-1.434982335210	0.169843609129

Atom	X	Y	Z
C	0.725965463392	-0.293890307082	0.713769627331
C	-0.616116842942	0.183698268667	0.126083685521
C	-1.329310553818	-0.856410022103	-0.729937470971
Cl	1.886136701747	-0.802009077464	-0.555090499502
F	1.265495345821	0.689417006587	1.455556995932
H	0.536177139476	-1.169494178180	1.337258956440
Cl	-0.413288799355	1.680577350703	-0.843263031230
F	-1.392331203669	0.471314204037	1.206001204935
H	-2.337737083013	-0.492418160788	-0.948762354776
H	-0.780026339784	-1.033596795592	-1.656682239802
F	-1.408174827854	-2.024673288786	-0.006422873878

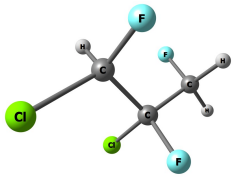
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
69.3344	0.164
114.1212	0.556
168.9904	0.194
184.3145	0.0747
205.5662	0.491
308.5440	0.685
327.3914	0.167
377.5528	0.0255
414.6927	0.154
506.8951	3.12
571.3253	6.50
661.5640	10.4
833.5707	7.80
947.5904	9.40
1000.3104	13.0
1091.2433	7.05
1130.6979	17.9
1177.1735	7.31
1199.0971	8.43
1282.0485	3.31
1303.2382	1.45
1366.4563	1.84
1411.4489	1.01
1489.4071	0.770
3068.2165	1.51
3113.5102	0.570
3132.9925	1.29

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
64.7662	0.161
112.2521	0.401
168.7330	0.115
181.3493	0.308
229.8866	0.755
311.0980	0.236
334.8790	0.417
380.7166	0.0781
410.1251	0.720
449.0943	0.321
599.2525	7.39
681.1542	6.97
821.0987	16.7
940.9014	6.99
999.0185	15.9
1090.6316	6.39
1146.0739	17.7
1172.5884	8.92
1198.0466	6.81
1266.1271	3.81
1301.0823	0.188
1371.5823	2.83
1417.0965	0.662
1491.1144	1.19
3068.7960	1.53
3114.9485	0.604
3136.5576	1.37



$\Delta E = 0.78$ kcal mol^{-1}
Population = 0.106



$\Delta E = 0.85$ kcal mol^{-1}
Population = 0.095

Optimized Coordinates (Angstroms)

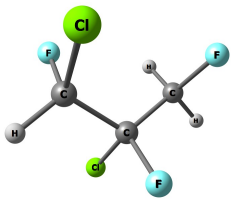
Atom	X	Y	Z
C	0.709883416455	0.405436650740	-0.569053676009
C	-0.426206270983	0.002432594215	0.388317194656
C	-0.690802976079	-1.501134479258	0.438867142071
Cl	2.264270637758	-0.336179858006	-0.031997400174
H	0.511703555005	0.033846226444	-1.574142031535
F	0.853715335470	1.742013463784	-0.574743036417
Cl	-1.916250723781	0.849821630675	-0.193566215826
F	-0.149677459369	0.426363871407	1.639971407551
H	0.180585378736	-1.999533822478	0.874676275859
H	-1.575559738447	-1.685224923070	1.055111503750
F	-0.897319154764	-1.968450354453	-0.833196163926

Atom	X	Y	Z
C	0.681341799819	-0.586702659288	-0.433554580085
C	-0.457265280122	0.054170244169	0.383437422327
C	-1.734254457814	-0.788477373769	0.316444778424
Cl	2.243470180558	0.235496564459	-0.167926438823
F	0.792508808324	-1.880762896293	-0.035306200596
H	0.456755879507	-0.549038033110	-1.499176647414
Cl	-0.782015183745	1.702180199984	-0.260097496887
F	-0.102644694376	0.140853370730	1.684664814546
H	-1.526765310000	-1.762544749987	0.769903595215
H	-2.529110435844	-0.276425320450	0.866078789572
F	-2.101645306307	-0.960339346446	-0.992216036279

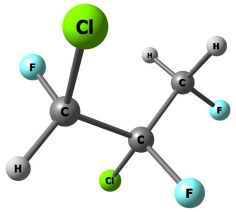
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
59.5488	0.131
95.5363	0.335
163.2191	0.0500
204.4870	0.668
253.8750	0.374
270.0102	0.217
326.0902	0.493
387.3297	0.191
401.3293	0.572
482.1240	0.699
604.4870	4.89
706.1323	28.3
777.5197	5.38
858.1684	2.07
1072.5199	10.7
1115.0715	14.2
1145.9754	14.8
1168.7748	0.706
1211.7548	11.2
1264.8906	2.84
1286.2574	0.721
1379.6823	1.13
1420.2864	0.403
1500.3404	1.42
3060.1944	2.04
3119.2416	1.78
3135.0172	0.447

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
64.2915	0.117
95.8518	0.388
156.1598	0.103
206.1315	0.549
228.2257	0.105
304.8105	0.845
326.6966	0.168
383.2057	0.0242
427.4229	1.06
484.0221	1.63
552.0966	7.90
749.5367	12.2
790.3596	5.35
890.5283	9.04
1079.9009	14.8
1096.5837	10.3
1117.4137	18.9
1145.7630	0.178
1207.3995	10.8
1267.2988	1.60
1290.5501	1.75
1367.9638	0.438
1415.5160	1.53
1499.5900	0.949
3060.3020	2.32
3121.2497	1.55
3134.9015	0.541



ΔE = 1.00 kcal mol^{-1}
Population = 0.073



ΔE = 1.05 kcal mol^{-1}
Population = 0.068

Optimized Coordinates (Angstroms)

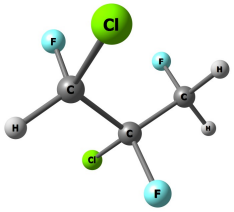
Atom	X	Y	Z
C	0.452406178570	0.941048644152	0.090232005002
C	-0.533217626922	-0.230004535413	0.281227483546
C	-0.461328291447	-1.347586069629	-0.759268876098
Cl	2.140153535994	0.457877663702	0.452457647014
F	0.372065817371	1.372045968437	-1.188322999254
H	0.207587114964	1.754536705900	0.774530698004
Cl	-2.199046618542	0.485397089329	0.147715871954
F	-0.378716323868	-0.726769546009	1.523622767514
H	-1.289424185998	-2.039550620858	-0.577790697495
H	-0.549459104442	-0.914537067243	-1.759396628429
F	0.725437504319	-2.018220232367	-0.642065271758

Atom	X	Y	Z
C	0.950852870922	0.698187036483	0.071998710891
C	-0.371566849080	-0.066314356243	0.266129917526
C	-0.655241646741	-1.098748518948	-0.822937060186
Cl	2.357210731101	-0.420207460503	0.209820951523
F	0.965166530952	1.275891878311	-1.147056591023
H	1.073749438455	1.451424891323	0.851224709666
Cl	-1.686235514959	1.176700959561	0.282919352374
F	-0.344547828263	-0.659440938275	1.479912997546
H	-0.603258702551	-0.616884042196	-1.803107866459
H	0.099990704898	-1.888695280830	-0.754616133080
F	-1.893166734734	-1.640529168684	-0.627838988779

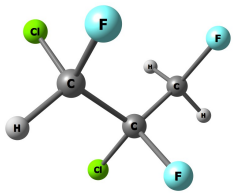
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
54.0438	0.0950
117.5113	0.420
174.5258	0.269
183.3891	0.0727
248.0157	0.264
271.7707	1.62
324.6502	0.120
378.6258	0.296
403.3067	0.274
459.5160	4.21
537.1275	0.778
755.1709	26.8
813.1946	8.75
889.6891	4.91
980.8943	5.42
1114.5815	11.0
1126.6689	16.0
1198.2712	6.41
1219.8383	7.09
1292.0892	4.15
1310.2162	2.43
1365.3665	0.369
1428.4883	0.771
1491.2896	0.732
3061.8115	1.71
3116.9095	0.680
3122.9390	1.59

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
71.4605	0.365
92.0012	0.299
159.3291	0.353
177.7350	0.189
254.0550	0.231
267.0223	0.385
321.8487	0.185
381.3862	0.101
393.8800	0.370
499.3074	1.11
612.4138	6.64
671.6232	10.5
758.7762	23.5
901.1725	4.34
1055.6484	3.56
1127.0403	16.5
1130.4260	11.4
1179.1018	0.842
1193.8026	13.8
1287.2790	0.173
1294.2708	6.66
1367.0197	0.412
1427.4601	0.392
1499.9586	0.449
3057.3849	1.90
3118.0693	1.34
3122.1401	0.737



$\Delta E = 1.07$ kcal mol^{-1}
Population = 0.066



$\Delta E = 1.71$ kcal mol^{-1}
Population = 0.022

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	0.719151650791	0.446896520762	-0.635634733566
C	-0.424849389725	0.289956493840	0.385799613578
C	-0.554991090424	-1.080966447503	1.052032804617
Cl	2.314366071068	0.221334027283	0.175519913703
F	0.592247396391	-0.456306280816	-1.621470855359
H	0.722764053775	1.459683272011	-1.042424112251
Cl	-1.953192581344	0.689664061639	-0.489778984034
F	-0.238146573688	1.205895942910	1.365820730830
H	0.394264984979	-1.322906277101	1.542098145314
H	-1.350544016480	-1.014657723378	1.801414225151
F	-0.854647505344	-2.041787589645	0.131278252017

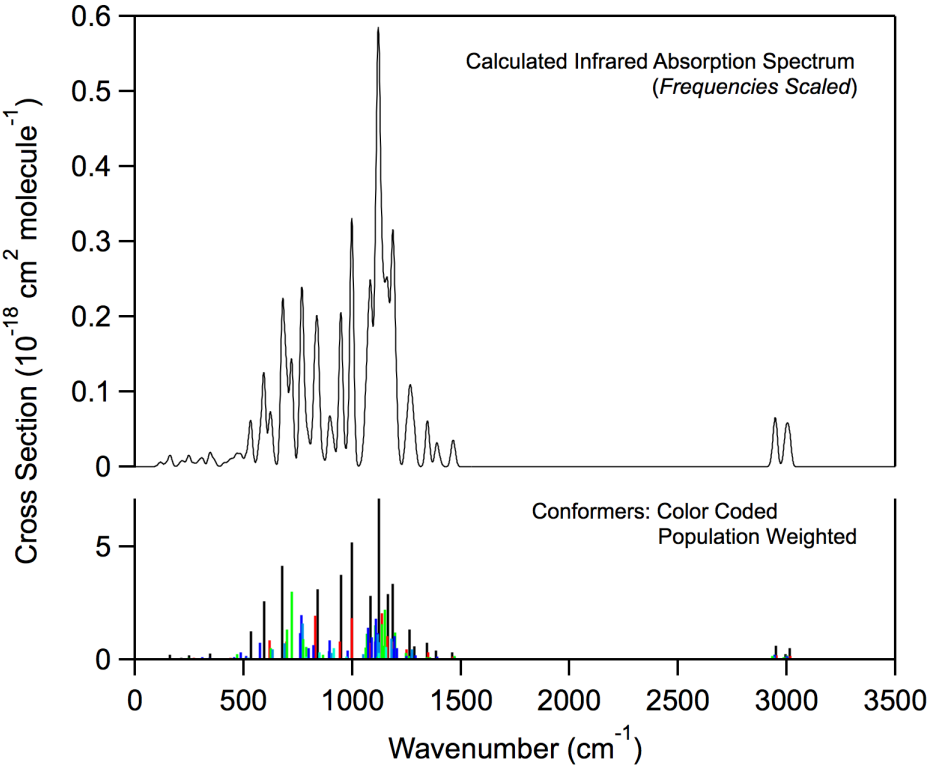
Atom	X	Y	Z
C	0.797675855395	-0.004269247021	0.730799636049
C	-0.651202478964	-0.014344788761	0.191957727814
C	-0.895313329075	-0.775928020046	-1.108060818546
Cl	1.974648708365	0.579538816879	-0.491335251372
H	0.867437149624	0.667889955242	1.588248199733
F	1.126207901507	-1.255989664254	1.104288576763
Cl	-1.198581425097	1.686704947304	-0.050573869579
F	-1.397565435283	-0.568278169631	1.180337600293
H	-1.970186493114	-0.755347780709	-1.315508363326
H	-0.347353790972	-0.305428994526	-1.927885208856
F	-0.480948662387	-2.071912054476	-0.952583228972

Infrared Absorption Spectrum (unscaled frequencies)

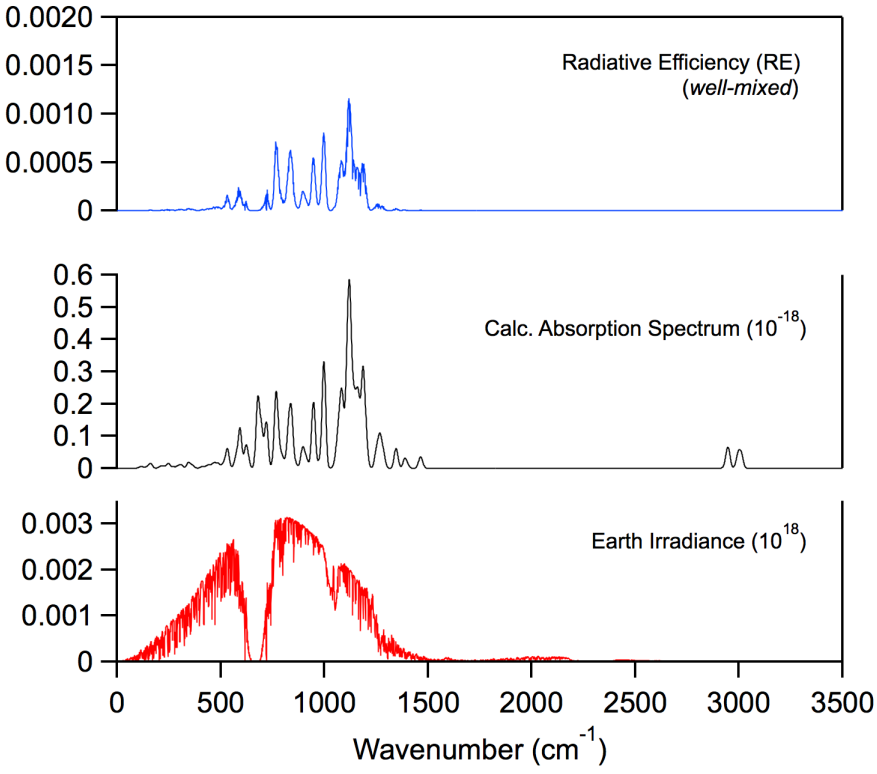
Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
52.8680	0.135
116.7104	0.315
166.0933	0.0901
192.5428	0.141
253.6854	0.764
275.4400	0.860
357.5417	0.0430
374.3354	0.722
425.1249	0.498
440.0110	3.58
576.6008	0.00722
682.4773	20.3
762.6332	13.7
901.6733	0.295
1066.6637	8.15
1127.3852	1.89
1156.4620	9.28
1160.5943	33.8
1220.0698	0.898
1277.9191	2.51
1290.5739	0.348
1365.9007	1.46
1429.8976	0.519
1499.8915	1.22
3049.9539	2.29
3106.0802	1.73
3113.3607	1.10

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
54.2587	0.0655
125.2623	0.432
166.3455	0.0315
186.7829	0.130
261.0167	1.52
309.7576	0.191
324.4138	0.224
383.0897	0.204
411.4054	0.361
439.9665	2.19
489.5688	3.39
778.4014	5.77
842.9357	14.0
910.8734	23.2
972.4968	5.67
1102.4028	3.04
1132.7384	13.1
1166.9421	24.7
1214.5610	0.478
1279.7758	2.57
1306.5662	0.977
1370.1913	1.81
1429.1442	1.54
1491.1233	1.05
3061.1999	1.76
3109.2683	0.954
3125.9752	1.58

Infrared Spectrum

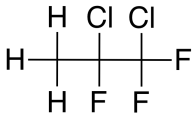


Radiative Efficiency



HCFC-243bc

Molecular Formula:	$CH_3CClFCF_2Cl$
Name:	1,2-Dichloro-1,1,2-trifluoropropane
CAS number:	7126-00-3
Molecular Weight:	166.96



Global Atmospheric Lifetime (years):	15.6
Tropospheric Atmospheric Lifetime (years):	18.7
Stratospheric Atmospheric Lifetime (years):	94.2
Ozone Depletion Potential (ODP):	0.088

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.273	0.264
Global Warming Potential (GWP_H):		
GWP_{20}	4142	4005
GWP_{100}	1549	1498
Global Temperature Potentials (GTP_H)		
GTP_{20}		3431
GTP_{50}		952
GTP_{100}		252

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

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

OH Reactivity

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

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

τ^{OH}_{Global} = 18.0 years
τ^{OH}_{Trop} = 18.7 years
τ^{OH}_{Strat} = 471.3 years

Fractional Atmospheric Loss: 0.868

O(^{1}D) Reactivity

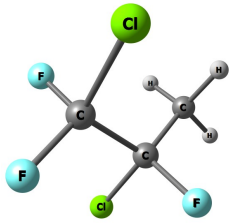
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 1.5 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)}$ = 250 years
Fractional Atmospheric Loss: 0.063

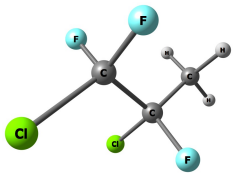
UV Photolysis

UV Spectrum: *No Recommendation*
τ_{hv} = 225 years
Fractional Atmospheric Loss: 0.069

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.591



$\Delta E = 0.41$ kcal mol^{-1}
Population = 0.297

Optimized Coordinates (Angstroms)

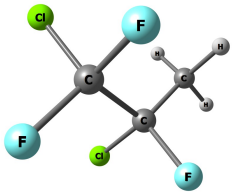
Atom	X	Y	Z
C	-0.627088891367	1.633927178527	0.911407533253
C	-0.587115988949	0.513679071098	-0.106857039730
C	0.579578321076	-0.493275076864	0.095397155453
H	-1.501571024031	2.256082583208	0.715497125961
H	-0.692555728023	1.226698361316	1.920768639299
H	0.276044364581	2.241235587032	0.820174141549
F	-0.477286447630	1.005882550103	-1.361324663766
Cl	-2.122131162276	-0.450688370449	-0.021468176218
F	0.530261197501	-1.006554659293	1.324821756147
F	0.510253791855	-1.481592571156	-0.788227484278
Cl	2.169289567262	0.332644346478	-0.116693987670

Atom	X	Y	Z
C	-1.616014787631	1.444781240353	0.156189848933
C	-0.767744134312	0.255091685024	-0.259225239946
C	0.695888088859	0.392713737207	0.249346061021
H	-1.189698506206	2.353797502001	-0.273584155604
H	-2.630063150030	1.304605396689	-0.220295507745
H	-1.642022797086	1.532443039664	1.242824301647
F	-0.715741713141	0.170622652488	-1.608573736691
Cl	-1.476853905725	-1.271885086101	0.384848633304
F	1.174074048408	1.568245830574	-0.183659728003
F	0.714232942004	0.406473600572	1.582833273579
Cl	1.769639914860	-0.902243598472	-0.348905750495

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
67.6771	0.0760
173.9669	0.123
214.4590	0.176
234.1843	0.170
254.0313	0.0781
308.2449	0.156
334.6473	0.122
356.2008	0.193
390.2631	0.160
420.1822	0.100
514.2043	0.0869
558.0003	2.82
669.5717	2.19
725.2267	30.5
929.5262	12.5
962.0192	15.4
1108.6908	5.19
1143.1778	19.3
1208.2382	36.0
1227.2172	6.11
1276.1277	4.44
1410.8381	2.85
1478.3001	0.257
1484.5685	1.05
3070.0335	0.234
3152.4694	0.549
3165.0359	0.272

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
69.2635	0.121
169.8459	0.162
199.9916	0.157
232.7216	0.00837
290.0787	0.388
311.9404	0.0357
318.6898	0.188
357.0793	0.0702
416.2754	0.443
428.9890	0.165
486.0815	1.72
552.5936	4.14
651.8325	2.72
771.9080	13.5
924.6161	13.3
1005.0979	27.2
1105.2071	22.7
1129.0407	7.65
1185.3557	11.1
1205.8901	26.5
1263.1738	4.01
1406.0718	1.60
1478.5489	0.211
1485.2059	1.02
3069.2768	0.370
3153.5695	0.495
3164.6362	0.318



$\Delta E = 0.99$ kcal mol^{-1}
Population = 0.112

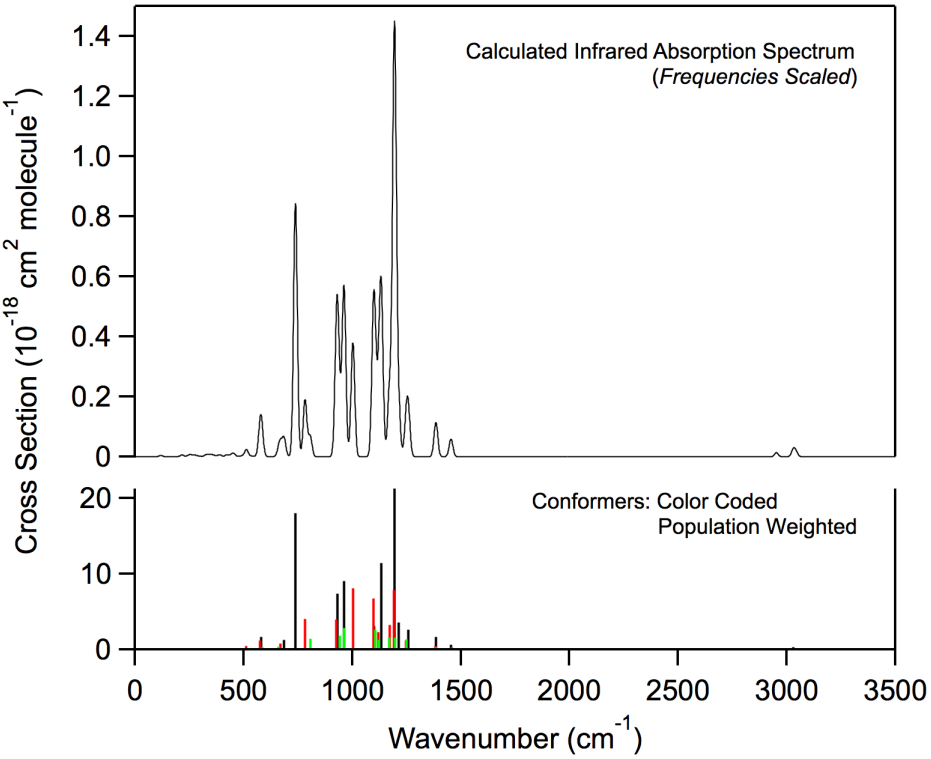
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-0.897604645275	0.496232054825	1.717801424148
C	-0.752364417368	0.319535411663	0.221055507179
C	0.720205452381	0.328331654175	-0.285027370472
H	-1.958539314764	0.594787080851	1.953144259147
H	-0.485241444334	-0.357403259948	2.254609270736
H	-0.374052160777	1.406709840031	2.020065848746
F	-1.335706953085	1.367811878457	-0.420741345615
Cl	-1.565105841454	-1.187399979676	-0.339443513132
F	0.754653696037	0.221845191095	-1.608072079681
F	1.259960200786	1.506375462321	0.053109063176
Cl	1.716826427852	-0.977491333794	0.435674935768

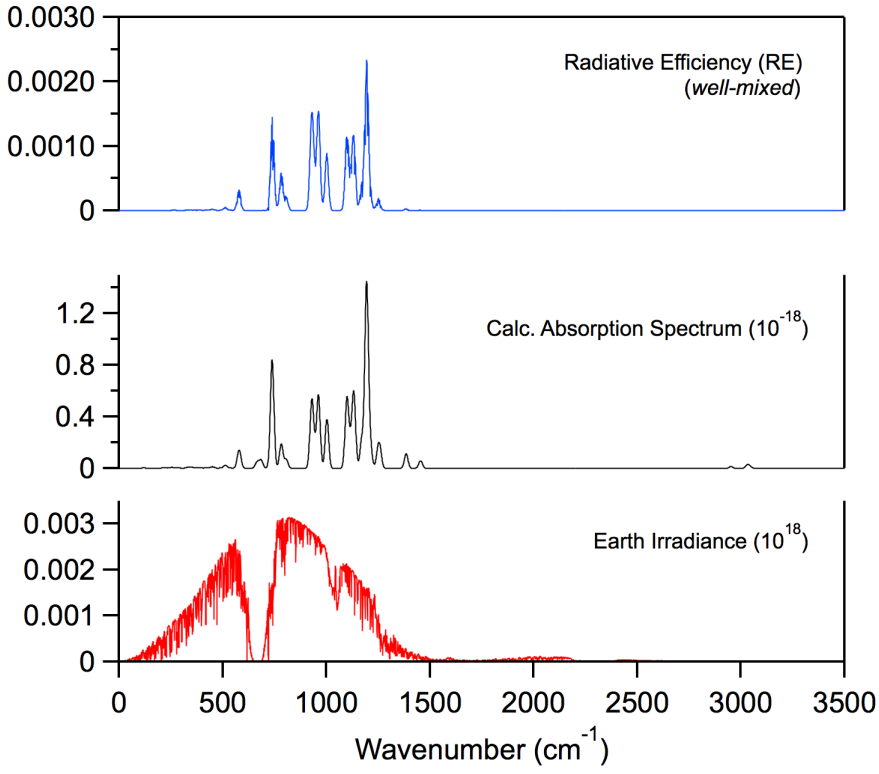
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
72.8419	0.0600
168.6937	0.0515
210.1978	0.301
232.6484	0.0197
290.2740	0.195
307.9281	0.165
316.6177	0.251
378.0333	0.0722
396.6870	0.447
426.3988	0.479
461.0018	0.528
563.5089	2.84
644.2061	3.40
797.0834	12.9
942.7514	16.6
960.7626	25.8
1113.5648	23.7
1131.4144	11.6
1180.3789	14.4
1211.3225	14.2
1267.4496	12.2
1409.9408	2.90
1478.6221	0.414
1483.8431	0.927
3067.7823	0.311
3148.4740	0.485
3170.8138	0.341

Infrared Spectrum

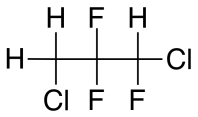


Radiative Efficiency



HCFC-243ca

Molecular Formula:	CH_2ClCF_2CHClF
Name:	1,3-Dichloro-1,2,2-trifluoropropane
CAS number:	67406-68-2
Molecular Weight:	166.96



Global Atmospheric Lifetime (years):	2.89
Tropospheric Atmospheric Lifetime (years):	3.14
Stratospheric Atmospheric Lifetime (years):	36.9
Ozone Depletion Potential (ODP):	0.035

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.206	0.182
Global Warming Potential (GWP_H):		
GWP_{20}	803	708
GWP_{100}	218	192
Global Temperature Potentials (GTP_H)		
GTP_{20}		297
GTP_{50}		35
GTP_{100}		27

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 1.87 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 1.19 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 3.04$ years

$\tau^{OH}_{Trop} = 3.14$ years

$\tau^{OH}_{Strat} = 94.5$ years

Fractional Atmospheric Loss: 0.952

O(^{1}D) Reactivity

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

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

$\tau_{O(^1D)} = 250$ years

Fractional Atmospheric Loss: 0.012

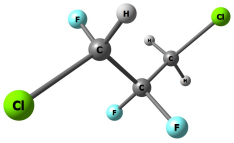
UV Photolysis

UV Spectrum: *No Recommendation*

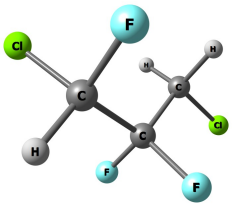
$\tau_{hv} = 80$ years

Fractional Atmospheric Loss: 0.036

Molecular Structure and Infrared Spectrum (6 conformers)



E = 0
Population = 0.447



$\Delta E = 0.18$ kcal mol^{-1}
Population = 0.327

Optimized Coordinates (Angstroms)

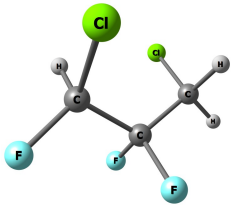
Atom	X	Y	Z
C	-1.514853179060	-0.424431684434	0.668440601065
C	-0.102047541212	-0.640304145405	0.126742624711
C	0.716732504204	0.656203213317	-0.003453733257
Cl	-2.507847258858	0.601001514394	-0.418488049828
H	-2.000266779386	-1.396351794417	0.752710377008
H	-1.462885121638	0.061680720588	1.640667466707
F	-0.145381384899	-1.242661740827	-1.078353247015
F	0.514728102965	-1.475330711821	0.996707687536
H	0.293462158207	1.306416967466	-0.769343719984
F	0.702015463040	1.286496086044	1.196260162581
Cl	2.400329036639	0.295909575095	-0.478290169523

Atom	X	Y	Z
C	0.905852102830	-0.368526232197	-0.721930459174
C	0.146615581318	0.353292595281	0.382852423057
C	-1.356674666869	0.538659643317	0.084200241438
Cl	2.657878310364	-0.432899537593	-0.362041412257
H	0.541454729896	-1.390177674016	-0.814124924372
H	0.767835248437	0.164060411072	-1.661714309821
F	0.638489604668	1.605916258333	0.548353716695
F	0.263632660252	-0.292022559590	1.560858228443
H	-1.816525500782	1.116768936833	0.888333281919
F	-1.489148900915	1.193354035180	-1.090813796949
Cl	-2.215893169201	-1.031944876619	-0.000983988979

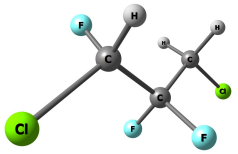
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
53.0143	0.179
86.5334	0.363
159.5272	0.218
191.8181	0.389
238.0334	0.215
306.7247	0.599
355.6916	0.159
383.2999	0.144
467.9993	0.990
561.1257	5.51
601.1452	4.13
761.7752	1.48
807.8428	14.6
849.7138	4.64
905.9813	4.70
1085.3648	8.01
1114.9138	19.5
1161.1018	13.1
1218.1184	15.1
1269.6182	5.66
1311.0218	2.39
1318.9040	0.485
1378.3287	1.27
1460.3231	1.46
3109.2592	0.871
3129.1980	0.863
3181.7292	0.00125

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
69.4857	0.256
73.0890	0.413
140.5776	0.282
189.9585	0.0603
225.4088	0.413
313.2701	0.278
338.5617	0.0967
411.3762	0.108
480.7376	0.372
535.1123	4.36
603.8628	6.45
759.5728	3.56
812.2626	10.3
845.2883	7.56
906.3439	2.02
1100.9580	10.2
1121.2611	20.1
1165.7792	10.9
1198.1871	7.70
1273.5375	11.3
1296.4520	1.51
1333.9428	1.20
1375.7144	4.22
1466.0872	1.55
3110.1228	1.05
3113.2942	1.00
3179.7415	0.0101



$\Delta E = 0.84$ kcal mol^{-1}
Population = 0.107



$\Delta E = 1.25$ kcal mol^{-1}
Population = 0.054

Optimized Coordinates (Angstroms)

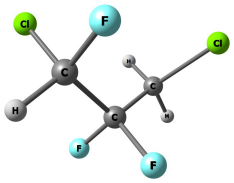
Atom	X	Y	Z
C	-1.256247815658	0.041660428411	-0.870549041613
C	-0.085146048128	-0.727566851326	-0.269998461430
C	0.873105525201	0.066268157120	0.639423471086
Cl	-2.312618580762	0.755024223985	0.392805967602
H	-0.893475492417	0.847521677930	-1.505091649388
H	-1.854381309387	-0.659616222970	-1.452339978170
F	0.619592360080	-1.251786166539	-1.299906887218
F	-0.546489213139	-1.758853452630	0.477113827378
H	0.342844080900	0.487545417033	1.493726517779
F	1.839299718592	-0.773042234594	1.059223498202
Cl	1.616289774719	1.436383023579	-0.253032264227

Atom	X	Y	Z
C	-1.336914654341	0.702243538903	-0.424263371278
C	-0.142573432202	-0.168020354241	-0.035622588408
C	1.182019619876	0.493132933597	-0.474680484538
Cl	-2.881062618869	-0.077525480621	0.030861511544
H	-1.270293481545	1.659090523499	0.090341377789
H	-1.347494304243	0.859614219916	-1.503397379315
F	-0.217538130489	-1.371922577728	-0.643756087693
F	-0.129714677149	-0.363998090864	1.295961901887
H	1.249473790404	0.525002329708	-1.564392145000
F	1.225699859028	1.753564326381	0.022472354199
Cl	2.585942029530	-0.438631368551	0.110628910811

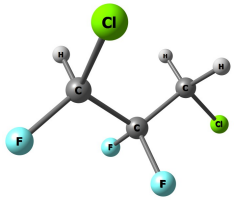
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
50.2721	0.166
95.4849	0.336
161.9028	0.186
198.6143	0.594
249.4555	0.230
312.3473	0.253
349.1734	0.154
403.0776	0.271
410.6638	1.07
558.7283	1.48
628.3305	4.39
761.7265	3.56
803.8222	13.9
850.4678	9.27
893.8335	2.07
1076.5620	9.21
1132.9350	19.1
1171.7220	24.1
1217.8737	7.18
1252.5427	6.97
1302.4215	0.750
1322.5198	2.22
1390.5271	2.59
1463.1270	2.83
3109.0850	0.850
3129.4952	0.794
3181.7833	0.0185

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
58.7021	0.0739
76.3138	0.507
123.0181	0.178
222.6439	0.274
237.0359	0.109
264.3941	0.132
346.0799	0.0737
381.4079	0.0211
464.1233	0.500
554.3119	1.86
680.6111	19.0
750.0441	5.83
818.8608	5.43
852.9596	2.70
907.3870	1.15
1081.3258	8.97
1113.7985	9.67
1132.0743	16.6
1249.1395	10.3
1266.0131	10.3
1315.1233	2.26
1326.4617	1.26
1367.3670	1.05
1463.6784	1.14
3097.9380	1.27
3103.5265	1.72
3171.7906	0.0629



$\Delta E = 1.41$ kcal mol^{-1}
Population = 0.042



$\Delta E = 1.99$ kcal mol^{-1}
Population = 0.016

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.047410917078	-0.314193066499	0.957368814738
C	-0.065249005918	-0.889381340781	-0.058212526006
C	0.992739991056	0.044058286580	-0.682177175005
Cl	-2.192029309058	0.865696325399	0.249752095437
H	-1.627212937301	-1.147377487906	1.355050702057
H	-0.503295115483	0.176980153466	1.761927485203
F	-0.731140941593	-1.448793930079	-1.093905188151
F	0.616302626129	-1.880634042822	0.574706480222
H	1.676303238070	-0.562022175525	-1.281721674639
F	0.405242679411	0.974639487839	-1.453550066280
Cl	1.983761691765	0.840349790328	0.586233052423

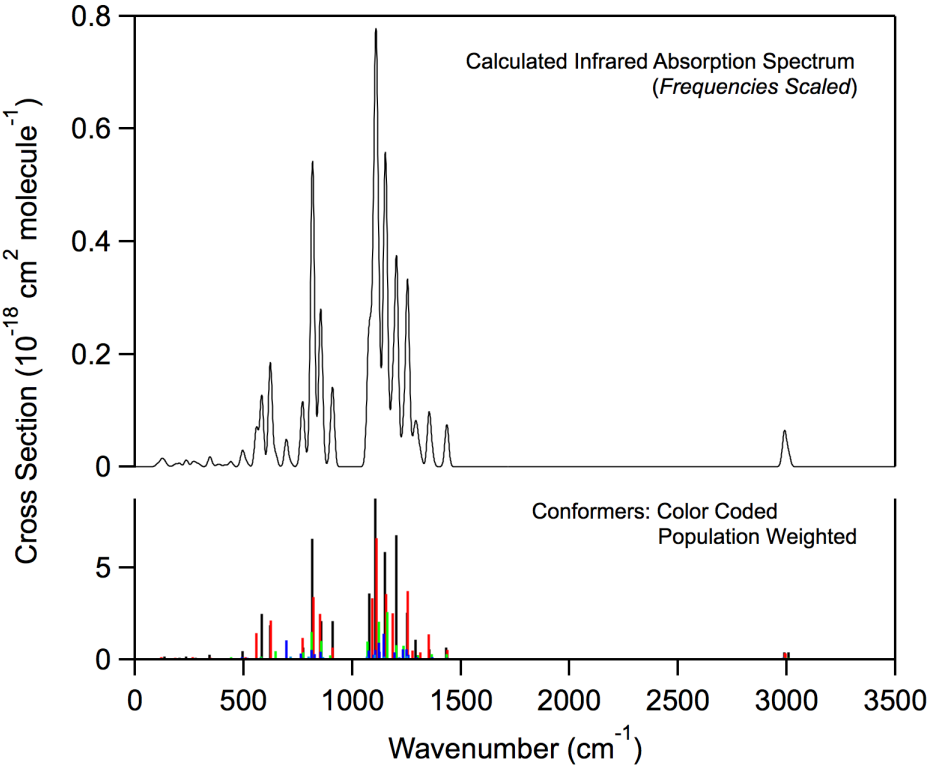
Atom	X	Y	Z
C	-1.058443964314	0.684824046302	0.521225046415
C	-0.144430505662	-0.418396614500	-0.000206281705
C	1.314905317516	-0.305884849462	0.496688665540
Cl	-2.760355301982	0.375577271505	0.059324216991
H	-1.010815223252	0.727478577201	1.610060479996
H	-0.763169742461	1.642781352286	0.098378738484
F	-0.145668534027	-0.440694851554	-1.346036475356
F	-0.578556447720	-1.627258546476	0.435890986081
H	1.358178810251	-0.367327075903	1.586351338030
F	2.023320616031	-1.311703415619	-0.046192452191
Cl	2.049651975619	1.264774106219	0.027114737715

Infrared Absorption Spectrum (unscaled frequencies)

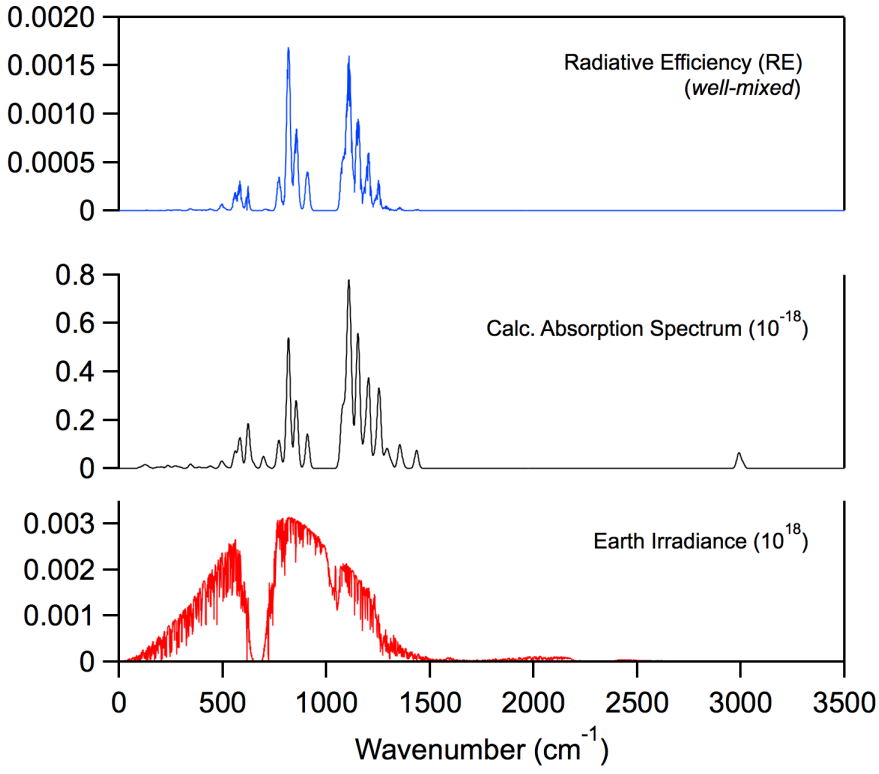
Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
37.7147	0.0912
109.6610	0.247
167.5034	0.184
187.6896	0.139
254.8340	1.56
315.6718	0.137
332.1134	0.0208
411.0751	0.406
463.0502	3.22
490.0498	2.02
609.0961	1.17
758.5848	2.37
803.6364	12.9
847.8013	10.4
908.0062	1.47
1104.5092	5.96
1134.4848	10.6
1155.6314	33.8
1207.5539	9.31
1276.3495	6.07
1307.3782	1.73
1318.3473	0.645
1392.2433	2.86
1464.8536	2.74
3100.2268	1.34
3105.2821	1.19
3174.7082	0.0146

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
65.1419	0.293
73.1666	0.357
131.0317	0.124
199.5562	0.200
247.9383	0.145
306.4868	0.250
332.6466	0.102
392.7802	0.0670
419.6210	0.646
534.7120	1.68
700.6955	9.59
776.0621	4.97
787.9120	10.8
859.1059	9.42
904.5290	2.45
1072.7833	9.74
1111.1979	15.9
1158.2413	11.3
1231.9185	8.51
1268.7740	13.6
1297.0514	3.63
1327.7161	0.973
1391.4990	1.99
1462.6524	1.16
3098.3288	1.43
3104.1887	1.71
3175.8259	0.0791

Infrared Spectrum

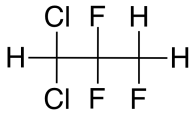


Radiative Efficiency



HCFC-243cb

Molecular Formula:	$CHCl_2CF_2CH_2F$
Name:	1,1-Dichloro-2,2,3-trifluoropropane
CAS number:	70192-70-0
Molecular Weight:	166.96



Global Atmospheric Lifetime (years):	1.46
Tropospheric Atmospheric Lifetime (years):	1.54
Stratospheric Atmospheric Lifetime (years):	27.3
Ozone Depletion Potential (ODP):	0.020

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.184	0.147
Global Warming Potential (GWP_H):		
GWP_{20}	360	289
GWP_{100}	98	78
Global Temperature Potentials (GTP_H)		
GTP_{20}		99
GTP_{50}		14
GTP_{100}		11

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 3.82 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 2.44 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 1.49$ years

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

$\tau^{OH}_{Strat} = 49.7$ years

Fractional Atmospheric Loss: 0.976

$O(^1D)$ Reactivity

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

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

$\tau_{O(^1D)} = 250$ years

Fractional Atmospheric Loss: 0.006

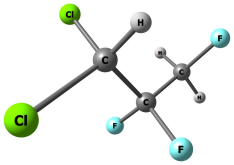
UV Photolysis

UV Spectrum: *No Recommendation*

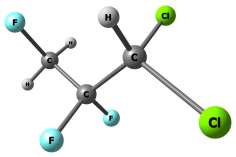
$\tau_{hv} = 80$ years

Fractional Atmospheric Loss: 0.018

Molecular Structure and Infrared Spectrum (5 conformers)



E = 0
Population = 0.432



E = 0
Population = 0.432

Optimized Coordinates (Angstroms)

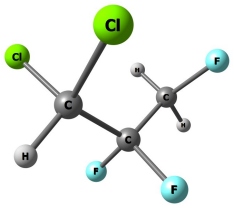
Atom	X	Y	Z
C	-0.517715906006	-0.146633462316	-0.468183804767
C	0.648079926782	0.448737143032	0.346413073562
C	1.949641667589	-0.343656902798	0.233660839906
Cl	-0.912906333232	-1.792918894541	0.111269124461
Cl	-1.940782653237	0.922712426162	-0.399847228081
H	-0.214304323521	-0.234949536708	-1.508012940997
F	0.323351909891	0.541357797980	1.652162341041
F	0.864602431825	1.701244791694	-0.123134292456
H	2.740380462822	0.239377307280	0.717236826472
H	1.846284346647	-1.315682397731	0.721244638693
F	2.247708470439	-0.517552272053	-1.095821577836

Atom	X	Y	Z
C	-0.517106029463	0.163047745661	-0.466829359567
C	0.635460705931	-0.478372797800	0.331471348884
C	1.947157014152	0.301957098923	0.259363086028
Cl	-1.953264251763	-0.890748982516	-0.450973784209
Cl	-0.896956258219	1.789708321473	0.174954054268
H	-0.204974773725	0.288897189192	-1.500192314069
F	0.840532674634	-1.713785169198	-0.186055492592
F	0.300000094362	-0.618825113920	1.630219647180
H	1.851768839364	1.255034231173	0.784529147714
H	2.727303699475	-0.309417030335	0.724804127708
F	2.257097285251	0.524881507346	-1.060049461345

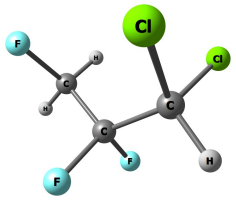
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
51.3752	0.110
95.8005	0.455
182.6478	0.290
200.6935	0.516
210.7396	0.0363
275.3221	0.372
351.0789	0.231
367.5088	0.409
448.4862	0.869
567.7264	1.45
592.5861	9.30
747.4148	1.80
796.1520	15.5
843.9689	2.70
955.9049	8.60
1109.6560	14.9
1139.8480	7.65
1206.9129	9.38
1217.5676	10.1
1239.5641	1.56
1278.9534	4.12
1319.9400	4.70
1424.1060	0.375
1497.5475	1.18
3061.5380	2.38
3128.4168	1.88
3163.0899	0.324

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
51.3741	0.110
95.8008	0.455
182.6479	0.290
200.6936	0.516
210.7393	0.0363
275.3222	0.372
351.0793	0.231
367.5091	0.409
448.4868	0.869
567.7263	1.45
592.5861	9.30
747.4147	1.80
796.1521	15.5
843.9694	2.70
955.9055	8.60
1109.6549	14.9
1139.8486	7.65
1206.9138	9.38
1217.5679	10.1
1239.5652	1.56
1278.9542	4.12
1319.9409	4.70
1424.1066	0.375
1497.5483	1.18
3061.5377	2.38
3128.4167	1.88
3163.0897	0.324



$\Delta E = 1.50$ kcal mol^{-1}
Population = 0.034



$\Delta E = 1.50$ kcal mol^{-1}
Population = 0.034

Optimized Coordinates (Angstroms)

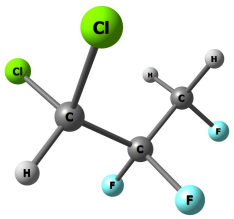
Atom	X	Y	Z
C	-0.694405434461	-0.079792650753	0.537092178504
C	0.791979521084	-0.457145787394	0.348611079447
C	1.441839503550	-0.230048661555	-1.014868981824
Cl	-0.968024679584	1.672835111405	0.389732268938
Cl	-1.729737442104	-1.007585760471	-0.589364309198
H	-0.983364852098	-0.370931173086	1.545239359403
F	0.889968281062	-1.786580555277	0.614398780657
F	1.490684719433	0.202785489069	1.299265213610
H	2.430579762338	-0.701021999605	-0.975855553892
H	0.840971077704	-0.702068262405	-1.797446265855
F	1.577159543075	1.105495250072	-1.268904769790

Atom	X	Y	Z
C	-0.691716261015	0.098652389194	0.544686083069
C	0.813197006378	0.402048824040	0.370190995912
C	1.442507651791	0.234299130718	-1.011402545430
Cl	-1.676572886589	1.161467550464	-0.505122463570
Cl	-1.067354224357	-1.620590201057	0.277501315178
H	-0.958640557640	0.334348512567	1.573189180087
F	1.476745328629	-0.362242985248	1.266295856259
F	0.989459966567	1.701648453921	0.727422093025
H	0.866476513992	0.793984593912	-1.753839691753
H	2.457095175093	0.643630661347	-0.948116077956
F	1.498884287152	-1.085655929859	-1.359342744821

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
43.4523	0.146
109.9215	0.399
180.7861	0.251
185.1376	0.160
234.8205	0.352
273.8148	1.17
350.4321	0.239
368.9597	0.201
443.5973	2.50
499.1051	2.07
600.1828	1.24
745.0596	3.38
805.9355	21.9
841.0302	3.22
970.7996	4.27
1131.1305	23.2
1135.1250	4.34
1176.4580	15.2
1222.5900	4.09
1229.0827	0.504
1297.3176	4.76
1328.0579	4.56
1437.8106	0.490
1498.3522	0.993
3051.7155	2.67
3113.0833	2.10
3140.4923	0.455

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
43.4531	0.146
109.9203	0.399
180.7850	0.251
185.1369	0.160
234.8202	0.352
273.8131	1.17
350.4320	0.239
368.9596	0.201
443.5967	2.50
499.1074	2.07
600.1816	1.24
745.0588	3.38
805.9357	21.9
841.0299	3.22
970.7988	4.27
1131.1311	23.2
1135.1253	4.34
1176.4570	15.2
1222.5896	4.09
1229.0833	0.504
1297.3180	4.76
1328.0585	4.56
1437.8102	0.490
1498.3528	0.993
3051.7153	2.67
3113.0827	2.10
3140.4925	0.455



$\Delta E = 1.54$ kcal mol^{-1}
Population = 0.032

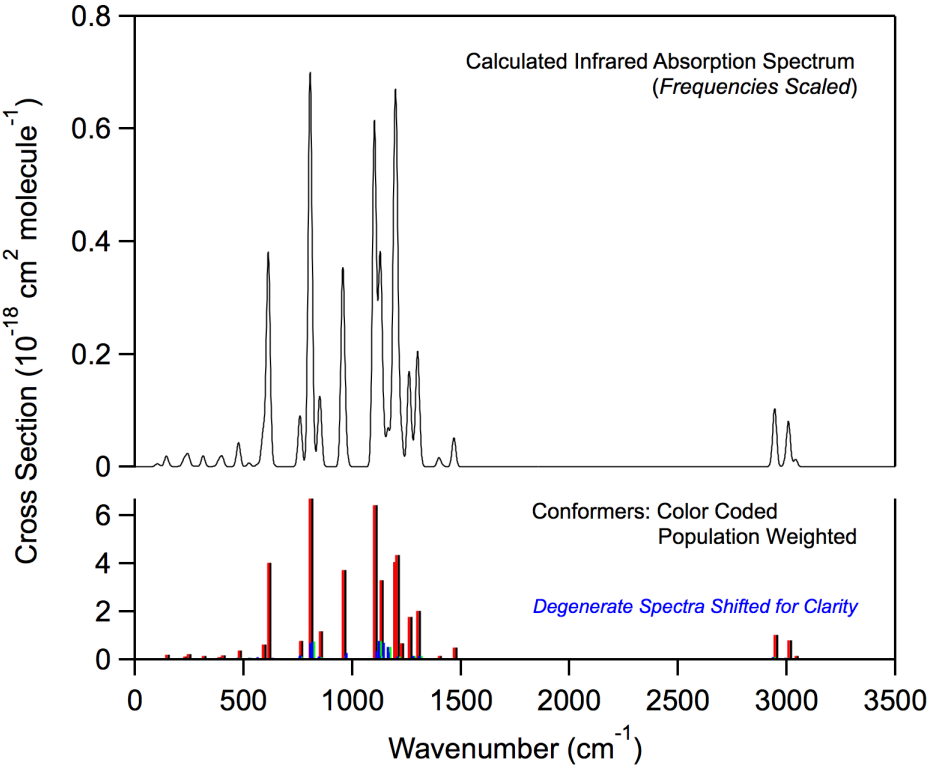
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-0.842161353004	0.001324886835	0.476883581439
C	0.699758219840	-0.008471230330	0.384486524268
C	1.298934818696	0.037659762120	-1.018090431352
Cl	-1.522177303504	1.510549319273	-0.195582535778
Cl	-1.547406558405	-1.443017113884	-0.303432500193
H	-1.114558488963	-0.034798194804	1.529869712161
F	1.125884721133	-1.125439622559	1.020674572219
F	1.144484444736	1.051657901664	1.100223705269
H	0.970187377861	-0.834724741323	-1.589856296385
H	0.985442437223	0.954906051965	-1.524477818662
F	2.661443684388	0.021368981043	-0.890097512985

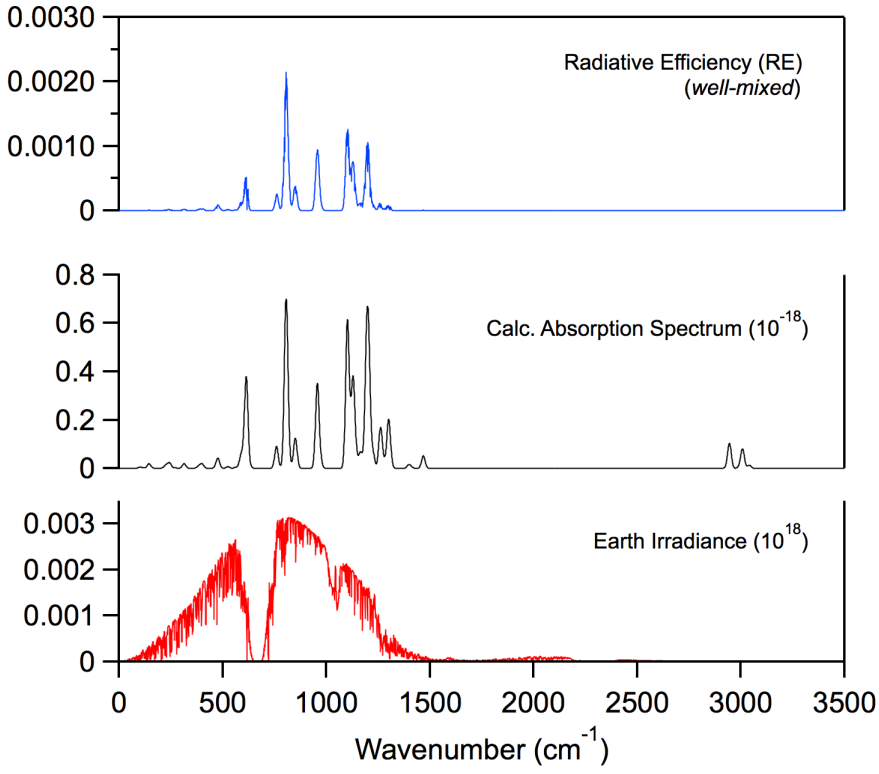
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
63.6801	0.632
78.9224	0.166
159.1928	0.428
183.2620	0.0536
235.3650	0.0820
280.6079	0.387
322.8285	0.311
368.9486	0.180
433.0272	0.228
540.7831	2.95
615.0768	2.46
749.5971	5.32
796.8200	21.2
839.8273	4.35
973.2741	8.52
1121.0309	10.7
1155.9207	22.3
1178.2091	9.74
1182.6873	1.93
1226.6931	1.69
1299.3461	3.77
1330.0071	4.28
1440.1290	0.745
1500.7280	0.356
3064.8595	2.00
3122.5769	1.71
3144.4119	0.410

Infrared Spectrum

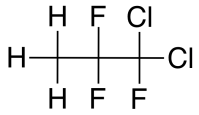


Radiative Efficiency



HCFC-243cc

Molecular Formula:	$CH_3CF_2CFCl_2$
Name:	1,1-Dichloro-1,2,2-trifluoropropane
CAS number:	7125-99-7
Molecular Weight:	166.96



Global Atmospheric Lifetime (years):	13.8	19.5 #
Tropospheric Atmospheric Lifetime (years):	18.7	27.1 #
Stratospheric Atmospheric Lifetime (years):	53.5	~70 #
Ozone Depletion Potential (ODP):	0.134	

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.295	0.284
Global Warming Potential (GWP_H):		
GWP_{20}	4209	4057
GWP_{100}	1491	1437
Global Temperature Potentials (GTP_H)		
GTP_{20}		3374
GTP_{50}		809
GTP_{100}		226

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

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

OH Reactivity

$k_{Rec}(T) = 7.7 \times 10^{-13} \exp(-1720/T)$; $k_{Rec}(272\ K) = 1.38 \times 10^{-15}$ cm^3 $molecule^{-1}$ s^{-1}

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

$\tau^{OH}_{Global} = 18.0$ years

$\tau^{OH}_{Trop} = 18.7$ years

$\tau^{OH}_{Strat} = 471.3$ years

Fractional Atmospheric Loss: 0.771

O(^{1}D) Reactivity

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

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

$\tau_{O(^1D)} = 250$ years

Fractional Atmospheric Loss: 0.056

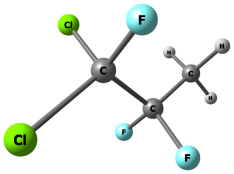
UV Photolysis

UV Spectrum: *No Recommendation*

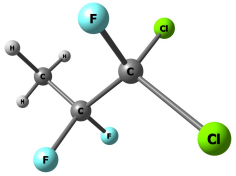
$\tau_{hv} = 80$ years

Fractional Atmospheric Loss: 0.173

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.436



E = 0
Population = 0.436

Optimized Coordinates (Angstroms)

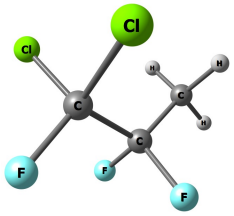
Atom	X	Y	Z
C	2.022639898997	-0.946581761986	-0.319536337743
C	1.073788796335	0.134027377583	0.156738090031
C	-0.400740784177	-0.052047422433	-0.320569403785
H	1.993576483280	-1.015189521712	-1.407707002512
H	3.029532732090	-0.668250833476	-0.001338785608
H	1.758504010783	-1.910323575070	0.115491004142
F	1.478311440849	1.334802836452	-0.326408270195
F	1.072598978990	0.214188014844	1.503702655291
F	-0.398853182323	-0.130823156275	-1.658196720517
Cl	-1.092665904767	-1.566730098195	0.339902674218
Cl	-1.401034470057	1.339665140269	0.172181096678

Atom	X	Y	Z
C	2.022512341546	-0.946630262770	0.318790554706
C	1.073215307845	0.133350925199	-0.158020237746
C	-0.400638650768	-0.051480736861	0.321848791388
H	3.028993330235	-0.669138176627	-0.001435934633
H	1.995077530979	-1.013245261153	1.407127250784
H	1.757474354329	-1.911096468084	-0.114077548065
F	1.070013124726	0.211057878612	-1.505125298903
F	1.478767298782	1.334902062165	0.322326801317
F	-0.396752810871	-0.127828080704	1.659612542960
Cl	-1.401324543170	1.339588885898	-0.171919348190
Cl	-1.093939283633	-1.567184765677	-0.334827573618

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
66.9711	0.180
183.8471	0.206
194.9693	0.0595
201.7816	0.0408
265.5649	0.159
305.1276	0.252
313.1775	0.232
363.4789	0.0836
384.6352	0.0306
441.5993	0.243
516.2330	0.981
550.1684	4.26
634.7497	4.53
834.9785	26.5
886.3501	20.3
979.1742	4.56
991.7729	9.94
1139.3973	18.7
1215.5282	13.3
1237.9725	14.8
1259.7096	10.2
1411.2805	3.73
1478.7059	0.347
1487.1260	0.188
3073.3397	0.233
3155.7322	0.567
3169.9707	0.437

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
66.9714	0.180
183.8476	0.206
194.9695	0.0595
201.7809	0.0408
265.5649	0.159
305.1278	0.252
313.1776	0.232
363.4789	0.0836
384.6352	0.0306
441.5993	0.243
516.2328	0.981
550.1685	4.26
634.7496	4.53
834.9785	26.5
886.3498	20.3
979.1742	4.56
991.7729	9.94
1139.3976	18.7
1215.5281	13.3
1237.9724	14.8
1259.7100	10.2
1411.2803	3.73
1478.7059	0.347
1487.1260	0.188
3073.3400	0.233
3155.7326	0.567
3169.9705	0.437



$\Delta E = 0.72$ kcal mol^{-1}
Population = 0.128

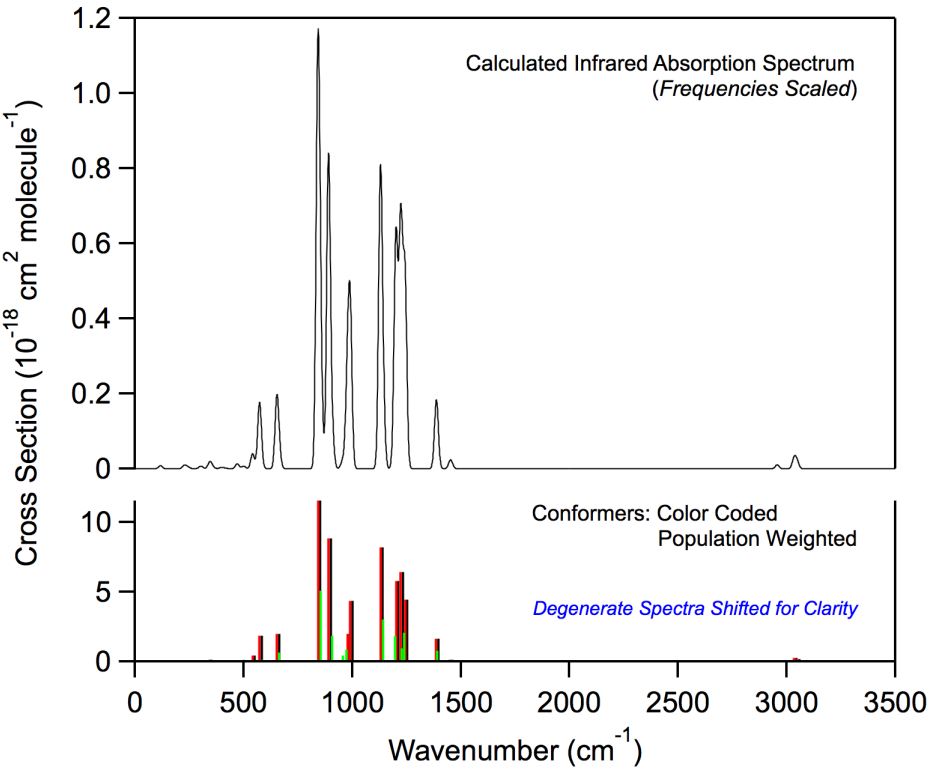
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.889564025092	0.933220166072	0.000000000000
C	0.381928685259	1.029641906114	0.000000000000
C	-0.414297045139	-0.316065854063	0.000000000000
H	2.284779168714	1.951513179169	0.000000000000
H	2.239575806612	0.411920201245	0.891265854223
H	2.239575806612	0.411920201245	-0.891265854223
F	-0.047426198429	1.711575178047	-1.089794685767
F	-0.047426198429	1.711575178047	1.089794685767
F	-1.715856379107	-0.024463510274	0.000000000000
Cl	-0.047276835593	-1.271821822778	-1.469119978060
Cl	-0.047276835593	-1.271821822778	1.469119978060

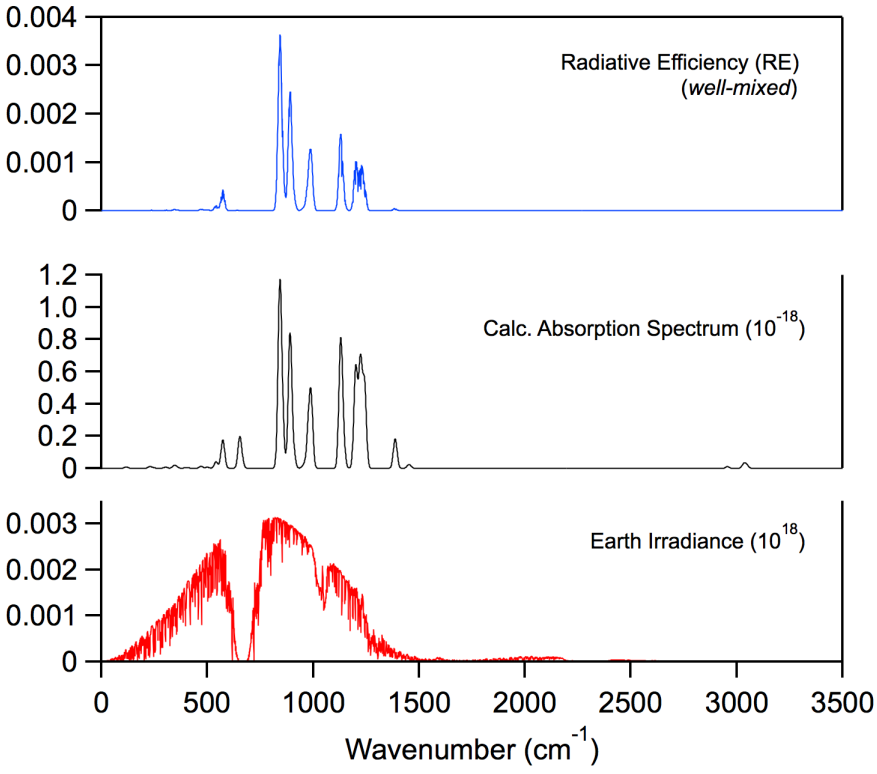
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
70.9006	0.121
178.5999	0.0469
193.4172	0.00385
206.7179	0.215
255.1608	0.191
310.9200	0.164
326.0284	0.398
369.0666	0.0501
376.6766	0.0776
441.0350	0.520
472.2020	1.15
561.4286	0.875
647.0568	4.89
848.1337	39.6
904.6310	14.5
955.0414	3.37
974.6204	6.72
1153.3885	23.6
1210.2599	14.6
1243.6141	7.49
1255.1758	16.1
1416.8518	6.00
1479.7594	0.453
1485.7380	0.135
3073.7662	0.152
3154.8409	0.682
3170.1386	0.395

Infrared Spectrum

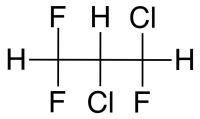


Radiative Efficiency



HCFC-243da

Molecular Formula: $CHF_2CHClCHFCl$
Name: 1,2-Dichloro-1,3,3-trifluoropropane
CAS number: –
Molecular Weight: 166.96



Global Atmospheric Lifetime (years): 1.97
  Tropospheric Atmospheric Lifetime (years): 2.07
  Stratospheric Atmospheric Lifetime (years): 41.9
Ozone Depletion Potential (ODP): 0.022

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.192	0.162
Global Warming Potential (GWP_H):		
GWP_{20}	512	430
GWP_{100}	139	116
Global Temperature Potentials (GTP_H)		
GTP_{20}		158
GTP_{50}		21
GTP_{100}		16

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 2.83 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 1.81 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 2.01$ years
$\tau^{OH}_{Trop} = 2.07$ years
$\tau^{OH}_{Strat} = 65.0$ years

Fractional Atmospheric Loss: 0.983

$O(^1D)$ Reactivity

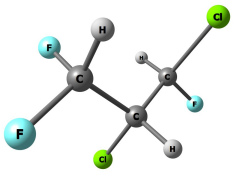
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 1.5 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)} = 250$ years
Fractional Atmospheric Loss: 0.008

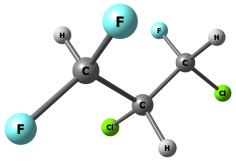
UV Photolysis

UV Spectrum: *No Recommendation*
$\tau_{hv} = 225$ years
Fractional Atmospheric Loss: 0.009

Molecular Structure and Infrared Spectrum (11 conformers)



E = 0
Population = 0.242



$\Delta E = 0.23$ kcal mol^{-1}
Population = 0.165

Optimized Coordinates (Angstroms)

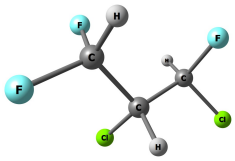
Atom	X	Y	Z
C	0.902800677502	1.138720833879	-0.109573839635
C	0.252437089923	-0.209610438086	-0.430777032357
C	-1.053669418615	-0.434571939878	0.328544937313
F	1.109616199680	1.240564085654	1.224876081207
F	2.091790508323	1.232912353320	-0.736533940121
H	0.266874191721	1.970895764425	-0.430454969452
Cl	1.382552110264	-1.542618818617	-0.001497824438
H	0.067235619609	-0.275807374478	-1.504048622487
F	-1.580059609379	-1.629799614391	0.003479137401
H	-0.917703759043	-0.365150120117	1.408218648305
Cl	-2.252117609984	0.849910268290	-0.123521575735

Atom	X	Y	Z
C	1.630897829580	0.418793920586	0.146992133267
C	0.291715527508	-0.136981011774	-0.356103327952
C	-0.857473737874	0.758423142638	0.099415731564
F	2.646040794034	-0.269206051312	-0.406838312697
F	1.729479282837	1.713087280378	-0.262472525329
H	1.716139942698	0.381885063349	1.237642810672
Cl	0.110388331679	-1.815832555147	0.239939614424
H	0.318084958291	-0.169222464612	-1.446359497676
F	-0.928476125571	0.768573237841	1.451611851896
H	-0.692089503009	1.776671290740	-0.257885785201
Cl	-2.432748300173	0.236114147314	-0.581791692969

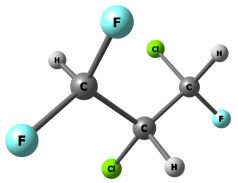
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
63.2046	0.259
78.2136	0.177
151.8929	0.194
199.5923	0.102
216.6399	0.724
284.4127	0.311
344.9919	0.134
416.4227	0.443
465.4377	2.18
553.4162	1.08
656.7159	9.87
742.7241	19.1
810.4821	1.75
972.3483	1.72
1068.4786	3.67
1125.0183	18.2
1163.6050	21.9
1175.5270	12.3
1210.7784	3.18
1277.3086	1.85
1302.4564	3.05
1386.5342	0.266
1393.9475	7.60
1414.7879	3.78
3075.7416	3.00
3115.5938	0.349
3131.4186	0.685

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
67.8377	0.197
73.4824	0.198
148.8057	0.300
181.4142	0.0194
208.1321	0.409
284.3376	0.237
374.9101	0.126
405.6509	0.127
460.8301	4.74
567.0511	1.01
641.1856	4.97
781.7736	14.8
832.1115	4.45
968.5469	5.96
1070.0456	5.24
1112.8767	21.0
1135.2725	12.5
1158.7729	22.0
1236.2315	1.07
1277.0099	0.383
1299.2015	4.78
1376.6678	2.20
1390.5547	3.91
1415.3892	7.66
3085.9630	2.98
3108.2366	0.354
3121.9814	0.920



$\Delta E = 0.47$ kcal mol^{-1}
Population = 0.110



$\Delta E = 0.55$ kcal mol^{-1}
Population = 0.095

Optimized Coordinates (Angstroms)

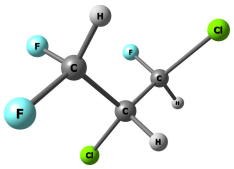
Atom	X	Y	Z
C	1.510156332524	0.732546242317	-0.203245045887
C	0.235947297214	-0.094078971331	-0.416906050879
C	-0.951494140300	0.572743772129	0.281765483874
F	1.771423479699	0.846924715287	1.119663747652
F	2.556588877022	0.125909442795	-0.796536497679
H	1.393502882384	1.736341668640	-0.626890843644
Cl	0.466133372752	-1.755304280471	0.208716311009
H	0.042070527553	-0.167360462467	-1.488255624764
H	-0.875436339662	0.503516154551	1.367261499084
F	-0.973799625073	1.883519411325	-0.087714145686
Cl	-2.509327664113	-0.178556692775	-0.189401833080

Atom	X	Y	Z
C	1.380691518307	0.597556969001	0.206095998332
C	0.348306488369	-0.297872716457	-0.481970057627
C	-1.001099729952	0.390101688004	-0.676183139137
F	2.598740957753	0.029868609597	0.115898152726
F	1.418408967269	1.780998969343	-0.464879362727
H	1.144490079078	0.788757533412	1.257012803019
Cl	0.195128594182	-1.842513633139	0.408928805263
H	0.728405619435	-0.543617388438	-1.477499922583
H	-0.864910075390	1.310228899878	-1.247790454169
F	-1.841813202804	-0.432942823677	-1.335317311280
Cl	-1.761416216248	0.885836892476	0.880412488184

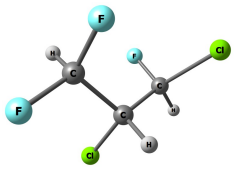
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
63.2648	0.125
75.6019	0.285
147.6632	0.167
193.8773	0.160
217.7908	0.519
275.5839	0.555
347.0978	0.0238
427.0912	0.340
478.2646	1.66
538.3522	2.77
673.0692	8.63
770.8655	14.8
822.4625	2.69
972.7585	3.10
1069.5120	11.2
1104.9730	8.20
1142.2546	20.5
1174.2643	17.9
1213.2960	1.81
1272.1217	2.98
1322.3133	5.29
1371.7240	0.640
1387.9675	9.42
1412.7348	3.63
3070.9986	3.10
3113.1318	0.543
3130.0055	0.782

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
64.6154	0.161
81.9496	0.200
146.1956	0.116
179.1751	0.208
203.6512	0.346
315.1427	0.313
369.1805	0.180
415.4684	1.41
480.4595	2.10
565.1197	1.91
619.4620	6.38
685.9314	6.46
845.3650	8.40
1039.9721	7.20
1080.0628	4.68
1110.3970	16.3
1129.1129	22.0
1164.6357	16.9
1240.8103	1.25
1265.6783	4.15
1306.3764	6.08
1370.7147	2.05
1390.5891	2.17
1418.1467	6.30
3085.7382	0.802
3098.6449	1.82
3109.6944	1.27



$\Delta E = 0.56$ kcal mol^{-1}
Population = 0.094



$\Delta E = 0.74$ kcal mol^{-1}
Population = 0.069

Optimized Coordinates (Angstroms)

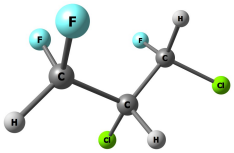
Atom	X	Y	Z
C	0.715464858750	1.151823591278	0.018287995900
C	0.278014119462	-0.194159413848	-0.571271093971
C	-1.050299618873	-0.714912905904	-0.026385859791
F	1.037743147098	1.029534925894	1.319469011327
F	1.805355356984	1.587641601538	-0.652732676538
H	-0.082413290247	1.897299501706	-0.082733820519
Cl	1.541614565341	-1.440566433961	-0.270053056366
H	0.193655657913	-0.082318169427	-1.652395435759
H	-1.277600249388	-1.706454824581	-0.419698066264
F	-1.051866236906	-0.746763088330	1.318302301686
Cl	-2.400047310134	0.362508215635	-0.590714299704

Atom	X	Y	Z
C	0.772511918758	1.046023257701	0.421979190124
C	0.408191560752	-0.145062763566	-0.476412845760
C	-0.883228657899	-0.859321006760	-0.072240890831
F	1.907626474779	1.612065737348	-0.038507267994
F	-0.209128066890	1.972724753904	0.357501458516
H	0.916060382429	0.743187119825	1.463680423202
Cl	1.754201663141	-1.345754675546	-0.374898066066
H	0.349454862250	0.185621979908	-1.512953169129
H	-0.947945386785	-1.842066326054	-0.539777687410
F	-0.931315078780	-0.999619863023	1.274177868590
Cl	-2.338632671756	0.048348786263	-0.626074013244

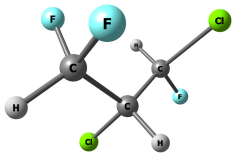
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
53.2516	0.304
90.6557	0.0538
161.2382	0.429
184.5792	0.176
202.1670	0.0618
284.3279	0.291
319.1238	0.156
391.3506	0.214
496.0479	3.09
644.0672	6.01
679.4028	7.44
747.7961	17.6
798.1530	1.45
950.0429	1.70
991.4081	2.14
1138.2129	13.3
1159.9128	26.2
1180.8208	11.0
1240.0049	6.16
1277.9938	1.87
1308.8201	1.99
1386.1263	5.03
1406.4815	4.99
1413.6204	2.92
3062.8801	3.18
3117.9532	1.13
3127.9021	0.267

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
46.9054	0.140
80.9032	0.104
158.5789	0.0275
187.4043	0.285
230.0424	0.523
268.8495	0.573
374.7331	0.521
389.3889	0.505
430.6674	2.95
561.4230	1.40
669.2605	1.76
755.1657	25.2
832.6794	2.33
927.5903	1.75
1092.0604	12.9
1134.2544	16.5
1135.5198	11.1
1153.0213	19.5
1226.5148	2.98
1286.8062	3.36
1289.2157	1.38
1373.6881	2.59
1400.4203	2.21
1426.0496	5.23
3088.9642	2.95
3121.0561	0.915
3137.3535	0.266



$\Delta E = 0.84$ kcal mol^{-1}
Population = 0.059



$\Delta E = 0.89$ kcal mol^{-1}
Population = 0.054

Optimized Coordinates (Angstroms)

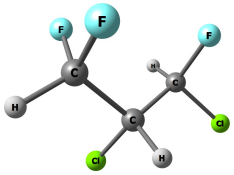
Atom	X	Y	Z
C	1.730181900275	0.094025732761	-0.401162000615
C	0.248813892827	-0.269148124817	-0.566159453697
C	-0.657613294086	0.767450254431	0.100843276651
F	1.929282813513	1.296493820260	-1.007983238640
F	2.060484977215	0.224515348175	0.896580476716
H	2.383887905600	-0.651392589594	-0.867079763156
Cl	-0.028288960591	-1.916666492623	0.077037157095
H	0.029242660249	-0.292375553951	-1.633983905140
F	-0.601280869865	0.673260179981	1.442275118575
H	-0.352468708454	1.769929854162	-0.208375274374
Cl	-2.366424316683	0.577033571214	-0.437682393416

Atom	X	Y	Z
C	0.723969234336	1.345035588778	-0.246079133500
C	0.442951824463	-0.140417102140	-0.519872352156
C	-0.610534263189	-0.770842637438	0.393677456057
F	-0.256539238035	2.110267422797	-0.771716685309
F	0.764916330558	1.567114524838	1.089032572981
H	1.680892948278	1.647768873651	-0.684343383221
Cl	1.993553882601	-1.036863814171	-0.276610282933
H	0.158481099463	-0.270366561948	-1.564364224736
F	-0.707513274440	-2.090892316166	0.128867826664
H	-0.373826294263	-0.620166179058	1.446778693336
Cl	-2.224498249772	-0.021407799145	0.108889512818

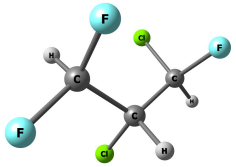
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
53.2041	0.226
88.3405	0.0523
157.3462	0.235
181.5940	0.256
204.5839	0.102
262.5420	0.0436
366.1513	0.401
385.4177	0.356
529.6856	4.91
577.7360	5.58
668.2659	7.12
791.0291	4.34
845.0254	5.44
937.4497	3.34
1002.6321	3.74
1102.1994	19.4
1161.2991	10.0
1178.9296	24.6
1237.7667	3.25
1276.3496	0.746
1326.7729	10.1
1377.0935	1.14
1383.7067	5.33
1419.2269	4.63
3073.6015	4.44
3100.0389	0.581
3123.1796	0.492

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
46.5726	0.133
85.2899	0.139
155.9941	0.0446
203.4472	0.185
239.4256	0.877
276.2990	0.633
351.4710	0.515
397.1399	0.943
441.7467	1.59
550.7736	1.00
671.7763	7.54
764.2020	20.0
824.8562	2.94
923.9600	1.21
1092.8253	8.36
1121.7636	17.1
1140.1455	9.72
1168.3338	19.2
1212.9255	3.31
1265.6379	4.18
1312.2222	3.02
1383.4869	5.37
1400.0559	1.83
1420.9154	2.16
3075.3724	4.09
3123.6106	0.233
3136.7839	0.527



$\Delta E = 0.95$ kcal mol^{-1}
Population = 0.049



$\Delta E = 1.27$ kcal mol^{-1}
Population = 0.028

Optimized Coordinates (Angstroms)

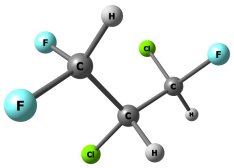
Atom	X	Y	Z
C	1.722489005188	0.069164635424	-0.262842643929
C	0.239508014167	-0.265371616048	-0.496244691729
C	-0.688071588790	0.572493258017	0.391018528393
F	2.007537203193	1.266950100522	-0.817838587881
F	1.977054483407	0.143977176878	1.064308375845
H	2.373177171325	-0.693002706402	-0.705545172967
Cl	-0.000565938764	-2.011594608004	-0.151157041702
H	0.003418851940	-0.099994522830	-1.547932140683
H	-0.593931944634	0.301311896949	1.442713320384
F	-0.382307872287	1.880406980630	0.227092139073
Cl	-2.412287384747	0.327656404864	-0.059060084804

Atom	X	Y	Z
C	1.122311376879	0.642426126438	0.506390089682
C	0.405163672103	-0.174196834659	-0.574232832507
C	-1.098601711838	0.088352012859	-0.703611274327
F	2.453736487633	0.455224553490	0.382327240923
F	0.860879767642	1.953196744075	0.298010042635
H	0.812047560411	0.366407341781	1.518409244737
Cl	0.694135379409	-1.921631025128	-0.290119253334
H	0.856413634318	0.075285187282	-1.537986501663
F	-1.286945379000	1.319495099170	-1.228377843669
H	-1.564028605291	-0.659388775274	-1.347639586033
Cl	-1.964898182266	-0.014074430034	0.875194673556

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
55.4222	0.103
80.7567	0.145
151.9464	0.0438
198.9343	0.136
219.1396	0.488
295.9747	0.382
363.6884	1.18
398.9920	1.73
443.5038	0.733
539.8416	2.78
630.5738	9.21
811.0484	7.94
860.1667	6.62
921.0582	1.24
1088.0495	12.0
1110.7489	5.87
1139.2035	22.2
1167.7946	23.5
1211.4655	0.637
1254.2013	1.87
1326.5029	7.40
1368.7523	4.60
1399.6668	3.77
1418.2870	2.78
3070.9449	4.18
3119.8915	0.371
3132.7050	0.632

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
53.8377	0.127
86.5945	0.0721
151.1437	0.0963
181.5561	0.0274
225.6432	0.621
318.8174	0.342
376.5989	0.210
409.5699	3.58
431.0810	0.215
541.3552	3.30
625.4455	3.95
720.4628	5.92
854.5023	9.91
994.4748	7.32
1102.8101	3.45
1125.6800	5.32
1138.7545	31.4
1140.5137	21.9
1227.8313	1.42
1264.5194	5.25
1320.1156	3.21
1365.5864	1.49
1399.2428	2.37
1423.1205	5.55
3089.5103	1.61
3101.6524	1.71
3112.3337	0.981



$\Delta E = 1.97$ kcal mol^{-1}
Population = 0.009

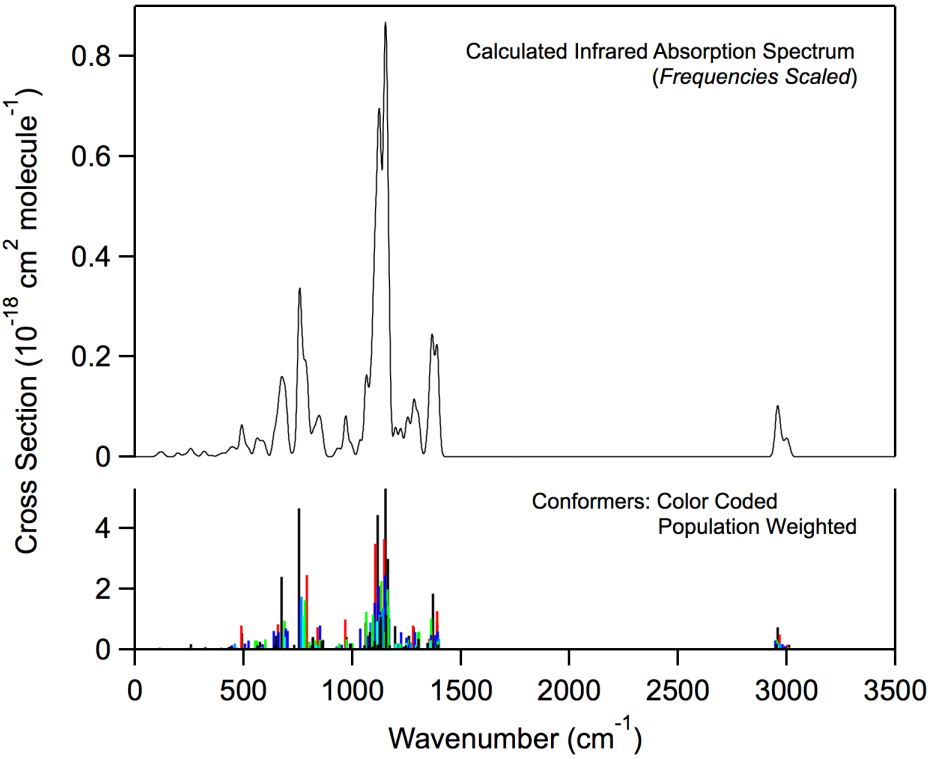
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.040105631617	1.012906257520	0.016290207097
C	0.402142178699	-0.193859635236	-0.680698818843
C	-1.123543412793	-0.125432899530	-0.784166134890
F	0.928961013438	0.935147164283	1.354194962793
F	2.356341332268	1.048592366188	-0.295729081839
H	0.567539819407	1.940547344247	-0.330452135462
Cl	0.927707505117	-1.736322550476	0.054064845440
H	0.771473050616	-0.192031289719	-1.709584583793
F	-1.425462575630	0.981633164769	-1.518891170932
H	-1.518993637662	-1.010987394068	-1.283410412009
Cl	-1.965779905076	-0.016491527978	0.793762322439

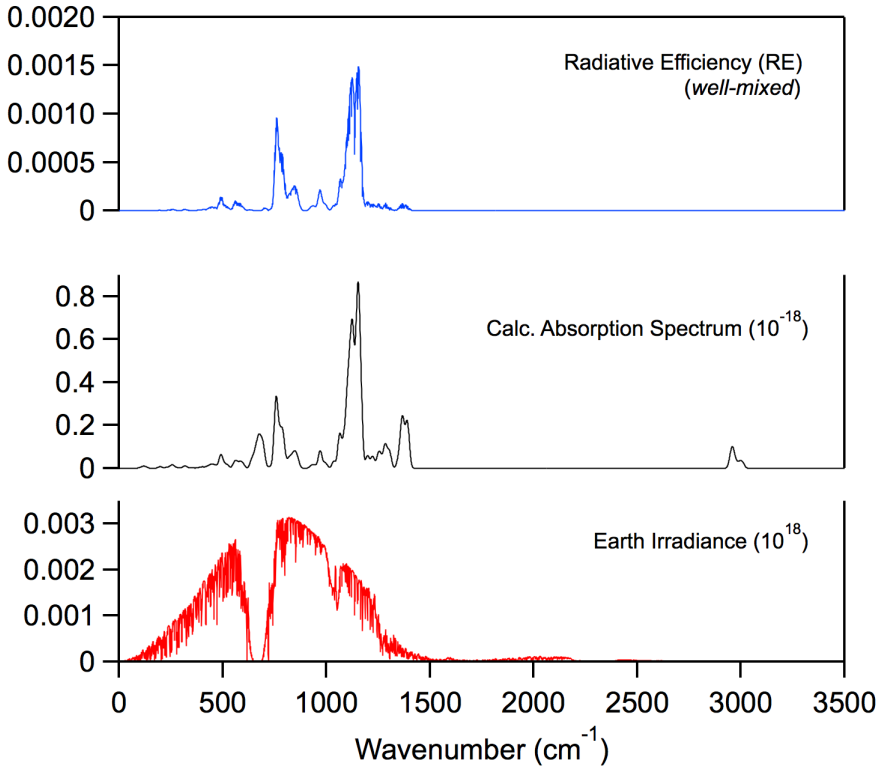
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
54.6156	0.232
84.4791	0.0413
152.8390	0.109
174.1865	0.408
199.1801	0.0733
282.4333	0.436
346.0739	0.114
428.9816	0.206
503.3260	3.23
640.7125	7.30
653.9801	4.37
706.5797	5.67
818.5873	2.72
980.9054	2.68
1060.9499	16.3
1087.0251	12.1
1132.6074	16.3
1184.1132	16.2
1241.9614	0.986
1270.1173	7.83
1338.8756	4.36
1359.4880	0.564
1399.7215	7.17
1415.6802	2.80
3055.9813	3.05
3091.3468	0.852
3115.7642	1.06

Infrared Spectrum

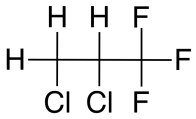


Radiative Efficiency



HCFC-243db

Molecular Formula:	$CH_2ClCHClCF_3$
Name:	2,3-Dichloro-1,1,1-trifluoropropane
CAS number:	338-75-0
Molecular Weight:	166.96



Global Atmospheric Lifetime (years):	1.44
Tropospheric Atmospheric Lifetime (years):	1.51
Stratospheric Atmospheric Lifetime (years):	34.5
Ozone Depletion Potential (ODP):	0.018

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.172	0.138
Global Warming Potential (GWP_H):		
GWP_{20}	335	268
GWP_{100}	91	73
Global Temperature Potentials (GTP_H)		
GTP_{20}		92
GTP_{50}		13
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*

$k_{SAR}(298\ K) = 3.89 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 2.49 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 1.46$ years

$\tau^{OH}_{Trop} = 1.51$ years

$\tau^{OH}_{Strat} = 48.8$ years

Fractional Atmospheric Loss: 0.988

O(^{1}D) Reactivity

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

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

$\tau_{O(^1D)} = 250$ years

Fractional Atmospheric Loss: 0.006

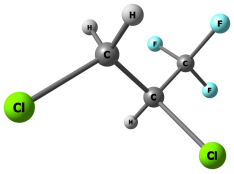
UV Photolysis

UV Spectrum: *No Recommendation*

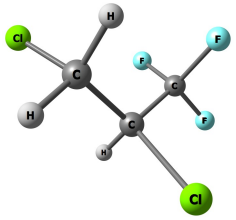
$\tau_{hv} = 225$ years

Fractional Atmospheric Loss: 0.006

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.492



ΔE = 0.05 kcal mol^{-1}
Population = 0.449

Optimized Coordinates (Angstroms)

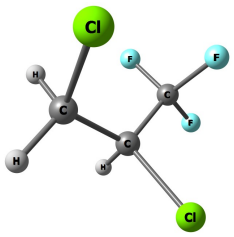
Atom	X	Y	Z
C	1.008554835105	-0.841926846551	0.324966442358
C	0.018883647566	0.083088802567	-0.372983286171
C	-1.422367636010	-0.347973258061	-0.067415955554
Cl	2.685245657021	-0.598065250670	-0.267950515779
H	1.008816764164	-0.672696630602	1.400779582333
H	0.743012272613	-1.878388882742	0.114166301219
H	0.149729511117	0.043763555498	-1.455009584702
Cl	0.244769862119	1.794448062005	0.118965882144
F	-2.311413978804	0.447037779194	-0.654974823176
F	-1.612024996818	-1.594809622048	-0.534540538655
F	-1.667083938072	-0.362921708588	1.245226495985

Atom	X	Y	Z
C	0.991672203442	1.082814343320	0.266976130426
C	-0.205972454570	0.476706668768	-0.461256397825
C	-0.591969262382	-0.928696828844	0.025467104455
Cl	2.550786059352	0.331468734338	-0.238845980679
H	1.063019040705	2.141199378246	0.026334337240
H	0.894303834577	0.955318246580	1.344383598138
H	-0.034428754719	0.429393028453	-1.536615629968
Cl	-1.613525352147	1.576433508983	-0.198533019271
F	-1.718886643742	-1.344098383330	-0.553128816353
F	0.370217779382	-1.804298264904	-0.280847875744
F	-0.765914449899	-0.951869431610	1.350831549581

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
61.2798	0.00611
81.8436	0.496
158.2602	0.657
185.2428	0.200
252.6191	0.0125
296.1881	0.123
355.4548	0.0331
431.8743	1.25
538.3196	0.796
560.5658	0.0298
668.5871	7.82
722.2995	2.91
777.6542	4.36
871.7048	0.955
949.6397	5.30
1065.4734	0.898
1145.1607	25.8
1172.1078	3.13
1220.5996	23.6
1269.7717	22.1
1287.2458	12.5
1310.4739	7.65
1363.0444	13.5
1470.0961	0.759
3099.0170	0.928
3120.6855	0.380
3167.3730	0.0314

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
41.8015	0.0966
107.5036	0.432
168.7781	0.310
209.5627	0.421
237.4067	0.388
273.1819	0.0251
361.9079	0.0294
428.2650	1.77
531.3746	0.959
566.9440	0.671
641.0190	2.07
736.8891	12.3
793.8990	1.46
828.7072	1.98
953.3100	4.46
1067.1824	0.637
1150.1501	14.5
1183.1178	17.5
1226.4968	12.6
1238.6373	21.8
1272.8647	19.4
1321.0960	5.56
1383.6781	7.75
1477.3076	1.35
3111.9140	0.437
3129.5850	0.387
3180.1479	0.0115



$\Delta E = 1.26$ kcal mol^{-1}
Population = 0.059

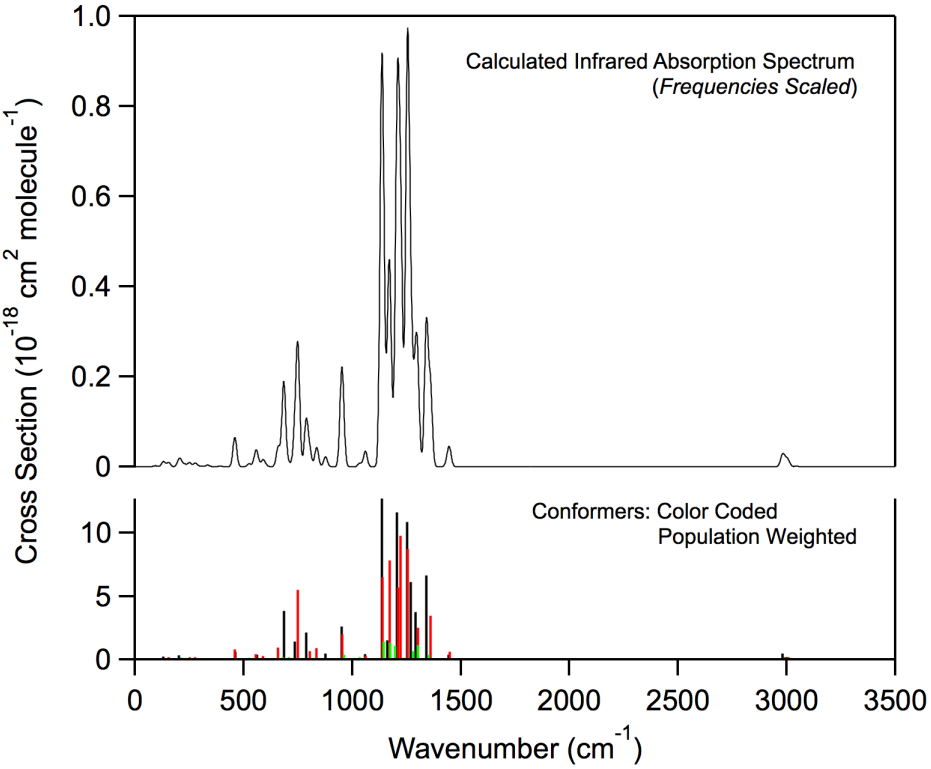
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.194359317984	-0.146613901123	-1.068581213938
C	-0.160043020614	0.442817984053	-0.694778458503
C	-1.104479212224	-0.525268883111	0.033184739961
Cl	2.231694738985	-0.607695194297	0.323275399196
H	1.034439296047	-1.048377737677	-1.660946271144
H	1.753683207249	0.581905357575	-1.653997525184
H	-0.664891548752	0.702413996011	-1.629370659382
Cl	-0.015828606443	1.969189761892	0.236017198584
F	-2.340823120328	-0.022168699814	0.076633747984
F	-1.155905899933	-1.677555860837	-0.658901335173
F	-0.724280151973	-0.802676822671	1.273980377600

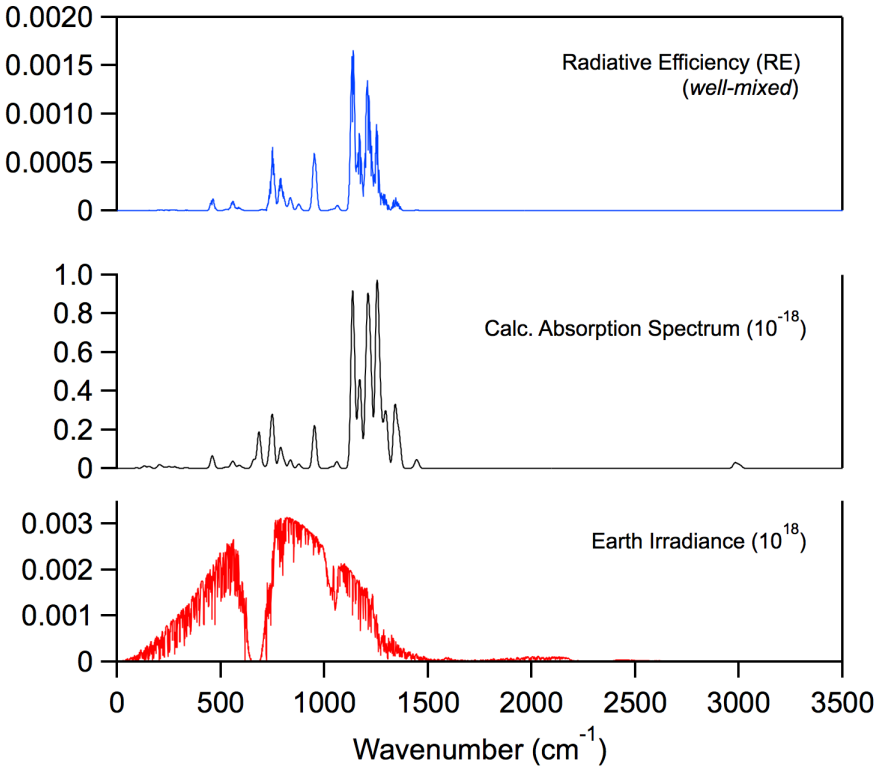
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
52.6497	0.0899
95.5389	0.0852
154.5027	0.0506
196.8399	0.266
258.9601	0.256
301.0224	0.291
361.4092	0.00681
499.3970	2.34
523.3215	1.05
580.6928	1.14
663.8689	3.36
691.9550	3.43
799.1924	1.67
827.1999	0.528
961.2450	6.24
1039.2165	2.86
1155.2339	24.5
1187.1958	22.2
1211.0281	18.4
1253.5008	2.03
1298.1901	11.5
1321.6680	19.7
1376.2520	6.08
1463.2953	1.90
3085.3489	0.380
3099.3012	1.26
3160.5628	0.0770

Infrared Spectrum

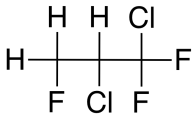


Radiative Efficiency



HCFC-243dc

Molecular Formula:	$CH_2FCHClCF_2Cl$
Name:	1,2-Dichloro-1,1,3-trifluoropropane
CAS number:	199171-49-8
Molecular Weight:	166.96



Global Atmospheric Lifetime (years):	2.03
Tropospheric Atmospheric Lifetime (years):	2.13
Stratospheric Atmospheric Lifetime (years):	42.6
Ozone Depletion Potential (ODP):	0.023

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.241	0.203
Global Warming Potential (GWP_H):		
GWP_{20}	659	556
GWP_{100}	178	151
Global Temperature Potentials (GTP_H)		
GTP_{20}		206
GTP_{50}		27
GTP_{100}		21

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 2.75 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 1.76 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 2.07$ years

$\tau^{OH}_{Trop} = 2.13$ years

$\tau^{OH}_{Strat} = 66.7$ years

Fractional Atmospheric Loss: 0.983

O(^{1}D) Reactivity

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

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

$\tau_{O(^1D)} = 250$ years

Fractional Atmospheric Loss: 0.008

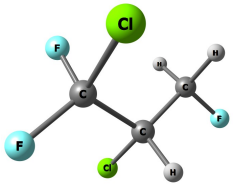
UV Photolysis

UV Spectrum: *No Recommendation*

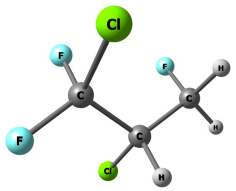
$\tau_{hv} = 225$ years

Fractional Atmospheric Loss: 0.009

Molecular Structure and Infrared Spectrum (9 conformers)



E = 0
Population = 0.227



$\Delta E = 0.12$ kcal mol^{-1}
Population = 0.184

Optimized Coordinates (Angstroms)

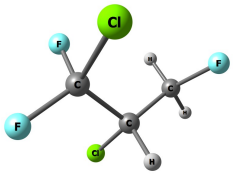
Atom	X	Y	Z
C	1.008544199748	-1.332298209919	0.361268380543
C	0.520857388875	-0.095606389129	-0.389319442038
C	-0.865601541608	0.372040561070	0.066209480724
F	2.202355710568	-1.733716940988	-0.177052128673
H	1.144979532939	-1.101263717160	1.422119034036
H	0.278493376310	-2.141490752614	0.252633199489
H	0.484894046234	-0.291790562906	-1.460992412260
Cl	1.690097462748	1.257028411880	-0.154128885721
F	-0.908153945494	0.537310370028	1.390646805743
F	-1.210225321634	1.517935033615	-0.512518659220
Cl	-2.114862908685	-0.864729803876	-0.386653372624

Atom	X	Y	Z
C	0.817954105257	-1.516803097177	-0.571446116585
C	0.519899101946	-0.025542960042	-0.672755144775
C	-0.670851058012	0.455893764696	0.170634266944
F	1.123381938673	-1.869299517746	0.715026073461
H	-0.056984803837	-2.087184282410	-0.902595216078
H	1.668383939420	-1.748438079117	-1.221315714167
H	0.307255592497	0.228978029651	-1.712221549871
Cl	1.972991801543	0.928300111497	-0.187766819143
F	-0.511651647149	0.198860436206	1.462854768795
F	-0.853549311476	1.767670826001	0.019677257793
Cl	-2.190276658863	-0.368348231559	-0.392879806374

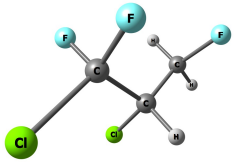
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
60.3721	0.0939
96.2219	0.647
173.8983	0.408
184.2527	0.394
257.3032	0.296
287.6934	0.110
334.4201	0.102
389.2383	0.353
414.3474	0.447
495.1863	1.66
608.9981	1.79
695.9442	11.4
803.3854	18.8
937.0362	23.6
1014.5470	1.66
1083.3437	5.62
1114.4343	10.9
1188.8177	17.7
1237.8858	12.1
1248.3410	6.00
1305.2150	3.42
1317.5054	7.03
1429.8567	1.70
1507.4046	0.588
3050.7277	2.68
3105.4109	1.51
3131.1149	0.764

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
51.3035	0.164
109.3890	0.183
177.2738	0.153
200.4243	0.255
260.8993	0.377
290.6184	0.125
329.9761	0.221
399.6537	0.228
413.4298	0.534
525.3382	3.36
658.3943	3.66
715.6660	17.0
800.8447	1.50
918.7997	30.3
965.2344	1.19
1050.5016	2.51
1132.2062	8.30
1184.8970	21.7
1235.9740	7.20
1258.6589	11.8
1292.7062	4.62
1349.5246	6.15
1429.3596	1.90
1501.0143	1.49
3045.8519	2.89
3096.6999	2.65
3117.2046	0.411



$\Delta E = 0.21$ kcal mol^{-1}
Population = 0.158



$\Delta E = 0.51$ kcal mol^{-1}
Population = 0.096

Optimized Coordinates (Angstroms)

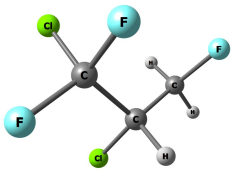
Atom	X	Y	Z
C	0.565106808061	-1.706704159020	0.205531890180
C	0.599277264206	-0.333632887465	-0.473361717429
C	-0.383006597883	0.694573621280	0.107632613938
F	-0.572506694729	-2.387621329815	-0.147394869361
H	1.437806572044	-2.277706240811	-0.123649233638
H	0.598939253117	-1.587474540217	1.293090645482
H	0.412901375462	-0.425671203836	-1.543243314895
Cl	2.271455306991	0.317950496280	-0.273199371976
F	-0.236649514622	0.796999701472	1.432320934941
F	-0.181646833071	1.898788479521	-0.428816391701
Cl	-2.086757939575	0.220466062610	-0.240256185541

Atom	X	Y	Z
C	1.987754694171	-0.019194098094	0.018349040446
C	0.574272363439	0.353925995113	-0.448023918530
C	-0.500756228393	-0.541699539755	0.189902958609
F	2.338572732749	-1.241292359456	-0.497797510111
H	2.688351937904	0.739126522969	-0.343333546527
H	2.027104430917	-0.057033660123	1.111849874199
H	0.497676877401	0.263884235907	-1.531694894535
Cl	0.292796607028	2.072406714359	-0.016601136718
F	-0.234700772350	-1.818421272320	-0.106261088418
F	-0.495006983314	-0.418323408173	1.520174166953
Cl	-2.153203659552	-0.168072130429	-0.416063945368

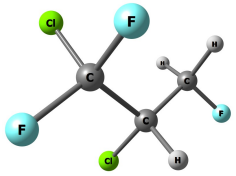
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
40.4813	0.0986
121.2063	0.759
169.6550	0.100
219.1461	0.324
247.2715	0.526
255.5960	0.211
352.1195	0.579
378.6967	0.0941
421.9478	0.195
499.8937	3.07
582.3131	0.947
733.9987	12.5
802.1436	11.6
930.2196	21.6
1011.8691	4.45
1084.3791	6.64
1107.9607	13.9
1187.3443	19.2
1216.3243	5.53
1235.1950	12.7
1278.9045	2.75
1365.1414	2.85
1427.1480	1.25
1508.8388	0.585
3057.7884	2.24
3111.5822	2.21
3134.1091	0.300

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
43.7431	0.0789
127.7773	0.696
168.1916	0.143
200.9619	0.268
224.9727	0.0478
305.2630	0.0447
360.7109	0.774
405.0055	0.987
419.2133	0.227
444.0710	4.59
582.9881	1.85
721.0306	4.57
846.9478	7.28
949.1474	27.0
1009.6182	6.36
1088.0835	6.87
1103.7098	9.87
1159.8307	31.2
1224.0172	5.95
1232.4465	12.6
1273.1246	2.57
1360.4162	1.41
1420.8111	2.51
1508.6943	0.574
3054.4064	2.37
3108.1618	2.19
3130.7989	0.437



$\Delta E = 0.58$ kcal mol^{-1}
Population = 0.085



$\Delta E = 0.61$ kcal mol^{-1}
Population = 0.081

Optimized Coordinates (Angstroms)

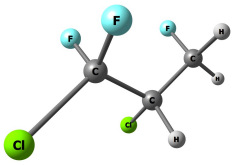
Atom	X	Y	Z
C	1.388941634094	-1.106433431014	0.462034112790
C	0.780776435269	-0.029402393412	-0.435626075265
C	-0.756856750881	0.024296590156	-0.437999041985
F	0.981719040589	-2.344824365314	0.030523448845
H	2.479599763990	-1.041000503697	0.397846228660
H	1.077778344657	-0.960138699139	1.500705141055
H	1.065570167321	-0.207367189408	-1.475750918924
Cl	1.469169057222	1.557484790444	0.035435146204
F	-1.181143866472	1.017535439785	-1.221670492213
F	-1.225656634917	-1.122473892857	-0.940134274210
Cl	-1.468208190871	0.254790654454	1.199957725042

Atom	X	Y	Z
C	1.283418281403	-1.178478150857	0.234037567671
C	0.594832054531	-0.019687550089	-0.478416389077
C	-0.935391887272	-0.122302143279	-0.455811606715
F	2.618770430567	-1.154697062778	-0.073597538787
H	1.158738649817	-1.097731363613	1.317404701096
H	0.849844963176	-2.122405827606	-0.116730791205
H	0.876272377423	-0.032407643784	-1.534684049998
Cl	1.143813928454	1.558014311044	0.171367094181
F	-1.490563940262	0.899752576540	-1.101969167255
F	-1.285576089366	-1.252473773738	-1.094713440694
Cl	-1.623738768471	-0.188827371839	1.205451620783

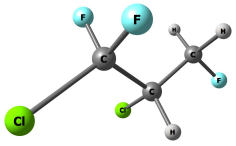
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
45.8811	0.0778
125.5648	0.498
176.2609	0.0210
202.0235	0.378
225.8593	0.510
302.5342	0.0108
380.2837	0.118
401.2067	0.865
416.7077	0.266
493.7928	2.05
558.5418	6.07
660.8455	3.36
851.8770	11.4
918.2836	15.8
1087.0580	5.27
1089.3464	23.2
1107.5766	2.54
1185.2257	23.0
1200.4067	21.4
1228.9001	1.81
1267.8902	2.15
1363.7174	3.54
1425.4739	1.83
1508.3831	0.973
3056.2609	2.20
3093.5148	0.876
3115.5617	2.00

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
66.5445	0.0353
97.2616	0.638
154.1379	0.219
185.2200	0.380
248.4468	0.375
318.5404	0.0432
337.8354	0.192
408.1109	0.285
439.1425	1.10
470.0057	1.00
630.6206	2.30
658.6797	10.7
754.5955	8.46
1010.9828	6.51
1035.8351	25.9
1089.2449	8.56
1116.7491	14.3
1166.1064	20.5
1208.4866	11.9
1249.1177	0.663
1305.5487	7.21
1309.9059	5.17
1429.1891	1.67
1505.8926	0.555
3045.4072	2.72
3091.5693	0.194
3112.7003	1.99



$\Delta E = 0.64$ kcal mol^{-1}
Population = 0.077



$\Delta E = 0.73$ kcal mol^{-1}
Population = 0.066

Optimized Coordinates (Angstroms)

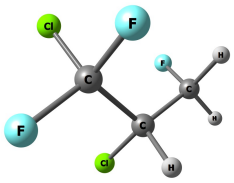
Atom	X	Y	Z
C	1.777149716494	-0.664764604875	-0.706245541243
C	0.522159085558	0.203640073839	-0.656774742921
C	-0.647846241938	-0.511963841922	0.043517210367
F	2.208419429213	-0.974935861646	0.555202210040
H	1.548164851024	-1.591381493224	-1.245090436508
H	2.565941526386	-0.120292369597	-1.235679102399
H	0.210483167904	0.426732847689	-1.678405970221
Cl	0.867611127879	1.768211105590	0.149212948692
F	-0.785553280859	-1.730185337159	-0.509638457246
F	-0.430808897940	-0.671313286077	1.343122539445
Cl	-2.205141483723	0.366236767381	-0.178793658007

Atom	X	Y	Z
C	1.663757281172	-0.967279116450	0.065347260088
C	0.560379936924	-0.002425095153	-0.374531589517
C	-0.810410023082	-0.495723026107	0.108801505082
F	2.850348635238	-0.573805368616	-0.491973964831
H	1.754665422300	-0.969243217691	1.156005267351
H	1.419791066521	-1.976069483227	-0.285030119125
H	0.537498797667	0.063365220203	-1.462692490559
Cl	0.901233949539	1.645787544472	0.243334186236
F	-0.995191469702	-1.746047017883	-0.353861759836
F	-0.859573075887	-0.546299161621	1.442243313792
Cl	-2.168412520690	0.513691722073	-0.483967608680

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
56.2802	0.103
105.5446	0.301
158.4861	0.0434
206.1465	0.248
252.7095	0.0191
309.0780	0.903
324.9032	0.0231
417.2635	0.119
426.5716	0.192
524.9321	7.06
609.9628	3.92
751.8379	6.72
807.9311	0.955
943.3111	17.4
975.6140	13.1
1048.7402	4.36
1133.2593	17.6
1143.8429	23.9
1236.5529	7.99
1257.7876	10.2
1290.8000	4.16
1336.4576	4.12
1425.6123	2.84
1500.0322	1.10
3043.0239	3.32
3095.8401	2.36
3114.8797	0.539

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
59.3353	0.0233
98.4633	0.778
154.8408	0.369
186.6098	0.248
261.8187	0.269
304.1251	0.383
328.7649	0.0356
399.7778	0.596
423.8148	0.196
471.8822	2.49
607.3777	1.73
729.4985	4.16
804.5644	16.1
959.0842	25.0
1007.7415	5.45
1095.3011	9.93
1124.3898	8.07
1134.0141	23.4
1231.0361	18.9
1248.7666	1.73
1300.6972	2.16
1313.2007	4.80
1426.8124	2.12
1509.4573	0.389
3048.0239	2.81
3102.3675	1.49
3126.9089	0.979



$\Delta E = 1.30$ kcal mol^{-1}
Population = 0.025

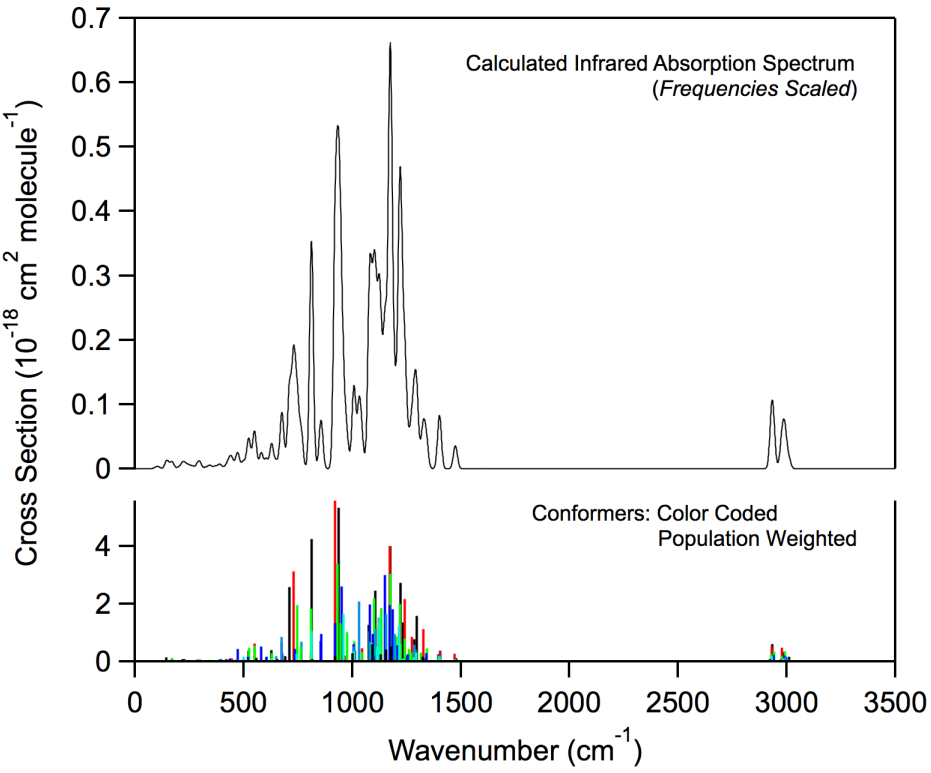
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.265791843474	-1.152028278483	-0.820336976734
C	0.662013736453	0.239090349079	-0.662589440887
C	-0.851125835641	0.258496907869	-0.385322233477
F	1.309777914375	-1.827670166431	0.367342519184
H	0.659620152069	-1.718829160416	-1.537325027587
H	2.284615718766	-1.049265072560	-1.208738611397
H	0.772374704450	0.762351421364	-1.617215821023
Cl	1.551408251688	1.203773811115	0.556784357856
F	-1.303405544156	1.514200565533	-0.413862797579
F	-1.452126500936	-0.413444780902	-1.386202672558
Cl	-1.341943440543	-0.487252596167	1.163429704200

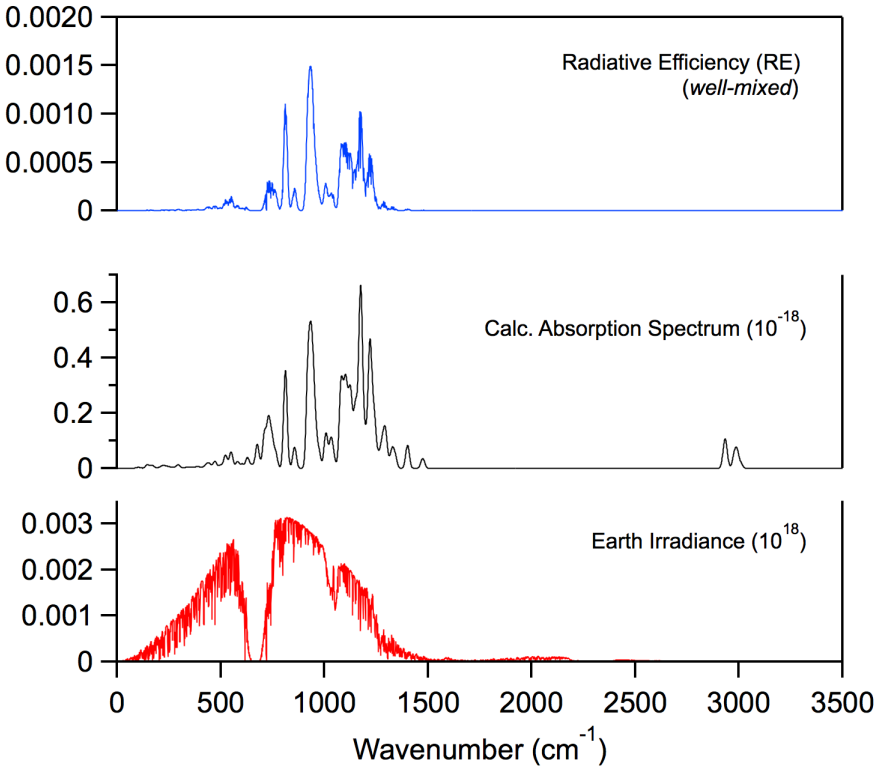
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
56.2019	0.198
111.8389	0.293
170.1549	0.121
178.1769	0.0443
254.9811	0.559
308.1334	0.258
324.2627	0.0400
422.1813	0.0419
438.3133	0.385
534.1345	4.81
636.4510	3.36
674.9156	7.67
806.5290	3.48
918.1271	7.49
1002.8365	11.4
1100.4886	24.0
1139.4292	10.2
1167.4600	16.4
1191.4602	20.7
1246.0132	1.16
1295.8342	0.990
1345.5349	6.31
1429.8027	1.21
1500.9154	0.930
3038.6564	3.07
3081.7959	1.21
3091.7548	2.33

Infrared Spectrum

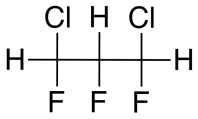


Radiative Efficiency



HCFC-243ea

Molecular Formula:	CHFClCHFCHFCl
Name:	1,3-Dichloro-1,2,3-trifluoropropane
CAS number:	151771-08-3
Molecular Weight:	166.96



Global Atmospheric Lifetime (years):	1.57
Tropospheric Atmospheric Lifetime (years):	1.64
Stratospheric Atmospheric Lifetime (years):	36.3
Ozone Depletion Potential (ODP):	0.019

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.212	0.172
Global Warming Potential (GWP_H):		
GWP_{20}	448	363
GWP_{100}	121	98
Global Temperature Potentials (GTP_H)		
GTP_{20}		127
GTP_{50}		17
GTP_{100}		14

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 3.58 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 2.29 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

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

$\tau^{OH}_{Trop} = 1.64$ years

$\tau^{OH}_{Strat} = 52.6$ years

Fractional Atmospheric Loss: 0.987

O(^{1}D) Reactivity

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

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

$\tau_{O(^1D)} = 250$ years

Fractional Atmospheric Loss: 0.006

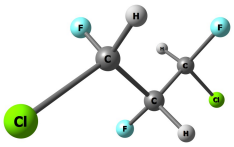
UV Photolysis

UV Spectrum: *No Recommendation*

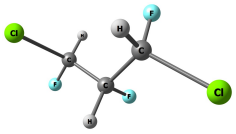
$\tau_{hv} = 225$ years

Fractional Atmospheric Loss: 0.007

Molecular Structure and Infrared Spectrum (8 conformers)



E = 0
Population = 0.322



$\Delta E = 0.29$ kcal mol^{-1}
Population = 0.197

Optimized Coordinates (Angstroms)

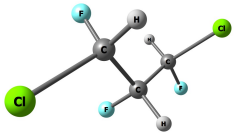
Atom	X	Y	Z
C	1.260233318461	0.458062735789	-0.185311761082
C	0.008697681239	-0.320397520523	0.233823765934
C	-1.234715512818	0.546766917676	0.030436661171
Cl	2.734576606898	-0.508034369119	0.132916929638
H	1.251446727333	0.687268991939	-1.251654273776
F	1.309117346289	1.610205891469	0.532903280618
H	0.086544013086	-0.600418832779	1.289715931776
F	-0.079365168293	-1.439316306615	-0.541417670718
H	-1.205945363755	1.430762132563	0.669128452354
F	-1.310399591890	0.928500200850	-1.269091191036
Cl	-2.714500056550	-0.368686841250	0.467375875122

Atom	X	Y	Z
C	0.984240502882	-0.543104980327	0.141323526493
C	0.011199723033	0.539166764918	-0.320436488638
C	-1.385684362616	0.367372447909	0.284723552213
Cl	2.634798069328	-0.194341819439	-0.472515909619
F	1.008188021538	-0.573097434357	1.497919605301
H	0.708034451505	-1.526132205485	-0.240330375941
H	-0.062031020125	0.533453476296	-1.413041749392
F	0.461650087976	1.761703155907	0.103364561324
H	-1.355324547207	0.349904511684	1.374907470854
F	-2.167232625242	1.381544065598	-0.135735365167
Cl	-2.110872301072	-1.196261982705	-0.250241827427

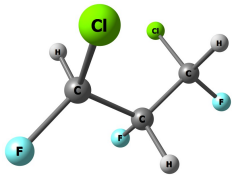
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
60.3531	0.163
69.0463	0.174
124.4580	0.321
217.3206	0.478
232.4454	0.232
240.3634	0.0519
372.1233	0.153
392.5969	0.484
435.2023	4.07
493.6791	0.495
698.9197	29.0
770.5202	5.00
851.4089	3.56
905.6618	4.84
1088.2336	9.97
1098.2859	12.3
1117.9130	12.1
1173.9604	14.4
1237.1018	1.73
1281.8946	1.02
1333.8427	2.43
1358.1495	1.81
1381.4036	2.69
1397.0258	0.366
3074.4660	0.871
3117.4875	0.929
3124.3613	1.30

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
53.6345	0.187
81.8998	0.229
130.4560	0.183
199.8802	0.475
234.7087	0.246
295.9336	0.294
366.8422	0.589
391.2147	0.618
415.9106	1.23
456.2197	2.91
736.0617	9.35
787.2307	13.2
803.1233	19.9
914.4060	4.73
1076.4244	2.60
1090.3799	9.20
1145.1426	24.4
1161.8651	13.5
1237.3311	1.80
1276.9805	0.147
1323.4509	2.78
1365.7984	0.0718
1383.6499	1.62
1403.2482	2.45
3076.8472	0.665
3125.2233	0.668
3127.7605	1.46



$\Delta E = 0.29$ kcal mol^{-1}
Population = 0.197



$\Delta E = 0.65$ kcal mol^{-1}
Population = 0.108

Optimized Coordinates (Angstroms)

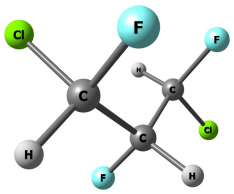
Atom	X	Y	Z
C	1.386951121171	-0.368669931011	-0.283829375111
C	-0.009129597652	-0.533380683008	0.325141659232
C	-0.984211458964	0.540340496477	-0.152023948984
Cl	2.110278350540	1.203935755232	0.226802384822
F	2.170394160769	-1.375217679317	0.151171343441
H	1.355585080249	-0.367708496826	-1.374124371856
H	0.065072462203	-0.511051841464	1.417468096124
F	-0.458120593480	-1.762850608113	-0.079727485617
H	-0.709141483163	1.529435727359	0.214471239624
F	-1.009425651683	0.549786146580	-1.508896085010
Cl	-2.633691389991	0.198442114091	0.468538543335

Atom	X	Y	Z
C	1.103030905592	0.277719373917	0.606387411600
C	-0.016574997079	-0.738113526864	0.388067312167
C	-1.210381621297	-0.232417122894	-0.420153732649
Cl	1.828529501440	0.797608967489	-0.959298543109
H	0.745712081364	1.181656542661	1.099861676868
F	2.061131212978	-0.307680355441	1.359417990091
H	-0.370820908742	-1.058754387775	1.376462495946
F	0.488563397791	-1.824536104369	-0.274130712493
H	-0.926095197822	0.104590204015	-1.417820910743
F	-2.111953583013	-1.231279398682	-0.516246883622
Cl	-1.975120791212	1.172845807943	0.415099895945

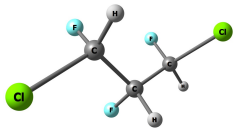
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
53.6354	0.187
81.8998	0.229
130.4557	0.183
199.8793	0.475
234.7089	0.246
295.9343	0.294
366.8425	0.589
391.2146	0.618
415.9105	1.23
456.2204	2.91
736.0606	9.35
787.2309	13.2
803.1232	19.9
914.4037	4.73
1076.4241	2.60
1090.3800	9.20
1145.1432	24.4
1161.8628	13.5
1237.3302	1.80
1276.9790	0.147
1323.4503	2.78
1365.7963	0.0718
1383.6478	1.62
1403.2476	2.45
3076.8475	0.665
3125.2228	0.669
3127.7621	1.46

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
49.1016	0.126
90.6315	0.240
137.0066	0.179
193.3266	0.377
246.0621	0.335
297.4861	0.355
365.3355	0.280
393.3130	0.736
436.5333	2.24
474.6475	1.18
652.5255	11.6
754.5929	4.85
804.1596	18.2
973.4072	4.09
1084.1737	12.9
1122.4125	10.7
1140.1599	8.58
1155.6497	25.2
1240.9427	0.767
1284.0426	4.26
1306.4395	1.12
1368.5759	1.37
1375.8115	1.99
1413.5595	1.83
3048.4695	0.947
3125.2445	0.929
3127.8488	1.01



$\Delta E = 0.97$ kcal mol^{-1}
Population = 0.063



$\Delta E = 1.22$ kcal mol^{-1}
Population = 0.041

Optimized Coordinates (Angstroms)

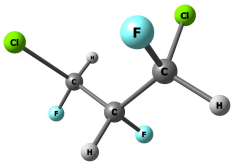
Atom	X	Y	Z
C	0.929639136592	0.254237752157	-0.419721429455
C	0.084714111947	-0.277028498343	0.739492611713
C	-1.400060343790	0.106845290755	0.675375001534
Cl	2.652124280403	-0.199298341738	-0.166721537949
H	0.632234827762	-0.178235171866	-1.375430623097
F	0.820431364104	1.600041667076	-0.464577059009
H	0.480547935255	0.124388361753	1.681049955406
F	0.159099221308	-1.642045805828	0.754586964097
H	-1.950656946361	-0.446535389303	1.439638857588
F	-1.544058714772	1.432892699191	0.874309940798
Cl	-2.152860872447	-0.354329563853	-0.896152681626

Atom	X	Y	Z
C	1.434306957111	0.477717043894	-0.351074268798
C	-0.047401533446	0.312716547656	-0.706655765786
C	-0.873053346663	-0.384182583653	0.375805628701
Cl	2.244045028615	-1.137899492168	-0.331521594139
H	1.938200283477	1.067900980354	-1.119838241809
F	1.590920382283	1.073375460127	0.845616399699
H	-0.117549082483	-0.259547821296	-1.636777274271
F	-0.546524554512	1.574309441898	-0.903629757675
H	-0.465522535236	-1.365660025988	0.623432408149
F	-0.933055646257	0.384032674067	1.481804502534
Cl	-2.547229952888	-0.665523224891	-0.233948036604

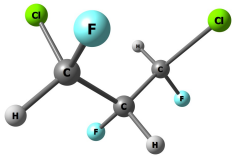
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
39.2613	0.131
84.8736	0.0445
149.2010	0.124
184.2325	0.135
220.3180	0.270
331.6199	0.203
360.9246	2.87
389.8348	1.65
445.5183	0.118
542.8640	3.70
565.2836	9.03
695.5693	6.80
831.6197	14.8
989.4067	3.68
1114.2070	5.58
1132.1836	0.837
1147.6206	1.85
1154.5664	43.1
1242.8904	0.818
1292.5078	7.85
1322.4383	1.76
1340.8040	0.365
1371.7551	3.35
1417.6732	0.451
3050.5556	1.32
3098.4568	1.73
3128.4874	1.01

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
41.4017	0.205
84.7594	0.137
157.9340	0.281
189.5356	0.307
235.2317	0.0944
270.0797	0.0241
338.6680	0.377
380.2267	0.789
403.0679	0.614
561.9424	11.0
746.0254	4.36
794.8512	22.3
846.4077	4.14
862.5940	7.60
988.9604	0.197
1104.7955	9.31
1163.3364	35.3
1166.4072	0.716
1254.3318	3.78
1268.7999	2.39
1348.3302	3.28
1361.3419	0.267
1391.6947	1.61
1409.8058	2.46
3081.6732	0.917
3102.3241	1.48
3115.6803	1.20



$\Delta E = 1.62$ kcal mol^{-1}
Population = 0.021



$\Delta E = 1.62$ kcal mol^{-1}
Population = 0.021

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.222871593447	-0.178805819218	-0.692266074505
C	-0.048785039247	0.676230642824	-0.688423506700
C	-1.077166751299	0.417987606529	0.413527242904
Cl	2.005516026656	-0.242632713680	0.931160215764
F	0.964019027071	-1.430640370761	-1.118751591357
H	1.955553605706	0.291751853144	-1.351849904201
H	-0.537731387476	0.549904432411	-1.662656898783
F	0.355481935509	1.982771211895	-0.553877567908
H	-0.645993169903	0.515648513774	1.410046697481
F	-2.074816874331	1.318817967569	0.261749676735
Cl	-1.756574966132	-1.238586324488	0.286115710569

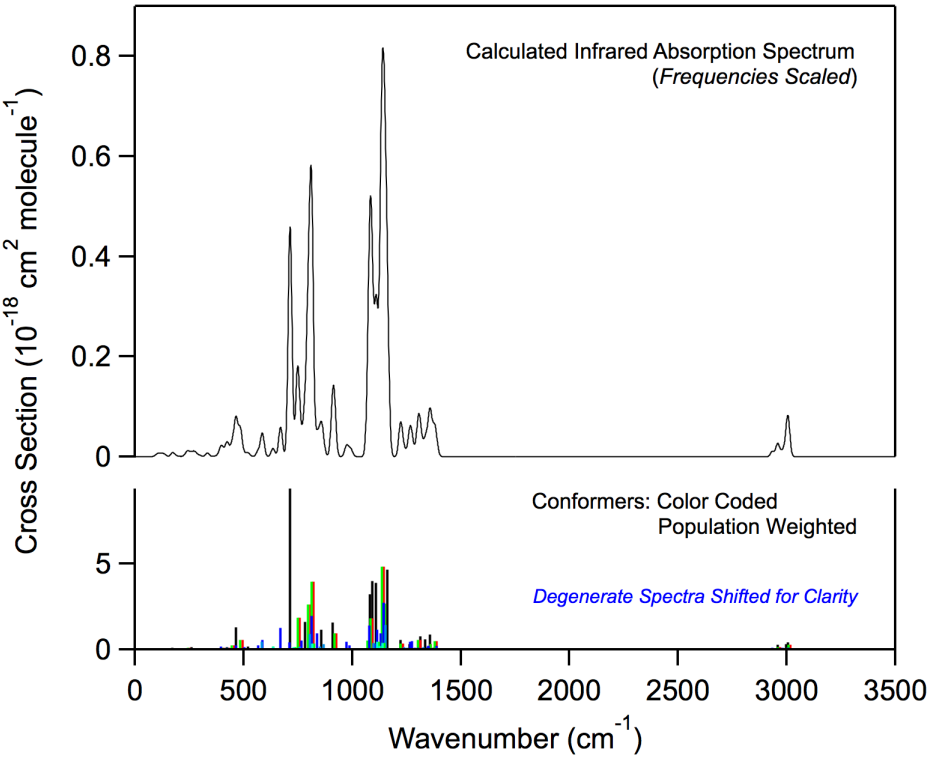
Atom	X	Y	Z
C	1.076094484086	-0.425913889245	-0.416550148930
C	0.050799144289	-0.674200545999	0.690552350718
C	-1.213018808735	0.192335654855	0.700067948714
Cl	1.771096049226	1.224506789597	-0.293458686000
F	2.066269432699	-1.335662948758	-0.269082233151
H	0.639201386346	-0.520226626467	-1.410898454980
H	0.545614195861	-0.551764346800	1.662316176733
F	-0.365947668857	-1.977096462213	0.558770362331
H	-1.946710889832	-0.271182617061	1.363502504129
F	-0.940748164789	1.442012938065	1.124520472419
Cl	-2.002964160294	0.262335054027	-0.919563291982

Infrared Absorption Spectrum (unscaled frequencies)

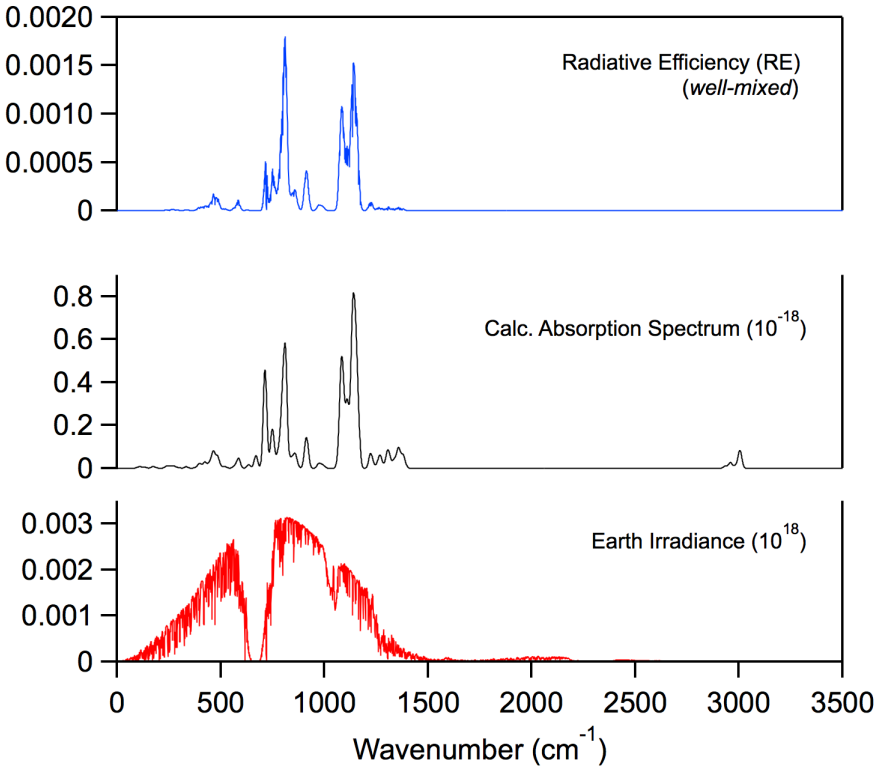
Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
41.1136	0.108
97.4197	0.0620
145.2728	0.0901
184.4535	0.174
259.3836	1.20
311.5424	0.132
352.1396	1.33
400.8928	0.725
424.5445	2.38
514.1186	0.377
615.6322	8.46
714.7176	6.37
805.9960	16.2
999.2352	3.89
1103.4515	3.74
1121.6927	22.5
1135.4193	10.7
1148.8604	17.7
1249.5871	3.70
1285.4181	3.31
1325.7609	2.16
1337.1672	1.02
1382.6509	2.45
1417.7000	1.15
3052.8421	1.07
3099.5536	1.74
3129.9132	0.989

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
41.1136	0.108
97.4202	0.0620
145.2745	0.0901
184.4541	0.174
259.3833	1.20
311.5420	0.132
352.1397	1.33
400.8927	0.725
424.5440	2.38
514.1188	0.377
615.6331	8.46
714.7176	6.37
805.9957	16.2
999.2357	3.89
1103.4525	3.74
1121.6937	22.5
1135.4197	10.7
1148.8606	17.7
1249.5868	3.70
1285.4184	3.31
1325.7609	2.16
1337.1671	1.02
1382.6508	2.45
1417.7002	1.15
3052.8424	1.07
3099.5519	1.74
3129.9145	0.989

Infrared Spectrum

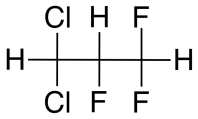


Radiative Efficiency



HCFC-243eb

Molecular Formula:	$CHCl_2CHFCHF_2$
Name:	1,1-Dichloro-2,3,3-trifluoropropane
CAS number:	1081835-90-6
Molecular Weight:	166.96



Global Atmospheric Lifetime (years):	0.898
Tropospheric Atmospheric Lifetime (years):	0.938
Stratospheric Atmospheric Lifetime (years):	20.9
Ozone Depletion Potential (ODP):	0.014

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.195	0.141
Global Warming Potential (GWP_H):		
GWP_{20}	236	170
GWP_{100}	64	46
Global Temperature Potentials (GTP_H)		
GTP_{20}		55
GTP_{50}		8
GTP_{100}		6

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 6.25 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 3.99 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 0.910$ years

$\tau^{OH}_{Trop} = 0.938$ years

$\tau^{OH}_{Strat} = 31.8$ years

Fractional Atmospheric Loss: 0.985

$O(^1D)$ Reactivity

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

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

$\tau_{O(^1D)} = 250$ years

Fractional Atmospheric Loss: 0.004

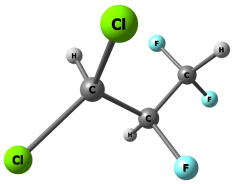
UV Photolysis

UV Spectrum: *No Recommendation*

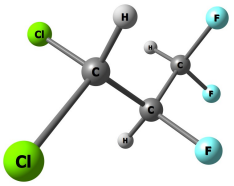
$\tau_{hv} = 80$ years

Fractional Atmospheric Loss: 0.011

Molecular Structure and Infrared Spectrum (5 conformers)



E = 0
Population = 0.573



$\Delta E = 0.63$ kcal mol^{-1}
Population = 0.197

Optimized Coordinates (Angstroms)

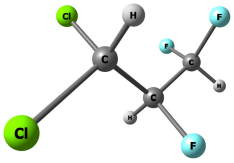
Atom	X	Y	Z
C	-0.761961742493	-0.113855028176	0.479055078131
C	0.458494041992	0.622918793123	-0.066770408903
C	1.745692228220	-0.200266608879	0.041916386833
H	-0.582933867544	-0.425170316464	1.504994520287
Cl	-2.183193443390	0.974351131331	0.491122224385
Cl	-1.104397276321	-1.599173850233	-0.467070981163
H	0.596151974059	1.537436084106	0.523975419399
F	0.278245765716	0.955666821769	-1.377824221034
H	1.750167985091	-1.070947985724	-0.621289949830
F	2.789760151013	0.596608089114	-0.265593280345
F	1.885226183656	-0.611453129967	1.328831212240

Atom	X	Y	Z
C	-0.803929797270	-0.057711697591	-0.335901141864
C	0.432033202395	0.436900167851	0.419458216370
C	1.680736120883	-0.398029244551	0.108839675465
H	-0.615762642275	-0.096405626359	-1.406066716810
Cl	-1.211363050359	-1.724475319989	0.193827486971
Cl	-2.177443871397	1.051826157604	-0.075130831942
H	0.243083571731	0.422869766179	1.498466710779
F	0.691429806809	1.719521775312	0.017498888275
H	1.595110848669	-1.433268054587	0.453172588790
F	1.895239853510	-0.394225299339	-1.229866597372
F	2.739495957305	0.183129375470	0.710814721338

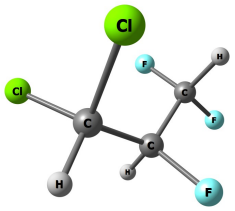
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
53.9047	0.0935
82.0064	0.287
136.6634	0.223
195.5079	0.217
208.2200	0.135
265.7733	0.340
336.9280	0.0480
440.0315	1.68
462.4422	4.23
567.1157	2.46
655.5430	6.04
732.1941	1.15
770.2772	16.8
978.1366	2.24
1100.6930	6.08
1130.3688	15.6
1150.0514	19.3
1161.8639	15.5
1228.5377	3.97
1274.1749	0.202
1304.4121	0.0832
1356.9694	3.83
1398.8790	0.598
1429.2181	5.14
3051.4061	0.767
3090.1599	3.79
3159.0329	0.244

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
55.3048	0.193
77.8485	0.189
140.8811	0.213
217.7708	0.462
233.4186	0.403
264.4288	0.211
324.3571	0.180
383.2609	1.01
451.1462	1.49
540.9334	2.40
741.7935	11.0
773.1993	19.0
804.6231	2.61
898.2733	6.58
1085.9849	0.190
1110.9854	10.8
1145.7326	15.6
1178.4291	20.7
1226.4820	1.50
1237.0299	3.80
1341.5178	0.185
1373.4360	2.05
1408.6333	4.14
1419.5436	2.81
3070.1377	0.787
3087.1206	4.45
3158.2597	0.177



$\Delta E = 0.91$ kcal mol^{-1}
Population = 0.123



$\Delta E = 1.43$ kcal mol^{-1}
Population = 0.051

Optimized Coordinates (Angstroms)

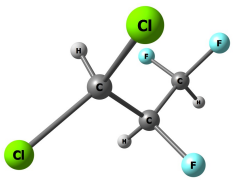
Atom	X	Y	Z
C	-0.678141764769	-0.016362690881	-0.374521497775
C	0.340939788468	0.634604825036	0.565239919097
C	1.802684317003	0.274384455257	0.251860507314
H	-0.430468120650	0.185452378732	-1.413090780902
Cl	-0.683520833683	-1.790775613785	-0.160069617310
Cl	-2.304459250653	0.671066541502	-0.077663097931
H	0.118382796179	0.374540246073	1.605010196716
F	0.254031033343	1.998104162721	0.406145946208
H	2.462267627678	1.035080086873	0.687474251466
F	2.125436352453	-0.933909390953	0.754467141474
F	1.999992054630	0.248625999424	-1.088498968356

Atom	X	Y	Z
C	-0.929454560739	0.187566967589	0.548748445200
C	0.591011918553	0.256946618495	0.720878903569
C	1.447175565726	-0.118998366679	-0.492469531097
H	-1.391993795833	0.681468785093	1.400515551581
Cl	-1.482499332306	1.091253911367	-0.901137714732
Cl	-1.520264243049	-1.498112717458	0.541139927296
H	0.872258080169	-0.392884609400	1.558200301256
F	0.901298215074	1.557927346130	1.036219957243
H	1.277425361874	0.549670689022	-1.342372025679
F	2.743510665233	-0.031271732652	-0.116951156254
F	1.196924125298	-1.392644891508	-0.862388658383

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
39.8896	0.139
86.9524	0.124
147.9779	0.0671
217.9373	0.417
228.4361	0.353
268.3681	0.573
352.7523	0.110
368.0354	2.56
470.4861	1.13
556.5528	3.43
635.7427	7.66
785.7672	10.9
808.3263	8.94
924.7560	1.97
1086.3135	3.90
1116.6359	7.30
1149.3780	23.1
1174.5687	12.7
1231.6736	3.46
1235.9506	0.502
1330.2213	0.354
1362.5653	4.17
1406.4009	3.91
1422.1092	3.31
3057.2351	5.42
3081.1229	1.34
3164.2554	0.151

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
36.6310	0.119
88.8583	0.0659
149.6281	0.0403
183.8910	0.206
235.3734	0.490
274.6103	0.564
348.0467	0.0957
410.1216	3.98
471.5101	1.52
561.8106	2.82
622.0274	2.16
689.9089	4.69
798.2017	15.4
1003.9969	4.44
1103.1532	7.84
1136.9269	2.84
1142.3868	26.0
1154.6535	20.2
1229.3745	2.53
1259.0395	1.80
1323.2175	1.33
1343.4013	2.03
1400.6957	1.55
1441.4293	2.69
3059.8008	0.457
3088.0633	4.02
3142.9660	0.289



$\Delta E = 1.77$ kcal mol^{-1}
Population = 0.029

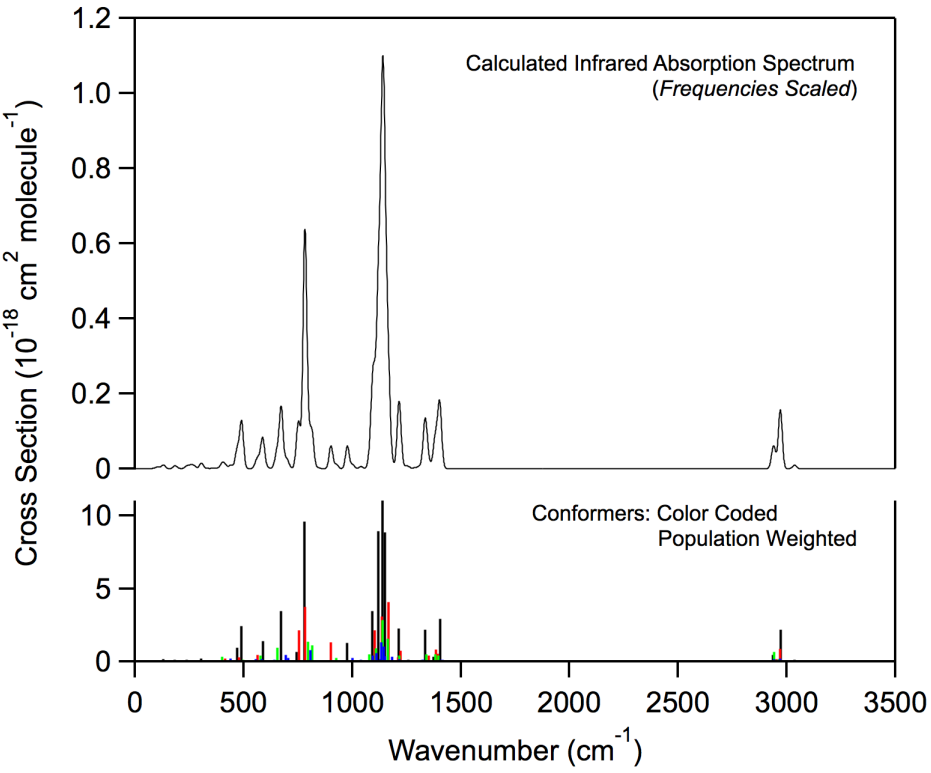
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-0.652795977880	-0.025494253107	0.479533520018
C	0.347801174778	0.851847821480	-0.277464144197
C	1.815818274837	0.512780478175	0.010737710170
H	-0.348461872334	-0.113709541040	1.519983841354
Cl	-2.269600277702	0.763478101427	0.477856162834
Cl	-0.762458495393	-1.673529109447	-0.192687943081
H	0.192526395593	1.884440092034	0.058905796212
F	0.146568222291	0.787616178804	-1.625397984438
H	2.480110233987	1.201460399934	-0.526187410465
F	2.020427944574	0.650683515930	1.347525540771
F	2.127298377251	-0.747384684191	-0.340473089179

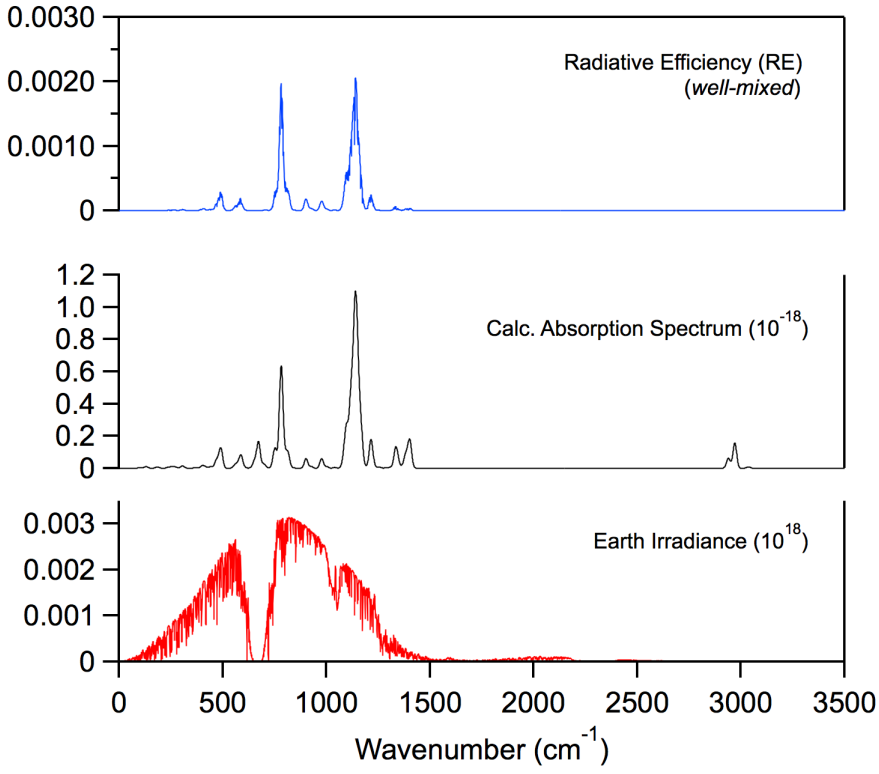
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
36.2036	0.173
89.1678	0.115
156.3062	0.364
196.1318	0.207
206.6483	0.0198
252.5207	0.0629
296.7567	0.652
422.4410	0.603
530.5093	5.62
587.4532	2.84
678.5498	15.1
736.4693	3.53
835.1595	2.01
878.2693	0.274
1044.7373	4.20
1121.3669	20.6
1161.6725	12.5
1195.6099	12.0
1232.2939	5.53
1277.2537	0.422
1349.4145	4.75
1355.7589	1.46
1405.7308	2.27
1429.2813	4.31
3047.8470	2.27
3058.6681	5.41
3151.0676	0.187

Infrared Spectrum

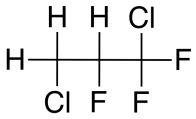


Radiative Efficiency



HCFC-243ec

Molecular Formula:	$CH_2ClCHFCF_2Cl$
Name:	1,3-Dichloro-1,1,2-trifluoropropane
CAS number:	149329-27-1
Molecular Weight:	166.96



Global Atmospheric Lifetime (years):	1.70
Tropospheric Atmospheric Lifetime (years):	1.78
Stratospheric Atmospheric Lifetime (years):	38.3
Ozone Depletion Potential (ODP):	0.020

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.221	0.182
Global Warming Potential (GWP_H):		
GWP_{20}	507	417
GWP_{100}	137	113
Global Temperature Potentials (GTP_H)		
GTP_{20}		148
GTP_{50}		20
GTP_{100}		16

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 3.29 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 2.10 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 1.73$ years

$\tau^{OH}_{Trop} = 1.78$ years

$\tau^{OH}_{Strat} = 56.8$ years

Fractional Atmospheric Loss: 0.986

O(^{1}D) Reactivity

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

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

$\tau_{O(^1D)} = 250$ years

Fractional Atmospheric Loss: 0.006

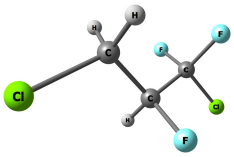
UV Photolysis

UV Spectrum: *No Recommendation*

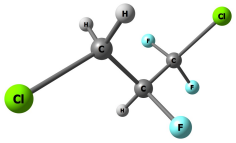
$\tau_{hv} = 225$ years

Fractional Atmospheric Loss: 0.008

Molecular Structure and Infrared Spectrum (7 conformers)



E = 0
Population = 0.335



$\Delta E = 0.06$ kcal mol^{-1}
Population = 0.305

Optimized Coordinates (Angstroms)

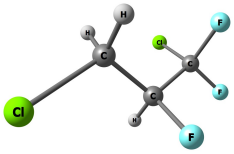
Atom	X	Y	Z
C	1.441302445199	0.638210929351	-0.162516109562
C	0.297960220017	-0.288547010866	0.229884924475
C	-1.053722511297	0.398478404703	-0.033278516667
Cl	3.021721245842	-0.072698831287	0.310500377583
H	1.454300179237	0.783705900243	-1.242201659930
H	1.344534436851	1.598591709996	0.342602156342
H	0.347163516590	-0.542673676042	1.293377356471
F	0.348144077889	-1.432977997077	-0.513256725022
F	-1.149187862057	1.488530721470	0.742763823700
F	-1.146786319988	0.788531610444	-1.309109027501
Cl	-2.427131428285	-0.692071760933	0.334465400110

Atom	X	Y	Z
C	1.233305218507	0.500494681655	0.475986577565
C	0.317350485457	-0.566672555936	-0.097493015894
C	-1.158294464909	-0.347780376477	0.279181406708
Cl	2.956665022362	0.039543336657	0.246861778394
H	1.079820655371	1.451328679200	-0.032776471298
H	1.060820075047	0.616210469494	1.545388017133
H	0.582351175115	-1.554521293297	0.300706639236
F	0.406668189990	-0.600963392180	-1.459047113592
F	-1.896249642555	-1.350462499253	-0.196688268618
F	-1.275261403807	-0.338532629016	1.614882050382
Cl	-1.814974310578	1.195354579154	-0.368983600016

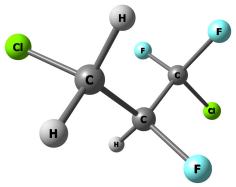
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
63.4674	0.0289
75.2431	0.622
130.5050	0.569
217.2285	0.238
249.1728	0.180
272.7243	0.130
346.3155	0.153
414.9144	0.262
432.5122	1.31
512.1874	2.15
623.6455	2.47
716.5153	20.4
838.5468	1.86
873.1650	0.345
966.8856	27.0
1055.4691	9.29
1140.3525	7.46
1161.7519	24.1
1215.8046	6.25
1243.7301	10.3
1281.8028	5.18
1364.3349	2.93
1388.9002	0.508
1466.7701	0.850
3080.6810	1.22
3104.3490	0.882
3171.4650	0.0829

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
69.5885	0.237
70.7951	0.383
143.1050	0.543
201.4091	0.216
228.0490	0.190
309.2000	0.0677
339.3261	0.260
414.5503	0.0494
481.6348	0.992
493.2291	1.03
631.6097	9.40
670.9938	11.4
773.2294	5.06
872.2513	1.21
1040.7884	12.4
1059.2184	19.8
1148.7011	13.4
1187.5416	18.1
1194.6493	13.7
1238.2766	6.68
1279.2980	6.49
1367.4516	3.54
1387.8034	1.86
1466.0677	0.833
3050.0464	1.58
3106.3704	1.04
3174.0402	0.0382



$\Delta E = 0.29$ kcal mol^{-1}
Population = 0.206



$\Delta E = 0.99$ kcal mol^{-1}
Population = 0.063

Optimized Coordinates (Angstroms)

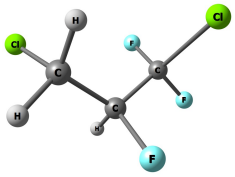
Atom	X	Y	Z
C	1.206792053294	0.521660365394	-0.461843622886
C	0.306387935580	-0.363592512719	0.384410678011
C	-1.170761677646	-0.279130779566	-0.041963331038
Cl	2.904126870381	0.421636699745	0.120578556457
H	1.194095217126	0.186704508826	-1.498713893030
H	0.899622168932	1.564384085200	-0.402117989967
H	0.372354138391	-0.103165031384	1.445260272591
F	0.668705897059	-1.676453832103	0.222402148284
F	-1.302297225999	-0.511863430751	-1.351215299761
F	-1.885139870077	-1.188846296736	0.616287958541
Cl	-1.851539507043	1.353652224095	0.324772522796

Atom	X	Y	Z
C	1.547496295675	-0.890773505604	-0.159808008722
C	0.142966227942	-0.783090565835	0.438462536729
C	-0.718961852373	0.303416650633	-0.226326967171
Cl	2.652703690671	0.390466439951	0.441360938104
H	1.964733418762	-1.851210641973	0.141066176320
H	1.516232531266	-0.828431347140	-1.246925447311
H	0.185012466749	-0.587206458154	1.513755226816
F	-0.475967644637	-1.987923299941	0.212438665490
F	-0.209734431448	1.512668429575	0.012995469723
F	-0.757084124519	0.118710162988	-1.551263123404
Cl	-2.403380578088	0.256140135500	0.401651533426

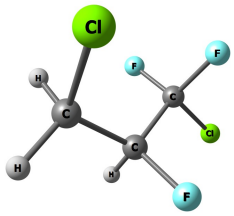
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
70.3201	0.452
71.6570	0.181
148.7192	0.673
197.0937	0.189
257.1964	0.00804
305.6062	0.241
329.7691	0.517
400.4195	0.213
422.0244	0.706
509.8195	1.44
599.1695	3.62
760.9392	12.7
827.0926	5.14
883.4851	4.66
952.0737	37.4
1045.9899	0.293
1130.6539	7.04
1176.4054	19.3
1214.3326	5.76
1252.9936	19.6
1282.7570	5.62
1370.3910	2.56
1384.2268	1.60
1467.5878	0.944
3083.2767	1.06
3107.5368	1.000
3175.3322	0.0924

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
37.5215	0.105
98.5556	0.315
178.7647	0.442
188.6874	0.387
247.1533	0.0731
313.9219	0.0438
375.3435	0.162
392.7940	2.76
433.9651	2.89
470.1910	0.389
618.8595	2.03
718.0958	6.06
785.7006	6.87
941.8652	24.3
963.1264	17.8
1072.0511	4.12
1110.5017	11.0
1164.8064	7.29
1195.2355	20.6
1244.3424	14.0
1286.7540	3.05
1363.2681	0.295
1389.8800	0.480
1479.4675	0.933
3088.5378	0.733
3103.7389	1.24
3169.3610	0.0853



$\Delta E = 1.16$ kcal mol^{-1}
Population = 0.047



$\Delta E = 1.49$ kcal mol^{-1}
Population = 0.027

Optimized Coordinates (Angstroms)

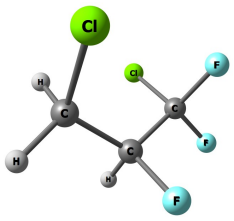
Atom	X	Y	Z
C	1.361054163559	-0.790869558429	-0.500265635721
C	0.144151943214	-0.946217973529	0.406949578092
C	-0.852744489655	0.225180928789	0.402985877615
Cl	2.609046360791	0.286837579099	0.213336731215
H	1.811370961857	-1.775680366163	-0.622953601238
H	1.087806900261	-0.390145891395	-1.475750969454
H	0.455711455773	-1.081784592042	1.449793694384
F	-0.543334679519	-2.061272012466	-0.002218251339
F	-1.845388743555	-0.045996965162	1.254259622189
F	-0.256117398846	1.349321795258	0.800126144415
Cl	-1.571864473880	0.495323056042	-1.227193190159

Atom	X	Y	Z
C	1.531287511321	-0.336701095028	0.962697705649
C	0.122515227034	-0.763550065227	0.564667550719
C	-0.778735545310	0.388707419436	0.085969347191
Cl	2.542665783915	0.219370191590	-0.413927996667
H	1.481983585684	0.471001170988	1.692781473054
H	2.042814029284	-1.194093223651	1.400425255930
H	-0.355476137976	-1.181258605377	1.460607422065
F	0.159525927759	-1.717012128868	-0.409459258615
F	-0.771828047481	1.356620883704	1.015339212414
F	-0.369108694995	0.905732234913	-1.066334995029
Cl	-2.474586639234	-0.185181782480	-0.123578716711

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
36.3852	0.125
103.8040	0.293
184.9905	0.352
196.5821	0.234
226.2210	0.731
321.8197	0.169
355.3816	0.266
412.9352	0.0394
447.0761	1.84
513.9582	0.997
592.0953	9.23
660.3209	2.15
785.0575	6.82
877.6069	13.5
1040.9675	9.92
1098.7328	14.3
1114.5995	9.40
1181.4437	19.3
1205.1257	18.3
1214.3188	11.6
1286.2365	1.73
1365.7862	0.461
1389.5414	3.56
1480.3610	1.87
3057.5471	1.24
3102.2741	0.971
3167.2241	0.0699

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
38.1279	0.150
99.2346	0.0909
169.0928	0.209
191.7780	0.165
241.3288	0.207
297.3735	0.588
345.4530	0.198
415.7837	0.0702
463.2391	0.396
535.5022	8.32
631.8890	4.82
684.6246	1.94
820.0690	3.01
898.6727	4.93
943.3720	23.8
1021.1638	19.9
1147.2151	8.75
1170.3581	22.6
1202.5972	7.11
1285.9507	7.13
1305.3636	9.79
1364.0113	2.67
1390.2050	0.0100
1461.2063	1.30
3040.2956	1.33
3098.3993	1.54
3160.7767	0.0921



$\Delta E = 1.77$ kcal mol^{-1}
Population = 0.017

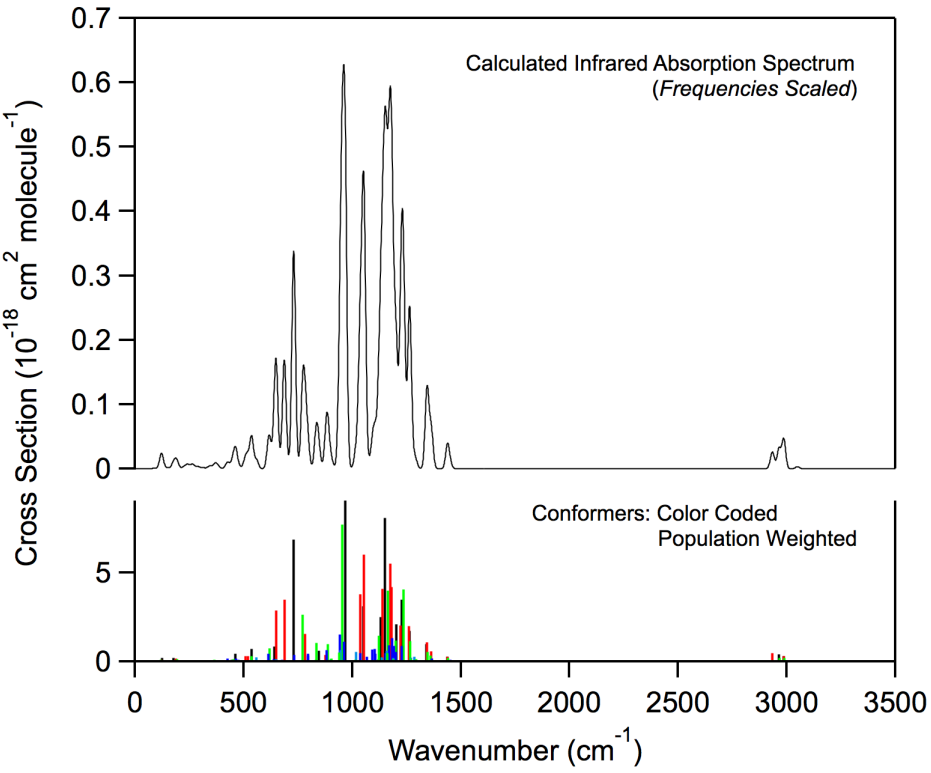
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.306392872522	0.245358680357	1.030686412450
C	0.153156381902	-0.707297805200	0.756616124273
C	-0.939560101168	-0.236485540303	-0.220875933611
Cl	2.337242199387	0.568421665549	-0.405426604057
H	0.935682129471	1.200307619885	1.400280156016
H	1.952332874618	-0.210271203167	1.781580541723
H	-0.356206347211	-0.900289992961	1.710244468495
F	0.626413127911	-1.893802592209	0.260811784659
F	-0.476794072346	-0.041467818143	-1.449298353875
F	-1.890836366549	-1.172943790720	-0.281170253253
Cl	-1.699234698537	1.295379776912	0.371057657179

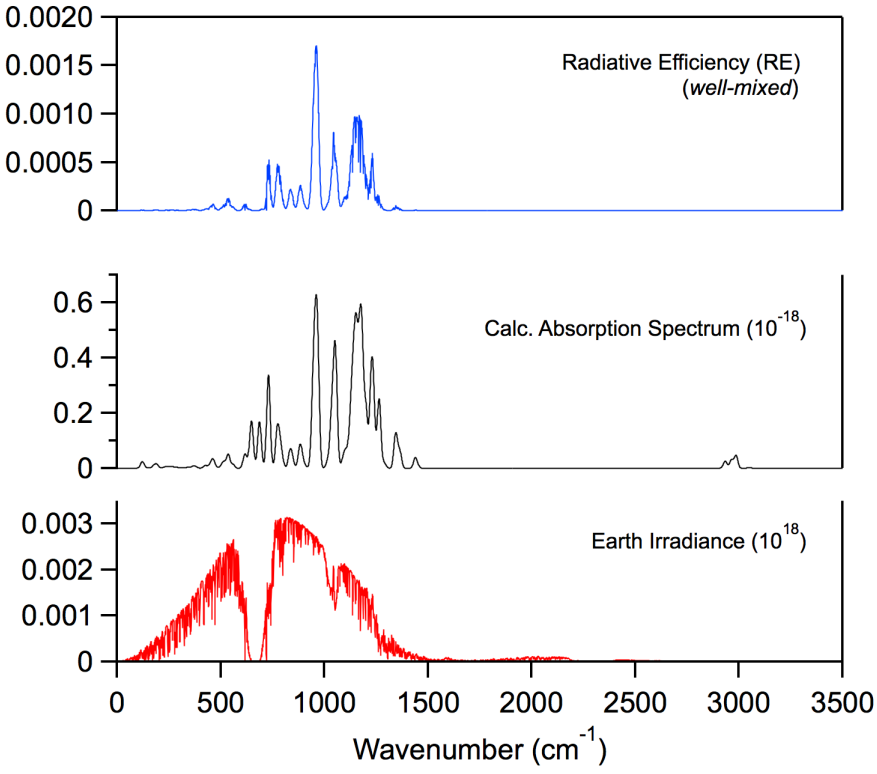
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
38.4752	0.175
106.4702	0.0456
174.3377	0.148
197.6509	0.419
254.9557	0.143
312.1623	0.431
343.7114	0.238
400.5880	0.383
419.4109	0.851
536.3305	3.83
661.6343	4.80
689.7822	1.24
825.7798	5.39
901.4523	9.28
937.5186	29.2
1016.7652	6.40
1128.9320	7.20
1173.5754	28.8
1203.2025	7.30
1286.4557	9.67
1313.4157	8.45
1361.2245	2.33
1391.2886	1.34
1462.4283	2.35
3039.6256	1.29
3101.8421	1.38
3166.0386	0.149

Infrared Spectrum

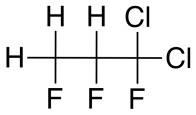


Radiative Efficiency



HCFC-243ed

Molecular Formula:	$CH_2FCHFCFCl_2$
Name:	1,1-Dichloro-1,2,3-trifluoropropane
CAS number:	–
Molecular Weight:	166.96



Global Atmospheric Lifetime (years):	2.03
Tropospheric Atmospheric Lifetime (years):	2.17
Stratospheric Atmospheric Lifetime (years):	31.9
Ozone Depletion Potential (ODP):	0.026

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.254	0.215
Global Warming Potential (GWP_H):		
GWP_{20}	696	587
GWP_{100}	188	159
Global Temperature Potentials (GTP_H)		
GTP_{20}		218
GTP_{50}		28
GTP_{100}		22

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 2.70 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 1.73 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 2.10$ years

$\tau^{OH}_{Trop} = 2.17$ years

$\tau^{OH}_{Strat} = 67.7$ years

Fractional Atmospheric Loss: 0.967

O(^{1}D) Reactivity

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

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

$\tau_{O(^1D)} = 250$ years

Fractional Atmospheric Loss: 0.008

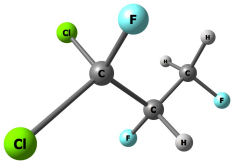
UV Photolysis

UV Spectrum: *No Recommendation*

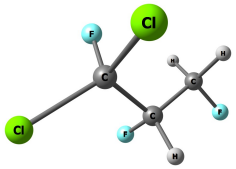
$\tau_{hv} = 80$ years

Fractional Atmospheric Loss: 0.025

Molecular Structure and Infrared Spectrum (9 conformers)



E = 0
Population = 0.270



$\Delta E = 0.29$ kcal mol^{-1}
Population = 0.166

Optimized Coordinates (Angstroms)

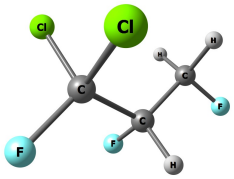
Atom	X	Y	Z
C	1.935024830750	0.391527976974	0.360754902905
C	0.780627207425	-0.543463781265	0.021055883833
C	-0.595435634420	0.050541387762	0.365427029751
F	3.097772536891	-0.339408512941	0.332871205825
H	1.997285333737	1.195599218348	-0.378445870485
H	1.796098423714	0.816547664095	1.360129446495
H	0.882505217207	-1.462896006079	0.611119735538
F	0.812773697576	-0.862050310404	-1.306011053237
F	-0.626856887699	0.308336264133	1.683634884777
Cl	-0.895118477792	1.582250420768	-0.519901800435
Cl	-1.891582247389	-1.123722321390	-0.013607364967

Atom	X	Y	Z
C	1.910260203970	0.517936063693	-0.217518660999
C	0.784870073241	-0.339349452222	0.353355676331
C	-0.596679627526	0.060598080638	-0.195613932033
F	3.069693440654	0.181355601035	0.435204528200
H	2.021052946935	0.305229769235	-1.285669154769
H	1.707714392337	1.582881674659	-0.071810178480
H	0.764977562358	-0.265103112718	1.444903490141
F	1.018239809573	-1.642820535209	-0.001941537004
F	-0.552898105130	0.133220176915	-1.534707480192
Cl	-1.835790991082	-1.143101414418	0.262229148985
Cl	-1.060437705330	1.678347148393	0.442979099819

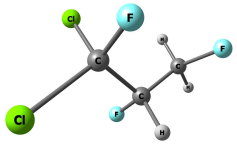
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
70.6790	0.164
86.0568	0.615
146.5785	0.450
191.3033	0.116
263.0692	0.279
275.3254	0.462
311.3306	0.187
373.4769	0.0383
407.2136	0.671
479.7223	2.97
551.6784	0.411
659.8017	13.6
814.9077	32.3
913.9168	5.28
1065.1596	13.5
1108.7643	13.9
1117.9839	4.39
1152.2917	19.6
1177.5627	0.340
1280.9244	0.413
1305.2049	2.34
1387.3812	1.59
1432.6365	1.13
1501.2085	0.368
3052.1718	1.00
3055.7122	2.38
3114.4225	2.43

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
65.0700	0.277
84.9254	0.510
157.6808	0.578
208.2779	0.206
246.3610	0.257
309.0544	0.135
318.6118	0.155
333.6392	0.575
394.6143	0.830
460.8497	0.596
505.8248	2.80
782.4389	17.9
833.9048	29.7
910.0607	10.7
967.0100	13.4
1112.9876	8.59
1114.2095	5.23
1141.7484	6.42
1193.9449	13.9
1279.8978	0.678
1310.2228	1.13
1385.6206	0.732
1433.9573	1.17
1503.4969	0.452
3055.8349	2.23
3084.5562	0.675
3115.7028	2.93



$\Delta E = 0.36$ kcal mol^{-1}
Population = 0.146



$\Delta E = 0.50$ kcal mol^{-1}
Population = 0.115

Optimized Coordinates (Angstroms)

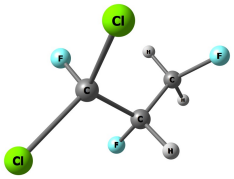
Atom	X	Y	Z
C	1.661305578703	0.482255998872	-0.652858247191
C	0.837478899191	-0.001235341675	0.530510552382
C	-0.683829034178	-0.046442228653	0.305568310393
F	2.945521300801	0.693836093856	-0.211384724814
H	1.672062664957	-0.283546344320	-1.434554103214
H	1.258271797683	1.416098170364	-1.055761267620
H	1.008508070028	0.656832135393	1.391423248203
F	1.229778140552	-1.270780013982	0.867338287092
F	-1.261626206918	-0.564874068347	1.393387986307
Cl	-1.323812575764	1.618224657278	0.073485696075
Cl	-1.119006635055	-1.076975058787	-1.096271737613

Atom	X	Y	Z
C	2.065453859296	-0.281175130241	-0.264697560079
C	0.664845606636	-0.876527999576	-0.107606705447
C	-0.423081935022	0.152760135110	0.251927773617
F	2.556928644802	0.064107271950	0.968553489959
H	2.701519060967	-1.053418279947	-0.712290852357
H	2.054975422675	0.598190220117	-0.916049774127
H	0.677867312409	-1.615323609021	0.702890965145
F	0.322123732729	-1.487811408410	-1.280922789478
F	-0.061427973199	0.793862673129	1.368160522021
Cl	-0.643205820825	1.359076540279	-1.058541736404
Cl	-1.980708910467	-0.687104413391	0.553302667151

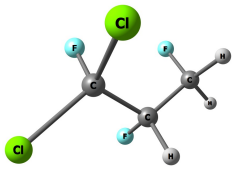
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
70.6034	0.510
82.7140	0.203
163.4555	0.447
188.0609	0.180
252.3660	0.316
292.2301	0.305
313.2194	0.369
373.6492	0.0517
400.3441	0.607
479.1093	1.73
519.7005	1.15
667.6467	14.8
840.4584	32.4
914.1857	5.68
1056.2465	11.8
1095.9981	16.8
1120.2824	8.09
1142.5061	2.93
1186.1558	13.8
1282.0910	0.801
1306.2292	1.91
1381.4670	1.93
1437.2636	0.561
1500.2120	0.546
3054.5312	0.736
3059.8316	2.45
3116.2560	2.34

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
43.6792	0.129
117.2721	0.498
185.1459	0.283
190.9342	0.127
214.2856	0.303
280.4055	0.121
360.8439	0.491
371.8092	0.0135
431.8924	4.72
461.0459	1.66
561.2023	1.96
585.3670	6.00
801.0814	30.7
950.6318	7.28
1095.6862	4.90
1108.1392	2.17
1119.7292	13.5
1150.0193	21.0
1184.0983	11.1
1252.1993	0.508
1330.9466	0.337
1375.0835	1.68
1428.2962	1.13
1512.7018	0.871
3045.6262	2.99
3056.3257	1.56
3104.7987	2.89



$\Delta E = 0.66$ kcal mol^{-1}
Population = 0.088



$\Delta E = 0.79$ kcal mol^{-1}
Population = 0.071

Optimized Coordinates (Angstroms)

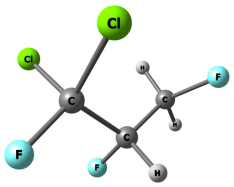
Atom	X	Y	Z
C	2.003971260047	-0.623789091527	-0.038808838922
C	0.573640900312	-0.804746300683	0.483199265054
C	-0.472797572692	0.054985037714	-0.247474654564
F	2.589284994596	0.477331812726	0.529806893898
H	2.562410006223	-1.521761094654	0.246911398200
H	2.012316851933	-0.523946966245	-1.128664381505
H	0.531301409701	-0.582790951730	1.553641675071
F	0.231169448377	-2.117002394357	0.263378636444
F	-0.419275223615	-0.197287318243	-1.563909346724
Cl	-2.121783633547	-0.350203618235	0.329952336011
Cl	-0.146348441337	1.795087885233	0.014948017038

Atom	X	Y	Z
C	1.993531809306	0.264938955901	0.601492469785
C	0.671257607375	-0.484369911262	0.713306042313
C	-0.463253675709	0.059693806095	-0.178714761865
F	2.445161388846	0.270309522524	-0.691636611428
H	1.882370488496	1.293695602464	0.957810435549
H	2.721882035428	-0.259452325826	1.231814767597
H	0.325386678585	-0.444244047348	1.752437559819
F	0.875935749258	-1.790769460848	0.348780597468
F	-0.115753519945	0.038447841033	-1.463649396572
Cl	-1.932976249396	-0.953942238847	0.021540148253
Cl	-0.842697312245	1.757002256116	0.291179749081

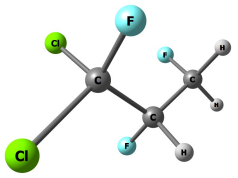
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
46.4881	0.148
113.0539	0.661
166.4216	0.247
209.8645	0.318
244.2638	0.0604
268.6539	0.293
328.6662	0.137
377.3977	0.383
426.5466	4.47
447.8046	1.96
491.0940	0.750
712.1286	6.57
846.4516	36.7
940.7162	10.2
1011.5885	6.85
1099.1452	7.38
1117.9772	11.9
1120.2139	6.45
1200.6956	13.4
1258.5034	1.05
1325.4040	0.210
1378.3564	0.512
1427.6117	0.984
1512.7618	0.627
3049.0719	3.15
3085.9211	0.929
3108.0475	2.88

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
42.6161	0.228
115.6553	0.215
181.1968	0.286
215.4236	0.313
228.7873	0.0520
296.7861	0.0993
321.6080	0.387
350.5245	0.223
396.8005	0.776
445.9784	1.16
571.4683	10.1
819.6403	30.4
833.8952	3.66
886.4392	13.2
969.2873	8.82
1010.3442	4.58
1123.4294	7.99
1155.3108	9.57
1220.3366	15.9
1288.7308	2.97
1355.1373	0.434
1373.4885	0.767
1428.8467	2.17
1496.7056	1.35
3040.5319	2.80
3066.4565	2.10
3099.8236	2.89



$\Delta E = 0.82$ kcal mol^{-1}
Population = 0.067



$\Delta E = 1.04$ kcal mol^{-1}
Population = 0.047

Optimized Coordinates (Angstroms)

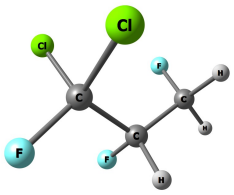
Atom	X	Y	Z
C	1.918896963208	-0.274373696716	-0.340624617697
C	0.791836081825	-0.561704929020	0.651105347556
C	-0.611749085018	-0.057045850957	0.271920720184
F	2.382516894815	1.005836513560	-0.174447885187
H	2.723857050495	-0.984494412205	-0.120612372635
H	1.589490293142	-0.413128204926	-1.374975760291
H	1.033887062924	-0.109074528661	1.620593733765
F	0.693706029826	-1.922933849421	0.800284977917
F	-1.458584621467	-0.383075585619	1.256969931202
Cl	-0.611053752291	1.723255224677	0.093079552667
Cl	-1.199926917458	-0.833308680712	-1.236783627482

Atom	X	Y	Z
C	1.967967082923	-0.629872559418	0.577440573264
C	0.570571581357	-0.985864954418	0.085286616238
C	-0.501630143486	0.093337391694	0.340321952980
F	2.493936251327	0.438113043831	-0.097301375033
H	1.929929152600	-0.408035001012	1.649770512107
H	2.610913455463	-1.502997291650	0.413029945715
H	0.241535849019	-1.871484157252	0.646080224808
F	0.596550470390	-1.280746094084	-1.246641597711
F	-0.454494527645	0.422997890444	1.643553324430
Cl	-0.259227507220	1.561123856908	-0.638399833767
Cl	-2.130465664729	-0.590595125043	-0.003020343031

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
49.9818	0.188
113.9516	0.611
176.9245	0.271
194.5828	0.112
236.3552	0.412
282.0141	0.661
322.4930	0.239
382.9954	0.112
429.3855	1.87
474.5001	0.849
526.6867	1.49
614.2957	10.2
842.6676	33.5
922.5626	6.48
1086.8547	2.39
1104.5402	7.25
1114.9735	24.4
1142.7300	3.49
1169.2020	13.1
1257.3842	0.388
1327.1621	0.125
1374.7181	2.71
1431.4861	0.368
1511.7605	0.874
3047.6105	2.44
3056.2747	1.74
3105.6160	2.81

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
43.6928	0.328
117.3009	0.357
171.7145	0.0554
193.9883	0.239
236.6394	0.0797
269.0842	0.357
309.2572	0.453
376.8516	0.0454
411.2812	0.180
515.4346	5.39
560.4648	3.03
702.8933	23.0
846.5244	10.8
886.7947	1.25
980.1443	9.94
1093.4438	16.7
1127.8896	14.5
1169.0823	6.60
1179.3887	10.8
1292.4789	0.957
1358.4850	1.19
1377.0740	1.77
1431.0994	1.46
1496.0082	0.922
3029.3871	0.763
3042.6269	4.98
3090.2997	2.85



$\Delta E = 1.32$ kcal mol^{-1}
Population = 0.029

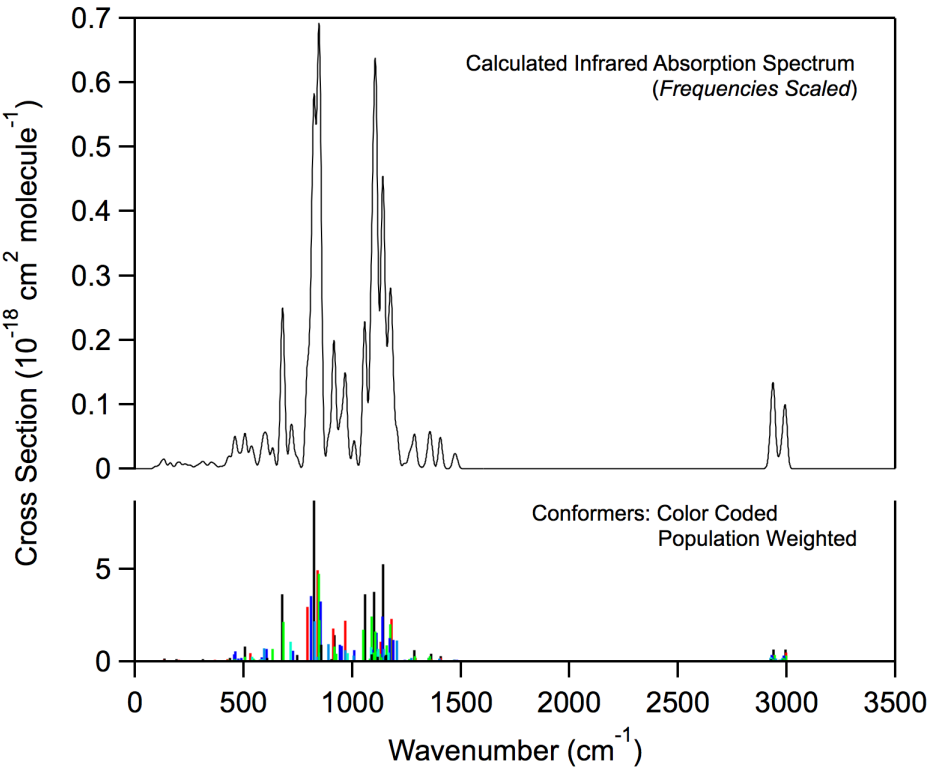
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.674675819304	1.090555424025	0.013305726942
C	0.732806442422	0.273755834257	0.883802664923
C	-0.614421223383	-0.165875039846	0.274719799253
F	2.070712952092	0.392771063479	-1.096124430751
H	1.193199463767	2.025316145205	-0.290771641316
H	2.559614049554	1.322307422604	0.618325183977
H	0.468165005537	0.878100532210	1.762516958363
F	1.368694537161	-0.865295403505	1.304860623516
F	-1.317133077411	-0.780024869183	1.238103145525
Cl	-1.546470681777	1.288014854236	-0.241814228113
Cl	-0.435263287266	-1.304389963483	-1.082713802320

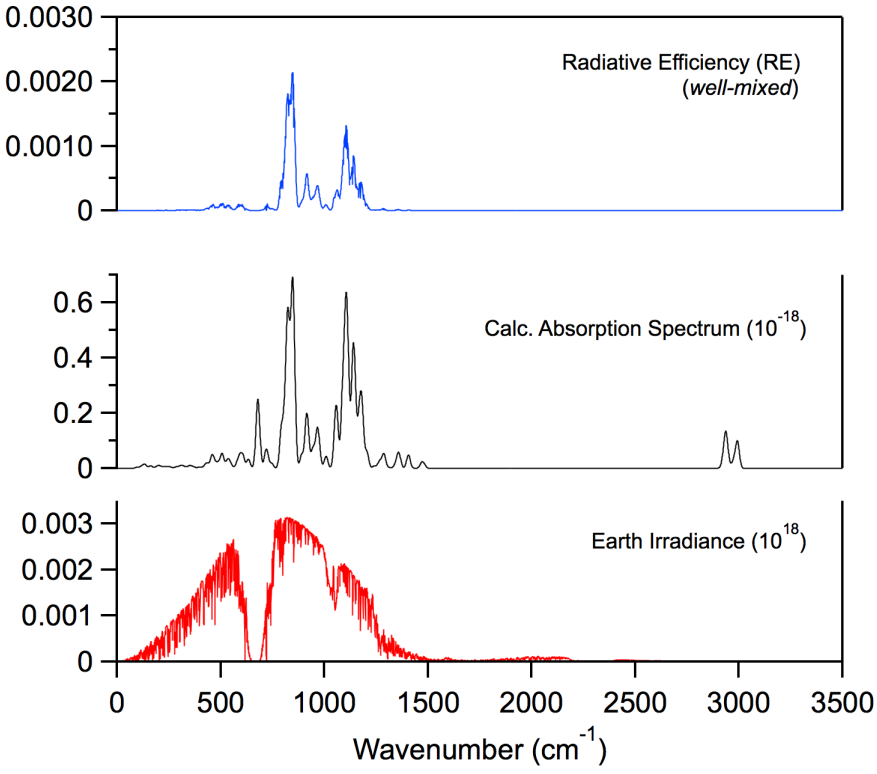
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
45.7108	0.332
118.5770	0.266
185.1832	0.131
188.4597	0.229
235.4572	0.166
294.8180	0.342
315.4727	0.355
376.1452	0.0578
400.5223	0.508
456.5249	1.62
588.6666	6.87
733.2016	12.2
849.9091	31.3
900.9641	4.60
946.9356	1.76
1095.9116	13.8
1125.6365	9.37
1163.5498	10.3
1168.2872	12.2
1291.8739	0.894
1362.1796	0.666
1371.6532	2.70
1434.1974	1.14
1496.9849	1.18
3030.9521	0.921
3044.8716	4.50
3098.3382	2.86

Infrared Spectrum

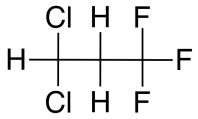


Radiative Efficiency



HCFC-243fa

Molecular Formula:	$CHCl_2CH_2CF_3$
Name:	3,3-Dichloro-1,1,1-trifluoropropane
CAS number:	460-69-5
Molecular Weight:	166.96



Global Atmospheric Lifetime (years):	0.780
Tropospheric Atmospheric Lifetime (years):	0.813
Stratospheric Atmospheric Lifetime (years):	20
Ozone Depletion Potential (ODP):	0.012

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.173	0.120
Global Warming Potential (GWP_H):		
GWP_{20}	182	126
GWP_{100}	49	34
Global Temperature Potentials (GTP_H)		
GTP_{20}		40
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*

$k_{SAR}(298\ K) = 7.21 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 4.60 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 0.790$ years

$\tau^{OH}_{Trop} = 0.813$ years

$\tau^{OH}_{Strat} = 28.0$ years

Fractional Atmospheric Loss: 0.987

O(^{1}D) Reactivity

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

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

$\tau_{O(^1D)} = 250$ years

Fractional Atmospheric Loss: 0.003

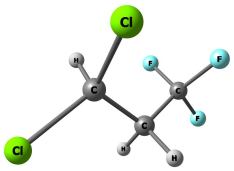
UV Photolysis

UV Spectrum: *No Recommendation*

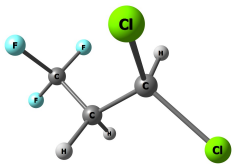
$\tau_{hv} = 80$ years

Fractional Atmospheric Loss: 0.010

Molecular Structure and Infrared Spectrum (2 conformers)



E = 0
Population = 0.492



E = 0
Population = 0.492

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	0.924189592060	-0.117585634441	0.383422492995
C	-0.232551300172	-0.766942248401	-0.367693712714
C	-1.603804641162	-0.216092847794	0.004839251339
Cl	2.411974520112	-1.104620011095	0.158980644618
Cl	1.216216765491	1.572133144254	-0.139962295313
H	0.740008398910	-0.080315797922	1.453880344356
H	-0.246444636265	-1.830483494452	-0.115978059187
H	-0.093199022312	-0.671524111000	-1.446278554431
F	-2.558523108729	-0.999910634234	-0.515118036554
F	-1.769915000191	-0.201236242773	1.338928232731
F	-1.812318567742	1.024121877856	-0.442222307841

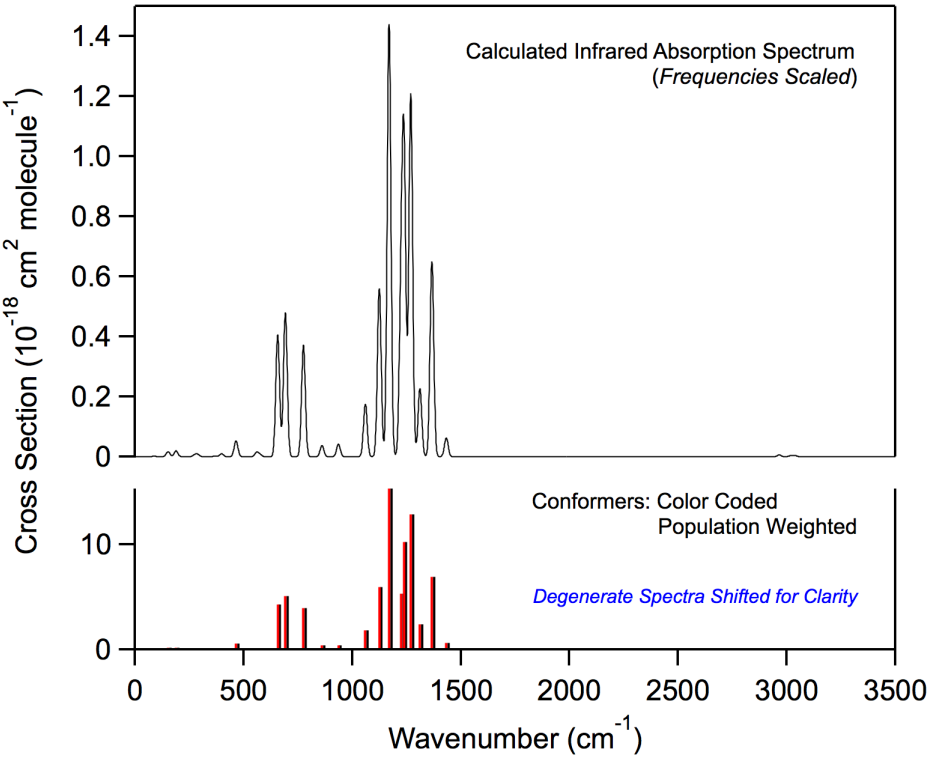
Atom	X	Y	Z
C	0.922975670512	0.118384785296	0.365134043342
C	-0.236481699159	0.750505103584	-0.396424381510
C	-1.606852443718	0.212824653813	-0.002049087730
Cl	1.208377358142	-1.585174272694	-0.115274311535
Cl	2.411660536448	1.095694798060	0.106681199981
H	0.744652323176	0.109668008830	1.437195807616
H	-0.103315228350	0.626488029255	-1.472879452830
H	-0.246650635523	1.820315924987	-0.172648829968
F	-2.562717076167	0.984970469297	-0.537144347009
F	-1.820563461175	-1.038194744601	-0.415271369774
F	-1.765593344186	0.233344244172	1.332861729417

Infrared Absorption Spectrum (unscaled frequencies)

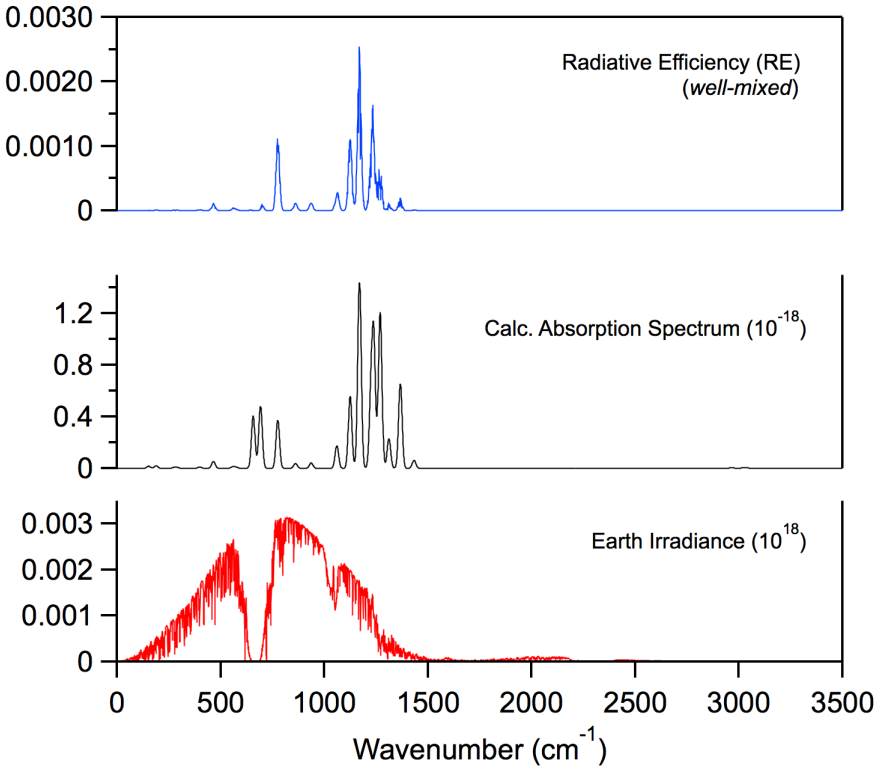
Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
35.7879	0.0394
104.2250	0.362
143.0014	0.419
233.9820	0.132
248.5577	0.154
330.4735	0.0323
365.0104	0.216
435.5410	1.14
536.3950	0.306
552.6596	0.151
638.5838	8.78
676.0870	10.4
764.1772	8.04
854.6177	0.809
934.6010	0.901
1065.9336	3.78
1133.9083	12.1
1181.5431	31.2
1240.1993	10.8
1254.3280	20.8
1287.3209	26.2
1331.9432	4.91
1390.3063	14.1
1460.5277	1.36
3083.1035	0.138
3137.9867	0.0677
3159.9509	0.0870

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
35.7881	0.0394
104.2262	0.362
143.0014	0.419
233.9820	0.132
248.5580	0.154
330.4737	0.0323
365.0107	0.216
435.5414	1.14
536.3951	0.306
552.6593	0.151
638.5844	8.78
676.0871	10.4
764.1775	8.04
854.6186	0.809
934.6017	0.901
1065.9336	3.78
1133.9082	12.1
1181.5430	31.2
1240.1987	10.8
1254.3290	20.8
1287.3222	26.2
1331.9436	4.91
1390.3069	14.1
1460.5282	1.36
3083.1025	0.138
3137.9858	0.0677
3159.9514	0.0870

Infrared Spectrum

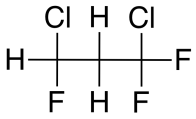


Radiative Efficiency



HCFC-243fb

Molecular Formula:	$CHFClCH_2CF_2Cl$
Name:	1,3-Dichloro-1,1,3-trifluoropropane
CAS number:	139754-78-2
Molecular Weight:	166.96



Global Atmospheric Lifetime (years):	2.24
Tropospheric Atmospheric Lifetime (years):	2.36
Stratospheric Atmospheric Lifetime (years):	45.1
Ozone Depletion Potential (ODP):	0.024

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.271	0.231
Global Warming Potential (GWP_H):		
GWP_{20}	817	699
GWP_{100}	221	189
Global Temperature Potentials (GTP_H)		
GTP_{20}		267
GTP_{50}		34
GTP_{100}		26

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 2.49 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 1.59 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 2.28$ years

$\tau^{OH}_{Trop} = 2.36$ years

$\tau^{OH}_{Strat} = 73.0$ years

Fractional Atmospheric Loss: 0.981

O(^{1}D) Reactivity

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

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

$\tau_{O(^1D)} = 250$ years

Fractional Atmospheric Loss: 0.009

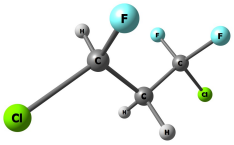
UV Photolysis

UV Spectrum: *No Recommendation*

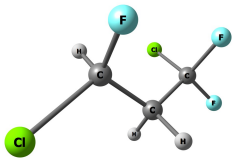
$\tau_{hv} = 225$ years

Fractional Atmospheric Loss: 0.010

Molecular Structure and Infrared Spectrum (5 conformers)



E = 0
Population = 0.460



$\Delta E = 0.29$ kcal mol^{-1}
Population = 0.284

Optimized Coordinates (Angstroms)

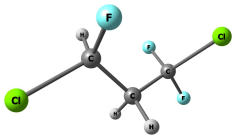
Atom	X	Y	Z
C	1.373811598552	0.259920946738	0.278742423070
C	0.157346507015	-0.563340381479	-0.129147135004
C	-1.143168748338	0.190535274582	0.126149732970
Cl	2.868780413107	-0.737013225215	0.081775601401
F	1.481183247259	1.365174527354	-0.493582276001
H	1.347911090065	0.559006399535	1.327764983843
H	0.138521132445	-1.488965882942	0.447203445996
H	0.220742406187	-0.812787654146	-1.189997369833
F	-1.216491642676	0.588068744327	1.407116438937
F	-1.247999674647	1.277613683765	-0.640704933577
Cl	-2.569186328969	-0.869882432519	-0.210286911801

Atom	X	Y	Z
C	1.199815544312	0.227271365913	-0.292191491202
C	0.203430171463	-0.330341750043	0.711712190435
C	-1.235994105342	-0.369974424417	0.210338222391
Cl	2.842013208818	0.283674094697	0.465929321906
F	1.255396185349	-0.559136904734	-1.391020592931
H	0.975940631936	1.250987890235	-0.594946262044
H	0.228754250462	0.265344171721	1.625032330594
H	0.483037717441	-1.359501604452	0.957845294445
F	-1.365479282529	-1.128168640530	-0.879312220510
F	-2.024074684398	-0.881455382414	1.163441954971
Cl	-1.862341637512	1.286894184023	-0.187210748055

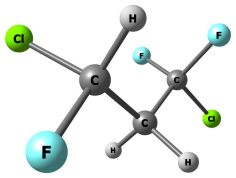
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
41.0476	0.0630
103.3711	0.561
127.5236	0.342
232.6205	0.0729
262.7685	0.0352
328.1656	0.285
382.4486	0.342
415.0068	0.289
422.3054	0.214
487.1069	3.68
572.1251	3.61
702.4019	26.0
844.0864	2.45
884.5818	6.67
961.4857	27.9
1016.8125	4.23
1122.0448	8.63
1170.1656	27.0
1229.3140	23.5
1261.2014	8.42
1301.7274	5.31
1361.0478	11.8
1399.6644	3.70
1451.7704	0.828
3097.6291	0.0751
3113.3895	1.18
3157.3601	0.0823

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
38.8264	0.0858
100.5039	0.367
143.4162	0.288
235.9623	0.195
287.4743	0.0596
321.5189	0.360
373.2487	0.382
411.7177	0.0357
417.9167	0.794
506.1744	1.72
584.8269	7.88
670.3344	11.1
780.9322	16.0
893.0487	4.62
968.5354	16.9
1079.8784	18.7
1130.5035	3.47
1178.0196	25.3
1208.8938	25.2
1259.9243	13.3
1295.0566	5.29
1367.6824	9.08
1403.3853	4.44
1452.0832	0.678
3076.2056	0.0699
3118.2848	1.01
3147.3436	0.160



$\Delta E = 0.80$ kcal mol^{-1}
Population = 0.119



$\Delta E = 1.06$ kcal mol^{-1}
Population = 0.076

Optimized Coordinates (Angstroms)

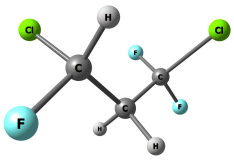
Atom	X	Y	Z
C	1.229216063381	0.123880833740	0.405180829415
C	0.227494647474	-0.673773829537	-0.416504156582
C	-1.218737730367	-0.514282710957	0.043852862837
Cl	2.906937419111	-0.405429673331	-0.019702973388
F	1.121527602443	1.447596844146	0.155689318280
H	1.123213266710	-0.048221780026	1.477399509416
H	0.457964135421	-1.737712570566	-0.314334572051
H	0.308447336554	-0.399987949596	-1.469811847563
F	-1.982737195256	-1.424434672783	-0.573529692671
F	-1.315043133916	-0.731112584266	1.366566191818
Cl	-1.912900411555	1.110490093177	-0.303481469511

Atom	X	Y	Z
C	1.440273547321	0.575159204003	0.347462903393
C	0.063773474428	0.831676761758	-0.261582515115
C	-1.008096901771	-0.143071023248	0.202357406590
Cl	2.247900186706	-0.872596850324	-0.360571819746
F	2.217709584677	1.659196741776	0.103844580517
H	1.396000207277	0.399441351623	1.423309898713
H	0.121246512332	0.815080902280	-1.351177370007
H	-0.238413651268	1.833613681669	0.054443602799
F	-0.810033380117	-1.378400005932	-0.259648506221
F	-1.035799630260	-0.210567001973	1.543851339072
Cl	-2.640155949326	0.401536238367	-0.359593519995

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
34.3421	0.0736
99.1385	0.335
147.0787	0.501
220.2778	0.0809
277.1559	0.194
330.6252	0.227
381.7327	0.237
412.6474	0.196
429.2486	0.192
509.8649	1.64
582.9388	6.19
669.1315	15.0
785.7817	12.7
895.1006	5.49
952.0173	7.79
1090.9534	18.4
1147.1511	26.0
1158.0771	28.3
1208.7520	17.8
1246.6348	6.92
1285.7325	2.67
1367.0440	8.63
1405.8248	4.07
1454.2672	0.781
3082.4977	0.0689
3113.2528	1.06
3146.3623	0.158

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
34.5260	0.0344
102.8286	0.365
140.9014	0.512
213.7062	0.0726
301.2908	0.241
340.3116	0.194
392.1498	0.708
416.7993	0.306
422.1543	0.519
456.3849	3.41
589.0761	1.35
678.5531	14.2
804.6636	11.7
919.4729	10.2
950.6652	20.3
1065.7272	21.3
1114.1686	10.6
1136.8630	20.2
1230.3632	17.2
1273.7961	19.2
1324.5865	1.95
1333.2737	4.36
1404.5354	6.14
1458.1041	1.03
3083.6769	0.0876
3113.1867	1.18
3145.7239	0.130



$\Delta E = 1.35$ kcal mol^{-1}
Population = 0.047

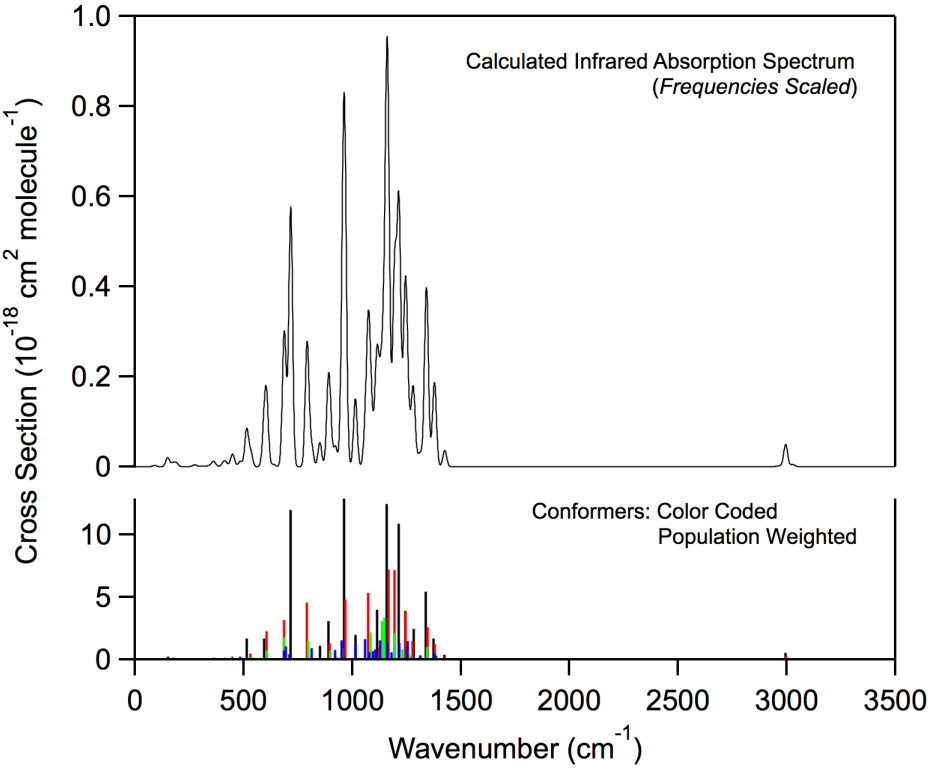
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.296177070451	0.574794658539	0.296964858483
C	0.127464489001	0.807695027413	-0.650800030929
C	-1.126712457388	-0.020023417039	-0.412679932020
Cl	2.098481727561	-1.015568002137	0.018478270271
F	2.208532522994	1.555782624348	0.079893705315
H	1.002459174506	0.584339706867	1.347313661009
H	0.448322973371	0.623570771021	-1.680446916105
H	-0.156783560546	1.859686402712	-0.560778966211
F	-2.072142294473	0.361836021006	-1.280892528387
F	-0.921266268414	-1.325641271350	-0.584702185941
Cl	-1.792534377063	0.221860478620	1.259318064515

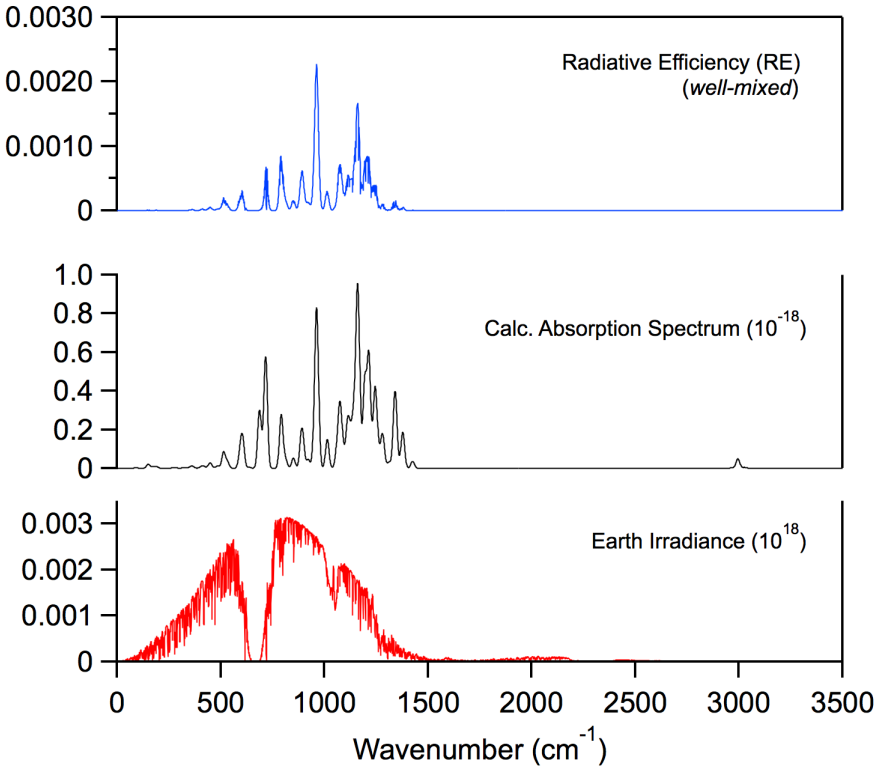
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
31.5221	0.0506
109.0780	0.311
139.7135	0.218
251.9931	0.247
308.6300	0.600
326.8194	0.0799
363.4178	0.499
415.5875	0.545
423.3080	0.771
491.8063	1.68
617.4411	2.44
669.3528	15.5
694.2926	8.74
922.0580	3.65
1017.7780	26.5
1085.6366	12.3
1102.5539	14.4
1174.1240	28.3
1192.5492	12.5
1270.3858	21.0
1320.9635	1.52
1336.2115	4.24
1409.8472	5.71
1458.1966	0.756
3069.7284	0.0981
3115.5652	0.569
3129.1805	0.653

Infrared Spectrum

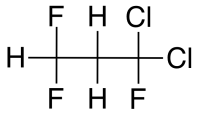


Radiative Efficiency



HCFC-243fc

Molecular Formula: $CHF_2CH_2CFCl_2$
Name: 1,1-Dichloro-1,3,3-trifluoropropane
CAS number: 213248-61-4
Molecular Weight: 166.96



Global Atmospheric Lifetime (years): 5.07
  Tropospheric Atmospheric Lifetime (years): 5.73
  Stratospheric Atmospheric Lifetime (years): 44.0
Ozone Depletion Potential (ODP): 0.056

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.285	0.263
Global Warming Potential (GWP_H):		
GWP_{20}	1907	1759
GWP_{100}	527	486
Global Temperature Potentials (GTP_H)		
GTP_{20}		973
GTP_{50}		103
GTP_{100}		68

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 1.02 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 0.654 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 5.53$ years
$\tau^{OH}_{Trop} = 5.73$ years
$\tau^{OH}_{Strat} = 162.5$ years

Fractional Atmospheric Loss: 0.916

O(^{1}D) Reactivity

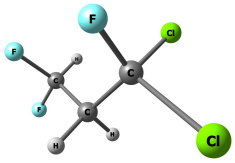
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 1.5 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)} = 250$ years
Fractional Atmospheric Loss: 0.021

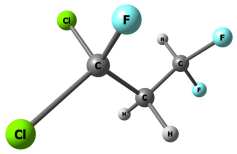
UV Photolysis

UV Spectrum: *No Recommendation*
$\tau_{hv} = 80$ years
Fractional Atmospheric Loss: 0.063

Molecular Structure and Infrared Spectrum (8 conformers)



E = 0
Population = 0.266



E = 0
Population = 0.266

Optimized Coordinates (Angstroms)

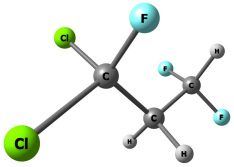
Atom	X	Y	Z
C	-1.846909882438	0.104457674521	-0.200896282687
C	-0.555593241244	-0.659289769685	-0.481002324152
C	0.685936515476	-0.060160009412	0.165448832436
F	-2.845052281977	-0.508058432616	-0.886642241279
F	-2.150219552722	0.046872785727	1.116687434957
H	-1.809482385607	1.156177275991	-0.504600988971
H	-0.402154423367	-0.711763345302	-1.559777171963
H	-0.676835771896	-1.675881721499	-0.095321005836
F	0.551348191810	0.017284343377	1.493020246540
Cl	2.117893835722	-1.096723873852	-0.186661183286
Cl	1.009763996242	1.607735072749	-0.451629315758

Atom	X	Y	Z
C	-1.848021091728	0.097008829846	0.210614238847
C	-0.555763764818	-0.672187336937	0.470769011598
C	0.684929544515	-0.055233073347	-0.160339942027
F	-2.151569060495	0.072908399359	-1.107951991212
F	-2.845303557196	-0.534051339831	0.880615834338
H	-1.811728320831	1.140630535196	0.541201733582
H	-0.675926374112	-1.678685002481	0.059147355413
H	-0.402018000000	-0.752153890388	1.547810998048
F	0.549952399694	0.056088302542	-1.485461651674
Cl	1.006975300878	1.596654747254	0.499261850036
Cl	2.118158924091	-1.098832171212	0.164779563051

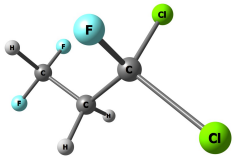
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
40.9447	0.0900
111.3846	0.417
142.3169	0.194
221.8700	0.0101
291.2087	0.384
312.2079	0.152
335.0154	0.226
386.8850	0.680
455.4749	0.281
494.9368	5.23
556.4315	2.20
660.7694	8.90
799.3578	29.2
890.3308	4.29
987.6735	10.0
1089.5108	12.4
1130.9334	17.0
1139.7723	17.9
1201.4036	26.7
1269.6157	2.87
1326.6637	1.99
1417.6783	4.60
1421.7460	9.89
1452.6002	0.617
3071.9637	3.07
3081.1966	1.33
3145.6085	0.163

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
40.9441	0.0900
111.3851	0.417
142.3161	0.194
221.8701	0.0101
291.2081	0.384
312.2074	0.152
335.0156	0.226
386.8850	0.680
455.4748	0.281
494.9361	5.23
556.4315	2.20
660.7692	8.90
799.3576	29.2
890.3298	4.29
987.6731	10.0
1089.5102	12.4
1130.9341	17.0
1139.7721	17.9
1201.4028	26.7
1269.6155	2.87
1326.6637	1.99
1417.6789	4.60
1421.7458	9.89
1452.6004	0.617
3071.9636	3.07
3081.1969	1.33
3145.6094	0.163



$\Delta E = 0.43$ kcal mol^{-1}
Population = 0.130



$\Delta E = 0.43$ kcal mol^{-1}
Population = 0.130

Optimized Coordinates (Angstroms)

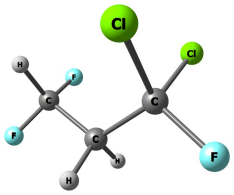
Atom	X	Y	Z
C	-1.854657389707	-0.249085190317	-0.252686470418
C	-0.545196379937	-0.781524075780	0.325733048401
C	0.703918943634	-0.119408827399	-0.241958873121
F	-2.843969472171	-1.106113045992	0.106082342978
F	-2.156910928571	0.964552271894	0.261373228523
H	-1.838141501167	-0.171558044604	-1.345710240670
H	-0.485603511534	-1.844338196535	0.076324638451
H	-0.562190593316	-0.678698012369	1.411991284412
F	0.677597192830	-0.178535810516	-1.586941391048
Cl	0.853667311136	1.605844931460	0.225870927745
Cl	2.171086328803	-1.007028999842	0.316117504746

Atom	X	Y	Z
C	-1.855385366719	-0.256051642982	0.251885423314
C	-0.544104110268	-0.786065708718	-0.324637781530
C	0.702997577017	-0.122017931890	0.245222524459
F	-2.158893650624	0.957245121972	-0.262237425146
F	-2.842663810510	-1.114642159955	-0.108745216804
H	-1.840737855430	-0.178873121970	1.344960154742
H	-0.559565637469	-0.682916347464	-1.410888455280
H	-0.483095396979	-1.848858838878	-0.075482023476
F	0.674678160525	-0.181627335633	1.590142615960
Cl	2.172536201516	-1.006972849472	-0.310847204568
Cl	0.850557888942	1.603637814990	-0.221815611672

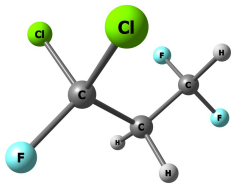
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
36.8592	0.0860
108.5012	0.443
145.3909	0.374
236.1304	0.106
240.6803	0.124
313.4282	0.123
371.3576	0.130
385.7531	0.345
451.8603	0.474
493.1548	5.06
569.2244	0.611
667.5631	11.7
785.8727	24.1
911.8520	5.13
961.4279	8.31
1095.9327	14.5
1127.6472	28.3
1153.1561	16.9
1179.8457	19.7
1259.7617	0.271
1325.4901	1.85
1419.7539	3.53
1423.0874	10.6
1455.0848	0.685
3067.9289	4.70
3082.0687	0.0670
3145.9892	0.144

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
36.8587	0.0860
108.4969	0.443
145.3867	0.374
236.1295	0.106
240.6795	0.124
313.4269	0.123
371.3565	0.130
385.7519	0.345
451.8609	0.474
493.1535	5.06
569.2241	0.611
667.5641	11.7
785.8716	24.1
911.8504	5.13
961.4268	8.31
1095.9329	14.6
1127.6470	28.3
1153.1562	16.9
1179.8466	19.7
1259.7655	0.271
1325.4915	1.85
1419.7541	3.53
1423.0853	10.6
1455.0842	0.685
3067.9312	4.70
3082.0679	0.0670
3145.9871	0.144



$\Delta E = 0.65$ kcal mol^{-1}
Population = 0.089



$\Delta E = 0.65$ kcal mol^{-1}
Population = 0.089

Optimized Coordinates (Angstroms)

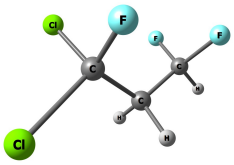
Atom	X	Y	Z
C	-1.722057602291	0.273617697791	-0.229324389343
C	-0.640601537410	0.355795499603	0.840483275623
C	0.798161384348	0.123656670052	0.396598229431
F	-1.919620748203	-1.006282673683	-0.619798174234
F	-2.879398689077	0.717475622809	0.325500047857
H	-1.505166969294	0.879705900639	-1.115644238276
H	-0.872145732999	-0.372798803787	1.622989155759
H	-0.674362651936	1.357817946529	1.277069521735
F	1.603468664574	0.311367648545	1.454331879715
Cl	1.083464550211	-1.537388011729	-0.214057724029
Cl	1.289854332077	1.316742503232	-0.870149584239

Atom	X	Y	Z
C	-1.720219483990	-0.267896153893	-0.232955910627
C	-0.639470230466	-0.353121833292	0.837332314154
C	0.799271983503	-0.116734471681	0.395626244727
F	-2.877290710322	-0.716049091811	0.318970083390
F	-1.919504707511	1.013415172009	-0.617889653323
H	-1.501674461080	-0.869688887188	-1.121792289986
H	-0.671984943283	-1.357125995727	1.269436494338
H	-0.872782847782	0.371621366583	1.622882799613
F	1.604041209441	-0.307848964051	1.453159452210
Cl	1.293869053755	-1.303412362887	-0.876000025302
Cl	1.082408137735	1.547451221937	-0.207441509194

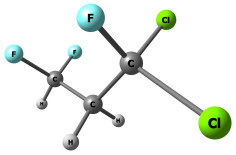
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
39.7648	0.0984
107.9590	0.324
149.1158	0.187
236.2391	0.104
275.0206	0.271
312.8776	0.432
351.3012	0.0880
389.5242	0.522
466.9334	1.52
522.8395	2.13
565.4329	1.81
636.6072	5.01
717.9127	27.0
915.8815	1.60
1059.1575	10.9
1094.5056	12.3
1114.6303	32.9
1151.2968	30.6
1164.1669	8.07
1250.3242	0.0436
1330.1365	1.47
1417.3920	3.29
1428.3497	8.37
1455.6091	0.562
3068.5093	0.497
3074.5085	3.51
3127.3824	0.352

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
39.7649	0.0984
107.9590	0.324
149.1155	0.187
236.2393	0.104
275.0197	0.271
312.8764	0.432
351.3010	0.0880
389.5241	0.522
466.9329	1.52
522.8381	2.13
565.4322	1.81
636.6070	5.01
717.9114	27.0
915.8783	1.60
1059.1578	10.9
1094.5023	12.3
1114.6311	32.9
1151.2944	30.6
1164.1673	8.07
1250.3237	0.0436
1330.1351	1.47
1417.3911	3.29
1428.3463	8.37
1455.6079	0.562
3068.5122	0.497
3074.5113	3.51
3127.3858	0.352



$\Delta E = 1.73$ kcal mol^{-1}
Population = 0.014



$\Delta E = 1.73$ kcal mol^{-1}
Population = 0.014

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.884477314309	-0.473178335330	0.484338826080
C	-0.413362587491	-0.716657850563	0.821013803062
C	0.615835401944	-0.128076978917	-0.143281127164
F	-2.196671233549	0.842721227774	0.499585131556
F	-2.185119575504	-0.959800423427	-0.742697987353
H	-2.521584832238	-0.982145607725	1.220561074271
H	-0.259007667829	-1.799688666193	0.831069923201
H	-0.211724136647	-0.337913736594	1.824659382803
F	0.377424109062	-0.518003603212	-1.399720426544
Cl	0.650570749012	1.666720451556	-0.112853163252
Cl	2.258016087550	-0.742342477368	0.316547563341

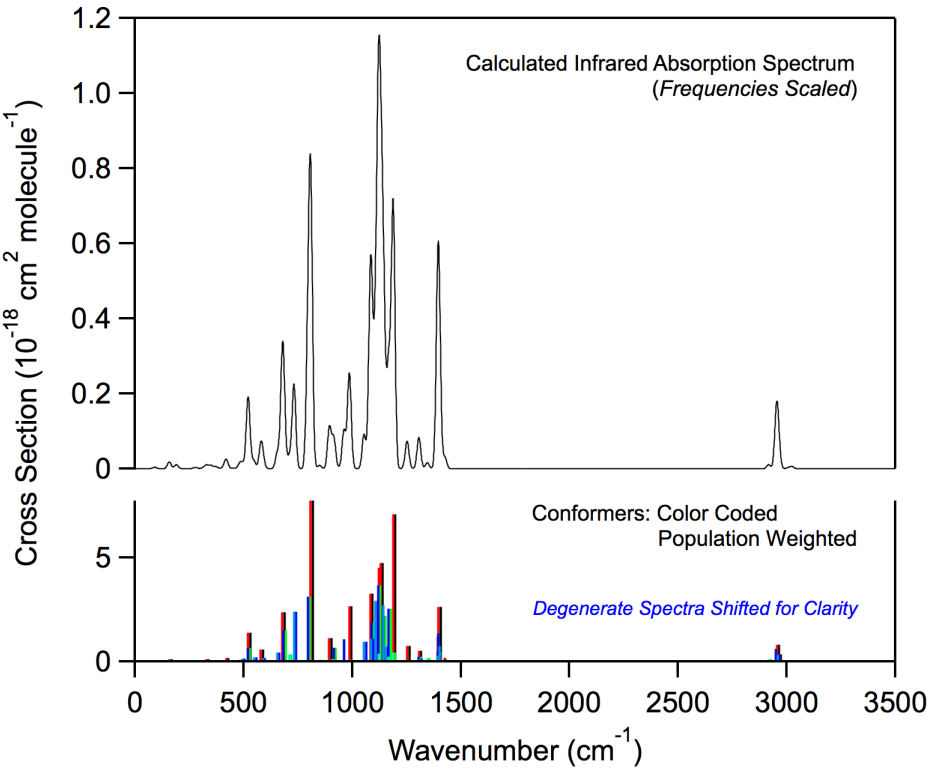
Atom	X	Y	Z
C	-1.884492658344	-0.476336557695	-0.481807435731
C	-0.413388777356	-0.717409425759	-0.820257479964
C	0.616020931576	-0.126837502866	0.142593186167
F	-2.182776865854	-0.963141669403	0.745731925332
F	-2.198941144234	0.839026335666	-0.497012545364
H	-2.521652524798	-0.986581451787	-1.217099564743
H	-0.213649051405	-0.338586519794	-1.824253125479
H	-0.257212308727	-1.800179931313	-0.830227249324
F	0.379845796220	-0.516839302633	1.399431301161
Cl	2.258659094221	-0.738449339421	-0.319138005410
Cl	0.647688508700	1.668007365006	0.111657993355

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
21.1308	0.173
135.4167	0.0323
161.8881	0.158
224.1296	0.00702
241.1523	0.145
320.8877	0.0177
370.9586	0.121
401.9081	0.309
424.2125	1.04
514.5836	4.56
558.4635	4.25
695.1502	23.6
842.6886	6.64
904.2486	7.68
932.5768	1.45
997.2321	6.16
1130.9823	26.3
1177.8644	15.8
1200.2697	29.3
1284.7246	0.591
1367.9552	12.1
1416.8192	4.36
1419.9354	3.57
1449.8413	1.28
3031.5255	7.88
3077.9950	0.472
3137.1999	0.116

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
21.1300	0.173
135.4129	0.0323
161.8856	0.158
224.1293	0.00702
241.1521	0.145
320.8876	0.0177
370.9582	0.121
401.9070	0.309
424.2125	1.04
514.5839	4.56
558.4634	4.25
695.1499	23.6
842.6884	6.64
904.2479	7.68
932.5764	1.45
997.2328	6.16
1130.9832	26.3
1177.8657	15.8
1200.2699	29.3
1284.7269	0.591
1367.9566	12.1
1416.8201	4.36
1419.9367	3.57
1449.8418	1.28
3031.5244	7.88
3077.9941	0.472
3137.1984	0.116

Infrared Spectrum



Radiative Efficiency