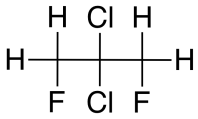
HCFC-252aa

Molecular Formula:	$CH_2FCCl_2CH_2F$
Name:	2,2-Dichloro-1,3-difluoropropane
CAS number:	154193-88-1
Molecular Weight:	148.97



Global Atmospheric Lifetime (years):	1.94
Tropospheric Atmospheric Lifetime (years):	2.07
Stratospheric Atmospheric Lifetime (years):	31.0
Ozone Depletion Potential (ODP):	0.029

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.125	0.105
Global Warming Potential (GWP_H):		
GWP_{20}	366	307
GWP_{100}	99	83
Global Temperature Potentials (GTP_H)		
GTP_{20}		113
GTP_{50}		15
GTP_{100}		12

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 2.83 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 1.81 \times 10^{-14}$ 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: 0.968

O(^{1}D) Reactivity

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

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

$\tau_{O(^1D)} = 230$ years

Fractional Atmospheric Loss: 0.008

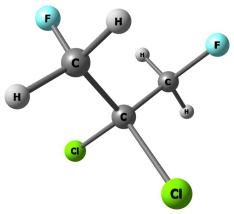
UV Photolysis

UV Spectrum: *No Recommendation*

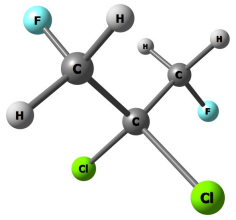
$\tau_{hv} = 80$ years

Fractional Atmospheric Loss: 0.024

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.919



$\Delta E = 1.98$ kcal mol^{-1}
Population = 0.032

Optimized Coordinates (Angstroms)

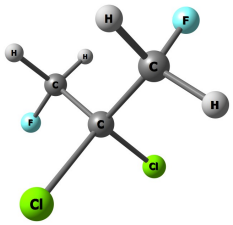
Atom	X	Y	Z
C	0.510991523817	0.738915169857	-1.161503054132
C	-0.001456070113	-0.112863139607	0.000179786658
C	-0.515606176976	0.735752579352	1.163424659660
F	1.511099696738	1.561213018660	-0.705264314643
H	0.894540079163	0.098392450053	-1.959774028221
H	-0.318114437876	1.351017375694	-1.529900264497
Cl	1.326347648460	-1.139849745865	0.648356305330
Cl	-1.327199944810	-1.141315454233	-0.649886371495
H	-0.897886275397	0.092998423486	1.960509597130
H	0.312276517716	1.348824573077	1.532958310050
F	-1.517346560721	1.556896749527	0.708691374159

Atom	X	Y	Z
C	0.373250037469	-0.880651274378	-1.125707450401
C	-0.041145639501	0.149771266321	-0.076239367387
C	-1.318747739987	0.886852385802	-0.482382336437
F	1.511689819085	-1.530241797268	-0.752152128678
H	-0.443733647763	-1.600095590281	-1.240393559668
H	0.546935320712	-0.362066200740	-2.076618616710
Cl	1.248472052548	1.397361781587	0.099475668199
Cl	-0.299166943263	-0.682000584923	1.497712181626
H	-1.608540526845	1.586590201121	0.305781899942
H	-1.136242131182	1.434974807756	-1.414179171809
F	-2.324836601273	-0.024563994997	-0.688519118676

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
100.1198	0.246
151.3662	0.630
165.0670	0.118
244.3495	1.90
248.6091	0.196
311.6176	0.437
333.6383	0.312
410.4656	0.0714
448.1456	3.38
677.2669	5.92
743.2881	15.4
916.4727	0.434
1020.1989	9.63
1092.7109	11.4
1095.7164	11.1
1127.6700	1.12
1192.5338	2.93
1281.7642	0.335
1284.5660	0.886
1398.8773	0.209
1423.2148	1.50
1489.2024	0.0998
1496.1738	1.69
3061.8392	3.25
3062.0102	0.0545
3124.0405	1.44
3125.7156	1.23

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
106.8308	0.448
117.0652	0.495
168.1558	0.188
213.5900	0.351
262.6543	0.301
312.1541	0.167
344.4334	0.185
388.6358	0.384
560.6887	4.13
592.9012	7.32
725.5405	14.3
931.8816	1.59
1049.8759	5.11
1089.2156	2.19
1111.5884	9.64
1139.1475	9.00
1170.8062	4.79
1272.5358	0.967
1290.0674	2.28
1408.6489	1.30
1423.1986	0.804
1496.9347	0.540
1499.0964	0.784
3035.4069	2.18
3046.3562	3.01
3099.7822	1.74
3115.0287	1.78



$\Delta E = 1.98$ kcal mol^{-1}
Population = 0.032

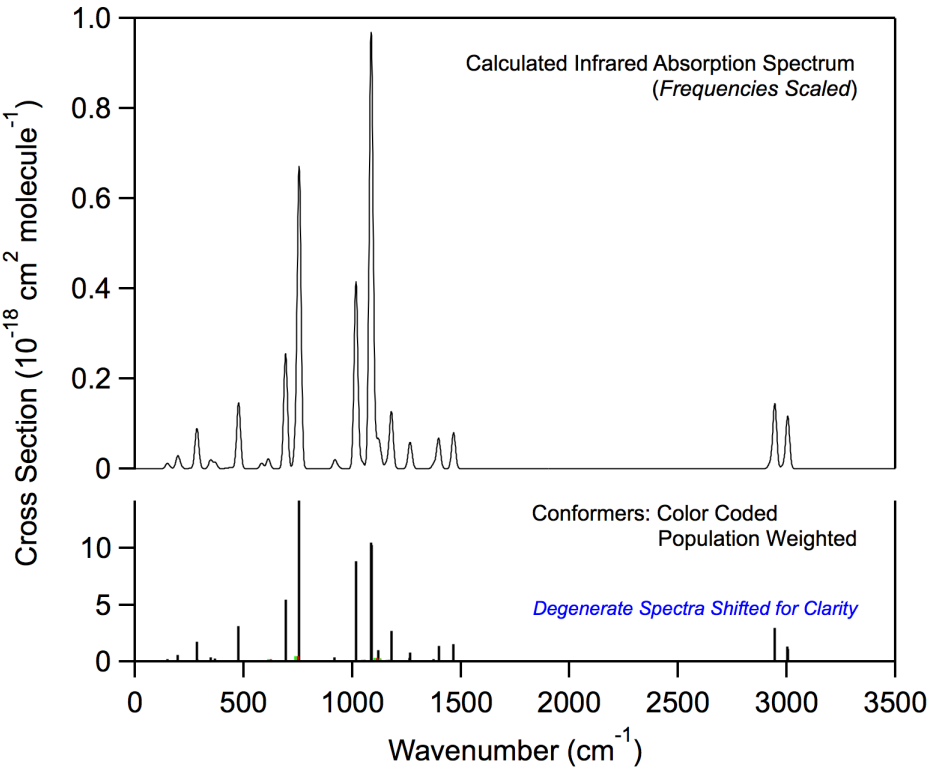
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.315694605965	-0.886987166723	0.489872621531
C	0.039576359721	-0.150466999918	0.078083081124
C	-0.381192996690	0.878143940641	1.126792201784
F	2.319883482571	0.025027488078	0.702523345591
H	1.128811827702	-1.436562617615	1.419944427050
H	1.610220104847	-1.585375960599	-0.297733576015
Cl	-1.248007785705	-1.398941183861	-0.106068277328
Cl	0.305063533793	0.683699541523	-1.493357357180
H	-0.559376517139	0.358095615420	2.076070585828
H	0.434547860651	1.598142677111	1.246726530251
F	-1.518241475717	1.527254665943	0.748199417363

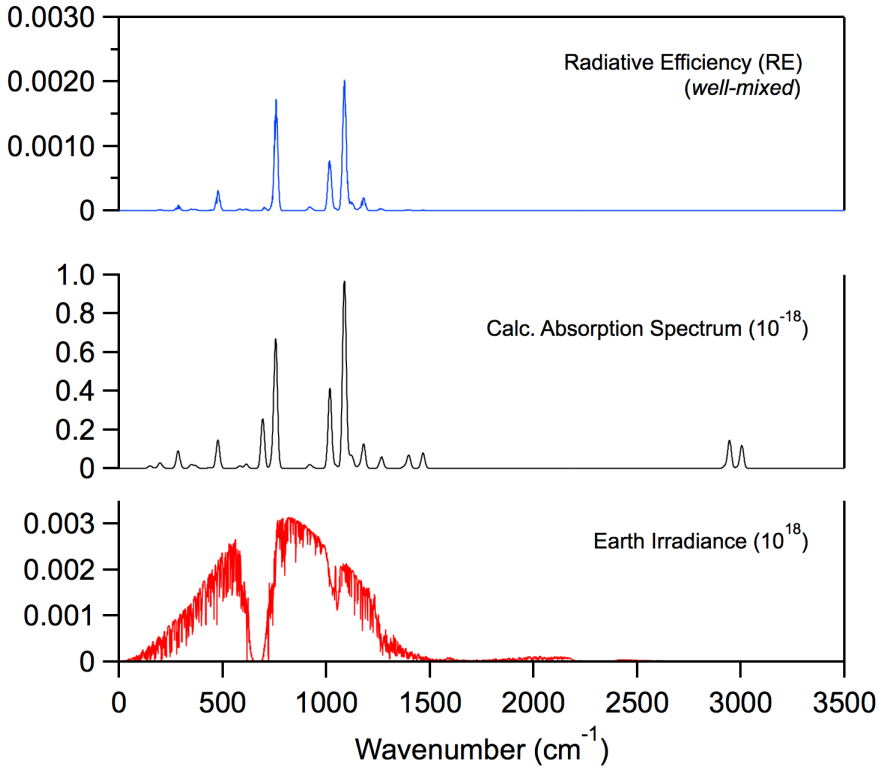
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
106.8304	0.448
117.0643	0.495
168.1560	0.188
213.5899	0.351
262.6545	0.301
312.1538	0.167
344.4337	0.185
388.6356	0.384
560.6887	4.13
592.9015	7.32
725.5395	14.3
931.8822	1.59
1049.8753	5.11
1089.2158	2.19
1111.5879	9.64
1139.1480	9.00
1170.8055	4.79
1272.5360	0.966
1290.0676	2.28
1408.6489	1.30
1423.1990	0.804
1496.9352	0.540
1499.0968	0.784
3035.4069	2.18
3046.3560	3.01
3099.7817	1.74
3115.0286	1.78

Infrared Spectrum

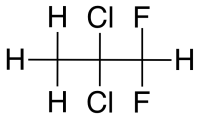


Radiative Efficiency



HCFC-252ab

Molecular Formula: $CH_3CCl_2CHF_2$
Name: 2,2-Dichloro-1,1-difluoropropane
CAS number: –
Molecular Weight: 148.97



Global Atmospheric Lifetime (years): 4.41
  Tropospheric Atmospheric Lifetime (years): 4.93
  Stratospheric Atmospheric Lifetime (years): 41.9
Ozone Depletion Potential (ODP): 0.056

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.167	0.153
Global Warming Potential (GWP_H):		
GWP_{20}	1100	1006
GWP_{100}	301	275
Global Temperature Potentials (GTP_H)		
GTP_{20}		517
GTP_{50}		55
GTP_{100}		39

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 1.19 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 0.760 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 4.76$ years
$\tau^{OH}_{Trop} = 4.93$ years
$\tau^{OH}_{Strat} = 141.9$ years

Fractional Atmospheric Loss: 0.926

O(^{1}D) Reactivity

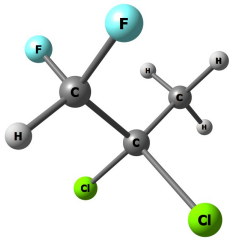
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 1.6 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)} = 230$ years
Fractional Atmospheric Loss: 0.019

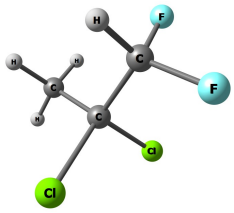
UV Photolysis

UV Spectrum: *No Recommendation*
$\tau_{hv} = 80$ years
Fractional Atmospheric Loss: 0.055

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.717



$\Delta E = 0.96$ kcal mol^{-1}
Population = 0.141

Optimized Coordinates (Angstroms)

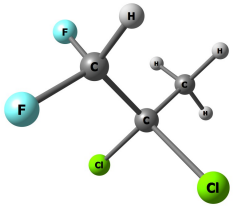
Atom	X	Y	Z
C	-1.734805519720	0.025659000777	0.000000000000
C	-0.236955230555	-0.223405190567	0.000000000000
C	0.580830932263	1.085937391761	0.000000000000
H	-2.274570401458	-0.921362656608	0.000000000000
H	-2.003115861508	0.598113504571	0.890512771937
H	-2.003115861508	0.598113504571	-0.890512771937
Cl	0.249282528892	-1.149962357838	-1.469229424188
Cl	0.249282528892	-1.149962357838	1.469229424188
H	1.658323397994	0.894355829254	0.000000000000
F	0.249138243350	1.811058665955	-1.090595809550
F	0.249138243350	1.811058665955	1.090595809550

Atom	X	Y	Z
C	-0.470835163813	0.769232669675	1.685069284464
C	-0.268861034400	0.149255103451	0.312028828671
C	0.972136606615	-0.765652602109	0.274529653872
H	-1.366701325223	1.390602609001	1.685649970636
H	-0.587111505814	-0.018651785881	2.435107647697
H	0.397459043151	1.381369951918	1.936554853830
Cl	-0.071990743944	1.440312813216	-0.924125244066
Cl	-1.689492292677	-0.884630747843	-0.110827169765
H	0.838106172471	-1.606152579520	0.967363170057
F	1.192190874123	-1.240687536637	-0.960569901275
F	2.055167369512	-0.049741895271	0.655573905879

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
90.2629	0.172
177.4919	0.117
226.9628	0.461
257.4774	0.00706
276.3324	0.667
312.1532	0.0409
324.5426	0.549
396.7348	0.891
434.6924	1.36
566.5795	2.00
716.8506	3.25
737.4939	16.9
911.1719	2.35
1088.0793	15.1
1096.2907	8.23
1132.2054	22.2
1139.5531	5.17
1213.7782	4.45
1379.5821	2.22
1385.4577	1.15
1412.2866	2.98
1478.3950	0.230
1485.3053	1.93
3065.2186	0.436
3088.8518	3.00
3146.6441	0.448
3161.3625	0.354

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
88.0060	0.124
190.4371	0.309
196.9062	0.0468
263.8104	0.0421
271.2934	0.187
301.7095	0.148
331.7794	0.0874
404.0088	0.410
505.4223	1.71
579.1823	2.11
626.2428	10.9
760.7478	10.4
928.2541	1.93
1082.4051	7.44
1097.6866	8.37
1128.0274	13.4
1168.9600	13.4
1210.6035	7.67
1376.0767	3.95
1397.7806	2.83
1411.6659	2.38
1481.3923	1.55
1482.5691	0.420
3051.1111	2.31
3057.6196	2.35
3135.8886	0.940
3159.8785	0.323



$\Delta E = 0.96$ kcal mol^{-1}
Population = 0.141

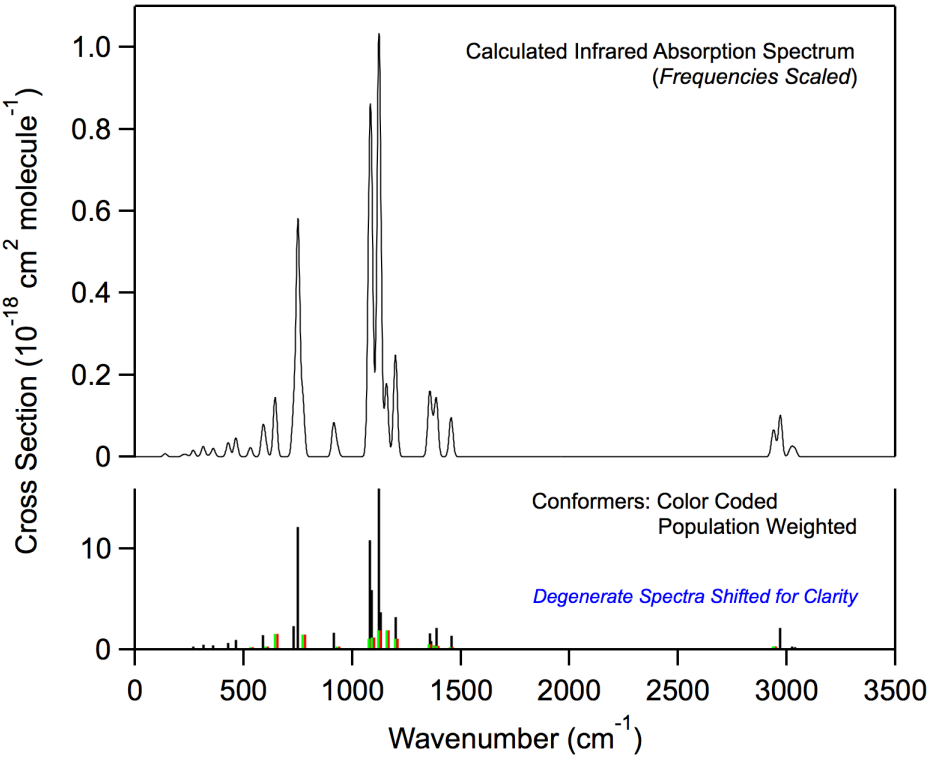
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-0.471592573545	-0.764957565152	1.686895763230
C	-0.269204786682	-0.147931446568	0.312587316380
C	0.972806415148	0.765512749933	0.273023546243
H	-0.586836432528	0.024542870688	2.435392632343
H	-1.368152163924	-1.385323620543	1.688889271513
H	0.396068317359	-1.377564612426	1.939421087165
Cl	-1.688766114816	0.886700256339	-0.112034033027
Cl	-0.074027789406	-1.441658317308	-0.921042085908
H	0.839855641370	1.607534944285	0.964214812764
F	2.055114156163	0.049149690100	0.655270053281
F	1.193140330862	1.237850050650	-0.963060363985

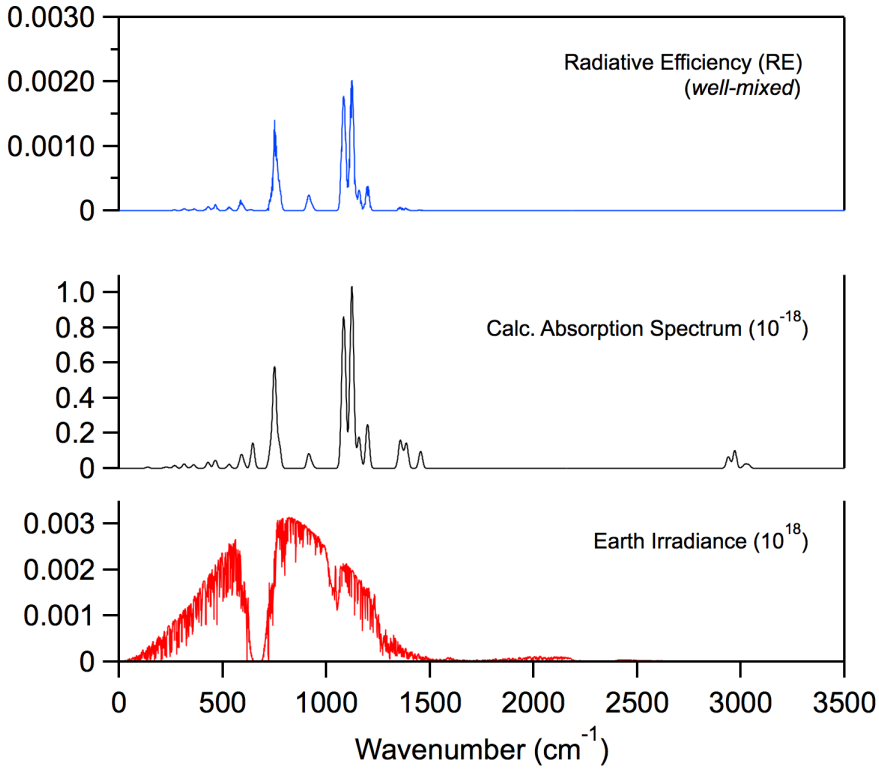
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
88.0060	0.124
190.4371	0.309
196.9062	0.0468
263.8103	0.0421
271.2934	0.187
301.7095	0.148
331.7794	0.0874
404.0088	0.410
505.4224	1.71
579.1823	2.11
626.2428	10.9
760.7478	10.4
928.2541	1.93
1082.4051	7.44
1097.6866	8.37
1128.0274	13.4
1168.9599	13.4
1210.6035	7.67
1376.0767	3.95
1397.7806	2.83
1411.6659	2.38
1481.3923	1.55
1482.5691	0.420
3051.1111	2.31
3057.6196	2.35
3135.8887	0.940
3159.8785	0.323

Infrared Spectrum

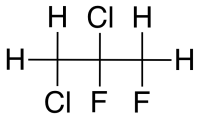


Radiative Efficiency



HCFC-252ba

Molecular Formula:	$CH_2ClCClFCH_2F$
Name:	1,2-Dichloro-2,3-difluoropropane
CAS number:	70192-74-4
Molecular Weight:	148.97



Global Atmospheric Lifetime (years):	2.19
Tropospheric Atmospheric Lifetime (years):	2.31
Stratospheric Atmospheric Lifetime (years):	44.0
Ozone Depletion Potential (ODP):	0.027

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.116	0.099
Global Warming Potential (GWP_H):		
GWP_{20}	386	329
GWP_{100}	104	89
Global Temperature Potentials (GTP_H)		
GTP_{20}		125
GTP_{50}		16
GTP_{100}		12

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 2.54 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 1.62 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 2.24$ years

$\tau^{OH}_{Trop} = 2.31$ years

$\tau^{OH}_{Strat} = 71.7$ years

Fractional Atmospheric Loss: 0.981

O(^{1}D) Reactivity

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

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

$\tau_{O(^1D)} = 230$ years

Fractional Atmospheric Loss: 0.009

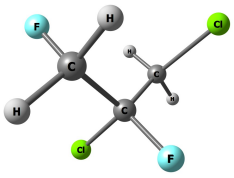
UV Photolysis

UV Spectrum: *No Recommendation*

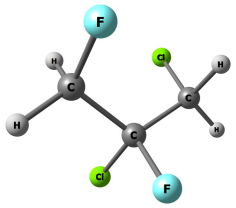
$\tau_{hv} = 225$ years

Fractional Atmospheric Loss: 0.010

Molecular Structure and Infrared Spectrum (4 conformers)



E = 0
Population = 0.683



$\Delta E = 0.79$ kcal mol^{-1}
Population = 0.180

Optimized Coordinates (Angstroms)

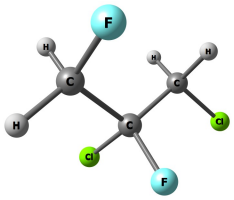
Atom	X	Y	Z
C	-0.707082923855	0.514065791182	-0.774982077841
C	0.338734407932	0.220079891159	0.293528874230
C	0.430499449528	-1.242575235548	0.722401031064
Cl	-2.371901034002	0.173333761631	-0.171206466460
H	-0.671625549710	1.565315602561	-1.053936256074
H	-0.531625214017	-0.120641701802	-1.641073520152
F	0.114599295235	0.959153253162	1.404856893578
Cl	1.933545144411	0.733114956981	-0.417535306887
H	1.258497030867	-1.361460401245	1.427176930134
H	-0.513076322867	-1.524126934925	1.201645068348
F	0.634914716477	-2.029918983155	-0.380185169938

Atom	X	Y	Z
C	-0.749407997283	-0.223037870010	0.960728946321
C	0.557272652817	0.090193921622	0.233966697044
C	0.908307382324	-0.863628100192	-0.902028958610
Cl	-2.188090694599	-0.193489078610	-0.106442114790
H	-0.664697992332	-1.229969663638	1.369264586638
H	-0.903713940659	0.500018283813	1.759926193985
F	1.528847313134	0.012166903996	1.186811621126
Cl	0.565749280212	1.767934075389	-0.434767702947
H	0.188332256671	-0.763946269870	-1.717527382858
H	1.918196301886	-0.637132129331	-1.256756371761
F	0.872198437829	-2.146621073168	-0.406624514150

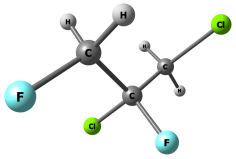
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
75.1772	0.228
132.2372	0.633
164.4185	0.184
224.9028	1.60
281.8909	0.118
310.7469	0.650
381.9163	0.195
439.5218	2.38
519.5569	0.713
673.0551	16.9
742.1273	5.86
853.4979	2.54
907.5475	1.15
1071.4137	7.46
1109.9064	13.5
1123.2787	5.60
1214.6713	7.39
1266.4795	2.89
1277.9795	2.09
1308.1287	0.725
1421.2747	0.413
1455.3791	1.72
1499.9558	1.36
3055.8770	2.23
3115.3337	1.72
3118.5997	0.870
3190.8048	0.0163

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
73.5657	0.173
136.2873	0.507
164.8605	0.299
226.0584	1.58
298.8345	0.487
327.3698	0.288
374.0418	0.364
442.1722	1.37
464.8255	1.84
693.5680	7.42
786.4913	6.61
856.3864	4.58
966.9535	4.54
989.5570	15.9
1091.7736	7.76
1147.9460	13.6
1182.0325	3.29
1252.5490	1.67
1280.6519	2.88
1320.5232	0.190
1417.8199	0.530
1460.7527	1.34
1491.2108	1.25
3067.3359	1.64
3104.6320	0.827
3131.8693	1.59
3174.8202	0.0251



$\Delta E = 1.44$ kcal mol^{-1}
Population = 0.060



$\Delta E = 1.59$ kcal mol^{-1}
Population = 0.046

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-0.560041990507	-0.816458938482	-0.592736430021
C	0.425756834954	0.112290510691	0.107422707579
C	1.863608357532	-0.125637924716	-0.359391609113
Cl	-2.224125797920	-0.680699513369	0.048786103129
H	-0.589017315254	-0.598653888561	-1.659689521789
H	-0.225690298034	-1.841500031268	-0.430790930504
F	0.365203441721	-0.080778258964	1.445144359231
Cl	0.052792666714	1.851682577052	-0.237180734970
H	1.965993896988	0.122316791309	-1.420109976112
H	2.534951474436	0.500219796622	0.235880608791
F	2.177939729371	-1.450439120313	-0.164119576224

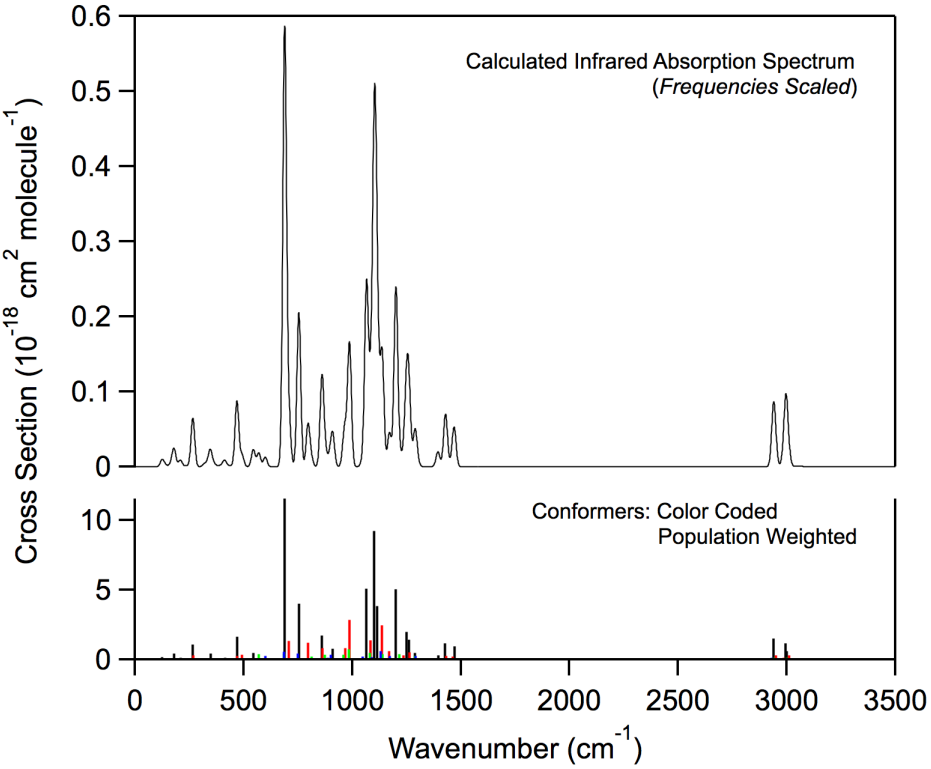
Atom	X	Y	Z
C	-0.966404014924	0.864027321682	-0.347195121834
C	0.260421804557	0.097504521038	0.135005578142
C	0.507864558190	-1.231872082608	-0.573273550793
Cl	-2.484454367310	-0.081922440529	-0.104273021929
H	-1.063263098885	1.783150228579	0.228167722520
H	-0.885679669721	1.093934902300	-1.408180069525
F	0.175890525385	-0.118311347688	1.467512144233
Cl	1.680157380889	1.200308968538	-0.158648297820
H	-0.320794726317	-1.907715400329	-0.337657656693
H	0.558406963029	-1.071135398468	-1.655527613120
F	1.676662645106	-1.780645272513	-0.129420113179

Infrared Absorption Spectrum (unscaled frequencies)

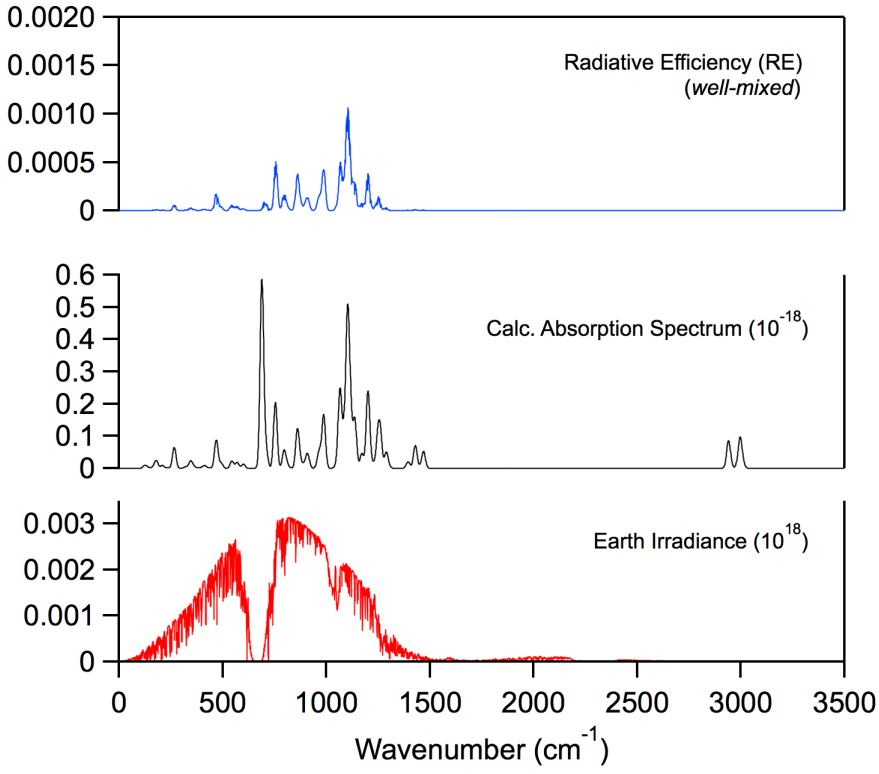
Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
87.9041	0.252
117.7360	0.869
168.1251	0.0491
193.5989	0.414
306.5477	0.155
328.6677	0.191
356.4573	0.330
410.7024	0.382
546.3885	6.50
670.4690	7.18
802.5213	3.71
869.0861	5.57
959.8474	5.87
984.5335	12.5
1088.3850	7.80
1150.0816	6.58
1188.2520	2.45
1232.1601	6.44
1307.6271	4.33
1321.8655	1.53
1412.7026	0.964
1462.8943	1.13
1492.7535	0.682
3058.8021	1.84
3099.9445	0.934
3119.6322	1.99
3166.2043	0.110

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
88.6793	0.936
112.1730	0.320
158.1971	0.207
207.6138	0.129
274.5871	0.0433
333.7055	0.376
358.5883	0.229
397.7791	0.227
578.0740	5.91
667.8530	11.7
737.7115	8.85
882.0337	3.22
897.6255	7.32
1053.4476	4.36
1096.9648	3.49
1140.4740	13.2
1184.4673	5.44
1270.1825	1.95
1299.4339	0.354
1309.3721	5.80
1429.1930	0.336
1461.6815	1.71
1496.0411	0.401
3047.5835	2.60
3104.4579	1.58
3112.7220	1.14
3181.3175	0.0205

Infrared Spectrum

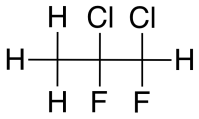


Radiative Efficiency



HCFC-252bb

Molecular Formula:	$CH_3CClFCHClF$
Name:	1,2-Dichloro-1,2-difluoropropane
CAS number:	362631-58-1
Molecular Weight:	148.97



Global Atmospheric Lifetime (years):	2.87
Tropospheric Atmospheric Lifetime (years):	3.04
Stratospheric Atmospheric Lifetime (years):	50.9
Ozone Depletion Potential (ODP):	0.032

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.167	0.147
Global Warming Potential (GWP_H):		
GWP_{20}	723	637
GWP_{100}	196	173
Global Temperature Potentials (GTP_H)		
GTP_{20}		266
GTP_{50}		32
GTP_{100}		24

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 1.93 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 1.23 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 2.94$ years

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

$\tau^{OH}_{Strat} = 91.8$ years

Fractional Atmospheric Loss: 0.975

O(^{1}D) Reactivity

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

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

$\tau_{O(^1D)} = 230$ years

Fractional Atmospheric Loss: 0.012

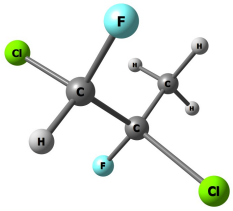
UV Photolysis

UV Spectrum: *No Recommendation*

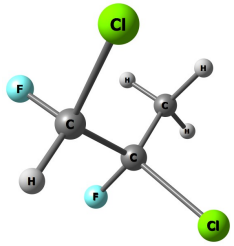
$\tau_{hv} = 225$ years

Fractional Atmospheric Loss: 0.013

Molecular Structure and Infrared Spectrum (5 conformers)



E = 0
Population = 0.716



$\Delta E = 1.06$ kcal mol^{-1}
Population = 0.120

Optimized Coordinates (Angstroms)

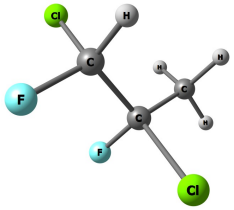
Atom	X	Y	Z
C	-0.480992871978	-0.863246898197	1.497280067146
C	-0.500114101702	-0.426246525982	0.048723874055
C	0.589972714832	0.589191067124	-0.344821986924
H	-1.322686057542	-1.531239563365	1.684783563621
H	0.453593736815	-1.392033716667	1.699503858092
H	-0.553563241101	0.006153158037	2.151336577800
Cl	-2.086821462137	0.391893183928	-0.329866972128
F	-0.389371344446	-1.490588264249	-0.780741690108
H	0.474122654354	0.900920091101	-1.383524873281
F	0.530980477507	1.657959157234	0.474739514157
Cl	2.224539495398	-0.160475688965	-0.215792932430

Atom	X	Y	Z
C	0.670981944327	0.640717602222	1.577288567514
C	0.660438050872	0.346160308838	0.093146324139
C	-0.735641416757	0.328323204337	-0.564705941039
H	1.704170199109	0.747010948607	1.911298541944
H	0.135272323460	1.577952881840	1.749198828580
H	0.187814926435	-0.160422692317	2.135953932847
Cl	1.490304365004	-1.219540132943	-0.272652933084
F	1.338816255088	1.326411668992	-0.569375696889
H	-0.652126608596	0.106856009686	-1.629816358527
Cl	-1.830509289303	-0.896365516995	0.151986518547
F	-1.280490749640	1.556305717734	-0.394786784031

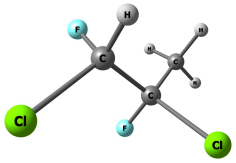
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
78.4124	0.199
171.8548	0.144
220.4698	0.161
249.3079	0.938
257.0028	0.00799
316.2619	0.177
379.3455	0.208
387.5482	0.407
445.5484	1.87
542.6538	0.629
675.6796	19.1
757.9407	15.7
865.0004	1.38
983.8664	4.45
1092.6648	11.1
1134.7958	15.4
1199.2915	16.9
1239.9268	2.09
1288.3563	2.67
1364.4869	0.350
1412.2745	3.51
1478.0129	0.234
1485.1631	0.802
3068.1698	0.305
3122.5111	0.837
3149.4903	0.581
3165.3448	0.317

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
81.6315	0.166
166.0156	0.0457
230.7387	0.218
238.5315	0.831
295.2418	0.186
313.8643	0.127
381.4664	0.0699
405.3857	0.970
425.4095	0.932
493.1422	2.23
712.5691	7.08
796.6405	12.9
878.4832	13.5
972.0405	2.99
1101.6486	21.3
1110.5385	7.54
1163.3582	17.7
1234.4415	3.46
1284.4555	0.888
1363.1565	1.19
1411.3140	3.58
1478.0180	0.372
1484.8143	0.744
3066.7316	0.370
3118.0108	0.973
3147.6361	0.534
3168.9505	0.393



$\Delta E = 1.40$ kcal mol^{-1}
Population = 0.068



$\Delta E = 1.70$ kcal mol^{-1}
Population = 0.040

Optimized Coordinates (Angstroms)

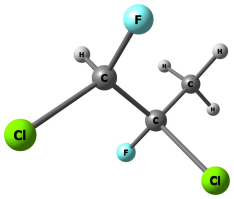
Atom	X	Y	Z
C	0.527743643459	1.807823455395	0.414496388876
C	0.502335534356	0.396718468962	-0.135632528025
C	-0.589377610439	-0.517406620799	0.451427309258
H	0.621949860402	1.797671591216	1.502186739231
H	1.382330710139	2.337751858342	-0.009063873597
H	-0.393155115546	2.323368673429	0.134496597519
Cl	2.087574553061	-0.426890119971	0.249138626360
F	0.367685751428	0.415577186301	-1.480530528072
H	-0.487632617734	-0.604671424682	1.534194545434
Cl	-2.226489318730	0.178051263572	0.137894201362
F	-0.528727390395	-1.731274331764	-0.122632478346

Atom	X	Y	Z
C	-1.617476504482	-1.404125423649	0.327412721197
C	-0.680920549802	-0.293108644166	-0.116131191007
C	0.705355966024	-0.401674159312	0.552902013813
H	-1.756743077559	-1.386587636752	1.410017285982
H	-2.585096061578	-1.269450683149	-0.158113080849
H	-1.189603685130	-2.364393891279	0.032268638000
Cl	-1.387444557699	1.319015107623	0.325942386477
F	-0.531972892582	-0.338398940334	-1.459625982539
H	0.640021866560	-0.169623248258	1.616956446986
F	1.151541121758	-1.674064469856	0.391677480085
Cl	1.897461374489	0.719434989133	-0.165830718145

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
70.7868	0.0852
180.5834	0.304
215.5510	0.0512
244.9355	0.0421
271.8442	0.0757
321.2282	0.336
355.6339	0.0512
393.0289	0.351
416.7833	0.391
579.0113	2.79
698.3757	29.3
777.2097	4.63
856.9876	4.24
961.4086	4.98
1095.9008	13.3
1146.2429	16.1
1171.6676	5.84
1250.1333	9.44
1276.3669	1.14
1383.6584	1.00
1412.7346	2.91
1477.5996	0.380
1485.1067	0.785
3065.7854	0.271
3115.4506	1.11
3150.1452	0.749
3153.9211	0.569

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
70.0301	0.124
169.4958	0.190
220.2093	0.0965
246.9666	0.0667
295.3197	0.351
328.1701	0.163
351.1989	0.123
399.3805	0.152
433.2128	0.929
528.7125	5.23
744.2818	12.3
790.7558	6.89
870.0256	11.4
975.2476	5.19
1094.7114	27.1
1106.3778	1.84
1149.5306	7.11
1243.9486	10.2
1295.8339	2.54
1363.7841	0.732
1407.5717	1.59
1479.3668	0.356
1484.1267	0.746
3065.5139	0.394
3115.3957	1.15
3150.4409	0.831
3155.9827	0.495



$\Delta E = 1.77$ kcal mol^{-1}
Population = 0.036

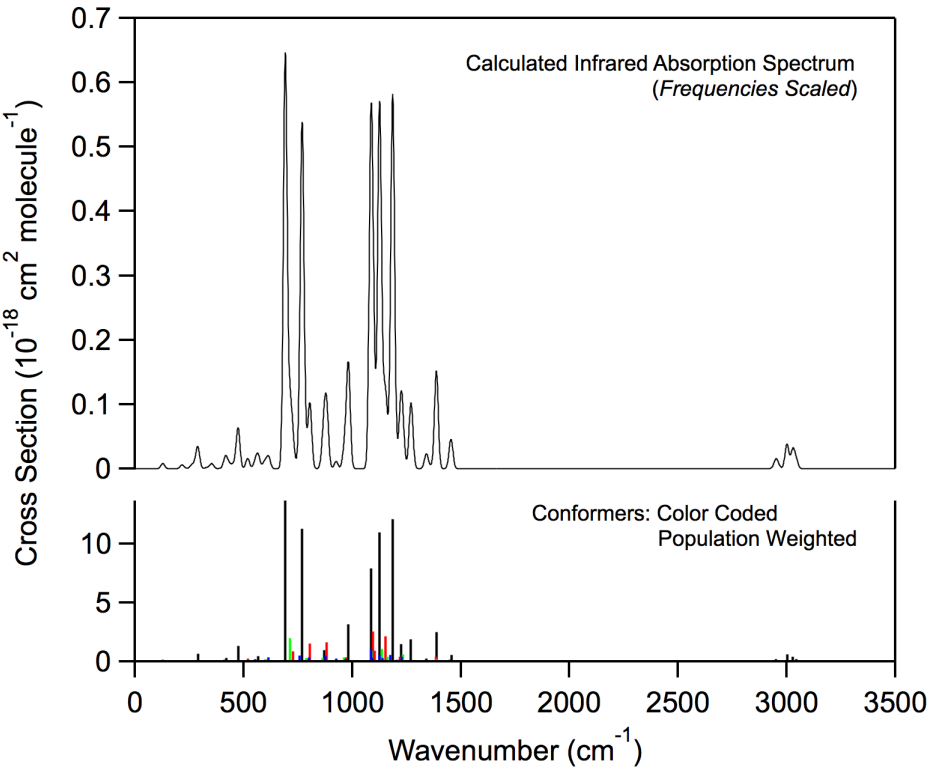
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.808800815034	1.207214553559	-0.235920249561
C	0.707455110402	0.166698152414	-0.351902527608
C	-0.673676887466	0.771566872384	-0.031844472299
H	2.768530819552	0.746376803010	-0.473687134579
H	1.616937270770	2.017170653537	-0.946974437248
H	1.840626110903	1.613430332781	0.775332977654
Cl	1.054959893115	-1.212622967177	0.761643684560
F	0.656388473595	-0.307981097766	-1.622232289147
H	-0.865506981131	1.595556369613	-0.725353069687
Cl	-2.012016780460	-0.390732246359	-0.258567592058
F	-0.677368844314	1.239866574005	1.235041109972

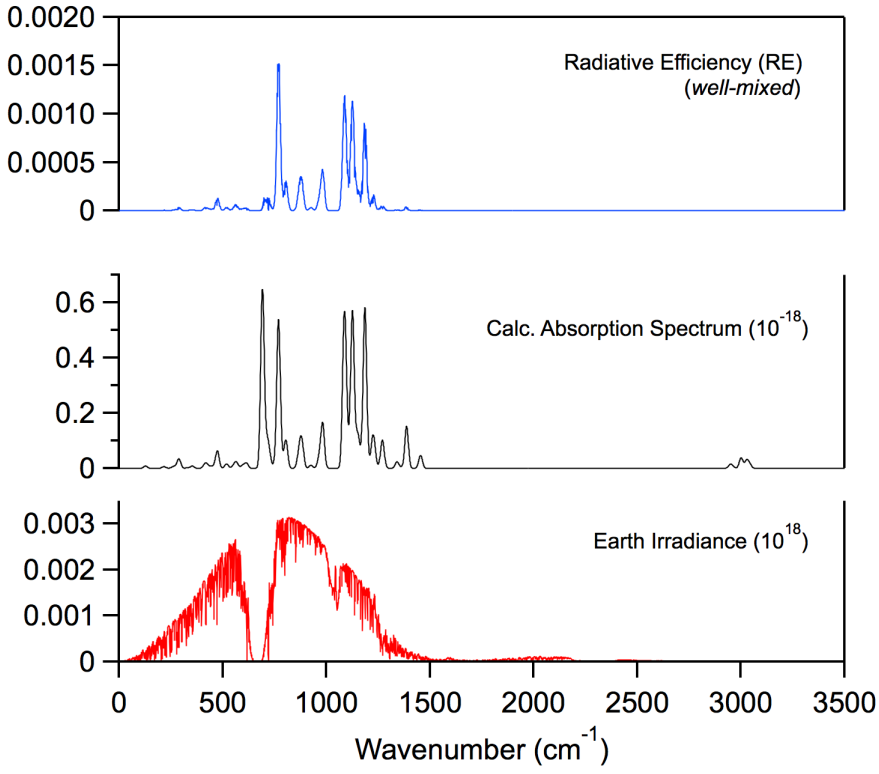
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
75.8024	0.0826
171.6114	0.0636
200.0573	0.258
235.8832	0.00166
286.6706	0.208
321.6728	0.177
371.3856	0.0463
405.9046	0.100
488.7879	2.19
568.1495	2.70
594.3554	10.7
792.9972	10.1
923.3117	6.83
966.5530	6.13
1099.4650	8.97
1134.4242	15.4
1188.8584	16.1
1219.4257	4.75
1296.7816	2.74
1357.8313	2.29
1407.0034	1.63
1480.8914	0.408
1483.1289	0.517
3054.3943	0.828
3081.4260	2.24
3136.9453	1.05
3166.1433	0.311

Infrared Spectrum

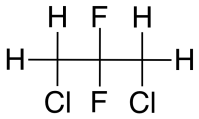


Radiative Efficiency



HCFC-252ca

Molecular Formula:	$CH_2ClCF_2CH_2Cl$
Name:	1,3-Dichloro-2,2-difluoropropane
CAS number:	1112-36-3
Molecular Weight:	148.97



Global Atmospheric Lifetime (years):	2.47
Tropospheric Atmospheric Lifetime (years):	2.61
Stratospheric Atmospheric Lifetime (years):	47.0
Ozone Depletion Potential (ODP):	0.029

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.145	0.126
Global Warming Potential (GWP_H):		
GWP_{20}	543	470
GWP_{100}	147	127
Global Temperature Potentials (GTP_H)		
GTP_{20}		186
GTP_{50}		23
GTP_{100}		18

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 2.25 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 1.44 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 2.52$ years

$\tau^{OH}_{Trop} = 2.61$ years

$\tau^{OH}_{Strat} = 80.0$ years

Fractional Atmospheric Loss: 0.978

O(^{1}D) Reactivity

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

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

$\tau_{O(^1D)} = 230$ years

Fractional Atmospheric Loss: 0.011

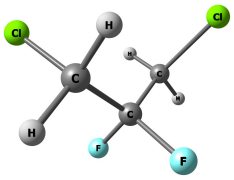
UV Photolysis

UV Spectrum: *No Recommendation*

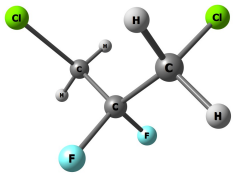
$\tau_{hv} = 225$ years

Fractional Atmospheric Loss: 0.011

Molecular Structure and Infrared Spectrum (6 conformers)



E = 0
Population = 0.375



E = 0
Population = 0.375

Optimized Coordinates (Angstroms)

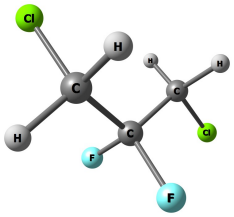
Atom	X	Y	Z
C	-0.960475250294	-0.030476078250	0.884002184218
C	-0.001321135157	-0.819361838900	-0.002454241166
C	0.955354878103	-0.021800303245	-0.883810600791
Cl	-2.061670337504	1.012444364304	-0.075357257156
H	-1.571417381955	-0.738284390216	1.443506868809
H	-0.399876571708	0.607384965005	1.564786740698
F	-0.708771768745	-1.624732186267	-0.838179212602
F	0.708650240427	-1.627874901282	0.828082318868
H	1.568497526077	-0.724084695965	-1.447850578755
H	0.392759397697	0.618672230689	-1.560483658472
Cl	2.053299403058	1.018361834126	0.082245436349

Atom	X	Y	Z
C	-0.960170601714	-0.030497644540	-0.882552040975
C	-0.000535847171	-0.822452270602	0.000641530372
C	0.958319052556	-0.027950859277	0.882393639730
Cl	-2.058804304139	1.011386129837	0.080861880617
H	-0.399909121028	0.608331042307	-1.562706484852
H	-1.572711588045	-0.736359087351	-1.442767619884
F	0.707318487154	-1.629808698330	-0.832822131138
F	-0.707596600310	-1.628988611217	0.835571372646
H	0.397429267405	0.611562229903	1.561386106977
H	1.571552832356	-0.732190496964	1.443890951400
Cl	2.055929422935	1.013259266235	-0.082913204895

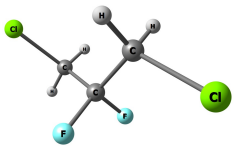
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
56.4573	0.176
132.3482	0.770
173.6376	0.169
205.3371	1.19
326.6431	0.369
336.6503	0.253
404.5069	0.831
510.0980	2.38
559.7428	0.771
741.1587	1.37
791.1309	9.22
828.4269	3.90
872.5045	2.20
926.8859	1.17
1077.5941	11.4
1110.6351	10.3
1184.9808	12.7
1251.0638	7.90
1271.0913	6.49
1327.0565	3.32
1338.0515	1.95
1462.6732	4.18
1463.7657	1.50
3109.2230	0.967
3109.5677	0.942
3179.6357	0.0367
3179.9555	0.0218

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
56.4570	0.176
132.3477	0.770
173.6375	0.169
205.3369	1.19
326.6430	0.369
336.6503	0.253
404.5069	0.831
510.0980	2.38
559.7428	0.771
741.1587	1.37
791.1308	9.22
828.4270	3.90
872.5047	2.20
926.8861	1.17
1077.5942	11.4
1110.6352	10.3
1184.9809	12.7
1251.0642	7.90
1271.0915	6.49
1327.0569	3.32
1338.0517	1.95
1462.6736	4.18
1463.7661	1.50
3109.2231	0.967
3109.5679	0.942
3179.6359	0.0367
3179.9558	0.0218



$\Delta E = 1.08$ kcal mol^{-1}
Population = 0.061



$\Delta E = 1.08$ kcal mol^{-1}
Population = 0.061

Optimized Coordinates (Angstroms)

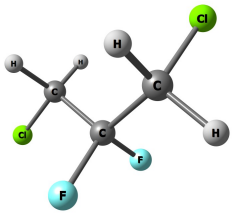
Atom	X	Y	Z
C	-1.451383320093	-0.661749223880	0.458412802913
C	0.003450904835	-0.561311754895	-0.009865798500
C	0.762751416091	0.636592989055	0.548776204356
Cl	-2.438179497444	0.753715203597	-0.035113255246
H	-1.890747478166	-1.550247371052	0.005361838911
H	-1.492916160633	-0.739772057865	1.544407348668
F	0.040567736894	-0.547430277578	-1.360167937820
F	0.598333208086	-1.714891554775	0.401844364287
H	0.303768861072	1.560643822430	0.202035510033
H	0.753571219326	0.602358126783	1.638530838051
Cl	2.472808110033	0.632554098179	0.015597084346

Atom	X	Y	Z
C	-1.449619992486	-0.658168339295	-0.461660468900
C	0.004629169051	-0.559638921850	0.008834613616
C	0.762709199075	0.644093584305	-0.538827521653
Cl	-2.438927158060	0.751601106031	0.043013838400
H	-1.490026418917	-0.726963826942	-1.548320987075
H	-1.888117707747	-1.551139871658	-0.016636191093
F	0.601569291795	-1.708796105984	-0.412161077995
F	0.040467925133	-0.557250105200	1.359240411156
H	0.754605519624	0.619158967162	-1.628843201614
H	0.302054177460	1.564481843995	-0.184642890071
Cl	2.472265995073	0.637974669436	-0.004067524769

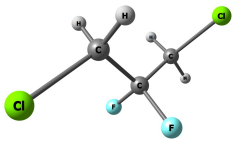
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
72.2724	0.588
88.9150	0.505
157.6018	0.0776
196.7586	0.187
318.9684	0.219
330.3736	0.134
404.8051	0.200
532.5409	1.32
571.4607	5.78
755.2147	0.956
786.5415	8.87
828.4957	2.10
901.3188	2.21
902.2301	1.61
1078.7186	11.6
1120.8893	5.66
1166.1224	14.3
1236.0438	6.64
1307.7366	4.85
1314.0720	2.68
1336.5955	3.63
1462.5988	1.73
1466.3747	1.24
3099.9024	1.43
3103.4955	1.23
3167.9682	0.0840
3173.3069	0.123

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
72.2724	0.588
88.9151	0.505
157.6025	0.0776
196.7586	0.187
318.9685	0.219
330.3738	0.134
404.8053	0.200
532.5410	1.32
571.4606	5.78
755.2151	0.956
786.5413	8.87
828.4960	2.10
901.3194	2.21
902.2300	1.61
1078.7184	11.6
1120.8891	5.66
1166.1227	14.3
1236.0444	6.64
1307.7363	4.85
1314.0721	2.68
1336.5967	3.63
1462.5996	1.73
1466.3750	1.24
3099.9024	1.43
3103.4950	1.23
3167.9684	0.0839
3173.3058	0.123



$\Delta E = 1.08$ kcal mol^{-1}
Population = 0.061



$\Delta E = 1.08$ kcal mol^{-1}
Population = 0.061

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-0.767244441609	0.632750617550	0.554678228515
C	-0.004149376018	-0.560610684850	-0.008499005341
C	1.449655576141	-0.660773546677	0.463023692698
Cl	-2.475896986206	0.628296861742	0.017019575798
H	-0.760832481740	0.592589095016	1.644250339705
H	-0.309171295836	1.559569612290	0.214179228610
F	-0.037780485007	-0.539435415620	-1.358797777310
F	-0.597841104581	-1.717573349913	0.395362631583
H	1.488515927179	-0.744638240890	1.548681694721
H	1.891935146103	-1.545931733451	0.006286574823
Cl	2.434959521574	0.759276784803	-0.020202183802

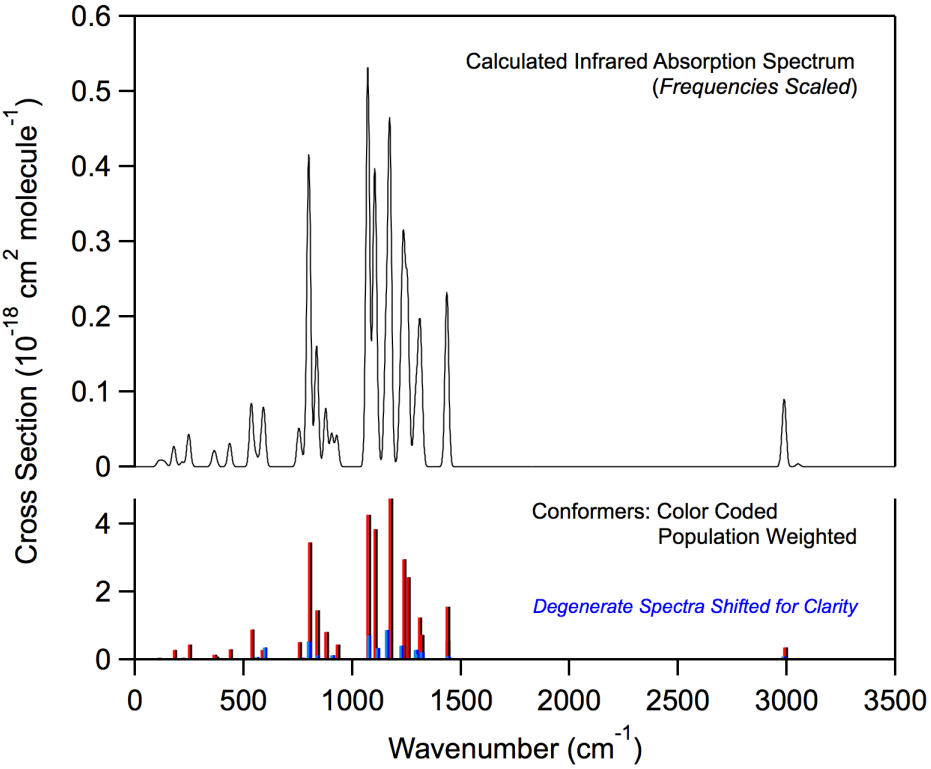
Atom	X	Y	Z
C	0.767005678769	-0.632726761252	-0.554563794415
C	0.003917776197	0.560567600324	0.008764973189
C	-1.450022558465	0.660540089492	-0.462380550492
Cl	2.475798622402	-0.628049902183	-0.017353417010
H	0.309130995448	-1.559585829904	-0.213906970433
H	0.760303272019	-0.592610363286	-1.644135818970
F	0.597367339080	1.717583729775	-0.395299353418
F	0.037905432213	0.539451225834	1.359055753998
H	-1.892286594106	1.545664739458	-0.005563415105
H	-1.489177459759	0.744356097994	-1.548031726671
Cl	-2.435032503797	-0.759606626253	0.021161319327

Infrared Absorption Spectrum (unscaled frequencies)

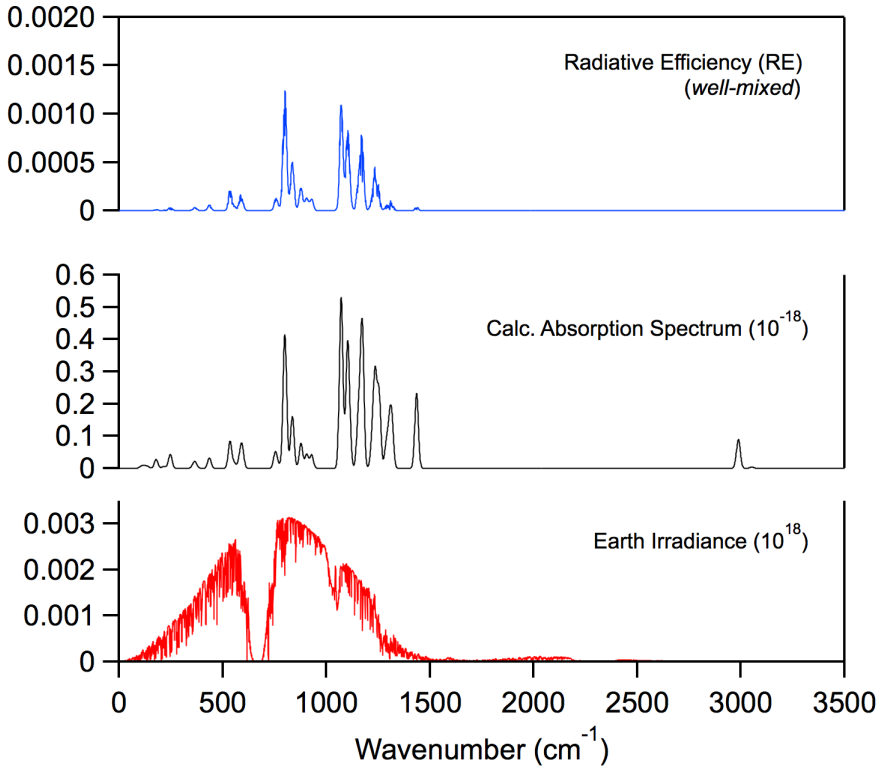
Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
72.2726	0.588
88.9150	0.505
157.6018	0.0776
196.7586	0.187
318.9684	0.219
330.3736	0.134
404.8051	0.200
532.5409	1.32
571.4607	5.78
755.2147	0.956
786.5414	8.87
828.4957	2.10
901.3188	2.21
902.2301	1.61
1078.7185	11.6
1120.8891	5.66
1166.1223	14.3
1236.0437	6.64
1307.7365	4.85
1314.0719	2.68
1336.5954	3.63
1462.5986	1.73
1466.3747	1.24
3099.9023	1.43
3103.4955	1.23
3167.9681	0.0840
3173.3069	0.123

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
72.2719	0.588
88.9145	0.505
157.6015	0.0776
196.7587	0.187
318.9682	0.219
330.3737	0.134
404.8050	0.200
532.5409	1.32
571.4607	5.78
755.2148	0.956
786.5415	8.87
828.4957	2.10
901.3190	2.21
902.2302	1.61
1078.7188	11.6
1120.8896	5.66
1166.1224	14.3
1236.0443	6.64
1307.7365	4.85
1314.0723	2.68
1336.5958	3.63
1462.5993	1.73
1466.3751	1.24
3099.9023	1.43
3103.4955	1.23
3167.9681	0.0840
3173.3069	0.123

Infrared Spectrum

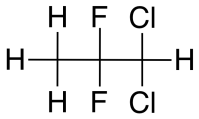


Radiative Efficiency



HCFC-252cb

Molecular Formula:	$CH_3CF_2CHCl_2$
Name:	1,1-Dichloro-2,2-difluoropropane
CAS number:	1112-01-2
Molecular Weight:	148.97



Global Atmospheric Lifetime (years):	1.19
Tropospheric Atmospheric Lifetime (years):	1.25
Stratospheric Atmospheric Lifetime (years):	24.4
Ozone Depletion Potential (ODP):	0.019

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.189	0.146
Global Warming Potential (GWP_H):		
GWP_{20}	341	263
GWP_{100}	92	71
Global Temperature Potentials (GTP_H)		
GTP_{20}		87
GTP_{50}		12
GTP_{100}		10

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

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

OH Reactivity

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

k_{SAR}(298 K) = 4.68×10^{-14}; k_{SAR}(272 K) ≈ 2.99×10^{-14} cm^3 $molecule^{-1}$ s^{-1}

τ^{OH}_{Global} = 1.22 years
τ^{OH}_{Trop} = 1.25 years
τ^{OH}_{Strat} = 41.3 years

Fractional Atmospheric Loss: 0.980

O(^{1}D) Reactivity

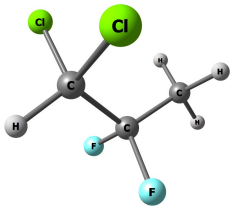
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 1.6 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)}$ = 230 years
Fractional Atmospheric Loss: 0.005

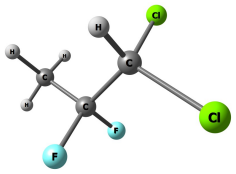
UV Photolysis

UV Spectrum: *No Recommendation*
τ_{hv} = 80 years
Fractional Atmospheric Loss: 0.015

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.662



$\Delta E = 0.81$ kcal mol^{-1}
Population = 0.169

Optimized Coordinates (Angstroms)

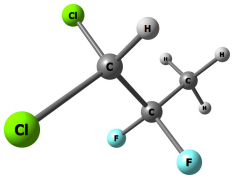
Atom	X	Y	Z
C	-1.705525642955	-0.946672201201	0.000000000000
C	-0.196141250197	-1.015228921244	0.000000000000
C	0.580381902810	0.323348235962	0.000000000000
H	-2.090788105105	-1.968452155419	0.000000000000
H	-2.060814812017	-0.426946458447	0.890597298300
H	-2.060814812017	-0.426946458447	-0.890597298300
F	0.240785368747	-1.701375172235	-1.090409753868
F	0.240785368747	-1.701375172235	1.090409753868
H	1.645117962473	0.099809802366	0.000000000000
Cl	0.239882509765	1.269688250508	-1.476722873041
Cl	0.239882509765	1.269688250508	1.476722873041

Atom	X	Y	Z
C	-2.003105604940	0.932535925658	0.394894903606
C	-1.013775245873	-0.136143938973	-0.028966491937
C	0.419865964156	0.053492572677	0.518085822616
H	-2.989066850260	0.638930672733	0.028046949761
H	-2.038894455361	1.009112828070	1.484068308771
H	-1.731864331182	1.899391385527	-0.028120390414
F	-0.970349439632	-0.218510419360	-1.377527554649
F	-1.440661568497	-1.342759088647	0.437130133396
H	0.397112544858	0.060709853000	1.605596722948
Cl	1.467825123613	-1.302503713956	0.023132305821
Cl	1.106719863119	1.621246923272	-0.006086709918

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
73.3770	0.205
178.3227	0.0398
200.8336	0.0393
219.7831	0.606
253.4263	0.273
333.8928	0.256
366.3447	0.108
441.1300	0.155
473.8930	2.80
579.1202	1.19
727.5907	1.74
797.2261	22.5
833.0321	4.38
966.9834	6.50
968.0925	2.30
1157.6427	13.9
1196.1515	18.2
1230.7068	0.355
1250.9012	11.2
1314.9343	3.68
1419.1388	6.91
1479.8779	0.439
1486.3900	0.0740
3072.5290	0.217
3147.2827	0.302
3154.5957	0.851
3164.7164	0.466

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
63.4632	0.129
185.6017	0.163
205.3466	0.105
213.2459	0.0257
265.4549	0.140
321.9624	0.108
355.9185	0.0974
414.7766	0.176
531.8706	2.54
590.5401	4.65
743.2645	1.62
786.3412	18.1
835.9661	4.63
951.1854	5.64
977.7377	4.19
1155.9507	13.1
1200.7579	13.1
1232.8004	1.36
1255.3745	15.2
1310.7473	2.63
1413.1368	3.68
1480.8871	0.334
1485.1095	0.222
3066.3585	0.395
3142.3750	1.05
3146.8753	0.489
3167.4424	0.597



$\Delta E = 0.81$ kcal mol^{-1}
Population = 0.169

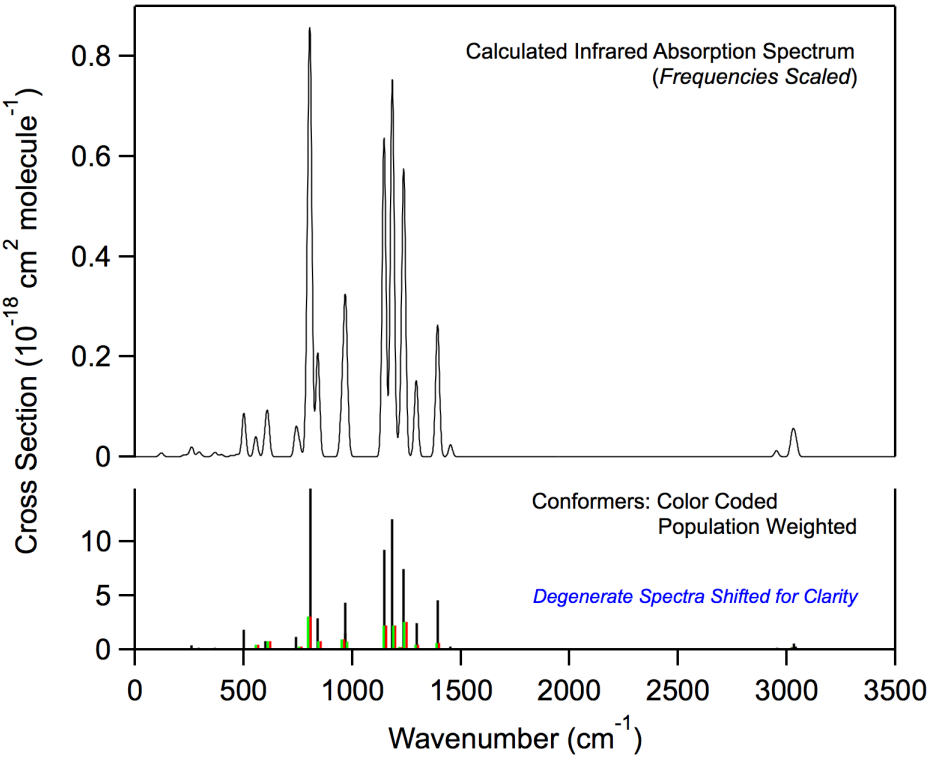
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-2.002433260243	0.934212337226	-0.394457513659
C	-1.014455403239	-0.136567382945	0.027279374334
C	0.420365268324	0.054488477990	-0.516173826149
H	-2.036007231506	1.014982245187	-1.483397677425
H	-2.989266080492	0.639688962102	-0.030703927095
H	-1.731576144667	1.899309534666	0.032798671874
F	-1.440972713404	-1.341182527180	-0.444294335688
F	-0.973757348897	-0.224131417278	1.375598341829
H	0.399790267864	0.065911733902	-1.603692278479
Cl	1.106901901752	1.619881717959	0.015418158214
Cl	1.466696744508	-1.303905681627	-0.024362987754

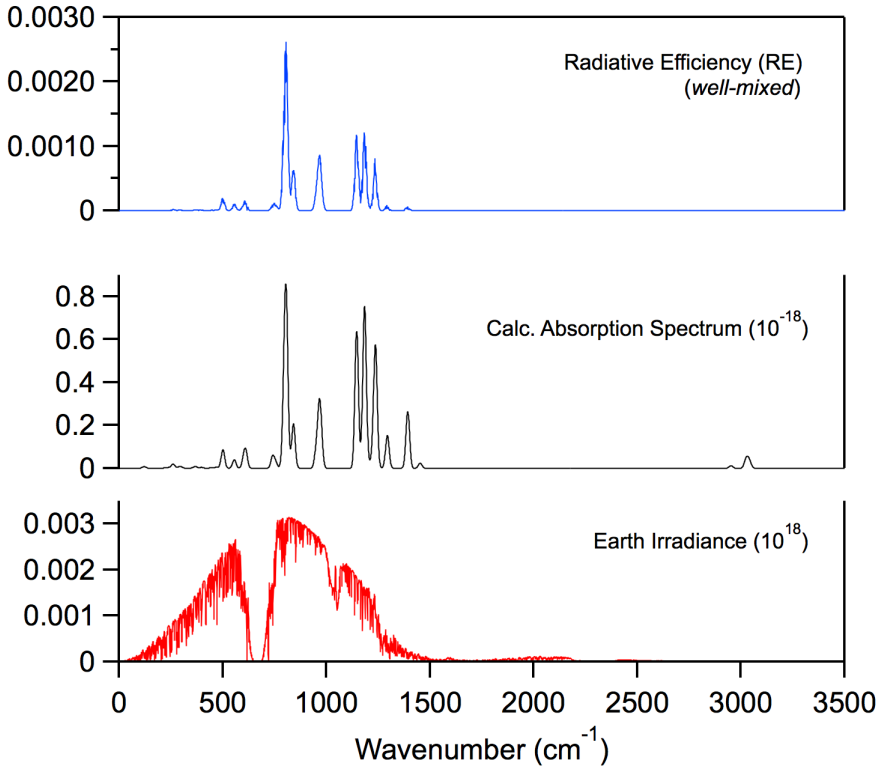
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
63.4682	0.129
185.5999	0.163
205.3416	0.105
213.2412	0.0257
265.4550	0.140
321.9623	0.108
355.9172	0.0974
414.7761	0.176
531.8696	2.54
590.5379	4.65
743.2656	1.62
786.3407	18.1
835.9636	4.63
951.1821	5.64
977.7335	4.19
1155.9474	13.1
1200.7529	13.1
1232.7994	1.36
1255.3744	15.2
1310.7460	2.63
1413.1324	3.68
1480.8849	0.334
1485.1103	0.222
3066.3635	0.395
3142.3803	1.04
3146.8761	0.489
3167.4404	0.597

Infrared Spectrum

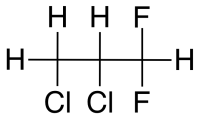


Radiative Efficiency



HCFC-252da

Molecular Formula:	$CH_2ClCHClCHF_2$
Name:	2,3-Dichloro-1,1-difluoropropane
CAS number:	82578-00-5
Molecular Weight:	148.97



Global Atmospheric Lifetime (years):	0.999
Tropospheric Atmospheric Lifetime (years):	1.04
Stratospheric Atmospheric Lifetime (years):	26.7
Ozone Depletion Potential (ODP):	0.016

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.121	0.090
Global Warming Potential (GWP_H):		
GWP_{20}	183	135
GWP_{100}	49	37
Global Temperature Potentials (GTP_H)		
GTP_{20}		44
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*

$k_{SAR}(298\ K) = 5.65 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 3.61 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

τ^{OH}_{Global} = 1.01 years
τ^{OH}_{Trop} = 1.04 years
τ^{OH}_{Strat} = 34.9 years

Fractional Atmospheric Loss: 0.991

O(^{1}D) Reactivity

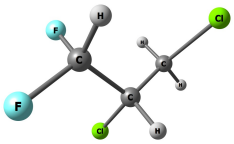
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 1.6 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)}$ = 230 years
Fractional Atmospheric Loss: 0.004

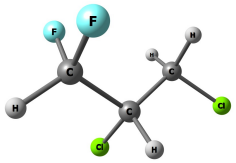
UV Photolysis

UV Spectrum: *No Recommendation*
τ_{hv} = 225 years
Fractional Atmospheric Loss: 0.005

Molecular Structure and Infrared Spectrum (6 conformers)



E = 0
Population = 0.500



$\Delta E = 0.60$ kcal mol^{-1}
Population = 0.182

Optimized Coordinates (Angstroms)

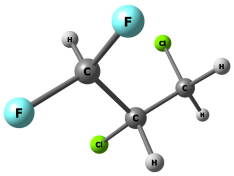
Atom	X	Y	Z
C	1.053907021241	0.866236313935	0.301381946281
C	-0.166343259593	0.344279145310	-0.445530205357
C	-0.511685711491	-1.101787629110	-0.091647570587
Cl	2.550481969356	-0.003048356769	-0.233369775547
H	1.210576470126	1.921864949876	0.091043635080
H	0.950642613329	0.706926420465	1.373708451796
H	-0.024709799825	0.415460732694	-1.524713066299
Cl	-1.559846095313	1.417525688189	-0.033259218860
H	0.311578519188	-1.773988901916	-0.361571872893
F	-0.741992834145	-1.213946259796	1.237572922166
F	-1.623110892871	-1.487808102880	-0.752383245780

Atom	X	Y	Z
C	0.667439280481	-0.822646734628	0.365032774881
C	-0.187827165771	0.115532408048	-0.473484578668
C	-1.677551474399	-0.168279433606	-0.261802869700
Cl	2.400781415095	-0.762836031893	-0.105456185050
H	0.602564228830	-0.574882670483	1.422845029908
H	0.327231499106	-1.846638202868	0.204671421504
H	0.034224505613	-0.004936966916	-1.534582077472
Cl	0.122779281217	1.846793596123	-0.079890138891
H	-2.316760905356	0.552264497414	-0.782749009727
F	-1.941143710389	-1.415497825293	-0.734277882067
F	-1.978964954427	-0.154300635898	1.055664515282

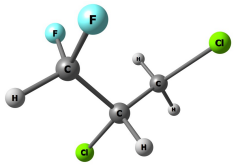
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
68.4336	0.410
109.3506	0.520
171.9459	0.528
200.2272	0.240
235.4131	0.380
301.9531	0.0808
463.1293	2.23
539.3499	0.519
643.2604	7.93
718.3179	9.17
738.7360	0.867
905.6373	1.78
986.7320	3.00
1071.2915	1.21
1131.6542	13.8
1171.9863	14.1
1184.1125	7.79
1235.6076	3.10
1307.2644	0.689
1343.3491	0.730
1396.4166	6.29
1414.5673	3.03
1477.6740	1.15
3063.0195	3.29
3112.8779	0.0716
3119.8503	0.979
3184.7607	0.0122

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
78.9870	0.0269
84.2730	0.567
160.5740	0.491
196.4008	0.754
254.4541	0.0303
333.2930	0.473
412.6290	1.43
538.0933	2.10
647.8553	6.22
709.3707	3.38
814.3792	1.43
921.3682	1.24
946.0934	4.94
1085.1287	9.24
1105.5003	14.9
1161.8466	11.4
1184.5993	4.80
1264.6265	1.05
1280.5560	3.00
1348.3587	7.89
1383.0956	3.59
1415.0415	3.01
1468.9103	0.961
3078.1909	4.36
3099.0890	0.798
3116.8020	0.509
3170.4396	0.0431



$\Delta E = 0.86$ kcal mol^{-1}
Population = 0.117



$\Delta E = 0.96$ kcal mol^{-1}
Population = 0.099

Optimized Coordinates (Angstroms)

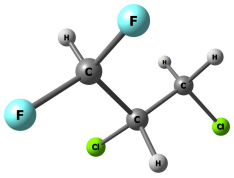
Atom	X	Y	Z
C	1.084523368792	-0.298950186083	-0.969252592251
C	-0.293212248171	0.242013157247	-0.623189091945
C	-1.087029945909	-0.657154320623	0.327004306123
Cl	2.144860952182	-0.549664526879	0.467917287255
H	0.972205463017	-1.271748700843	-1.448876976439
H	1.607554343789	0.386901550663	-1.633761812083
H	-0.866924732390	0.319645847924	-1.551467720516
Cl	-0.217244333059	1.904682364021	0.062857244148
H	-0.654278481201	-0.705605205767	1.330426775978
F	-2.360185042945	-0.219962605761	0.409029800974
F	-1.108681344106	-1.906904373899	-0.209634221244

Atom	X	Y	Z
C	0.520872103733	1.079070730965	0.376853168662
C	-0.419309346552	0.287377129787	-0.525640152182
C	-0.475094771707	-1.217937732462	-0.235784405358
Cl	2.251574591603	0.778367172559	-0.037488971388
H	0.349271088254	2.145767019385	0.249746671616
H	0.378111411151	0.800266729026	1.419474897720
H	-0.177645674364	0.435524968401	-1.578268010123
Cl	-2.092723861594	0.944751298970	-0.282357380636
H	-1.330162909584	-1.690660983971	-0.731716426236
F	0.662264124213	-1.806100279535	-0.670517495512
F	-0.574597755153	-1.429779053127	1.096853103437

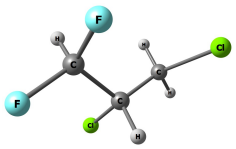
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
67.0773	0.259
92.5876	0.193
151.0462	0.0369
209.3803	0.721
293.8818	0.300
381.8554	0.689
406.8621	2.34
537.5104	2.11
596.5819	1.92
684.2005	3.08
761.5400	3.28
920.1910	4.96
1002.6160	3.63
1098.1372	3.84
1114.3367	17.5
1146.3216	22.1
1208.6996	0.646
1247.7998	1.94
1278.4039	2.43
1325.2453	3.82
1392.0184	1.66
1421.3163	4.63
1461.9928	1.93
3079.4121	0.497
3097.4934	1.44
3102.2916	2.44
3166.3783	0.0729

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
46.9525	0.0920
113.2710	0.480
169.6177	0.362
224.2038	0.276
268.9778	0.658
295.3233	2.43
374.7779	0.446
532.8096	1.10
649.5655	1.88
731.0540	11.5
809.2605	2.85
881.3610	2.94
953.4432	3.11
1082.5592	6.28
1130.7815	17.1
1168.2219	12.0
1186.9647	2.80
1222.3249	1.23
1300.7873	2.55
1359.0777	0.940
1400.5471	4.27
1416.6255	2.22
1477.2436	1.48
3069.2506	4.74
3114.4537	0.477
3125.8077	0.491
3182.4286	0.0229



$\Delta E = 1.31$ kcal mol^{-1}
Population = 0.055



$\Delta E = 1.69$ kcal mol^{-1}
Population = 0.029

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	0.901979905525	-0.833692066852	0.409155641918
C	-0.183147690929	0.035853450285	-0.207928936485
C	-1.577300017802	-0.401651868954	0.255111465240
Cl	2.515836191781	-0.526313819173	-0.318666311140
H	0.991918287461	-0.656506365781	1.481501867567
H	0.664537663832	-1.881808972128	0.227063125138
H	-0.153940713847	-0.023613054618	-1.297347425036
Cl	0.029502834366	1.771296411904	0.224984772000
H	-1.735330062335	-0.246172500271	1.329081790611
F	-2.519961573122	0.272244074954	-0.430771975049
F	-1.725648824929	-1.725039289366	-0.023449014764

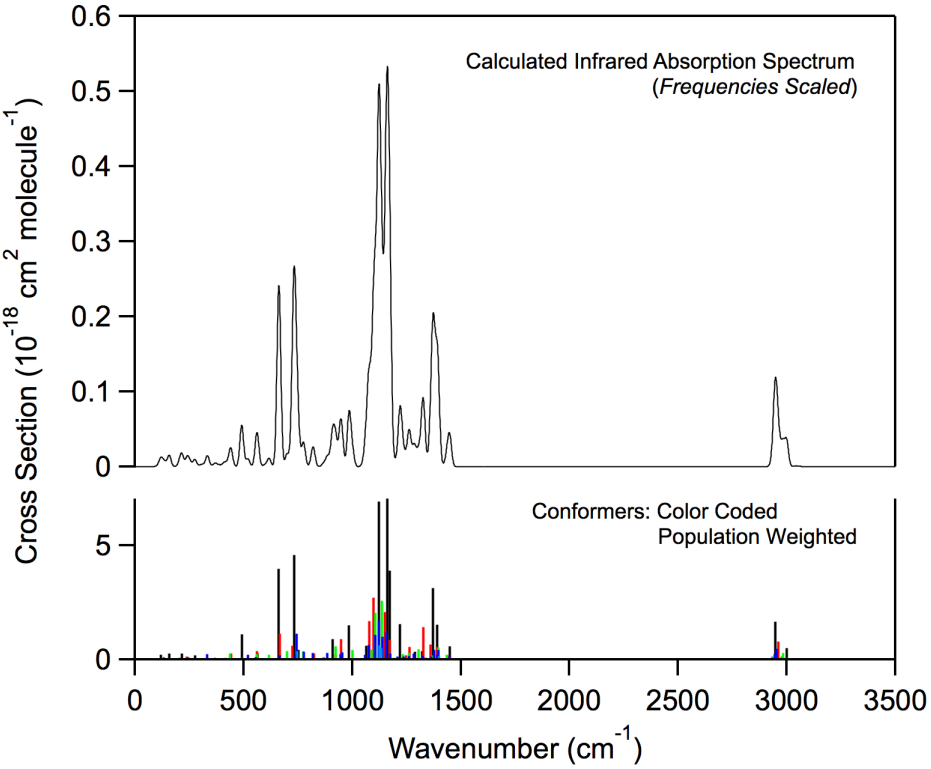
Atom	X	Y	Z
C	0.865310715686	1.064531149800	0.204572149644
C	-0.334363442899	0.293232850141	-0.339068576669
C	-0.613818655724	-1.038514715453	0.364240888372
Cl	2.432291574788	0.381749929821	-0.370408080572
H	0.829054121919	2.093818719328	-0.146274740823
H	0.883602932307	1.058142856922	1.295526047615
H	-0.238379238637	0.117490042308	-1.411208773122
Cl	-1.798899546474	1.335038829643	-0.106603353213
H	-0.843379205638	-0.897004091375	1.428279130879
F	-1.656904293698	-1.652985492902	-0.232238272943
F	0.463322038369	-1.847953078233	0.250629580832

Infrared Absorption Spectrum (unscaled frequencies)

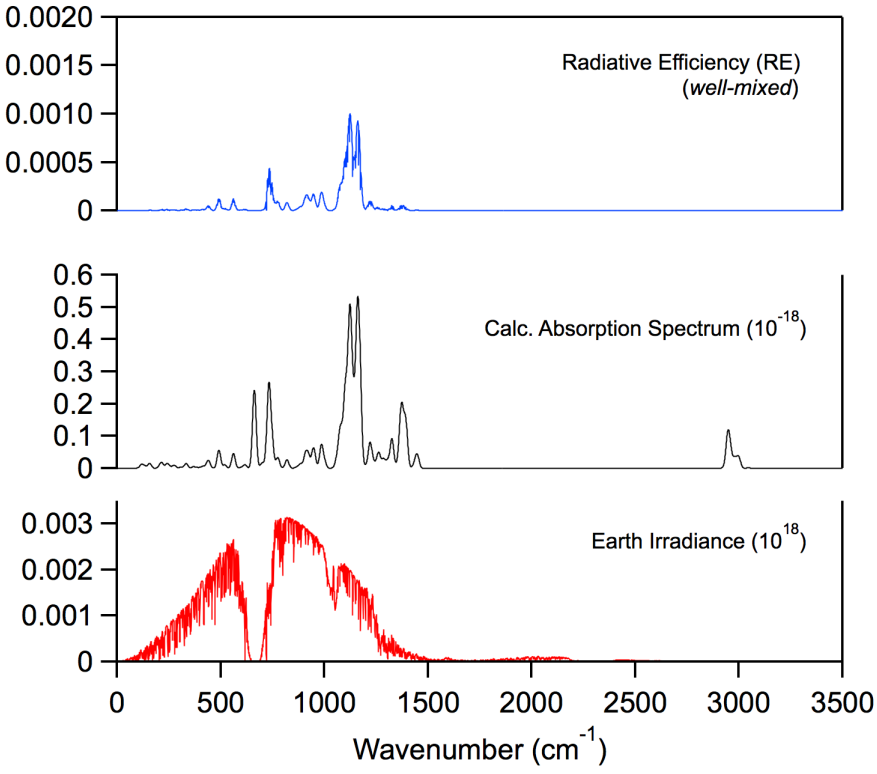
Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
70.2102	0.122
84.5257	0.429
165.0056	0.709
187.1245	0.213
294.2231	0.119
354.7427	0.889
404.1799	0.610
493.1736	4.09
575.2005	0.945
724.2935	4.01
766.9695	6.20
943.2112	4.52
1063.9691	3.80
1068.3904	1.01
1114.4497	19.9
1148.2664	18.5
1177.6761	0.757
1252.7680	2.49
1279.6776	2.99
1344.5429	2.71
1387.9082	2.38
1422.1072	7.51
1470.1297	0.666
3059.8298	4.37
3092.6460	1.27
3114.3451	0.608
3159.2211	0.143

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
46.9311	0.133
106.7675	0.543
170.8654	0.297
206.9605	0.679
267.6558	0.106
334.9957	0.746
390.6505	1.13
466.2602	2.45
590.5505	0.632
733.7745	13.2
804.5698	1.96
862.3179	3.36
1050.2674	1.02
1095.3820	0.968
1136.0680	21.8
1142.5626	17.8
1192.3625	1.57
1225.2671	1.60
1298.0914	1.96
1337.1540	0.546
1395.8140	2.30
1425.1081	5.73
1481.1800	1.48
3048.1549	4.67
3096.1779	0.932
3123.9982	0.573
3166.8133	0.116

Infrared Spectrum

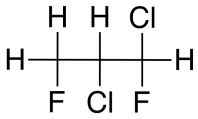


Radiative Efficiency



HCFC-252db

Molecular Formula:	$CH_2FCHClCHClF$
Name:	1,2-Dichloro-1,3-difluoropropane
CAS number:	–
Molecular Weight:	148.97



Global Atmospheric Lifetime (years):	1.15
Tropospheric Atmospheric Lifetime (years):	1.20
Stratospheric Atmospheric Lifetime (years):	29.4
Ozone Depletion Potential (ODP):	0.017

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.132	0.101
Global Warming Potential (GWP_H):		
GWP_{20}	230	176
GWP_{100}	62	48
Global Temperature Potentials (GTP_H)		
GTP_{20}		58
GTP_{50}		8
GTP_{100}		7

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 4.90 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 3.13 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 1.16$ years

$\tau^{OH}_{Trop} = 1.20$ years

$\tau^{OH}_{Strat} = 39.7$ years

Fractional Atmospheric Loss: 0.990

O(^{1}D) Reactivity

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

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

$\tau_{O(^1D)} = 230$ years

Fractional Atmospheric Loss: 0.005

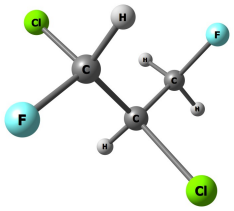
UV Photolysis

UV Spectrum: *No Recommendation*

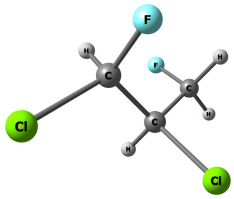
$\tau_{hv} = 225$ years

Fractional Atmospheric Loss: 0.005

Molecular Structure and Infrared Spectrum (13 conformers)



E = 0
Population = 0.287



$\Delta E = 0.34$ kcal mol^{-1}
Population = 0.161

Optimized Coordinates (Angstroms)

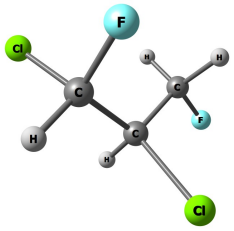
Atom	X	Y	Z
C	0.689440645678	-1.481668564618	0.508844671791
C	0.432754084374	0.016113606139	0.572274302739
C	-0.674818662437	0.483204030841	-0.371311161392
F	0.907147506154	-1.862686454606	-0.794640931785
H	1.569548448844	-1.732219410696	1.108880126570
H	-0.182997787851	-2.020435685398	0.893738056318
Cl	1.942285251837	0.912013876833	0.119549864309
H	0.188566802635	0.313213579564	1.593886298770
H	-0.486265533265	0.183357141720	-1.402004199375
Cl	-2.244529578469	-0.289189123515	0.109369966260
F	-0.828657177500	1.819179003737	-0.297241994206

Atom	X	Y	Z
C	1.950220065404	-0.160224308727	0.011012649538
C	0.532827175080	0.218185921855	0.444223276367
C	-0.481177679671	-0.762908473743	-0.135575841965
F	2.211034368121	-1.439567119284	0.461014374677
H	2.031620933835	-0.138940387218	-1.079829063589
H	2.675863223962	0.530941649385	0.448626706974
Cl	0.220832570949	1.902945517703	-0.097210655714
H	0.452831555759	0.205117208709	1.531816879856
H	-0.213388079532	-1.776800899672	0.170239139391
Cl	-2.142681363177	-0.471187751715	0.483713480796
F	-0.485706770730	-0.693297357292	-1.486765946330

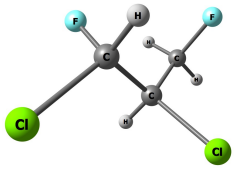
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
63.6803	0.267
97.4989	0.244
173.7067	0.0666
221.4475	1.25
274.7159	0.321
350.5980	0.0935
382.2146	1.04
435.1036	1.37
622.0727	4.26
698.0277	17.8
772.4212	6.32
919.7698	1.37
995.9352	3.03
1112.1070	9.61
1128.6400	1.33
1147.8012	17.8
1212.8606	3.87
1266.8319	0.304
1277.1955	2.40
1317.0988	1.06
1394.5664	2.41
1426.5232	1.19
1500.5215	1.43
3051.5162	2.78
3104.8310	2.52
3110.4850	0.295
3136.2461	0.651

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
68.1474	0.196
121.9958	0.774
173.6346	0.0763
191.5439	0.439
222.8683	0.0903
349.8249	0.977
385.5265	0.227
447.8959	4.01
621.2024	4.11
706.7298	4.91
821.4101	9.96
937.2116	5.68
1018.3976	5.28
1070.2929	9.80
1092.6541	6.52
1153.5161	13.6
1227.5784	1.08
1257.7717	1.18
1280.3159	2.85
1351.9406	1.02
1380.9099	2.55
1413.5370	1.89
1509.1127	0.467
3060.8103	2.45
3101.8967	0.607
3112.4887	1.28
3127.8106	1.61



$\Delta E = 0.38$ kcal mol^{-1}
Population = 0.151



$\Delta E = 0.60$ kcal mol^{-1}
Population = 0.104

Optimized Coordinates (Angstroms)

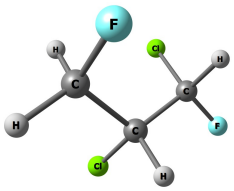
Atom	X	Y	Z
C	0.700082518993	1.225578368430	0.509530263420
C	0.393983007380	0.062883370981	-0.426825304376
C	-0.905632027597	-0.659062016666	-0.089072781809
F	1.820857745378	1.879109452033	0.066869512930
H	-0.145505870918	1.923037312795	0.506082191978
H	0.868041475954	0.861436617171	1.526948292906
Cl	1.734994972916	-1.155180905871	-0.355892998510
H	0.358236341573	0.409288648561	-1.459672193517
H	-1.026663304896	-1.576199289814	-0.665842287674
F	-0.961507221580	-0.943307363050	1.231139634183
Cl	-2.322664637202	0.389619805432	-0.517997329530

Atom	X	Y	Z
C	1.720508999997	0.792452340100	-0.518904510398
C	0.456727183389	-0.057395085287	-0.570478674352
C	-0.659574369937	0.568920800219	0.270914046647
F	2.112140178894	0.974019486291	0.785996130050
H	2.525708978189	0.299422244343	-1.072253159430
H	1.510183056010	1.770694998338	-0.965175198394
Cl	0.800588179052	-1.720212654466	0.031418298108
H	0.124438772959	-0.152494668241	-1.606169643481
H	-0.441629885114	0.518487173718	1.337632794261
F	-0.789227439511	1.869658178001	-0.104710996776
Cl	-2.235864653927	-0.253040813017	0.014067913766

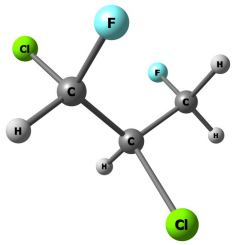
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
73.2819	0.307
95.3913	0.504
179.1331	0.231
189.0742	1.03
264.0432	0.233
289.5635	0.118
387.5620	0.274
442.4269	1.88
666.6071	3.73
680.1007	12.9
759.8023	14.2
929.6163	2.27
1001.3833	2.65
1098.6878	8.24
1115.8538	9.82
1158.0286	11.9
1236.7008	2.63
1273.5962	2.88
1286.5790	1.04
1311.0090	1.16
1387.6252	2.10
1433.0994	1.09
1506.6095	0.645
3047.2545	2.61
3105.8725	1.39
3123.2820	1.05
3131.5703	0.675

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
64.4833	0.200
97.8030	0.388
157.5699	0.0650
213.5314	0.495
312.3507	1.28
331.2831	0.705
374.3245	0.962
446.4838	0.574
593.3050	7.97
732.0732	5.93
816.1407	6.44
918.9806	3.81
1008.8798	3.50
1085.7772	15.3
1113.8669	12.8
1132.0308	4.90
1214.4983	1.74
1259.1416	0.754
1281.2776	2.24
1329.3000	4.04
1377.1333	0.857
1423.1022	2.06
1499.6737	1.03
3047.8418	3.24
3103.0053	2.31
3105.8799	0.515
3133.2321	0.777



$\Delta E = 0.81$ kcal mol^{-1}
Population = 0.073



$\Delta E = 0.97$ kcal mol^{-1}
Population = 0.056

Optimized Coordinates (Angstroms)

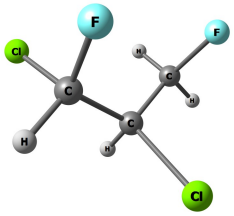
Atom	X	Y	Z
C	1.664773597630	0.542465774494	0.335590672662
C	0.655855938779	-0.312589231402	-0.423336494693
C	-0.669575791496	0.400258339823	-0.675801233396
F	1.848495025300	1.714976768794	-0.371176170914
H	1.295460576111	0.779695328610	1.337319774827
H	2.619491308617	0.013821511630	0.411145940701
Cl	0.437193542229	-1.870407054312	0.443513666224
H	1.054288319995	-0.565072492107	-1.409847897586
H	-0.475751637932	1.342737858502	-1.192675941065
F	-1.474045192842	-0.375751687524	-1.433501456942
Cl	-1.537345686393	0.841392883491	0.839724140182

Atom	X	Y	Z
C	0.503037287412	1.492873716143	0.349360798125
C	0.554182460433	0.222849941786	-0.502603325194
C	-0.378253266756	-0.898744861013	-0.043991046846
F	-0.690402818843	2.141670000056	0.149222230659
H	0.604826511897	1.234755769225	1.407603461436
H	1.323843112577	2.153825090958	0.055633543694
Cl	2.250519060749	-0.414757644668	-0.408337920250
H	0.361821008659	0.449151761850	-1.551056323787
H	-0.143138116523	-1.841260103286	-0.539675324094
F	-0.288113334470	-1.064493065898	1.295422081742
Cl	-2.090772905135	-0.524885605154	-0.476539175486

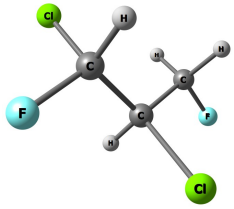
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
65.5977	0.197
120.0184	0.512
173.2825	0.120
196.9466	0.622
222.8873	0.544
363.9203	0.245
390.0807	0.488
508.1082	1.90
560.4264	5.31
664.9629	5.65
808.3874	11.3
932.5407	2.45
1065.6035	14.2
1093.8268	2.20
1103.8206	1.47
1141.4510	17.3
1230.7822	1.38
1250.1315	1.44
1297.3708	4.31
1336.2745	2.71
1380.8454	2.44
1418.7007	1.05
1509.9714	0.821
3061.3972	2.25
3084.0419	0.598
3104.5127	0.960
3121.4660	2.36

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
47.6454	0.0658
120.7080	0.600
171.2434	0.400
223.4423	0.286
256.2891	0.104
300.1482	3.07
378.5740	0.658
392.6457	0.294
631.9469	0.997
738.0490	23.6
820.6582	1.48
882.4025	3.34
1008.3690	3.69
1095.8630	17.0
1108.4584	3.80
1154.0086	9.80
1216.9627	1.69
1265.5631	1.18
1283.2803	2.16
1355.2927	0.783
1382.3204	1.24
1433.9305	0.852
1509.4772	0.528
3058.6385	2.70
3111.7837	2.07
3116.3589	0.993
3134.5035	0.559



$\Delta E = 1.07$ kcal mol^{-1}
Population = 0.047



$\Delta E = 1.31$ kcal mol^{-1}
Population = 0.031

Optimized Coordinates (Angstroms)

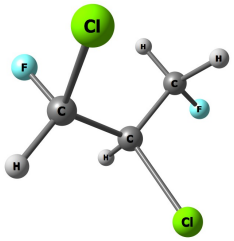
Atom	X	Y	Z
C	0.579352919005	1.385159537240	-0.613104476317
C	0.423468856665	-0.130181586568	-0.661432221439
C	-0.685399989017	-0.706207549884	0.218981117211
F	0.938214790921	1.808798232366	0.637425527537
H	1.350709993032	1.688217980466	-1.329295082467
H	-0.374209674853	1.849965498279	-0.891330738235
Cl	1.974298103321	-0.930642384673	-0.173824569380
H	0.231937121077	-0.434298053207	-1.691723548913
H	-0.693877811039	-1.796752844893	0.189102111795
F	-0.579610006175	-0.288547211073	1.491843928858
Cl	-2.300487302937	-0.188087618054	-0.436913048649

Atom	X	Y	Z
C	0.863042762685	-1.359995706105	-0.299141298737
C	0.405318979394	-0.020251585374	0.266947835914
C	-0.914545387970	0.483379291294	-0.308945803605
F	2.053121759516	-1.711362458716	0.282000106936
H	0.117132560099	-2.128557796272	-0.073009065081
H	0.999287789420	-1.292487327788	-1.385153761677
Cl	1.658897741472	1.237202317082	-0.087558109032
H	0.325393913917	-0.074001886769	1.354068145140
H	-0.880085997304	0.601923844942	-1.393925796517
Cl	-2.238632022347	-0.710317496649	0.028765753220
F	-1.255307098883	1.654326804354	0.262785993440

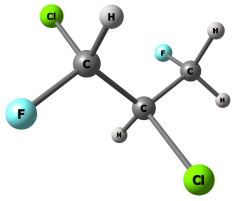
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
55.9164	0.248
121.8249	0.234
187.2378	0.703
199.4041	0.181
255.9339	0.492
307.0876	0.336
375.4092	0.503
450.7186	2.54
672.6080	13.9
750.6043	12.3
788.8383	2.33
876.2649	0.864
987.0787	1.32
1041.6947	2.33
1136.4902	20.8
1172.5997	6.97
1231.0490	3.59
1263.7946	3.03
1296.6164	0.0955
1339.5228	1.52
1400.1458	1.27
1431.7616	2.24
1500.6190	1.26
3038.5638	3.10
3089.1558	2.97
3110.3592	1.03
3117.7765	0.626

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
66.0546	0.134
102.5214	0.835
166.5795	0.412
208.7879	0.489
276.9886	0.384
344.6775	0.540
362.5620	0.405
437.6439	0.272
532.6299	3.64
688.4883	14.7
755.2514	12.2
999.4599	1.40
1061.4751	5.69
1094.3236	2.27
1116.9691	13.3
1149.5649	11.0
1212.6097	4.81
1251.9643	0.121
1300.0548	1.71
1310.5135	1.89
1401.1880	1.81
1432.0551	1.88
1505.2060	0.425
3038.1067	3.35
3095.2351	1.87
3102.2346	0.516
3120.9171	1.62



$\Delta E = 1.44$ kcal mol^{-1}
Population = 0.025



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

Optimized Coordinates (Angstroms)

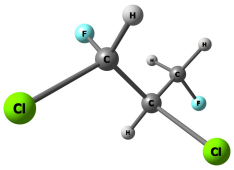
Atom	X	Y	Z
C	0.977092074681	-1.085847640325	-0.562032361405
C	0.499507812839	-0.143851221325	0.534102852805
C	-1.018707443472	-0.103335973344	0.698597062266
F	2.329253330959	-1.277687033022	-0.432516212463
H	0.463060403193	-2.047431861770	-0.442773498300
H	0.762016016456	-0.677001877492	-1.552657258597
Cl	1.139925406074	1.521915396515	0.297140096130
H	0.904692689736	-0.486476364102	1.489971337380
H	-1.325363421001	0.649690951512	1.425435711230
Cl	-1.885275772574	0.295905315520	-0.830507989940
F	-1.424926096890	-1.331119692168	1.116793260894

Atom	X	Y	Z
C	0.471218067944	-1.659148973168	-0.140684454309
C	0.553776872611	-0.213803366994	0.358416725949
C	-0.359006288480	0.783818902605	-0.350805877085
F	-0.655030688684	-2.270437267741	0.348397228579
H	0.455068092201	-1.688754215115	-1.237039736966
H	1.351045604641	-2.203774804040	0.214113578521
Cl	2.256664487394	0.346871707433	0.083995552874
H	0.373247188268	-0.171592186236	1.433657728181
H	-0.176685175344	0.805725332889	-1.427811203374
Cl	-2.092463561878	0.335859105089	-0.133233103384
F	-0.176469598672	2.019396765278	0.162286561013

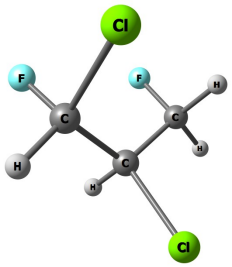
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
74.4851	0.152
97.7911	0.516
153.4306	0.184
200.5454	1.02
256.1814	0.289
333.2130	0.217
417.8711	1.06
434.3587	0.910
604.1303	6.96
710.6573	5.53
732.5058	7.37
992.1906	5.60
1015.9190	4.99
1092.8693	16.4
1110.8398	12.8
1132.4647	3.64
1240.2293	0.465
1257.9556	3.14
1298.3817	3.41
1333.2367	4.37
1361.5831	0.607
1429.8302	1.12
1504.9211	0.604
3042.6216	2.65
3087.5829	0.240
3113.9695	1.97
3119.0134	1.16

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
50.0774	0.0917
122.0684	1.00
166.6384	0.0890
227.3315	0.623
270.0634	0.372
328.3240	1.15
366.8985	0.137
396.6162	0.675
520.9163	2.97
739.0238	24.0
811.5795	0.429
899.5938	3.87
1081.6671	5.73
1094.1997	5.89
1135.0129	15.4
1137.1018	4.79
1204.4144	2.91
1241.3285	1.21
1289.0766	2.10
1336.7434	0.0439
1401.3603	2.53
1428.4390	1.33
1508.9212	0.474
3039.0872	3.00
3095.2526	1.57
3098.1596	2.46
3123.3836	0.767



$\Delta E = 1.80$ kcal mol^{-1}
Population = 0.014



$\Delta E = 1.92$ kcal mol^{-1}
Population = 0.011

Optimized Coordinates (Angstroms)

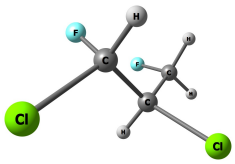
Atom	X	Y	Z
C	1.615217956147	0.967573565547	0.196953496265
C	0.455457983081	0.069516452977	-0.230039404705
C	-0.861924603990	0.533918013569	0.393167411542
F	2.764207104522	0.552753087861	-0.421886979168
H	1.396629007786	1.997212467602	-0.104752501355
H	1.756274386290	0.927977010926	1.283637805201
Cl	0.781060455828	-1.630614782572	0.265629717286
H	0.372275541577	0.067309460515	-1.317960005358
H	-0.905172521740	0.326726261847	1.464354207117
F	-0.988311769550	1.874261062699	0.190697317634
Cl	-2.277812539952	-0.287108600969	-0.344543064459

Atom	X	Y	Z
C	0.549292599198	-1.378678049861	-0.712950215940
C	0.617773816424	-0.405321465360	0.461399271619
C	-0.653177084920	0.407412243187	0.732476139993
F	-0.443883482459	-2.297285564730	-0.470728269204
H	0.332882691822	-0.844530074920	-1.642636223740
H	1.508578766721	-1.897887762792	-0.806931544962
Cl	2.008199318939	0.709155046602	0.205210088342
H	0.824117885270	-0.957081743167	1.382204233899
H	-0.467740157715	1.187374470816	1.473110824399
Cl	-1.272168524717	1.260859224041	-0.729906422554
F	-1.612307828563	-0.430623323816	1.188371118150

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
61.6572	0.0432
105.5643	0.831
156.4948	0.323
205.2495	0.566
289.2665	0.596
340.7378	0.0745
387.7665	1.25
429.0225	0.238
514.6356	3.54
728.4354	5.20
777.5563	17.2
1001.2707	3.62
1062.5718	7.35
1080.6898	2.28
1110.0691	9.85
1122.8011	14.6
1218.4598	1.87
1251.7434	0.377
1311.3626	3.24
1324.2132	4.84
1373.1986	1.05
1428.6733	2.25
1506.8872	0.353
3037.2333	3.42
3092.7280	1.81
3102.8026	0.646
3121.1780	1.73

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
48.8626	0.0587
127.2023	0.521
176.3162	0.00623
204.7174	0.541
269.7728	1.57
344.8185	1.47
383.5574	0.685
431.1289	0.270
528.7978	3.29
733.9484	8.58
843.2822	9.57
901.0105	4.24
1055.1657	3.21
1090.0599	2.59
1116.1588	27.0
1137.0052	4.51
1217.8981	0.715
1250.2032	1.42
1300.2840	3.43
1356.9780	0.831
1374.9177	2.15
1430.8612	1.49
1508.9027	0.803
3054.9247	2.73
3088.0978	0.706
3107.3763	1.19
3115.1415	2.56



$\Delta E = 1.97$ kcal mol^{-1}
Population = 0.010

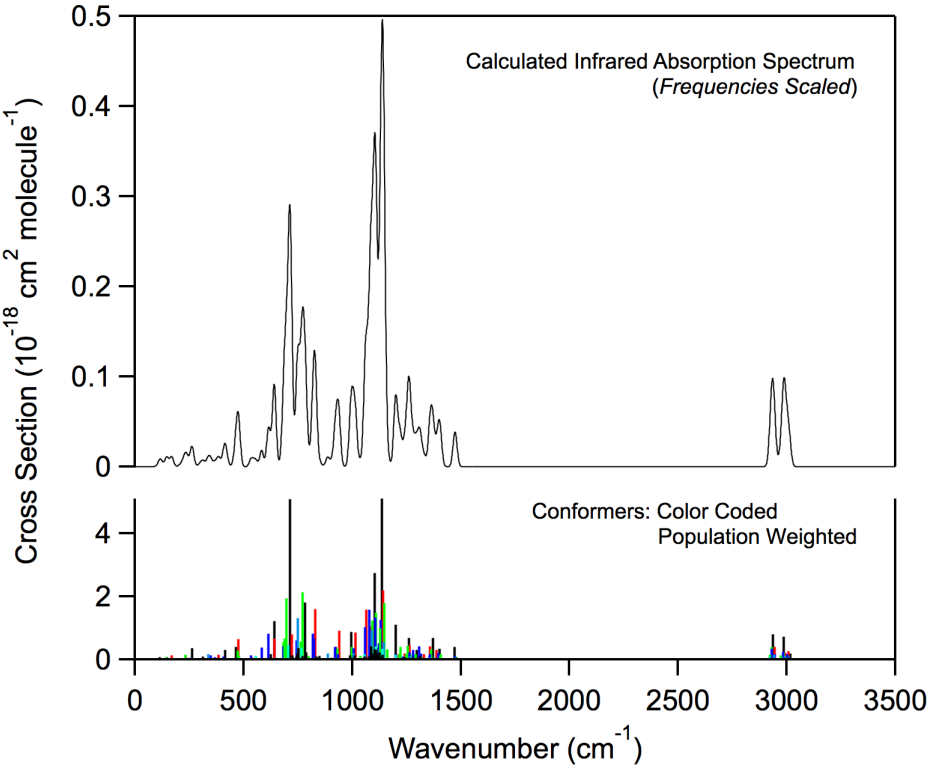
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.942393730907	-0.019260749349	0.077971694886
C	0.488694403761	-0.304691524015	-0.317227709642
C	-0.512145283950	0.577023144810	0.433781459978
F	2.335194473401	1.183227121808	-0.452275609459
H	2.050832169717	0.009391300586	1.168985458223
H	2.581520257740	-0.813259984469	-0.320592385523
Cl	0.143763438906	-2.031874330307	0.061743082714
H	0.366999673767	-0.173301652368	-1.393299780643
H	-0.589830324365	0.293116167117	1.485920114322
F	-0.121809981731	1.869538779917	0.342174050174
Cl	-2.169247558152	0.429461726270	-0.255970375028

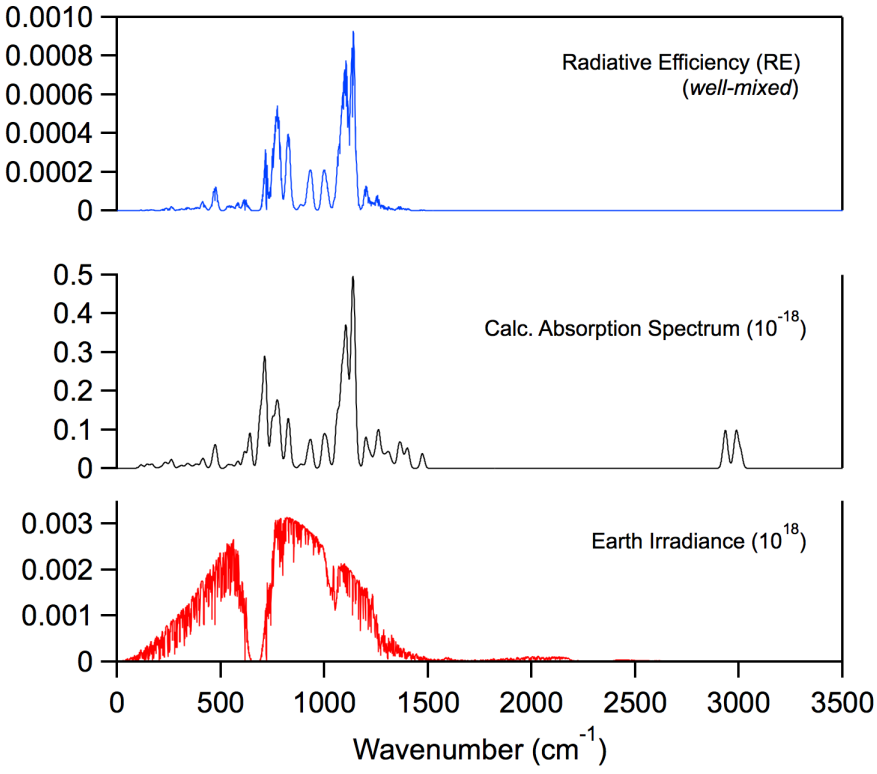
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
52.1950	0.0371
130.3058	0.885
165.1011	0.146
203.4682	0.353
290.9890	0.400
358.8938	0.625
369.9859	1.12
428.9724	2.78
446.8589	2.01
760.6646	11.2
827.6474	8.62
922.8365	3.49
1077.1997	3.17
1093.5957	1.08
1100.0267	18.1
1148.4772	15.5
1207.1594	1.84
1240.3354	1.10
1292.7632	3.61
1340.3353	1.51
1388.1507	1.18
1424.4502	2.41
1509.3258	0.449
3038.2077	3.14
3093.8260	3.04
3096.7473	1.02
3122.9168	0.898

Infrared Spectrum

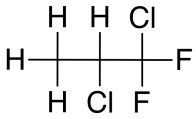


Radiative Efficiency



HCFC-252dc

Molecular Formula:	$CH_3CHClCClF_2$
Name:	1,2-Dichloro-1,1-difluoropropane
CAS number:	7126-15-0
Molecular Weight:	148.97



Global Atmospheric Lifetime (years):	0.771
Tropospheric Atmospheric Lifetime (years):	0.799
Stratospheric Atmospheric Lifetime (years):	22.2
Ozone Depletion Potential (ODP):	0.013

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.214	0.149
Global Warming Potential (GWP_H):		
GWP_{20}	250	173
GWP_{100}	68	47
Global Temperature Potentials (GTP_H)		
GTP_{20}		55
GTP_{50}		8
GTP_{100}		7

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 7.34 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 4.69 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 0.780$ years

$\tau^{OH}_{Trop} = 0.799$ years

$\tau^{OH}_{Strat} = 27.6$ years

Fractional Atmospheric Loss: 0.993

$O(^1D)$ Reactivity

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

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

$\tau_{O(^1D)} = 230$ years

Fractional Atmospheric Loss: 0.003

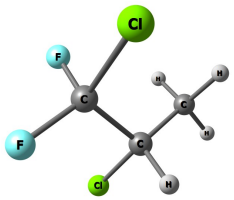
UV Photolysis

UV Spectrum: *No Recommendation*

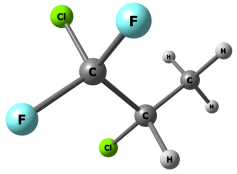
$\tau_{hv} = 225$ years

Fractional Atmospheric Loss: 0.004

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.660



$\Delta E = 0.79$ kcal mol^{-1}
Population = 0.174

Optimized Coordinates (Angstroms)

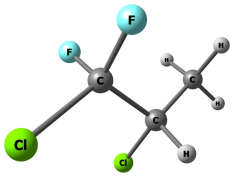
Atom	X	Y	Z
C	-0.624407171039	1.900613824822	0.176928523940
C	-0.598204954234	0.519145411898	-0.459397097216
C	0.499256875632	-0.395691479661	0.098965863039
H	0.310575580121	2.427752456893	-0.028313371203
H	-1.451570720303	2.477893790424	-0.238984481740
H	-0.758184477319	1.821128905679	1.257522024550
H	-0.465060139123	0.567369593002	-1.540098707878
Cl	-2.189431856389	-0.313330303427	-0.196565683244
Cl	2.132607314159	0.271565358011	-0.339029913302
F	0.433720950109	-0.488500530269	1.427432017697
F	0.423929598387	-1.622821027372	-0.411814174644

Atom	X	Y	Z
C	-0.926490043725	1.755906940954	0.586094739983
C	-0.760558061401	0.580759958063	-0.363240392730
C	0.677310014821	0.046475375583	-0.442851502442
H	-1.941329976869	2.149993759391	0.508725339930
H	-0.743840971332	1.452802752963	1.618539941396
H	-0.219604782439	2.545780352419	0.316754487302
H	-1.002855023918	0.869234953208	-1.389481306425
Cl	-1.897195225072	-0.757087632917	0.042797519954
Cl	1.326125672615	-0.534364418133	1.131702620709
F	0.767711473681	-0.947658892619	-1.326270391791
F	1.466825923639	1.046427851086	-0.872393055886

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
70.1581	0.170
182.2429	0.205
228.1987	0.0349
248.8649	0.103
261.4913	0.182
325.0020	0.0694
361.4886	0.270
412.4744	0.459
483.5635	1.32
588.4330	0.765
686.6393	13.4
741.4497	6.00
919.0509	32.7
991.8080	4.03
1065.6008	5.67
1105.6591	2.22
1195.2276	18.2
1250.1547	17.1
1266.8479	3.88
1354.7142	2.81
1412.6289	1.28
1489.0842	1.17
1493.0629	0.921
3063.1900	0.859
3122.7236	0.274
3141.9979	1.28
3153.0652	0.795

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
76.9916	0.135
174.8323	0.0795
212.2662	0.199
240.7669	0.00551
294.7315	0.124
321.5399	0.0318
408.4637	0.374
418.8239	0.329
487.9764	0.663
559.4779	5.56
641.4677	2.63
752.4842	7.47
929.4731	19.8
1020.7181	7.54
1107.2942	2.93
1110.8858	22.9
1176.4719	14.8
1205.1491	17.3
1268.8688	2.58
1349.4738	4.85
1411.6879	1.22
1487.0981	1.07
1493.3994	0.989
3059.1954	0.995
3087.6779	0.740
3136.5646	1.00
3151.9009	0.944



$\Delta E = 0.82$ kcal mol^{-1}
Population = 0.166

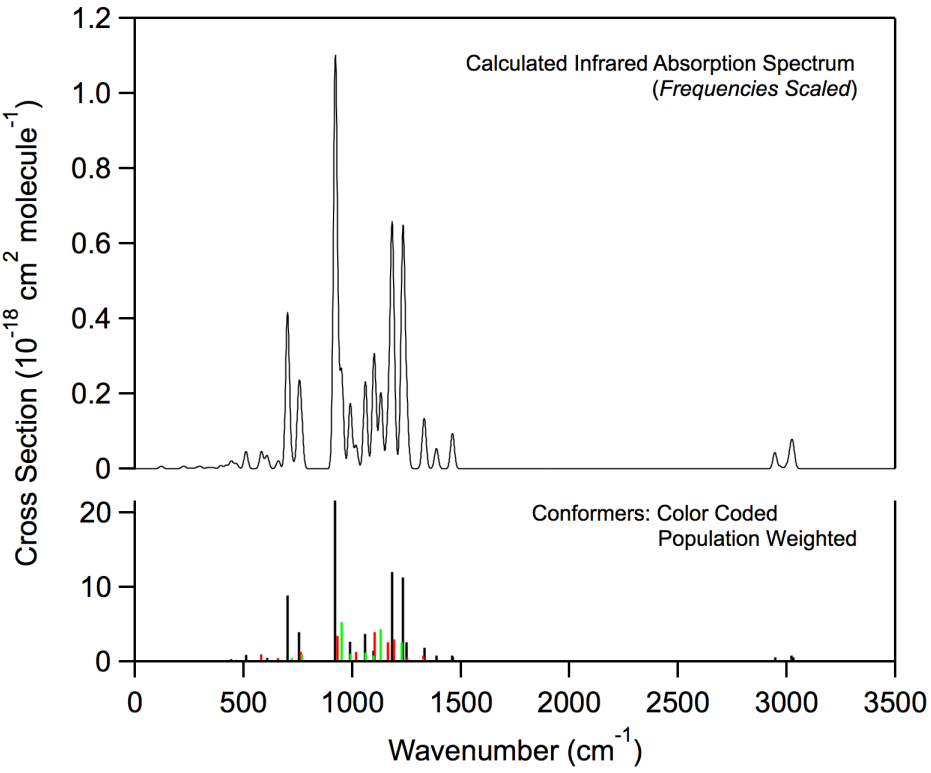
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.647050177757	1.496857796041	-0.236568028003
C	-0.792843932036	0.264145339049	-0.515072083134
C	0.607794530896	0.412371710912	0.099722386481
H	-2.631678469891	1.371671438153	-0.689516443063
H	-1.769791853256	1.644167822799	0.838409138611
H	-1.169169029667	2.381629675912	-0.664831300009
H	-0.664946936366	0.098317675145	-1.584862860539
Cl	-1.595466655460	-1.214024978675	0.133165018776
Cl	1.708895065147	-0.944318562168	-0.326896473536
F	1.157997806500	1.544385429551	-0.373184628923
F	0.549310651889	0.513315653281	1.428497273338

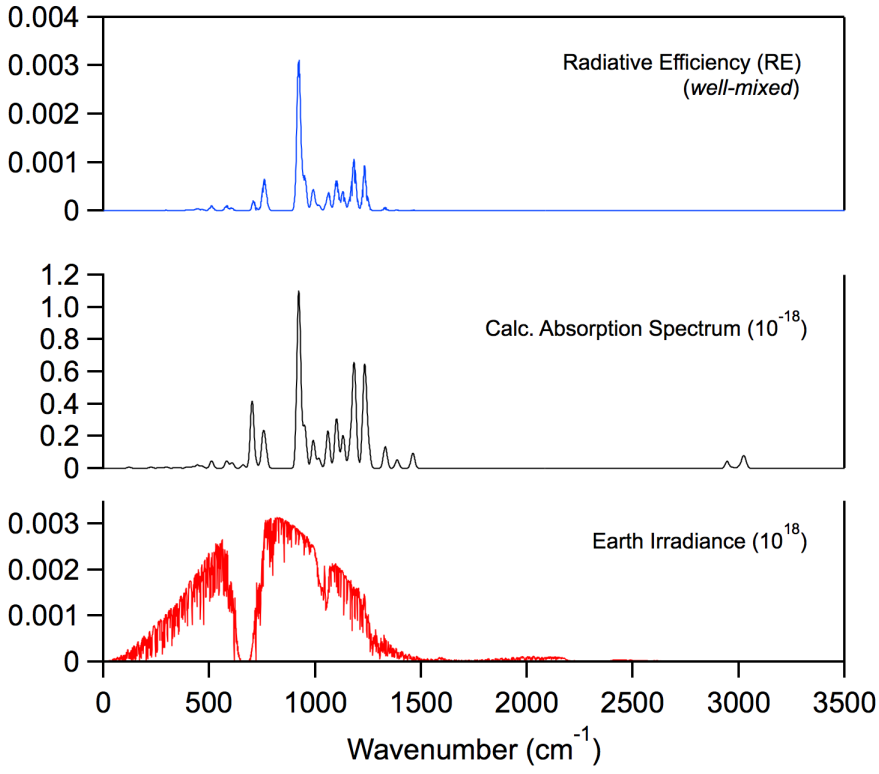
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
71.3953	0.125
168.4871	0.114
222.9576	0.0313
243.8179	0.00144
302.9726	0.384
322.8451	0.0761
387.6380	1.15
417.5527	0.210
436.7481	1.69
583.0394	1.64
707.9491	2.83
756.3160	6.02
950.2496	32.2
993.9649	6.35
1066.7541	7.31
1106.9147	4.77
1141.5861	26.1
1243.8196	15.7
1269.5809	1.53
1347.3843	1.90
1407.6804	0.610
1487.8906	1.07
1494.3785	0.931
3060.8157	1.20
3119.2750	0.265
3140.7146	1.22
3151.7079	0.873

Infrared Spectrum

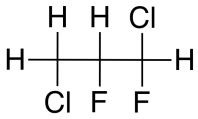


Radiative Efficiency



HCFC-252ea

Molecular Formula:	$CH_2ClCHFCHClF$
Name:	1,3-Dichloro-1,2-difluoropropane
CAS number:	111483-26-2
Molecular Weight:	148.97



Global Atmospheric Lifetime (years):	1.02
Tropospheric Atmospheric Lifetime (years):	1.06
Stratospheric Atmospheric Lifetime (years):	27.2
Ozone Depletion Potential (ODP):	0.016

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.150	0.112
Global Warming Potential (GWP_H):		
GWP_{20}	233	174
GWP_{100}	63	47
Global Temperature Potentials (GTP_H)		
GTP_{20}		57
GTP_{50}		8
GTP_{100}		7

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 5.51 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 3.52 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 1.03$ years

$\tau^{OH}_{Trop} = 1.06$ years

$\tau^{OH}_{Strat} = 35.7$ years

Fractional Atmospheric Loss: 0.991

O(^{1}D) Reactivity

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

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

$\tau_{O(^1D)} = 230$ years

Fractional Atmospheric Loss: 0.004

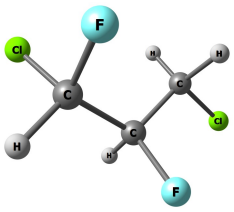
UV Photolysis

UV Spectrum: *No Recommendation*

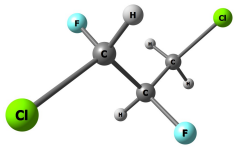
$\tau_{hv} = 225$ years

Fractional Atmospheric Loss: 0.005

Molecular Structure and Infrared Spectrum (12 conformers)



E = 0
Population = 0.203



$\Delta E = 0.01$ kcal mol^{-1}
Population = 0.201

Optimized Coordinates (Angstroms)

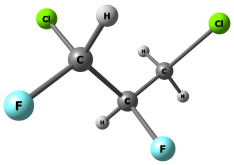
Atom	X	Y	Z
C	-0.934663352010	-0.388715073309	0.534147045447
C	-0.161685356380	0.369200736704	-0.532099343346
C	1.322583002298	0.517977980808	-0.187345124751
Cl	-2.652056366912	-0.600142943393	0.043063976214
H	-0.511408258572	-1.380933431673	0.685531188418
H	-0.926895863072	0.166583670063	1.470913428809
F	-0.656710645107	1.651075866390	-0.635195265221
H	-0.253132441535	-0.120642115107	-1.506636325169
H	1.807700968916	1.217903608081	-0.870498386016
F	1.468385019399	0.960421932854	1.082929307843
Cl	2.177226292975	-1.060475231419	-0.369613502228

Atom	X	Y	Z
C	1.482887394245	0.032627712793	-0.919881215286
C	0.070410292475	-0.484422914077	-0.687864362025
C	-0.772660500732	0.453037638125	0.178271623060
Cl	2.412867687430	0.216586832331	0.614860955630
H	2.034390249855	-0.674434977581	-1.539243304034
H	1.450338865567	1.008176833037	-1.403649135056
F	0.108693422672	-1.715679037034	-0.091485654193
H	-0.417026236496	-0.577114141656	-1.668391508028
H	-0.394777608957	0.525285816631	1.198468532620
F	-0.773763844508	1.680854109942	-0.400861134725
Cl	-2.460842721551	-0.149644872514	0.293817202037

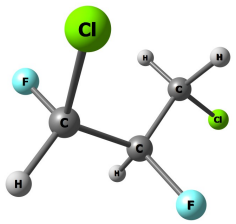
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
71.5224	0.216
81.5814	0.585
163.9077	0.798
195.7842	0.282
261.3191	0.000
324.9971	0.503
400.8502	0.755
461.3912	2.26
619.5378	5.67
788.2853	18.5
806.5059	0.896
862.2404	4.32
927.9139	3.44
1056.2729	1.83
1106.4663	16.1
1151.0065	10.6
1219.8945	1.44
1254.0802	1.92
1273.4284	2.33
1354.2390	2.23
1376.3124	0.586
1408.5920	1.92
1467.2390	1.29
3077.4468	1.40
3107.4515	0.975
3109.3145	1.53
3174.8129	0.0880

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
54.8745	0.255
90.8581	0.259
168.1104	0.161
191.7961	0.334
299.8635	1.04
374.5721	0.911
385.1951	1.74
490.9918	0.690
575.0408	7.63
690.5203	2.19
808.5734	10.9
896.5860	6.40
951.5796	1.07
1089.8886	8.74
1112.2980	9.62
1149.4057	11.4
1220.7768	1.53
1250.3084	2.89
1305.4824	4.47
1334.6716	1.91
1362.6262	2.08
1406.5446	0.220
1458.6198	1.37
3030.5645	1.64
3102.6201	1.41
3128.9124	1.02
3168.3778	0.0993



$\Delta E = 0.25$ kcal mol^{-1}
Population = 0.134



$\Delta E = 0.37$ kcal mol^{-1}
Population = 0.109

Optimized Coordinates (Angstroms)

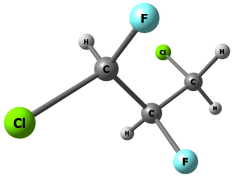
Atom	X	Y	Z
C	-1.211655222030	0.235947178286	0.933156280659
C	-0.071277072645	-0.720955161958	0.633405204132
C	0.938718270999	-0.249499288789	-0.413977848665
Cl	-2.175808970681	0.639901259305	-0.537883998220
H	-1.897774033738	-0.236240536561	1.636129226450
H	-0.837968756125	1.170564092524	1.348002992688
F	-0.579764783258	-1.913203407829	0.173085504879
H	0.474470641223	-0.912718038797	1.567555602251
H	0.471883507342	-0.022695548426	-1.372864346456
Cl	1.750314639825	1.263183312028	0.146015240465
F	1.870774779090	-1.212297859784	-0.576934858184

Atom	X	Y	Z
C	-0.968856451596	0.323063823952	-0.570006160011
C	-0.185504876643	0.065174239260	0.704696437823
C	1.305425029625	0.393328302282	0.569984918114
Cl	-2.740028899365	0.229317335917	-0.261967377596
H	-0.750277558946	1.321901740566	-0.946873802368
H	-0.731008407081	-0.422183393756	-1.327211986882
F	-0.298318982943	-1.244625946659	1.089653763557
H	-0.570804655520	0.701238824508	1.512557408242
H	1.841670517551	0.148485148130	1.488835786562
Cl	2.100114008058	-0.561630195727	-0.733627672304
F	1.436533276860	1.715924121527	0.301687684864

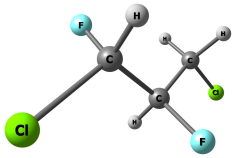
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
54.3337	0.268
101.1995	0.202
170.1928	0.118
208.7432	0.915
311.8308	0.364
375.9368	0.331
396.1038	1.12
430.8521	2.12
610.8529	4.19
696.8184	2.06
794.8052	18.5
880.1464	0.576
961.8428	2.31
1078.8544	2.34
1125.3513	14.3
1137.9467	18.0
1225.9403	1.00
1244.2924	3.20
1301.3118	3.13
1334.9614	1.72
1363.7951	1.62
1414.1304	1.47
1460.6307	2.34
3033.7867	1.45
3105.5304	1.26
3129.7140	0.935
3172.0385	0.156

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
73.4875	0.428
77.3488	0.214
152.7400	0.596
206.6821	0.536
227.8091	0.180
354.7241	0.334
426.4424	1.63
514.9088	0.459
573.4004	9.45
692.7902	7.15
808.3381	5.18
862.5478	1.25
984.1128	2.19
1086.0872	10.8
1114.2918	7.11
1148.2693	13.6
1223.1880	1.37
1258.5055	0.293
1300.5842	8.73
1336.0080	1.32
1372.3164	2.08
1405.2762	1.26
1465.1544	1.13
3039.4168	1.94
3106.6010	1.30
3107.6978	1.59
3175.7225	0.0594



$\Delta E = 0.37$ kcal mol^{-1}
Population = 0.109



$\Delta E = 0.59$ kcal mol^{-1}
Population = 0.075

Optimized Coordinates (Angstroms)

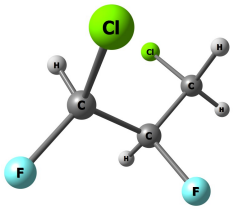
Atom	X	Y	Z
C	-1.523481238944	-0.772584850958	-0.151077479167
C	-0.111969393105	-0.661248935431	0.423577725963
C	0.685895134111	0.473498496975	-0.213543020482
Cl	-2.535035222465	0.635959064749	0.338363601917
H	-1.495136154286	-0.801297135610	-1.239471489660
H	-2.001805851419	-1.671291957157	0.235893964408
F	0.515494500480	-1.853861255401	0.151463055320
H	-0.146300506122	-0.509331747881	1.507360715864
H	0.245852343945	1.446536591169	0.009887526190
Cl	2.362551393373	0.503752728128	0.435052119205
F	0.733035994433	0.294632001417	-1.556880719559

Atom	X	Y	Z
C	1.347411303872	0.622635742123	0.357123711335
C	0.154614565132	-0.195402052250	-0.117833959529
C	-1.154634441228	0.444869516828	0.356530927576
Cl	2.883944812620	-0.041506474239	-0.299183870553
H	1.259150909402	1.653387850978	0.016945624664
H	1.423950666047	0.594444458770	1.445503472148
F	0.217393229266	-1.458247437661	0.410026759510
H	0.145770072515	-0.262608704979	-1.211130874838
H	-1.239173479122	0.440806727467	1.446135591879
F	-1.213330283530	1.721853377500	-0.099981291847
Cl	-2.566517354974	-0.472583004537	-0.263505090345

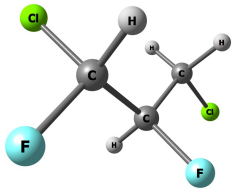
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
57.0942	0.263
95.9544	0.588
181.9097	0.523
201.3914	0.140
247.4100	0.128
373.0514	0.643
380.0628	0.809
430.1532	3.61
684.3252	4.38
755.8915	1.44
789.9328	14.3
863.1877	10.4
967.2746	4.02
1069.3231	1.81
1084.9237	11.8
1144.1209	7.97
1181.3535	6.96
1268.2749	3.17
1284.2684	0.331
1365.4019	0.473
1382.3873	0.303
1391.6981	1.45
1479.6990	1.02
3073.1861	1.39
3106.8528	1.10
3117.2442	1.32
3175.4593	0.0984

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
64.4684	0.0465
79.7921	0.541
133.8119	0.587
219.6957	0.367
263.1306	0.221
375.3886	0.0946
387.9123	1.95
463.6878	2.66
531.2145	2.67
719.8396	16.4
827.2652	6.02
867.6401	0.303
1034.9288	0.827
1082.1817	7.60
1121.3851	14.3
1132.7067	7.45
1200.7793	3.71
1250.2063	1.40
1304.8258	2.67
1334.0325	1.98
1374.9350	2.43
1400.3188	0.384
1466.3069	0.824
3068.6271	0.606
3090.4824	0.807
3097.9072	3.27
3164.4454	0.241



$\Delta E = 0.66$ kcal mol^{-1}
Population = 0.066



$\Delta E = 0.90$ kcal mol^{-1}
Population = 0.044

Optimized Coordinates (Angstroms)

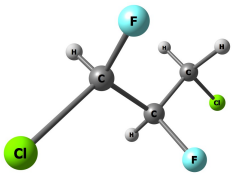
Atom	X	Y	Z
C	1.306051114455	-0.456943712112	0.691541222185
C	0.084734789188	-0.956395223985	-0.070830411667
C	-0.809433503401	0.139710646371	-0.645659761693
Cl	2.467023630857	0.360379359053	-0.418848881538
H	1.027595433614	0.256853062111	1.465944298157
H	1.822118996649	-1.306646974354	1.137135567721
F	-0.651750052015	-1.731975463370	0.791141156496
H	0.398003635883	-1.579576261372	-0.918652713264
H	-0.243990456786	0.831567100958	-1.271750943300
F	-1.790904633246	-0.439272678553	-1.375148304838
Cl	-1.562664955198	1.128254145253	0.660136771741

Atom	X	Y	Z
C	-1.073246583610	0.578601547476	-0.447518844604
C	-0.155868306910	-0.458034640300	0.180023712107
C	1.290014462880	-0.371803022674	-0.318767348226
Cl	-2.749936481081	0.398679607486	0.179591335922
H	-0.743236820337	1.588226377083	-0.211306481518
H	-1.121255167779	0.446042724861	-1.529819527225
F	-0.589210267236	-1.717829421701	-0.165577969850
H	-0.156501504727	-0.373810916532	1.272358555675
H	1.358346585224	-0.473607933876	-1.404709654167
Cl	2.020125530187	1.224576035852	0.101728756372
F	2.010442553389	-1.349561357675	0.267228465512

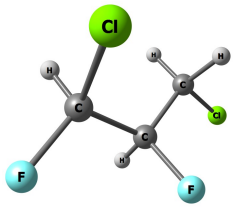
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
51.9336	0.248
105.0886	0.556
188.2927	0.641
200.9964	0.166
243.1635	0.368
368.5324	0.207
380.6737	0.867
503.1856	1.34
589.9373	7.70
750.1861	3.43
786.2113	10.9
844.3146	6.22
996.3341	0.807
1086.1984	3.58
1114.0538	14.2
1143.3408	14.4
1176.7372	2.67
1276.3806	2.62
1293.2616	1.90
1340.3975	0.692
1379.9779	2.29
1404.6177	1.52
1482.2651	1.87
3042.5995	1.85
3104.8353	0.978
3117.2256	1.19
3171.6685	0.119

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
72.5598	0.516
77.7616	0.206
146.2338	0.549
203.8315	0.349
304.6162	0.254
356.4997	0.870
404.4665	0.331
413.2273	1.64
535.6027	3.24
762.0301	9.98
786.4037	13.5
871.1015	3.61
1037.2983	2.51
1074.4985	1.66
1121.6332	7.62
1139.6673	21.9
1198.0416	4.19
1246.5019	0.983
1282.2994	1.34
1342.9149	1.08
1382.0101	0.672
1408.7228	2.44
1467.1643	0.857
3068.2029	0.532
3092.2728	0.912
3099.4121	3.23
3171.0503	0.239



$\Delta E = 1.33$ kcal mol^{-1}
Population = 0.022



$\Delta E = 1.52$ kcal mol^{-1}
Population = 0.016

Optimized Coordinates (Angstroms)

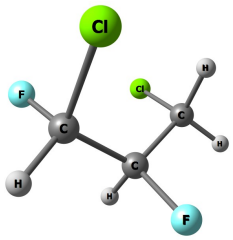
Atom	X	Y	Z
C	-1.353553297129	0.679185380822	0.270567674431
C	-0.160110611145	-0.265114157996	0.193800802543
C	1.140477026801	0.518474143082	0.383949479770
Cl	-2.900987833855	-0.234335288600	0.220802585336
H	-1.343232940163	1.247836915831	1.201776413781
H	-1.344562323169	1.361887821965	-0.578220299181
F	-0.144676373087	-0.876549134940	-1.030056334987
H	-0.222857019097	-1.031098343667	0.974928825945
H	1.206580616597	0.937834378071	1.391459316952
Cl	2.566165610237	-0.556023123089	0.189772831422
F	1.212445144011	1.523187408520	-0.524115296012

Atom	X	Y	Z
C	1.125410328920	0.562882960898	-0.478907180228
C	0.176792755324	-0.580482231366	-0.160748686932
C	-1.255266813638	-0.309823734124	-0.626308698349
Cl	2.833118643940	0.080147396876	-0.178378284886
H	1.051767155412	0.851735627448	-1.528633597736
H	0.914055435289	1.422749176816	0.155290411518
F	0.168463826046	-0.827680385417	1.184326989446
H	0.499543624477	-1.494720808756	-0.677460760838
H	-1.293867220189	-0.091390561575	-1.696797553119
F	-2.013836909903	-1.396050824947	-0.362039517076
Cl	-1.972548825678	1.117672384148	0.208083878201

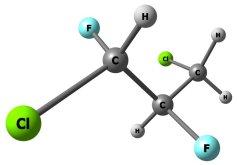
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
67.0467	0.0452
83.7715	0.624
131.5101	0.487
231.4203	0.0919
253.6329	0.0986
290.2141	0.0874
391.5235	0.321
475.5066	3.08
693.4956	18.7
762.1483	4.18
828.3940	3.49
864.7174	1.28
907.6798	6.27
1050.8774	0.387
1099.9054	11.2
1151.8559	11.7
1220.2439	1.51
1259.4669	3.16
1293.7775	2.76
1357.0892	2.42
1373.1882	0.758
1402.7957	1.64
1465.2614	0.809
3062.7962	1.31
3085.4563	2.01
3093.5865	2.20
3163.0519	0.276

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
73.3536	0.147
77.3908	0.584
143.5573	0.417
213.3329	0.0953
240.6613	0.154
325.2826	0.0311
408.5292	0.652
492.0496	1.43
632.9815	13.4
755.1587	8.87
775.3950	3.13
867.1906	1.51
967.3817	3.90
1062.6349	2.24
1121.0338	13.7
1147.5054	11.7
1226.4143	2.73
1259.8819	1.56
1285.5137	6.95
1346.4404	0.354
1384.7555	3.59
1405.0639	1.08
1463.9764	0.796
3034.2838	1.72
3085.2274	1.96
3094.4236	2.22
3164.5124	0.197



$\Delta E = 1.82$ kcal mol^{-1}
Population = 0.009



$\Delta E = 1.99$ kcal mol^{-1}
Population = 0.007

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.079331382095	-0.830092731114	-0.535645840889
C	-0.048540062028	-0.914018292491	0.585132534657
C	0.945863081298	0.245618630069	0.707576691375
Cl	-2.385242336442	0.347626844300	-0.159469597325
H	-0.622368123438	-0.532200506233	-1.478202964964
H	-1.544755713259	-1.809421829377	-0.645237073760
F	0.698698861729	-2.053188694786	0.374801139880
H	-0.557103929864	-1.000440442099	1.553854307693
H	1.717152781924	-0.005858704553	1.439212165900
Cl	1.828909266074	0.540330973144	-0.837425359098
F	0.309631556102	1.374104753140	1.083576996532

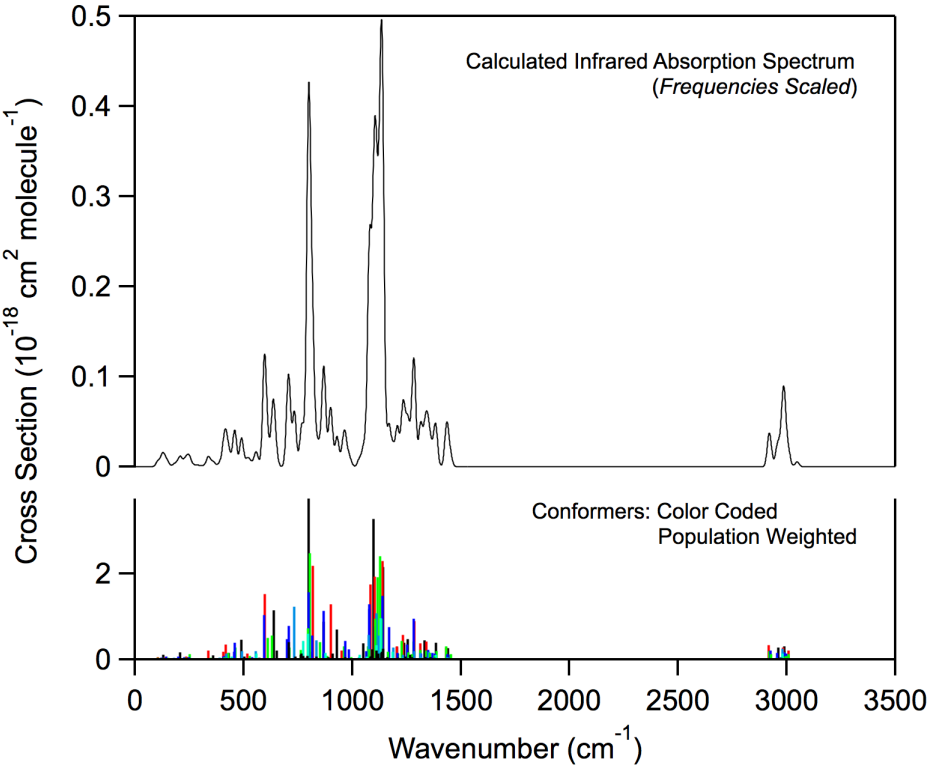
Atom	X	Y	Z
C	1.466943736745	-0.871538599175	0.198123261541
C	0.024965232907	-0.740158574604	-0.300134612458
C	-0.788308894584	0.310986147156	0.457020151581
Cl	2.551626972798	0.383276378874	-0.490813721366
H	1.528683759959	-0.803760348617	1.285546242429
H	1.845991683673	-1.841669854273	-0.122917768507
F	-0.584944265849	-1.954474671085	-0.067982772888
H	0.007084708148	-0.525611730366	-1.373241380539
H	-0.900987772252	0.034734817476	1.509148658172
F	-0.197458143851	1.520909630988	0.362918717641
Cl	-2.455429017694	0.410271803624	-0.215028775606

Infrared Absorption Spectrum (unscaled frequencies)

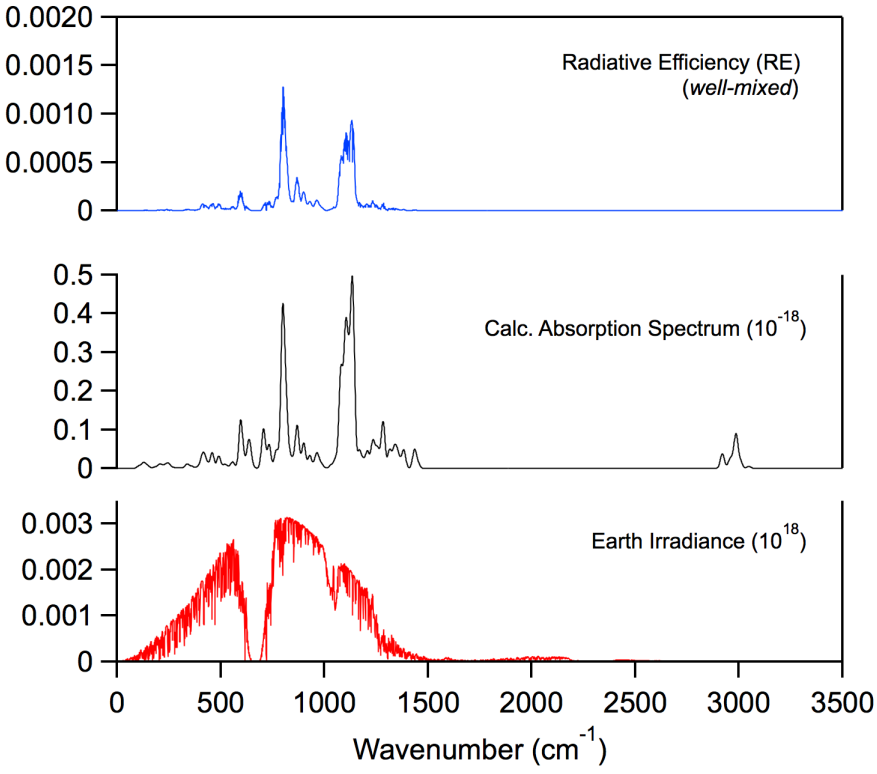
Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
33.4992	0.106
113.2439	0.242
182.3288	0.375
205.8826	0.367
281.0657	2.57
335.0128	0.986
382.5743	0.359
513.4289	0.0684
548.2463	5.08
725.7048	7.58
783.0260	8.27
877.9163	3.64
995.4949	0.928
1097.3248	9.11
1128.8301	14.8
1141.6143	4.60
1172.4567	5.58
1280.8331	2.73
1301.5215	3.29
1331.1043	1.16
1391.5687	2.32
1396.5588	1.46
1480.2774	1.90
3044.5957	1.80
3097.9337	2.25
3103.2597	1.21
3169.4080	0.103

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
39.7933	0.0897
97.0488	0.375
169.8258	0.320
198.4007	0.534
311.6973	0.142
358.3047	1.89
387.7975	1.05
419.3798	3.85
513.8321	0.0186
751.5203	15.6
791.0025	2.91
885.5662	8.24
1040.2595	0.791
1091.3762	9.62
1106.6910	0.418
1143.0766	22.2
1182.6490	0.353
1267.6191	4.93
1288.1617	2.36
1333.5062	1.97
1366.7765	0.353
1407.8386	0.155
1481.3410	0.930
3075.5128	0.0449
3086.2794	0.323
3093.2006	4.47
3153.1665	0.380

Infrared Spectrum

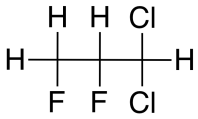


Radiative Efficiency



HCFC-252eb

Molecular Formula:	$CH_2FCHFCHCl_2$
Name:	1,1-Dichloro-2,3-difluoropropane
CAS number:	–
Molecular Weight:	148.97



Global Atmospheric Lifetime (years):	0.645
Tropospheric Atmospheric Lifetime (years):	0.670
Stratospheric Atmospheric Lifetime (years):	20
Ozone Depletion Potential (ODP):	0.011

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.140	0.092
Global Warming Potential (GWP_H):		
GWP_{20}	136	90
GWP_{100}	37	24
Global Temperature Potentials (GTP_H)		
GTP_{20}		28
GTP_{50}		4
GTP_{100}		3

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

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

OH Reactivity

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

k_{SAR}(298 K) = 8.75×10^{-14}; k_{SAR}(272 K) ≈ 5.58×10^{-14} cm^3 $molecule^{-1}$ s^{-1}

τ^{OH}_{Global} = 0.652 years
τ^{OH}_{Trop} = 0.670 years
τ^{OH}_{Strat} = 23.5 years

Fractional Atmospheric Loss: 0.989

O(^{1}D) Reactivity

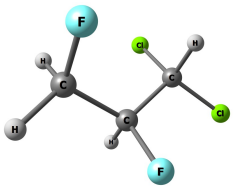
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 1.6 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)}$ = 230 years
Fractional Atmospheric Loss: 0.003

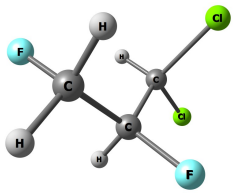
UV Photolysis

UV Spectrum: *No Recommendation*
τ_{hv} = 80 years
Fractional Atmospheric Loss: 0.008

Molecular Structure and Infrared Spectrum (6 conformers)



E = 0
Population = 0.533



$\Delta E = 0.53$ kcal mol^{-1}
Population = 0.216

Optimized Coordinates (Angstroms)

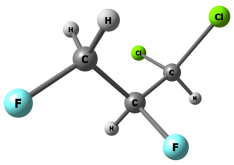
Atom	X	Y	Z
C	-1.959713803345	-0.271186701954	0.444833249711
C	-0.641412496276	0.470574518858	0.612177054408
C	0.457608540484	-0.056019052990	-0.318139635183
F	-2.296851865228	-0.320518009460	-0.889720754737
H	-1.885857307165	-1.289609505300	0.837002817704
H	-2.737594680563	0.277218299324	0.987772784013
H	-0.305369494983	0.400974551564	1.653617499351
F	-0.849752958805	1.793873673338	0.295584716330
H	0.122671023341	-0.052092575675	-1.351781418136
Cl	1.913414296113	0.975816506099	-0.223100203030
Cl	0.850757746426	-1.756065703804	0.104505889569

Atom	X	Y	Z
C	-2.040753805508	0.177656367677	-0.161718192071
C	-0.639522687659	0.782327558116	-0.229212974464
C	0.411355061390	-0.089541069307	0.456247823074
F	-2.381680803794	0.023645958474	1.165416876409
H	-2.750176435094	0.858238749238	-0.644248992578
H	-2.070549823052	-0.795070811419	-0.661602784519
H	-0.638073251057	1.750491060332	0.287489789310
F	-0.323024226506	0.980535936058	-1.545987767520
H	0.093601113003	-0.313860838126	1.471823678512
Cl	0.621095909993	-1.657815957104	-0.387289488553
Cl	1.973182948284	0.782870046061	0.565689032400

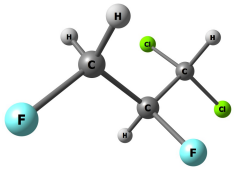
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
56.1208	0.273
101.0203	0.342
187.7478	0.300
213.9034	0.474
257.1814	0.646
340.5307	0.317
388.7836	0.315
395.9253	2.27
610.7335	6.99
773.8321	16.4
800.7316	3.59
887.0671	3.41
957.7608	6.92
1078.6561	3.35
1130.5756	5.53
1140.3723	8.85
1226.6772	0.0606
1235.0662	3.39
1279.9852	1.21
1360.6728	0.104
1380.5396	1.01
1423.3152	1.47
1496.6872	1.23
3047.2949	1.56
3060.3658	3.81
3108.4180	2.86
3166.4772	0.138

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
55.8804	0.148
105.8137	0.659
194.8638	0.437
204.5369	0.0636
210.7915	0.306
293.2109	0.579
435.1102	2.21
470.5956	2.64
584.2826	4.71
729.2349	1.01
760.0520	16.8
879.6432	1.63
1058.6576	1.65
1093.2359	14.4
1114.7409	0.578
1153.7431	9.62
1229.5240	2.52
1249.6137	1.45
1270.9156	0.281
1351.0242	0.674
1376.7678	2.35
1426.1683	0.637
1514.5905	0.821
3044.6676	1.55
3052.8271	3.76
3112.1302	3.17
3153.7252	0.200



$\Delta E = 0.89$ kcal mol^{-1}
Population = 0.118



$\Delta E = 1.44$ kcal mol^{-1}
Population = 0.047

Optimized Coordinates (Angstroms)

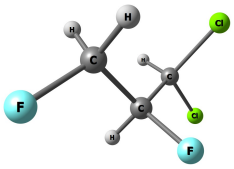
Atom	X	Y	Z
C	-1.440524435126	-0.392381571487	-0.733619820207
C	-0.765456782556	-0.083692303926	0.592643310292
C	0.757589392229	0.061589769156	0.543183461653
F	-2.743081113737	-0.752881433129	-0.478815048689
H	-1.433149312685	0.495466764272	-1.372763924526
H	-0.929329807047	-1.216218711312	-1.242136240433
H	-0.996863960993	-0.886181617852	1.304330380016
F	-1.268028917064	1.095302467967	1.095422321873
H	1.122076192442	0.407997146879	1.507394064793
Cl	1.528342432818	-1.528770645318	0.235381350376
Cl	1.281873311718	1.286381134750	-0.657795855147

Atom	X	Y	Z
C	-1.856640997422	-0.534220813923	-0.277463718381
C	-0.706212330527	0.343507861943	0.201720911096
C	0.649737850104	-0.052591923502	-0.392250959456
F	-3.002351402743	-0.116879004608	0.353098628863
H	-1.983909896762	-0.417676046963	-1.361265143687
H	-1.675711149857	-1.586149795150	-0.040500033297
H	-0.647916761608	0.320410229867	1.295708278518
F	-0.969146672174	1.633000960990	-0.198399307223
H	0.625863262153	-0.052317490965	-1.480634708550
Cl	1.907958283163	1.123513080311	0.089277741512
Cl	1.099341815673	-1.712531058001	0.122717310605

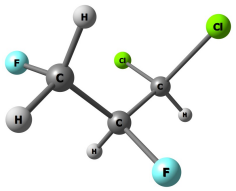
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
77.6172	0.398
81.3444	0.346
169.9647	0.478
197.2551	0.552
254.5727	0.378
293.5640	0.234
376.8244	0.559
475.6690	2.12
604.4488	5.42
686.0583	4.90
781.9915	16.6
900.7923	3.23
1008.6046	5.05
1103.0298	13.6
1118.4290	9.83
1146.9454	1.58
1226.3297	1.51
1252.2904	1.49
1283.5674	0.487
1331.6963	2.46
1385.0269	1.07
1441.8593	0.587
1499.8082	0.555
3048.5928	0.929
3055.8022	2.74
3113.3546	2.48
3148.9392	0.255

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
62.7694	0.206
90.5409	0.669
156.5975	0.500
237.0541	0.381
246.8650	0.527
331.7509	0.122
362.0780	0.854
417.1212	0.866
530.5022	3.55
756.4637	9.01
773.3580	17.4
907.0691	5.79
1081.3088	0.270
1091.8750	4.65
1115.9753	8.25
1124.8976	11.7
1220.6565	1.01
1237.4649	2.80
1287.6456	0.403
1338.5677	0.207
1388.2452	1.02
1436.1352	1.14
1502.4436	0.335
3034.0691	3.11
3067.6058	1.49
3107.6877	3.06
3136.8920	0.603



$\Delta E = 1.60$ kcal mol^{-1}
Population = 0.036



$\Delta E = 1.84$ kcal mol^{-1}
Population = 0.024

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.887645116551	-0.342818191917	0.486304105116
C	-0.698427441606	0.528697032705	0.101994078793
C	0.638379550965	-0.037815475865	0.577137744342
F	-3.037205261180	0.389249586252	0.315094538384
H	-1.925705534148	-1.229592309219	-0.153160756247
H	-1.813737290286	-0.654257731961	1.536021780377
H	-0.822088740347	1.513643863343	0.571766093280
F	-0.680709151316	0.697664355229	-1.256268725615
H	0.648195234118	-0.140325807930	1.660674350363
Cl	0.942075910538	-1.674339032150	-0.096777741726
Cl	1.973746839812	1.077962711512	0.154339532933

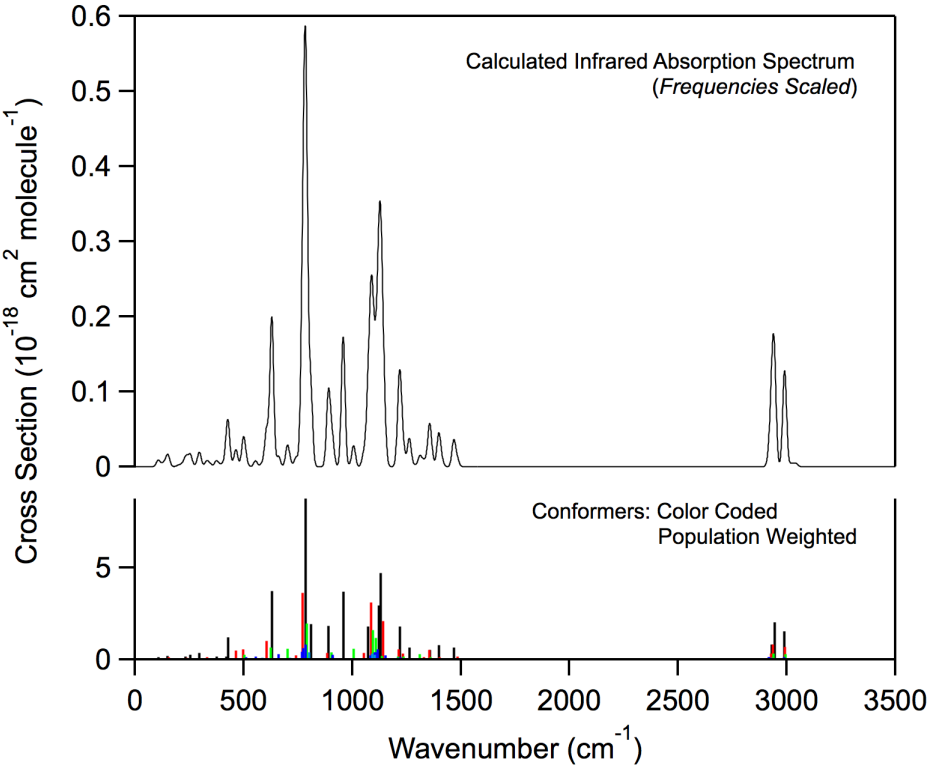
Atom	X	Y	Z
C	-1.719321769105	-0.171443426701	-0.543102795861
C	-0.911426518815	0.244507556310	0.686090076978
C	0.614901270324	0.248360879833	0.551415699187
F	-1.742856646762	-1.540309502108	-0.647084577419
H	-2.740510997248	0.200521221874	-0.402514127606
H	-1.303185267553	0.256743877391	-1.460119848113
H	-1.165684800239	-0.424326416049	1.518090872364
F	-1.281803867072	1.530240801875	1.017525033916
H	1.061435874627	0.629180628672	1.467231639604
Cl	1.238524114090	-1.410630673724	0.312921834378
Cl	1.161457607753	1.350913052628	-0.755007807428

Infrared Absorption Spectrum (unscaled frequencies)

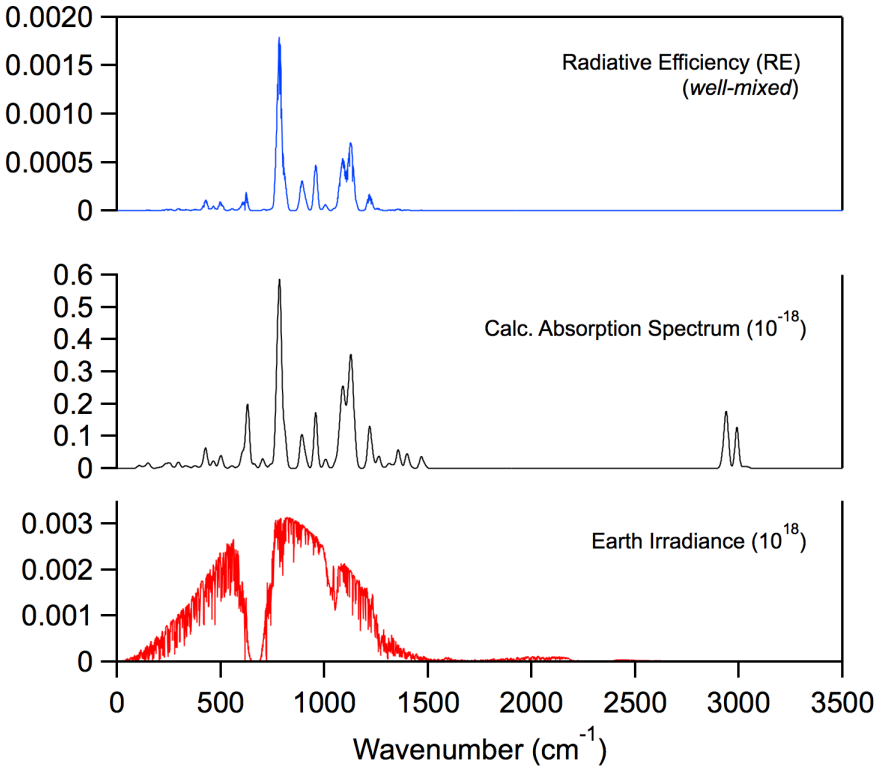
Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
71.3471	0.0579
93.8685	0.799
148.7073	0.448
201.2513	0.0221
262.7486	0.204
284.1864	0.334
353.7717	0.0168
484.0509	3.42
642.9675	8.17
727.2810	1.38
763.2351	17.2
906.9512	4.99
984.6999	0.781
1098.4438	7.06
1111.2344	10.9
1165.0285	6.43
1225.2716	3.03
1274.0718	0.551
1281.0483	0.543
1308.3493	1.25
1398.9842	2.03
1435.0174	1.34
1496.8945	0.347
3032.6851	3.88
3038.8068	1.32
3104.1151	2.66
3136.6797	0.657

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
43.6117	0.177
111.3601	0.439
182.0923	0.459
203.0798	0.355
259.2982	0.142
309.8032	3.03
359.0194	0.730
477.7967	0.134
562.8165	4.17
699.6152	4.55
791.5013	17.2
898.3951	1.11
1055.7172	0.760
1099.9086	14.5
1110.5503	11.4
1135.0568	0.131
1226.4090	1.98
1242.4338	1.18
1289.2375	1.54
1339.2156	0.427
1375.8954	2.50
1437.9527	0.152
1513.2592	0.776
3045.8085	1.08
3047.8368	4.10
3105.0683	3.02
3143.6148	0.363

Infrared Spectrum

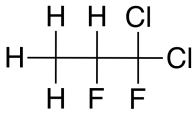


Radiative Efficiency



HCFC-252ec

Molecular Formula:	$CH_3CHFCCl_2F$
Name:	1,1-Dichloro-1,2-difluoropropane
CAS number:	151771-10-7
Molecular Weight:	148.97



Global Atmospheric Lifetime (years):	0.845
Tropospheric Atmospheric Lifetime (years):	0.882
Stratospheric Atmospheric Lifetime (years):	20.0
Ozone Depletion Potential (ODP):	0.015

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.245	0.175
Global Warming Potential (GWP_H):		
GWP_{20}	313	223
GWP_{100}	85	60
Global Temperature Potentials (GTP_H)		
GTP_{20}		71
GTP_{50}		10
GTP_{100}		8

* 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) = 6.65×10^{-14}; k_{SAR}(272 K) ≈ 4.24×10^{-14} cm^3 $molecule^{-1}$ s^{-1}

τ^{OH}_{Global} = 0.857 years

τ^{OH}_{Trop} = 0.882 years

τ^{OH}_{Strat} = 30.1 years

Fractional Atmospheric Loss: 0.986

O(^{1}D) Reactivity

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

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

$\tau_{O(^1D)}$ = 230 years

Fractional Atmospheric Loss: 0.004

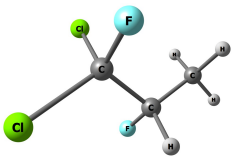
UV Photolysis

UV Spectrum: *No Recommendation*

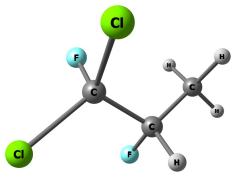
τ_{hv} = 80 years

Fractional Atmospheric Loss: 0.010

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.406



$\Delta E = 0.15$ kcal mol^{-1}
Population = 0.316

Optimized Coordinates (Angstroms)

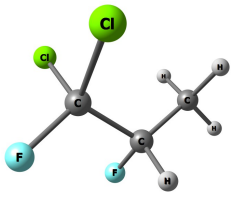
Atom	X	Y	Z
C	-2.293354996694	0.060962091851	0.485332299183
C	-1.001998571344	0.768859344603	0.114171685271
C	0.255876363770	-0.094382535642	0.338001791042
H	-3.126958896711	0.753540946274	0.346897544822
H	-2.451859840894	-0.813558680165	-0.148779157688
H	-2.267374074523	-0.253635066118	1.530853030132
H	-0.856677041695	1.663436486909	0.733221960646
F	-1.031448272562	1.153525749981	-1.200571290712
Cl	0.252715305118	-1.562972166546	-0.690533852037
Cl	1.734874128228	0.864153414275	-0.002092474322
F	0.288468897306	-0.474073585421	1.625308463664

Atom	X	Y	Z
C	-2.192196309622	0.755653327793	-0.124208280483
C	-1.095977813369	-0.216987432500	-0.529374500431
C	0.237080774480	0.032646082746	0.205535206508
H	-3.119510317768	0.454976985623	-0.616997897346
H	-2.340629712998	0.725140663443	0.957227442379
H	-1.948179841358	1.775621506974	-0.425023501093
H	-0.892667221889	-0.181739068147	-1.604383109631
F	-1.494377218400	-1.493230261646	-0.199857391977
Cl	1.414663457055	-1.269371768737	-0.155812533964
Cl	0.926581918137	1.617741796202	-0.300534726942
F	0.039853285731	0.060754168250	1.529077292981

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
78.4980	0.200
187.1064	0.187
198.5145	0.0119
214.8973	0.00417
271.4700	0.172
308.5079	0.235
373.0746	0.0138
409.4136	0.289
461.1639	2.94
550.7272	0.397
578.4609	7.08
804.7745	33.1
895.4564	3.26
988.0169	11.8
1103.8197	7.64
1129.2080	0.687
1157.2063	24.5
1188.1682	1.13
1358.4360	2.27
1373.6245	1.59
1407.7895	1.88
1484.8939	0.729
1494.8570	0.391
3042.0738	2.41
3061.5294	0.832
3139.6100	1.25
3149.8526	1.14

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
74.7181	0.222
182.2258	0.197
213.5105	0.00375
229.1606	0.0159
275.2931	0.108
324.8010	0.163
340.6839	0.419
396.4086	0.681
444.5675	1.47
473.6129	2.19
705.0341	4.32
832.1062	36.9
897.2128	9.41
965.5958	12.6
1030.1653	8.59
1123.6571	3.95
1150.5661	2.39
1213.6675	15.4
1357.5948	0.175
1374.7543	0.913
1407.5743	1.81
1486.7986	0.926
1494.9236	0.302
3064.6589	0.872
3073.9631	1.81
3143.1891	1.30
3154.6228	1.18



$\Delta E = 0.22$ kcal mol^{-1}
Population = 0.278

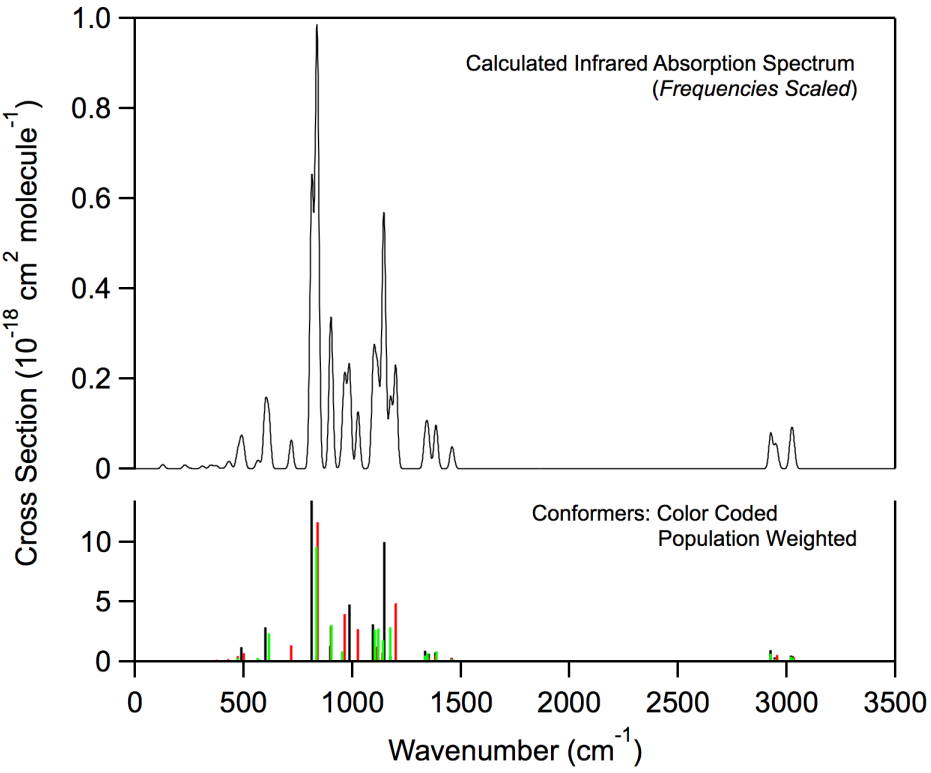
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.474212801271	1.290551458856	0.952697532234
C	-1.054567916624	0.626572191454	-0.343254432126
C	0.288377709061	-0.130410410266	-0.315633427963
H	-0.761757676050	2.063322450783	1.246195457889
H	-2.451777297744	1.754811733795	0.801790028066
H	-1.556169646178	0.553659284666	1.754386014477
H	-0.954443829732	1.359066773070	-1.154702673768
F	-2.003249914026	-0.296897843808	-0.720331514354
Cl	1.636023631897	1.014795553937	0.020493488028
Cl	0.289624171537	-1.455885638107	0.891050859315
F	0.500577569129	-0.672666554380	-1.520408331798

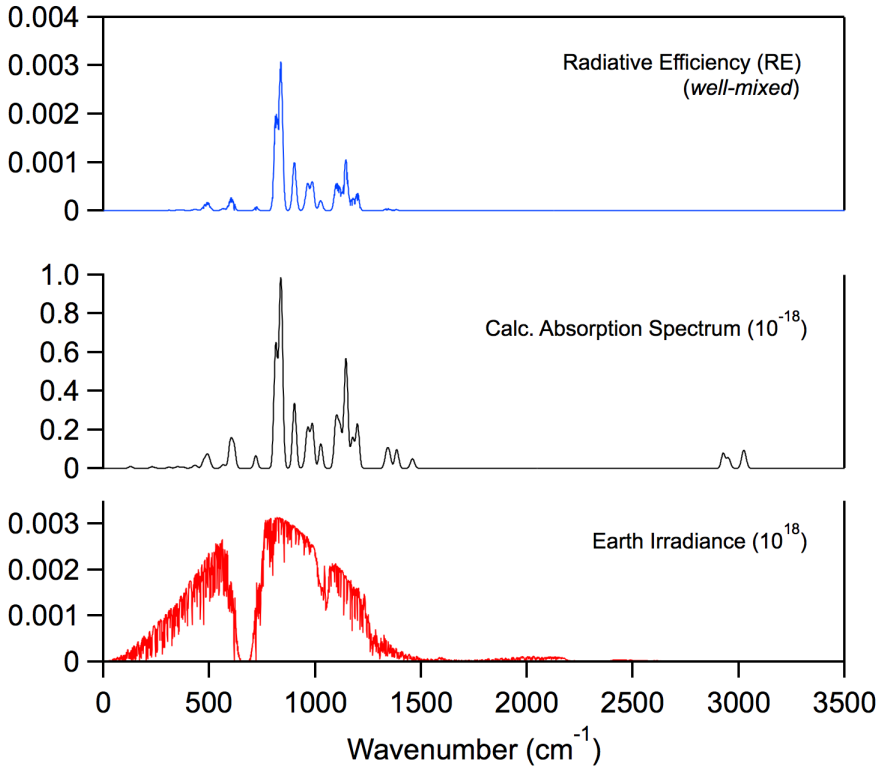
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
84.6546	0.223
188.0012	0.146
204.7626	0.0907
209.9427	0.0117
269.1213	0.107
316.3477	0.270
374.9163	0.0766
403.1679	0.321
443.8934	1.08
539.4926	1.12
595.7643	8.45
828.4493	34.5
900.4921	11.1
954.3638	2.98
1110.7302	9.53
1128.1618	9.92
1151.2906	6.52
1188.7618	10.2
1357.7399	1.76
1369.8091	2.54
1413.5192	3.03
1486.5402	0.714
1494.6695	0.407
3041.6713	2.37
3063.8834	0.673
3140.0721	1.44
3153.2908	1.01

Infrared Spectrum

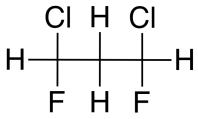


Radiative Efficiency



HCFC-252fa

Molecular Formula:	$CHClFCH_2CHClF$
Name:	1,3-Dichloro-1,3-difluoropropane
CAS number:	1378824-14-6
Molecular Weight:	148.97



Global Atmospheric Lifetime (years):	1.15
Tropospheric Atmospheric Lifetime (years):	1.19
Stratospheric Atmospheric Lifetime (years):	29.4
Ozone Depletion Potential (ODP):	0.017

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.187	0.143
Global Warming Potential (GWP_H):		
GWP_{20}	324	248
GWP_{100}	88	67
Global Temperature Potentials (GTP_H)		
GTP_{20}		82
GTP_{50}		12
GTP_{100}		9

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 4.91 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 3.14 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 1.16$ years

$\tau^{OH}_{Trop} = 1.19$ years

$\tau^{OH}_{Strat} = 39.5$ years

Fractional Atmospheric Loss: 0.990

O(^{1}D) Reactivity

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

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

$\tau_{O(^1D)} = 230$ years

Fractional Atmospheric Loss: 0.005

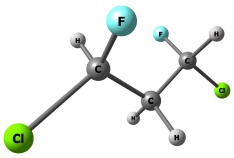
UV Photolysis

UV Spectrum: *No Recommendation*

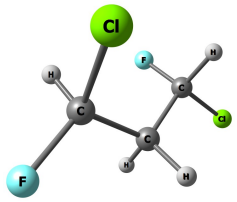
$\tau_{hv} = 225$ years

Fractional Atmospheric Loss: 0.005

Molecular Structure and Infrared Spectrum (9 conformers)



E = 0
Population = 0.397



$\Delta E = 0.44$ kcal mol^{-1}
Population = 0.188

Optimized Coordinates (Angstroms)

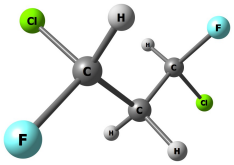
Atom	X	Y	Z
C	-1.245013402237	-0.377159447025	0.105050078083
C	-0.001399818461	0.494147327062	0.008309388853
C	1.243028162406	-0.374382746485	-0.101978274319
Cl	-2.725161883152	0.649177742756	0.213302336111
F	-1.338524848536	-1.167419121976	-0.997647592787
H	-1.250123880604	-1.011416960431	0.992435043296
H	0.073957879655	1.124895952864	0.896877437972
H	-0.077354300698	1.138585169080	-0.870329603953
H	1.248720906557	-0.994746622791	-0.999127695637
Cl	2.722213536754	0.654900805955	-0.194242174148
F	1.337294648317	-1.181621099009	0.988286056528

Atom	X	Y	Z
C	-1.346034144415	0.468870256909	0.352114525937
C	0.038111089712	0.750942481221	-0.215034205116
C	1.047417834688	-0.323274105132	0.145852924868
F	-2.159012705540	1.516954300344	0.085306542687
Cl	-2.069883327359	-1.020509683220	-0.389281060472
H	-1.334159352189	0.283457209232	1.426916447459
H	0.373271045204	1.705647087762	0.203679190857
H	-0.026066637114	0.853659870179	-1.300419538872
H	0.820331150134	-1.294479880606	-0.295107754365
Cl	2.686029974334	0.129004005533	-0.464358925833
F	1.106674072544	-0.458874542223	1.497848852849

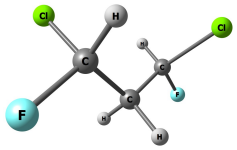
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
61.6554	0.122
95.3123	0.834
124.4621	0.428
232.6729	0.0227
307.4252	0.387
376.4984	0.465
391.7462	0.396
491.4258	3.15
495.6276	2.53
704.1365	25.1
842.3177	5.56
877.9365	5.12
952.5818	4.83
1093.8267	9.72
1122.5103	15.5
1123.9793	16.4
1223.8737	1.23
1243.5817	2.65
1303.2829	0.960
1357.8830	7.62
1388.2000	2.93
1399.6562	4.00
1458.2615	0.681
3084.6912	0.00996
3113.5064	1.23
3118.2330	0.850
3145.2248	0.761

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
55.6213	0.149
98.3610	0.705
136.4357	0.404
237.5901	0.284
333.2907	0.197
379.1149	0.440
411.7385	0.937
441.8421	2.84
524.2009	1.61
666.1147	12.2
775.1695	17.0
907.3057	7.07
1012.6374	7.16
1091.1728	5.49
1121.1475	16.1
1132.9020	18.7
1207.3905	1.30
1260.3779	5.28
1317.4595	3.83
1334.1300	3.53
1392.2889	2.19
1404.9061	5.20
1461.8664	0.723
3066.1029	0.187
3113.3600	0.912
3121.0449	0.673
3136.3185	1.06



$\Delta E = 0.44$ kcal mol^{-1}
Population = 0.188



$\Delta E = 0.87$ kcal mol^{-1}
Population = 0.091

Optimized Coordinates (Angstroms)

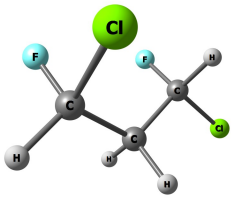
Atom	X	Y	Z
C	-1.046237807578	-0.331381632232	0.120692160461
C	-0.041488774413	0.764146277004	-0.184552931187
C	1.344500262671	0.458012016162	0.365357781788
F	-1.103086016783	-0.537944735528	1.463782523819
Cl	-2.687393035803	0.146000371804	-0.462981326039
H	-0.816111704274	-1.277240522677	-0.370886083426
H	-0.379653749588	1.694281286197	0.284069826102
H	0.020784225520	0.923901442014	-1.263131154913
H	1.334827186791	0.216419049356	1.428963614368
Cl	2.072909904590	-0.987641739831	-0.454026469366
F	2.153159508867	1.521753187732	0.152932058393

Atom	X	Y	Z
C	-1.164857872184	0.194369411028	-0.532660618473
C	0.001166241473	1.005828168047	0.002872960798
C	1.167130754313	0.193679075093	0.537489528425
Cl	-1.919918879481	-0.810634992632	0.776399453748
F	-2.104510935629	1.041828399759	-1.014343546780
H	-0.879469898186	-0.511167830685	-1.313778567211
H	-0.359369945345	1.646825769447	0.813998999416
H	0.361749524690	1.647715063519	-0.807528561410
H	0.881691000582	-0.512719023240	1.317810081301
Cl	1.922117643416	-0.809902246147	-0.772704742243
F	2.106846366351	1.040524205812	1.020129012430

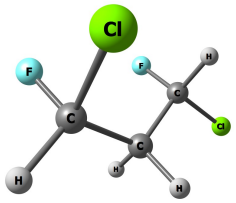
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
55.6215	0.149
98.3617	0.705
136.4374	0.404
237.5906	0.284
333.2910	0.197
379.1148	0.440
411.7386	0.937
441.8418	2.84
524.2011	1.61
666.1126	12.2
775.1705	17.0
907.3066	7.07
1012.6362	7.16
1091.1707	5.49
1121.1480	16.1
1132.9033	18.7
1207.3897	1.30
1260.3780	5.28
1317.4576	3.83
1334.1297	3.53
1392.2892	2.19
1404.9055	5.20
1461.8654	0.723
3066.1034	0.187
3113.3602	0.912
3121.0425	0.673
3136.3189	1.06

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
49.3919	0.142
110.2962	0.795
133.9323	0.126
294.4835	0.478
310.5193	0.459
380.2791	0.440
396.2868	1.67
469.9174	0.131
531.4251	2.79
651.4284	14.5
683.9822	8.35
961.0310	10.1
1061.8283	4.61
1074.6396	8.33
1113.4828	18.9
1140.1238	20.3
1189.0790	0.449
1280.9138	7.56
1312.5303	4.92
1325.8153	3.41
1379.9632	0.0573
1417.8657	4.59
1465.3214	0.593
3056.9180	0.307
3104.5325	0.0529
3121.9607	0.530
3126.3435	1.95



$\Delta E = 1.45$ kcal mol^{-1}
Population = 0.034



$\Delta E = 1.45$ kcal mol^{-1}
Population = 0.034

Optimized Coordinates (Angstroms)

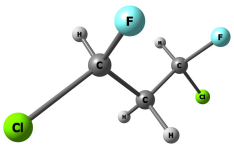
Atom	X	Y	Z
C	-0.944386948177	-0.031871916766	-0.324191634550
C	-0.088925252595	-0.066468895737	0.933077747498
C	1.382790541579	0.250268295118	0.698175802907
Cl	-2.634001106878	-0.551037561533	0.080396240009
F	-0.989210883778	1.220017822057	-0.833345514032
H	-0.600593494790	-0.721154558040	-1.096314822185
H	-0.164481257224	-1.052129300591	1.396298624311
H	-0.481220382844	0.674351799410	1.638252059970
H	1.953974830097	0.193927525969	1.627329718391
Cl	2.158513636262	-0.971825081696	-0.402080772016
F	1.541687318347	1.477177871810	0.155566549698

Atom	X	Y	Z
C	-1.390395303425	-0.263600025408	0.695498353591
C	0.085331222871	0.024769131973	0.941517010160
C	0.940680646954	0.024401471645	-0.316303506114
Cl	-2.149407937452	1.007843016339	-0.359563910744
F	-1.565442113033	-1.467783885481	0.108745145685
H	-1.961085640572	-0.233409959829	1.626172273796
H	0.467485961137	-0.746302596021	1.619298607416
H	0.173855180116	0.991885329867	1.440173846368
H	0.606358613817	0.745751453369	-1.062870077079
Cl	2.636920796586	0.506001462547	0.106606103691
F	0.969004573001	-1.208685399000	-0.870531846769

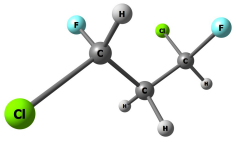
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
37.6197	0.207
103.9578	0.209
162.4570	0.258
242.5232	0.205
321.5386	0.589
365.8265	0.432
384.8322	0.421
459.8130	1.95
568.7983	10.2
680.9406	7.91
821.9301	15.2
868.9866	4.11
975.7573	5.22
1027.1255	1.48
1134.3644	3.23
1157.6188	33.3
1228.9488	3.16
1280.5872	4.48
1283.6428	7.81
1363.1899	5.77
1388.3052	1.46
1413.1922	2.16
1449.9284	1.21
3063.7078	0.0851
3097.2818	2.58
3118.7330	0.808
3134.1149	0.600

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
37.6182	0.207
103.9548	0.209
162.4563	0.258
242.5239	0.205
321.5367	0.589
365.8266	0.432
384.8323	0.421
459.8129	1.95
568.7986	10.2
680.9399	7.91
821.9288	15.2
868.9870	4.11
975.7567	5.22
1027.1268	1.48
1134.3654	3.23
1157.6192	33.3
1228.9498	3.16
1280.5883	4.48
1283.6437	7.81
1363.1905	5.77
1388.3067	1.46
1413.1940	2.16
1449.9301	1.21
3063.7069	0.0852
3097.2814	2.58
3118.7330	0.808
3134.1144	0.600



ΔE = 1.65 kcal mol^{-1}
Population = 0.024



ΔE = 1.89 kcal mol^{-1}
Population = 0.016

Optimized Coordinates (Angstroms)

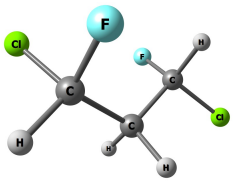
Atom	X	Y	Z
C	-1.262122977057	-0.230046116363	-0.398743489754
C	0.000485189008	0.488667153838	0.058572395153
C	1.262011982807	-0.237485871693	-0.389883752421
F	-1.368064178171	-1.442499553153	0.189597160516
Cl	-2.718921314198	0.754390367201	0.035466025598
H	-1.312456225615	-0.358336676478	-1.483594872809
H	-0.003112738476	0.566014021702	1.148937729195
H	0.004923297837	1.497069598381	-0.359006223161
H	1.319194946655	-0.366110765096	-1.474356072382
Cl	2.721502173068	0.738369669011	0.054536487808
F	1.356680844143	-1.450519827349	0.199181612258

Atom	X	Y	Z
C	-0.985922215179	0.012696751458	-0.375986638319
C	-0.126050002085	0.627477010942	0.719295881538
C	1.342815234182	0.776286024190	0.338175685895
F	-0.743519631942	-1.310273960648	-0.504790774743
Cl	-2.738763311494	0.234187312982	0.033305673334
H	-0.842506631693	0.499246236460	-1.341619814592
H	-0.219454554264	0.037678183127	1.633885463158
H	-0.502655109861	1.634708057787	0.922345411479
H	1.890966126207	1.347705251482	1.089822141672
Cl	2.212388378252	-0.800731866483	0.214030693017
F	1.440978717875	1.419751998704	-0.856712722439

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
38.7846	0.0125
109.7133	0.557
134.6883	0.672
248.9854	0.216
274.9787	0.0140
371.1808	0.368
398.1188	0.640
472.9809	1.22
500.9913	5.35
700.8087	22.3
826.8181	10.4
882.0203	1.21
969.1910	5.54
1084.6997	0.857
1119.0420	0.673
1162.1931	37.0
1210.3112	6.16
1276.4443	0.00971
1292.3622	3.45
1355.9544	7.71
1396.4368	4.72
1402.0670	2.91
1453.2117	0.697
3078.6763	0.145
3079.0278	2.84
3088.3105	2.25
3144.4418	0.424

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
33.8372	0.173
104.0237	0.125
160.1207	0.396
223.3812	0.0673
326.4965	0.870
378.4885	0.322
383.0185	0.324
458.4156	1.93
590.3693	10.9
674.1101	6.54
813.7517	14.8
892.6755	1.52
931.8622	2.63
1076.9517	15.1
1111.4411	9.42
1144.1494	21.4
1228.9155	1.42
1264.3918	2.78
1305.0149	11.2
1359.7658	4.99
1379.0398	0.503
1414.7883	1.67
1452.3372	1.14
3069.6552	0.0853
3100.1750	2.53
3115.4193	0.685
3133.9251	0.659



$\Delta E = 1.89$ kcal mol^{-1}
Population = 0.016

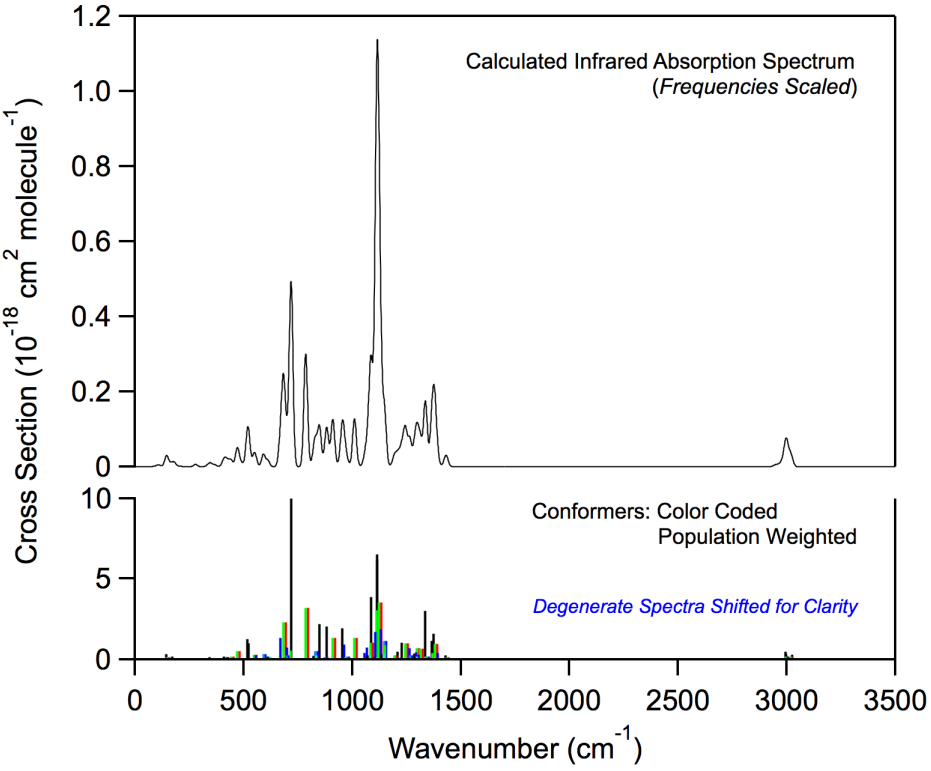
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.340806445059	0.771180643283	0.339592216981
C	0.126664848651	0.615721312107	0.723420747557
C	0.983196028352	-0.015035422429	-0.365376794445
F	-1.433479786191	1.404288563277	-0.861253329420
Cl	-2.221179577302	-0.800856559949	0.229149138159
H	-1.885631937861	1.353272154295	1.085445041610
H	0.215195871719	0.033719901878	1.643473716525
H	0.510064688494	1.622145572135	0.917558067601
H	0.843986627622	0.463603466794	-1.335568313002
Cl	2.737178108360	0.198062772104	0.043481943106
F	0.731737573215	-1.337423403494	-0.482253434672

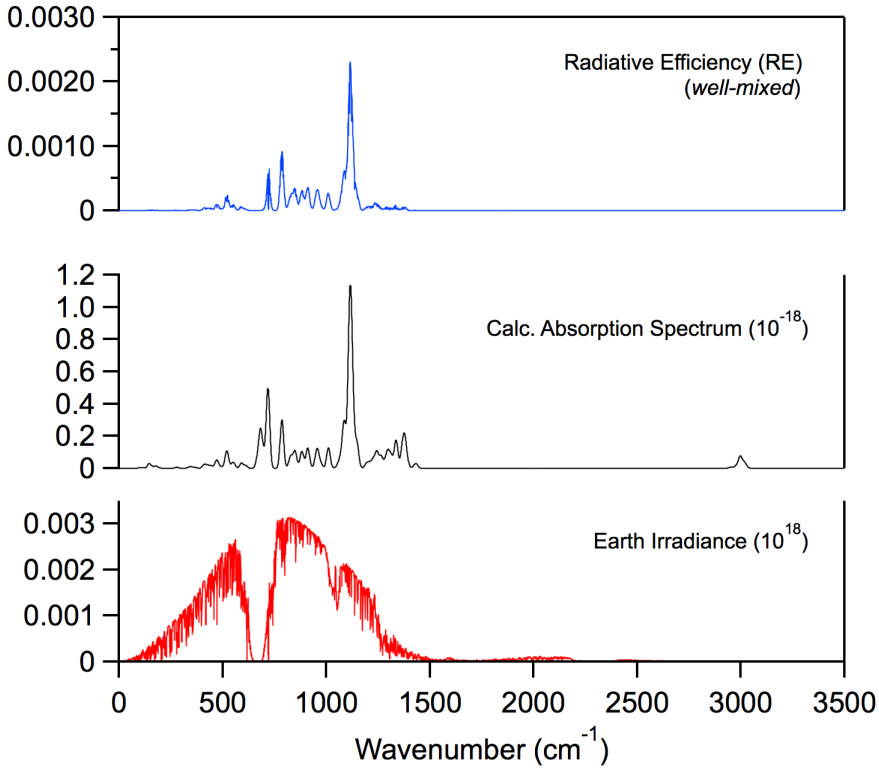
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
33.8370	0.173
104.0241	0.125
160.1215	0.396
223.3812	0.0673
326.4967	0.870
378.4884	0.322
383.0183	0.324
458.4150	1.93
590.3696	10.9
674.1094	6.54
813.7522	14.8
892.6748	1.52
931.8622	2.63
1076.9507	15.1
1111.4403	9.42
1144.1480	21.4
1228.9150	1.42
1264.3920	2.78
1305.0152	11.2
1359.7649	4.99
1379.0399	0.503
1414.7882	1.67
1452.3377	1.14
3069.6566	0.0853
3100.1749	2.53
3115.4190	0.685
3133.9262	0.659

Infrared Spectrum

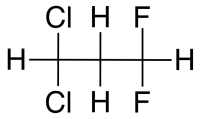


Radiative Efficiency



HCFC-252fb

Molecular Formula:	$CHCl_2CH_2CHF_2$
Name:	1,1-Dichloro-3,3-difluoropropane
CAS number:	131404-17-6
Molecular Weight:	148.97



Global Atmospheric Lifetime (years):	0.657
Tropospheric Atmospheric Lifetime (years):	0.684
Stratospheric Atmospheric Lifetime (years):	20
Ozone Depletion Potential (ODP):	0.011

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.172	0.114
Global Warming Potential (GWP_H):		
GWP_{20}	171	113
GWP_{100}	46	31
Global Temperature Potentials (GTP_H)		
GTP_{20}		35
GTP_{50}		5
GTP_{100}		4

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 8.58 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 5.47 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 0.665$ years

$\tau^{OH}_{Trop} = 0.684$ years

$\tau^{OH}_{Strat} = 23.9$ years

Fractional Atmospheric Loss: 0.989

$O(^1D)$ Reactivity

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

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

$\tau_{O(^1D)} = 230$ years

Fractional Atmospheric Loss: 0.003

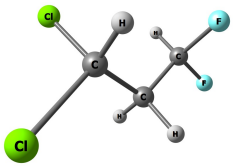
UV Photolysis

UV Spectrum: *No Recommendation*

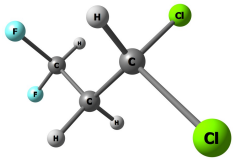
$\tau_{hv} = 80$ years

Fractional Atmospheric Loss: 0.008

Molecular Structure and Infrared Spectrum (6 conformers)



E = 0
Population = 0.435



E = 0
Population = 0.435

Optimized Coordinates (Angstroms)

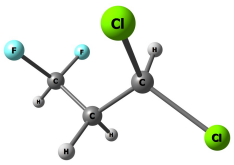
Atom	X	Y	Z
C	0.721959699064	0.068691836544	0.328300018921
C	-0.475736204164	0.652286182669	-0.403633468791
C	-1.771238176511	-0.088380312889	-0.102577309204
Cl	1.080314143329	-1.606923202563	-0.232929393475
Cl	2.161780640514	1.118897881074	0.111165876999
H	0.548628915800	-0.005129348674	1.398529732976
H	-0.297106240324	0.651067835740	-1.481502491264
H	-0.609225839389	1.688536662553	-0.077431657246
H	-1.778494095238	-1.127536093357	-0.448103036114
F	-1.990513655723	-0.085865017361	1.240861922651
F	-2.796754187358	0.571248576264	-0.693495195453

Atom	X	Y	Z
C	0.724398501896	-0.063413447204	0.339570307182
C	-0.469082205884	-0.675870050757	-0.375472159718
C	-1.767204749453	0.072826103992	-0.107368697362
Cl	2.167020979641	-1.118089616414	0.167330809307
Cl	1.082171476265	1.591118128637	-0.281398301289
H	0.546324123312	0.049382880915	1.405615067386
H	-0.602111249878	-1.699682403801	-0.011942388945
H	-0.285809522738	-0.713945456295	-1.451889275745
H	-1.774837806136	1.098561468621	-0.490896323614
F	-2.788964474921	-0.610087560734	-0.677994365135
F	-1.992286072104	0.119267953040	1.234308327933

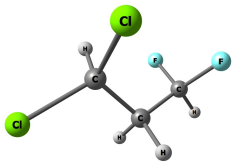
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
58.5266	0.143
103.3174	0.756
137.2075	0.261
234.0091	0.167
305.0106	0.407
334.4635	0.215
452.6829	1.24
498.5786	4.08
566.6498	1.10
663.6238	7.22
758.9844	14.9
889.5032	1.67
1029.6601	5.43
1094.4914	4.16
1124.0661	21.3
1142.1877	19.4
1216.1215	3.18
1238.7724	4.03
1290.7368	1.57
1345.7705	0.851
1414.4296	5.30
1423.1810	7.40
1462.9648	0.929
3067.5934	0.311
3077.0410	4.26
3126.8392	0.535
3161.5804	0.103

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
58.5261	0.143
103.3142	0.756
137.2057	0.261
234.0086	0.167
305.0113	0.407
334.4633	0.215
452.6818	1.24
498.5782	4.08
566.6501	1.10
663.6259	7.22
758.9824	14.9
889.5030	1.67
1029.6605	5.43
1094.4920	4.16
1124.0662	21.3
1142.1871	19.4
1216.1218	3.18
1238.7713	4.03
1290.7372	1.57
1345.7704	0.851
1414.4291	5.30
1423.1804	7.40
1462.9640	0.928
3067.5927	0.311
3077.0429	4.26
3126.8369	0.535
3161.5792	0.103



$\Delta E = 1.48$ kcal mol^{-1}
Population = 0.036



$\Delta E = 1.48$ kcal mol^{-1}
Population = 0.036

Optimized Coordinates (Angstroms)

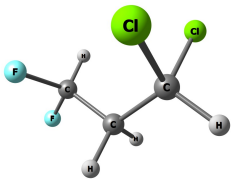
Atom	X	Y	Z
C	0.636921678565	0.152759195091	0.311317010408
C	-0.342005799063	0.845207347371	-0.630782519701
C	-1.808132028490	0.589064207928	-0.299335935832
Cl	0.713723745651	-1.617894475425	0.037849351002
Cl	2.276834150743	0.878150439850	0.127493239260
H	0.357657551994	0.291443442006	1.352039117974
H	-0.145595151663	0.555817800782	-1.666020019285
H	-0.178170212750	1.923881037096	-0.546117947048
H	-2.467874504701	1.242577050335	-0.884691083317
F	-2.167336988149	-0.692497596116	-0.537293848413
F	-2.027714442136	0.841386551083	1.020927634952

Atom	X	Y	Z
C	0.638105926106	-0.158535656217	0.329808688852
C	-0.337436439363	-0.864275321450	-0.605919776723
C	-1.804590274475	-0.593030919020	-0.291473400677
Cl	2.275098118879	-0.896928203931	0.173827916182
Cl	0.727538141708	1.605746317261	0.021249584817
H	0.349819637801	-0.274506887245	1.370849406363
H	-0.180662249031	-1.941938703806	-0.498168098194
H	-0.131152816083	-0.597047164091	-1.645186850895
H	-2.463550765817	-1.254448778480	-0.868775132745
F	-2.036080417552	-0.817298005671	1.031815961158
F	-2.154305862173	0.685499322651	-0.558144298137

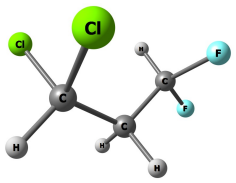
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
36.5170	0.266
116.8352	0.0706
157.0930	0.427
241.8155	0.0308
277.3866	0.763
358.2468	0.540
402.0993	0.587
515.6328	2.14
624.2836	4.02
680.3997	16.4
809.1991	2.76
880.7714	0.211
939.9143	1.40
1071.9656	10.1
1105.6183	14.1
1165.1710	14.1
1224.7064	6.41
1238.5529	5.66
1312.9594	1.19
1370.4138	8.88
1409.7742	2.97
1418.8087	4.37
1457.8235	1.27
3041.4077	7.21
3070.7994	1.63
3122.9976	0.317
3163.3604	0.0589

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
36.5171	0.266
116.8364	0.0706
157.0939	0.427
241.8151	0.0308
277.3860	0.763
358.2463	0.540
402.0992	0.587
515.6325	2.14
624.2829	4.02
680.3998	16.4
809.1996	2.76
880.7719	0.211
939.9137	1.40
1071.9634	10.1
1105.6173	14.1
1165.1710	14.1
1224.7060	6.41
1238.5538	5.66
1312.9587	1.19
1370.4134	8.88
1409.7741	2.97
1418.8079	4.37
1457.8235	1.27
3041.4079	7.21
3070.8004	1.63
3122.9985	0.317
3163.3609	0.0589



$\Delta E = 1.89$ kcal mol^{-1}
Population = 0.018



$\Delta E = 1.89$ kcal mol^{-1}
Population = 0.018

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	0.886020694313	0.131218799591	-0.680554373795
C	-0.605718334794	0.251849039307	-0.962313733177
C	-1.539121196805	0.238699984543	0.242000175592
Cl	1.472141103990	1.500202778492	0.342971796857
Cl	1.341415753423	-1.441775951748	0.053012311685
H	1.454133189494	0.201228883776	-1.604427515856
H	-0.904059226001	-0.564493039427	-1.628050241026
H	-0.764419336647	1.197741113624	-1.489365792755
H	-1.233228662201	0.927128445089	1.037282849403
F	-2.777722447834	0.599092029742	-0.187131710837
F	-1.634803536937	-1.006447082990	0.764178233910

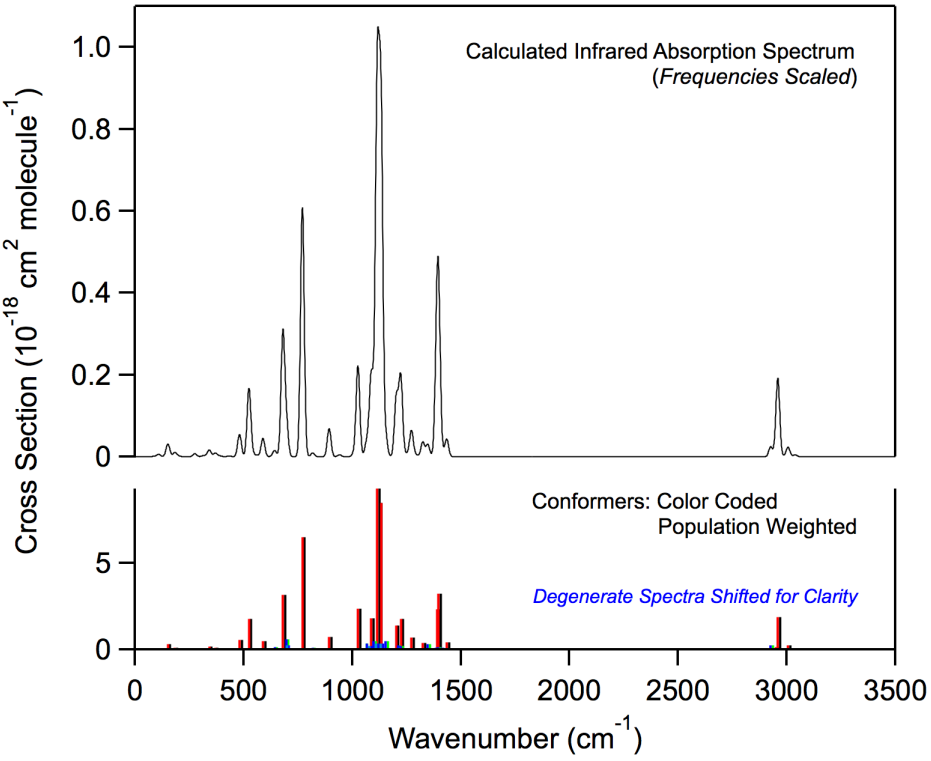
Atom	X	Y	Z
C	0.886151310401	-0.129373846042	-0.673651095803
C	-0.601306903691	-0.315588954072	-0.942010392769
C	-1.532298298561	-0.262206017101	0.263059363725
Cl	1.290527690658	1.498342208904	-0.035812185126
Cl	1.519345621567	-1.415477512401	0.426468017375
H	1.454485188693	-0.234994929927	-1.593996448601
H	-0.729559655771	-1.295656613843	-1.411797760786
H	-0.927854801395	0.449752035058	-1.653520257722
H	-1.202194782638	-0.892030987859	1.096324463150
F	-1.668224777160	1.007748898388	0.711339496999
F	-2.759090592104	-0.687976281105	-0.139271200444

Infrared Absorption Spectrum (unscaled frequencies)

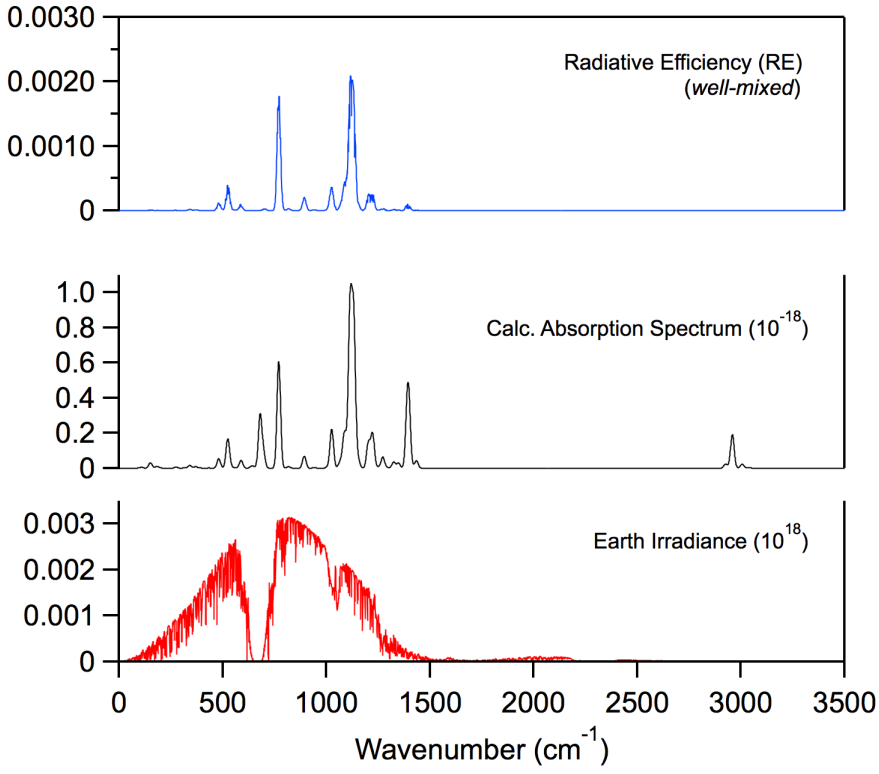
Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
39.4960	0.146
105.0942	0.220
154.7505	0.184
248.7019	0.253
287.8806	0.366
343.3703	0.438
449.6340	2.27
536.3341	2.05
617.1872	1.50
672.6226	3.78
682.5573	14.3
893.9627	0.225
1009.1702	4.43
1086.1849	11.0
1118.4496	19.2
1142.0523	19.8
1232.6630	5.75
1261.5889	2.27
1271.3281	2.60
1346.2270	0.570
1417.0936	3.27
1434.5593	5.20
1453.9023	1.52
3058.8183	0.187
3073.1675	3.98
3113.4426	0.841
3148.5171	0.281

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
39.4965	0.146
105.0949	0.220
154.7510	0.184
248.7018	0.253
287.8806	0.366
343.3702	0.438
449.6339	2.27
536.3340	2.05
617.1868	1.50
672.6223	3.78
682.5573	14.3
893.9622	0.225
1009.1703	4.43
1086.1843	11.0
1118.4497	19.2
1142.0520	19.8
1232.6627	5.75
1261.5886	2.27
1271.3278	2.60
1346.2266	0.570
1417.0937	3.27
1434.5588	5.20
1453.9021	1.52
3058.8189	0.187
3073.1674	3.98
3113.4432	0.841
3148.5172	0.281

Infrared Spectrum

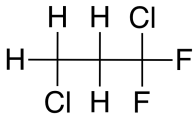


Radiative Efficiency



HCFC-252fc

Molecular Formula:	$CH_2ClCH_2CClF_2$
Name:	1,3-Dichloro-1,1-difluoropropane
CAS number:	819-00-1
Molecular Weight:	148.97



Global Atmospheric Lifetime (years):	0.937
Tropospheric Atmospheric Lifetime (years):	0.972
Stratospheric Atmospheric Lifetime (years):	25.5
Ozone Depletion Potential (ODP):	0.015

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.209	0.153
Global Warming Potential (GWP_H):		
GWP_{20}	296	216
GWP_{100}	80	59
Global Temperature Potentials (GTP_H)		
GTP_{20}		70
GTP_{50}		10
GTP_{100}		8

* 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) = 6.03×10^{-14}; k_{SAR}(272 K) ≈ 3.85×10^{-14} cm^3 $molecule^{-1}$ s^{-1}

τ^{OH}_{Global} = 0.945 years

τ^{OH}_{Trop} = 0.972 years

τ^{OH}_{Strat} = 32.9 years

Fractional Atmospheric Loss: 0.992

O(^{1}D) Reactivity

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

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

$\tau_{O(^1D)}$ = 230 years

Fractional Atmospheric Loss: 0.004

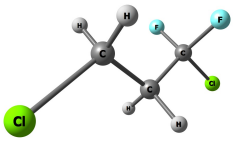
UV Photolysis

UV Spectrum: *No Recommendation*

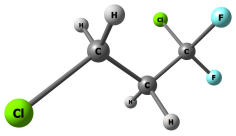
τ_{hv} = 225 years

Fractional Atmospheric Loss: 0.004

Molecular Structure and Infrared Spectrum (7 conformers)



E = 0
Population = 0.320



$\Delta E = 0.20$ kcal mol^{-1}
Population = 0.227

Optimized Coordinates (Angstroms)

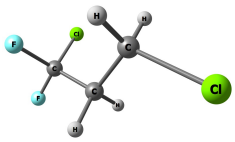
Atom	X	Y	Z
C	-0.961613821060	1.257386108492	0.000000000000
C	-0.531417394122	-0.208757324869	0.000000000000
C	0.985068407862	-0.321958488388	0.000000000000
Cl	-2.760808553299	1.381520641325	0.000000000000
H	-0.607720229385	1.778183780066	0.889015338078
H	-0.607720229385	1.778183780066	-0.889015338078
H	-0.914666809095	-0.722350718736	-0.883953503464
H	-0.914666809095	-0.722350718736	0.883953503464
Cl	1.515584099493	-2.049390017766	0.000000000000
F	1.514467169157	0.271919479346	-1.080689303285
F	1.514467169157	0.271919479346	1.080689303285

Atom	X	Y	Z
C	-1.297206917866	0.276502673177	0.439337597057
C	-0.350916142851	-0.525206764436	-0.445574984381
C	1.101231786580	-0.428979572600	-0.004091605634
Cl	-3.006318688342	0.012551953584	-0.078366920500
H	-1.230298125235	-0.036025286242	1.480842445732
H	-1.109634890536	1.347032438534	0.369467543213
H	-0.417765369715	-0.199842216679	-1.485575844235
H	-0.609649291685	-1.588469493060	-0.405897840712
Cl	1.757450897822	1.256396969636	-0.153456890322
F	1.243647311667	-0.806026879277	1.275050061512
F	1.868356430160	-1.228546822635	-0.752217561732

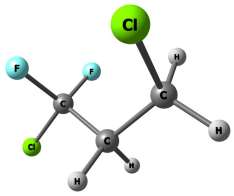
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
73.1415	0.791
99.5311	0.00231
123.5362	0.497
245.6956	0.122
322.8337	1.31
326.3241	0.0918
419.7234	1.05
424.6543	0.00128
570.2384	2.57
707.5700	16.8
778.5831	0.0258
826.2214	0.0826
942.9088	31.7
990.2172	5.48
1055.6670	8.82
1111.5014	7.63
1227.3115	11.7
1229.9966	22.5
1276.8715	0.309
1322.0995	3.64
1369.4727	8.11
1472.6711	0.691
1492.5327	0.356
3087.8300	0.244
3103.7147	1.33
3137.7411	0.0710
3168.6732	0.431

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
68.7891	0.693
100.8363	0.0151
144.5558	0.617
239.8897	0.176
321.3078	0.143
331.6173	0.295
417.2059	0.724
452.6469	0.348
584.7019	4.69
662.6717	11.4
762.0509	5.89
785.9743	0.911
935.3141	19.0
1053.9047	12.2
1063.4098	0.185
1154.8948	18.9
1187.1156	15.5
1230.6546	19.0
1283.2391	4.21
1312.3414	3.16
1378.9563	7.11
1472.9012	0.685
1492.8025	0.375
3066.8945	0.538
3104.8634	1.25
3128.0018	0.204
3169.9854	0.330



$\Delta E = 0.20$ kcal mol^{-1}
Population = 0.227



$\Delta E = 0.89$ kcal mol^{-1}
Population = 0.071

Optimized Coordinates (Angstroms)

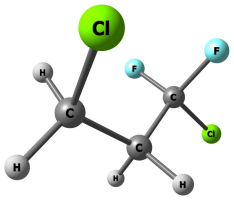
Atom	X	Y	Z
C	-1.297102518376	-0.276103573677	0.439238628889
C	-0.350676163075	0.525489580048	-0.445634391010
C	1.101457559208	0.428981762297	-0.004165539285
Cl	-3.006171058785	-0.011823586333	-0.078440658056
H	-1.109718827924	-1.346662311394	0.369307096372
H	-1.230132680374	0.036353888223	1.480760697856
H	-0.609221924057	1.588795566044	-0.405895400209
H	-0.417589046571	0.200195673026	-1.485653247173
Cl	1.757378942613	-1.256501802974	-0.153630924509
F	1.868718173473	1.228456527597	-0.752250889407
F	1.243947543867	0.805931277143	1.274996626532

Atom	X	Y	Z
C	-1.539148593646	-1.056233024380	0.135351921639
C	-0.129658707366	-0.989303032839	-0.448552322160
C	0.760316415421	0.051152377340	0.216810992457
Cl	-2.591699417350	0.320323893378	-0.375370544477
H	-2.037704452812	-1.961633013998	-0.209274902196
H	-1.518178547864	-1.051257543679	1.224852361768
H	-0.155516902542	-0.792169144744	-1.522034021051
H	0.347606572740	-1.962340434940	-0.296536271902
Cl	2.464127402551	-0.088537918668	-0.392370302242
F	0.348652097789	1.298646865135	-0.013809577387
F	0.788064133079	-0.127226022605	1.547253665550

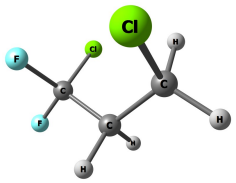
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
68.7891	0.693
100.8363	0.0151
144.5557	0.617
239.8897	0.176
321.3077	0.143
331.6173	0.295
417.2059	0.724
452.6469	0.348
584.7019	4.69
662.6717	11.4
762.0509	5.89
785.9743	0.911
935.3141	19.0
1053.9047	12.2
1063.4097	0.185
1154.8948	18.9
1187.1156	15.5
1230.6546	19.0
1283.2391	4.21
1312.3414	3.16
1378.9563	7.11
1472.9012	0.685
1492.8025	0.375
3066.8946	0.538
3104.8634	1.25
3128.0019	0.204
3169.9854	0.330

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
40.6358	0.308
110.0133	0.168
197.1269	0.117
236.6682	0.211
327.8279	0.388
390.1792	0.855
421.2091	0.199
432.9234	3.87
546.9153	1.20
672.5585	5.08
721.7019	3.63
903.9189	6.52
937.0871	9.92
951.0473	26.7
1047.0260	10.7
1119.5333	12.2
1203.4300	6.16
1235.2745	15.8
1293.1731	15.4
1336.9422	2.14
1383.0161	2.29
1456.0086	1.30
1479.1240	0.802
3071.5093	0.278
3099.1643	1.55
3131.2486	0.320
3160.5835	0.295



$\Delta E = 0.89$ kcal mol^{-1}
Population = 0.071



$\Delta E = 1.21$ kcal mol^{-1}
Population = 0.042

Optimized Coordinates (Angstroms)

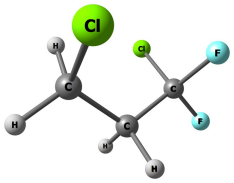
Atom	X	Y	Z
C	-1.539907043791	-1.056572945204	-0.133011252027
C	-0.130497556172	-0.988614347080	0.450968246097
C	0.759880850590	0.049970613085	-0.216773605318
Cl	-2.592160968583	0.321515555446	0.374180278247
H	-1.518750931102	-1.054255082989	-1.222516987328
H	-2.038773457089	-1.960992794701	0.213733302320
H	0.346522071129	-1.962151766046	0.301402200168
H	-0.156482832920	-0.788861159031	1.523962574212
Cl	2.463549166641	-0.088711195943	0.393036962861
F	0.787805259174	-0.131653226453	-1.546773402373
F	0.348525442123	1.298137348916	0.010739683142

Atom	X	Y	Z
C	-1.363020311986	-0.325508284015	-1.008003033458
C	-0.150991076733	0.593545972388	-1.074705167699
C	0.903847282927	0.409706550955	0.007925386813
Cl	-2.504858376855	0.098957750557	0.327093833568
H	-1.936228610073	-0.243036819989	-1.930960434052
H	-1.074593781822	-1.365561461824	-0.858413571098
H	-0.462333258255	1.642241046186	-1.030087049955
H	0.353635683036	0.435458706165	-2.033043852216
Cl	1.613376252990	-1.264612514347	-0.014176586869
F	1.908977355120	1.271467407208	-0.200472250879
F	0.427062841652	0.631208646717	1.232867725846

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
40.6358	0.308
110.0132	0.168
197.1268	0.117
236.6681	0.211
327.8279	0.388
390.1792	0.855
421.2091	0.199
432.9233	3.87
546.9153	1.20
672.5585	5.08
721.7019	3.63
903.9189	6.52
937.0871	9.92
951.0472	26.7
1047.0261	10.7
1119.5334	12.2
1203.4301	6.16
1235.2745	15.8
1293.1732	15.4
1336.9423	2.14
1383.0162	2.29
1456.0086	1.30
1479.1239	0.802
3071.5092	0.278
3099.1643	1.55
3131.2485	0.320
3160.5835	0.295

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
38.1166	0.275
117.6192	0.139
197.8501	0.274
253.4584	0.195
335.1037	0.215
364.2383	0.424
414.2512	0.801
482.9976	2.00
558.5150	2.89
655.8620	6.48
672.5415	3.97
861.9862	13.8
918.6173	0.848
1019.6020	21.4
1063.0187	2.67
1159.9248	24.7
1192.7102	7.96
1213.6538	13.4
1292.6840	14.4
1332.4238	2.41
1392.0747	3.14
1456.7930	0.912
1479.9577	1.46
3059.1424	0.544
3097.9148	0.801
3111.3795	1.05
3160.2585	0.335



$\Delta E = 1.21$ kcal mol^{-1}
Population = 0.042

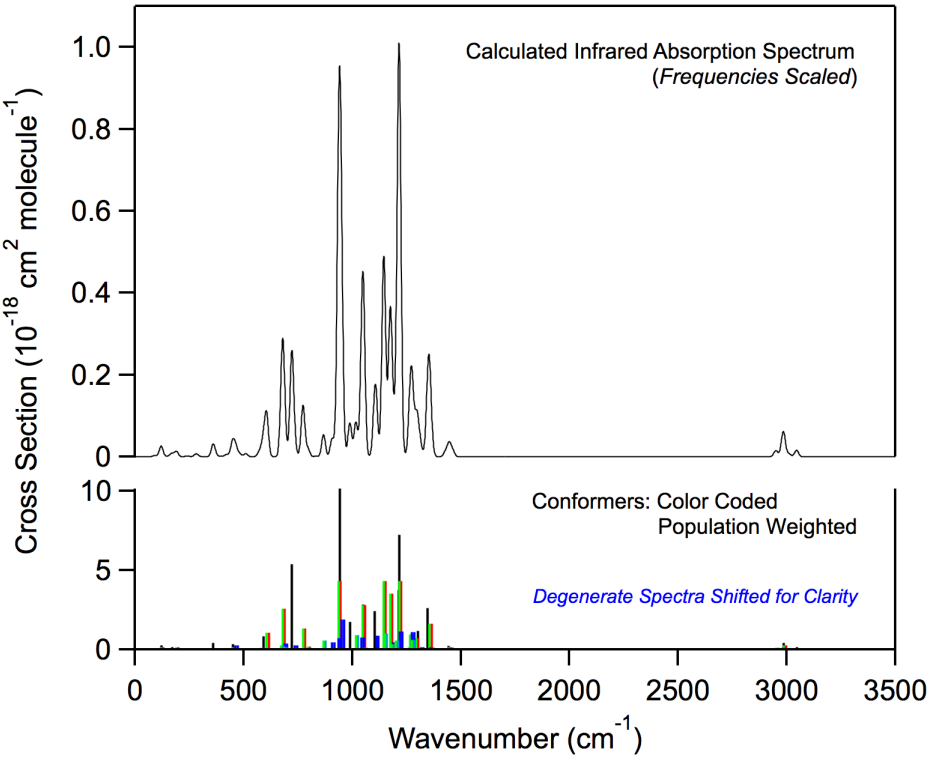
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.363211786129	0.325260449326	-1.007684895522
C	-0.150848045351	-0.593319897506	-1.074834649749
C	0.904038634906	-0.409461533626	0.007745605231
Cl	-2.504747994083	-0.100090888062	0.327388354704
H	-1.075155945561	1.365369154553	-0.857767581736
H	-1.936488870764	0.242894268379	-1.930608973049
H	0.353616508851	-0.434714450295	-2.033173109972
H	-0.461795388379	-1.642146019119	-1.030544708307
Cl	1.612942637665	1.265128787601	-0.013855469721
F	0.427468673307	-0.631563206400	1.232662843626
F	1.909466575536	-1.270776664849	-0.201057415503

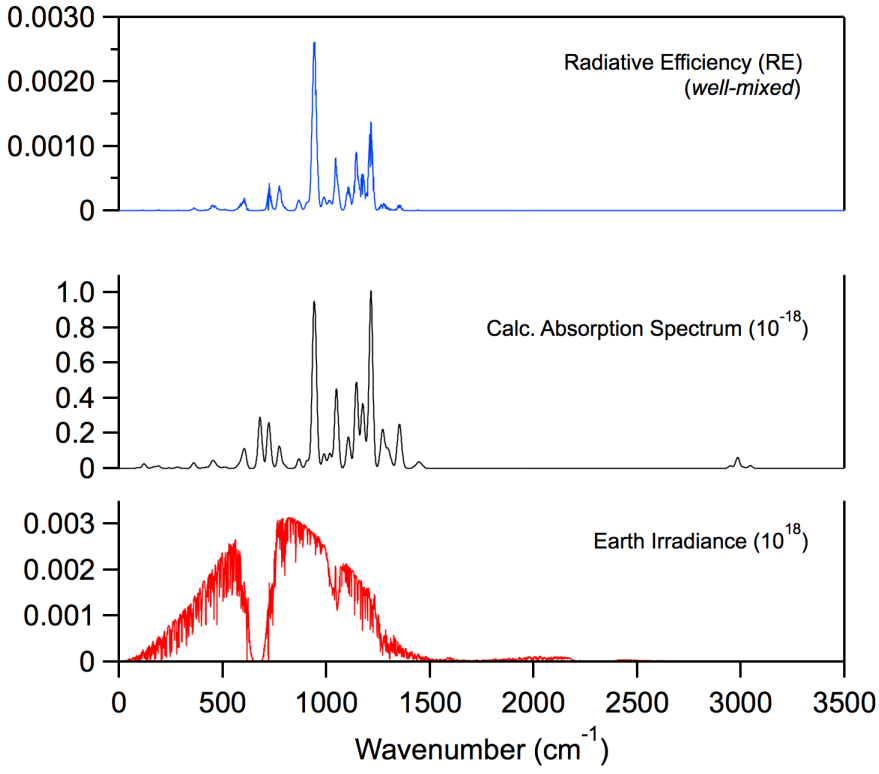
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
38.1167	0.275
117.6192	0.139
197.8501	0.274
253.4584	0.195
335.1037	0.215
364.2383	0.424
414.2512	0.801
482.9976	2.00
558.5150	2.89
655.8620	6.48
672.5415	3.97
861.9862	13.8
918.6173	0.848
1019.6019	21.4
1063.0187	2.67
1159.9248	24.7
1192.7102	7.96
1213.6538	13.4
1292.6839	14.4
1332.4238	2.41
1392.0746	3.14
1456.7929	0.912
1479.9577	1.46
3059.1424	0.544
3097.9148	0.801
3111.3795	1.05
3160.2585	0.335

Infrared Spectrum

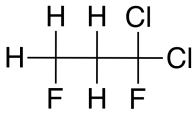


Radiative Efficiency



HCFC-252fd

Molecular Formula:	$CH_2FCH_2CCl_2F$
Name:	1,1-Dichloro-1,3-difluoropropane
CAS number:	121612-64-4
Molecular Weight:	148.97



Global Atmospheric Lifetime (years):	0.703
Tropospheric Atmospheric Lifetime (years):	0.732
Stratospheric Atmospheric Lifetime (years):	20
Ozone Depletion Potential (ODP):	0.012

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.229	0.155
Global Warming Potential (GWP_H):		
GWP_{20}	243	164
GWP_{100}	66	45
Global Temperature Potentials (GTP_H)		
GTP_{20}		52
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*

$k_{SAR}(298\ K) = 8.01 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 5.11 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 0.712$ years

$\tau^{OH}_{Trop} = 0.732$ years

$\tau^{OH}_{Strat} = 25.5$ years

Fractional Atmospheric Loss: 0.988

$O(^1D)$ Reactivity

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

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

$\tau_{O(^1D)} = 230$ years

Fractional Atmospheric Loss: 0.003

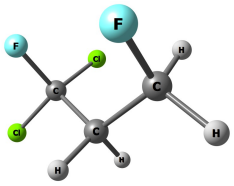
UV Photolysis

UV Spectrum: *No Recommendation*

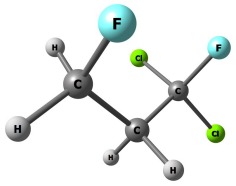
$\tau_{hv} = 80$ years

Fractional Atmospheric Loss: 0.009

Molecular Structure and Infrared Spectrum (9 conformers)



E = 0
Population = 0.180



E = 0
Population = 0.180

Optimized Coordinates (Angstroms)

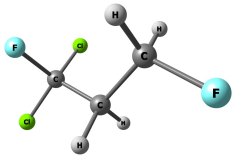
Atom	X	Y	Z
C	-2.070023792178	0.147225966952	-0.678285711440
C	-0.655757410771	0.692949386588	-0.844166527452
C	0.370587335156	0.084334294274	0.105538312074
F	-2.591637429782	0.530227877678	0.536130780010
H	-2.702576894233	0.555192446058	-1.476033235485
H	-2.087720170723	-0.946095926843	-0.741447182026
H	-0.664060673231	1.771514506170	-0.657381004852
H	-0.314698222413	0.529274115197	-1.868993203952
Cl	0.584016358889	-1.686061139654	-0.195238175994
Cl	1.968370282401	0.899720578303	-0.108401194585
F	0.001311616884	0.236806895278	1.380387143702

Atom	X	Y	Z
C	-2.068874196209	-0.150917532200	-0.678692134080
C	-0.654208235565	-0.696248428371	-0.842443956313
C	0.371246818852	-0.084779300771	0.106388320275
F	-2.590975577051	-0.531287069745	0.536341958619
H	-2.087142964244	0.942239142288	-0.744494847089
H	-2.700739286625	-0.561155632955	-1.475819679451
H	-0.312646889919	-0.534846150967	-1.867463865265
H	-0.662018320546	-1.774365977593	-0.653071225282
Cl	1.969609314831	-0.899780090557	-0.104671363228
Cl	0.583858728265	1.685008463836	-0.198514650656
F	0.001319608212	-0.234398422966	1.381386442470

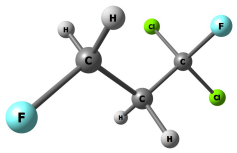
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
49.2736	0.340
141.6769	0.290
196.8920	0.198
231.2489	0.0906
306.0229	0.138
337.6592	0.187
388.2036	0.713
419.5257	0.950
480.2047	4.67
584.0639	5.35
785.6561	30.5
868.0556	5.00
964.0744	4.57
985.2392	5.57
1105.1458	6.62
1108.9768	17.0
1194.5228	18.1
1261.4085	1.96
1296.0141	3.20
1374.8769	1.31
1429.4119	3.01
1449.7941	0.824
1512.5791	0.868
3034.4563	5.25
3066.3525	0.0692
3088.5070	3.80
3127.0601	0.535

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
49.2732	0.340
141.6774	0.290
196.8924	0.198
231.2491	0.0906
306.0228	0.138
337.6594	0.187
388.2036	0.713
419.5255	0.950
480.2048	4.67
584.0638	5.35
785.6564	30.5
868.0555	5.00
964.0741	4.57
985.2389	5.57
1105.1458	6.62
1108.9767	17.0
1194.5225	18.1
1261.4085	1.96
1296.0138	3.20
1374.8767	1.31
1429.4118	3.01
1449.7942	0.824
1512.5790	0.868
3034.4565	5.25
3066.3526	0.0692
3088.5072	3.80
3127.0602	0.535



$\Delta E = 0.26$ kcal mol^{-1}
Population = 0.116



$\Delta E = 0.26$ kcal mol^{-1}
Population = 0.116

Optimized Coordinates (Angstroms)

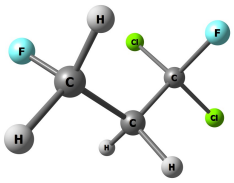
Atom	X	Y	Z
C	-2.058176640330	-0.136919534413	0.191957145409
C	-0.831483410941	0.621438261162	-0.317436997343
C	0.480359607779	0.075589974827	0.220520313652
F	-3.179246302912	0.509672795435	-0.279549924883
H	-2.068591379286	-1.170270447590	-0.168680655467
H	-2.085453169934	-0.141954098315	1.286777736481
H	-0.902508774307	1.664821737817	0.005482969992
H	-0.803116982752	0.606383158876	-1.408673622380
Cl	0.779645529820	-1.617050592635	-0.335959885125
Cl	1.859716792256	1.109136994601	-0.301664515305
F	0.466785730606	0.059797750234	1.564292434968

Atom	X	Y	Z
C	-2.057993286427	0.139850917073	0.189695730792
C	-0.831466620410	-0.625599485296	-0.309385633224
C	0.480277931997	-0.074911467907	0.223859590681
F	-3.179157003875	-0.510997753866	-0.275691101069
H	-2.086601828474	0.157567339221	1.284350374466
H	-2.066891424878	1.168974914261	-0.182873153572
H	-0.801744921996	-0.623178181044	-1.400687285629
H	-0.903971977615	-1.665109693934	0.025476005262
Cl	1.859207988903	-1.115830692188	-0.284628920343
Cl	0.781993488226	1.610880778839	-0.351768318729
F	0.465063654548	-0.043576675158	1.567341711366

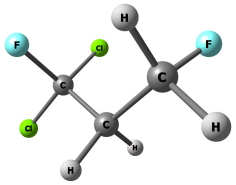
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
78.0156	0.805
106.6890	0.0177
143.3347	0.433
243.0230	0.0781
307.8467	0.790
315.4020	0.206
382.4886	0.351
394.0644	1.97
455.2305	0.243
647.0868	10.8
785.7899	18.2
815.8864	14.0
965.8177	13.6
1057.0259	9.73
1100.6781	16.6
1122.8331	4.60
1188.4451	13.5
1250.7130	1.17
1314.2816	0.792
1323.3116	2.12
1435.0167	3.07
1472.5417	0.595
1526.6481	0.146
3047.3859	3.50
3070.3613	0.646
3097.3463	2.77
3134.4970	1.14

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
78.0164	0.805
106.6909	0.0177
143.3364	0.433
243.0226	0.0781
307.8478	0.790
315.4027	0.206
382.4891	0.351
394.0647	1.97
455.2304	0.243
647.0870	10.8
785.7899	18.2
815.8875	14.0
965.8180	13.6
1057.0266	9.73
1100.6791	16.6
1122.8326	4.60
1188.4450	13.5
1250.7124	1.17
1314.2811	0.792
1323.3102	2.12
1435.0171	3.07
1472.5413	0.595
1526.6481	0.146
3047.3855	3.50
3070.3620	0.646
3097.3454	2.77
3134.4977	1.14



$\Delta E = 0.34$ kcal mol^{-1}
Population = 0.101



$\Delta E = 0.34$ kcal mol^{-1}
Population = 0.101

Optimized Coordinates (Angstroms)

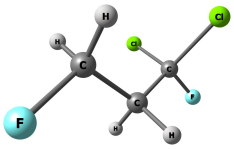
Atom	X	Y	Z
C	-1.997874406061	-0.949699312130	0.012976455950
C	-0.562163726765	-1.059417575776	-0.494184344294
C	0.431323786382	-0.153310307281	0.225969436700
F	-2.604965859220	0.195031865575	-0.447296854736
H	-2.567373906060	-1.812960832425	-0.351382401361
H	-2.023845050053	-0.949501957693	1.108263770665
H	-0.522823140619	-0.855903542645	-1.566168139365
H	-0.216146346790	-2.085700860565	-0.331542809534
Cl	2.113739184304	-0.537483742950	-0.311627030675
Cl	0.114559726367	1.590087341314	-0.058352804094
F	0.372218738516	-0.368800075423	1.552320720743

Atom	X	Y	Z
C	-1.992114778545	0.959235629502	0.012868172017
C	-0.557123361840	1.060452724316	-0.498081223327
C	0.432995113547	0.148902001553	0.219842744667
F	-2.607009415272	-0.182157532104	-0.445330255976
H	-2.015225849411	0.959639424064	1.108219712245
H	-2.557566947103	1.825623653099	-0.350371665748
H	-0.204760644264	2.084783347443	-0.336759535490
H	-0.521757978348	0.856297709657	-1.570081642115
Cl	0.105450287048	-1.592748569834	-0.062968118200
Cl	2.116192371265	0.523164159227	-0.322279627265
F	0.378586202924	0.365229453078	1.546258439193

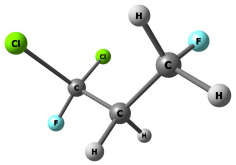
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
48.0943	0.473
133.3726	0.337
197.3342	0.202
249.1226	0.0890
260.2307	0.171
362.7136	0.527
378.5710	0.325
428.1898	0.687
470.3458	3.97
615.4260	5.58
760.1197	25.1
895.6821	2.03
929.8313	10.8
1005.7807	6.64
1098.4067	6.55
1115.2350	22.5
1179.3627	13.9
1258.8529	2.09
1300.4404	0.980
1372.2562	1.33
1430.7402	2.58
1451.1686	0.826
1513.5745	0.597
3034.6289	5.22
3064.6455	0.667
3085.4178	3.66
3131.0959	0.529

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
48.0914	0.473
133.3687	0.337
197.3355	0.202
249.1223	0.0890
260.2289	0.171
362.7127	0.527
378.5710	0.325
428.1890	0.687
470.3447	3.97
615.4275	5.58
760.1166	25.1
895.6821	2.03
929.8303	10.8
1005.7799	6.64
1098.4076	6.55
1115.2363	22.5
1179.3623	13.9
1258.8545	2.09
1300.4418	0.980
1372.2570	1.33
1430.7415	2.58
1451.1690	0.826
1513.5747	0.597
3034.6282	5.22
3064.6463	0.667
3085.4164	3.66
3131.0959	0.529



$\Delta E = 0.47$ kcal mol^{-1}
Population = 0.082



$\Delta E = 0.62$ kcal mol^{-1}
Population = 0.063

Optimized Coordinates (Angstroms)

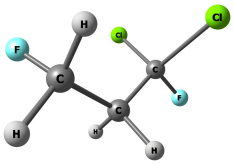
Atom	X	Y	Z
C	-1.866817727059	0.000217091520	0.453685831334
C	-0.905973180239	-0.011305728544	-0.730842793549
C	0.574241269573	-0.000299883672	-0.388727529600
F	-3.150163832142	-0.012067495898	-0.049597727535
H	-1.728227889998	-0.881907560384	1.087029609624
H	-1.736011006401	0.900014929993	1.063381576202
H	-1.092697804224	0.865221437013	-1.359347167577
H	-1.084962259541	-0.905799943572	-1.335844219421
Cl	1.037907532097	1.483686875273	0.529428915894
Cl	1.050748095364	-1.455298487054	0.568421854693
F	1.294224802570	-0.012156234675	-1.519442350066

Atom	X	Y	Z
C	-1.898624560524	0.818350796008	-0.184339025640
C	-0.705966816667	0.488405362542	-1.071252924445
C	0.566304572992	0.002490651035	-0.384146160757
F	-2.488648049709	-0.327138597272	0.298027734934
H	-1.603082782814	1.447716488282	0.661945545143
H	-2.640094681508	1.361918465369	-0.782038566931
H	-0.421557375355	1.385692645242	-1.631272814135
H	-0.991508215326	-0.282899702037	-1.793898007697
Cl	1.209025599892	1.248541056782	0.759455018413
Cl	0.335629868290	-1.542148903413	0.498164014984
F	1.509745440729	-0.201333262539	-1.318715813870

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
75.2455	0.760
106.2995	0.000
155.5767	0.386
259.7849	0.252
291.0464	0.206
312.0114	0.387
387.9900	0.494
405.9036	1.34
503.2195	0.0105
612.4777	6.74
699.5487	24.1
826.4352	8.74
1055.4613	11.4
1069.4712	4.31
1093.9965	25.0
1120.2140	10.9
1164.3598	11.3
1242.3058	0.503
1310.7740	0.385
1329.0076	2.40
1439.1858	2.13
1472.8947	0.425
1525.6888	0.274
3048.5932	2.33
3060.0175	1.63
3094.6267	1.23
3117.8673	2.45

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
51.1261	0.399
132.9423	0.321
200.2570	0.271
241.0378	0.142
281.0367	0.183
357.2653	0.0339
389.3279	0.497
432.2700	1.09
526.2283	2.99
559.0625	2.42
716.3028	27.5
901.1105	1.96
915.8886	8.18
1079.8099	6.81
1105.6729	18.5
1124.0263	10.4
1147.3548	18.5
1248.1387	1.04
1298.0239	0.744
1379.9223	2.01
1434.4210	1.87
1452.2577	0.491
1512.8817	0.803
3035.3789	4.90
3054.9059	0.511
3087.1274	3.59
3108.3026	1.10



$\Delta E = 0.62$ kcal mol^{-1}
Population = 0.063

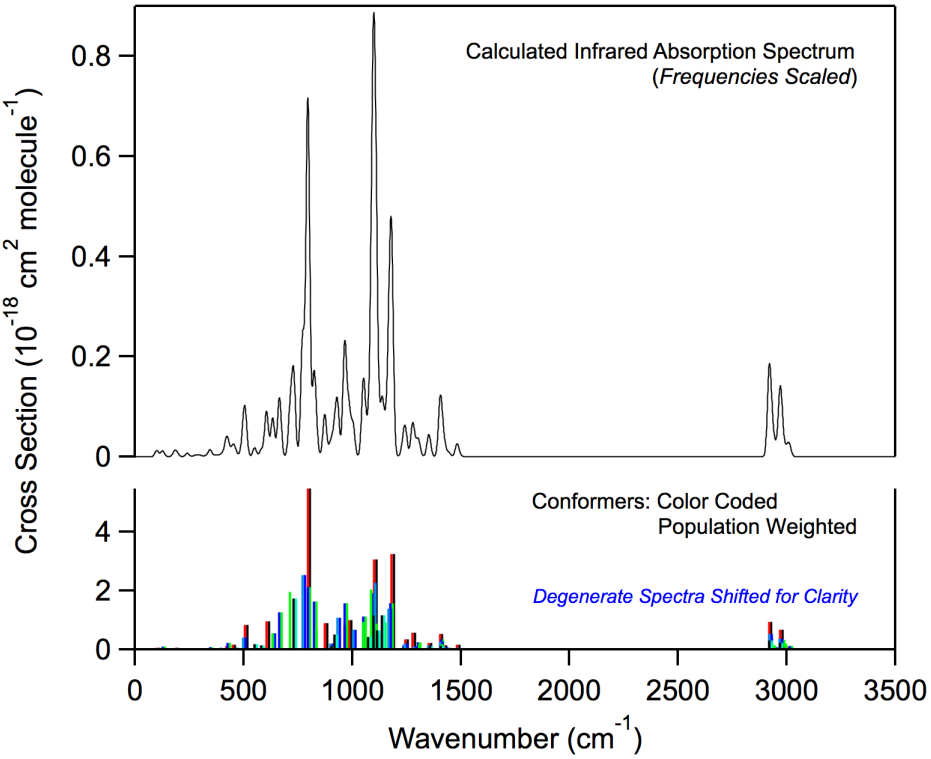
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.876371144016	-0.878111897600	-0.142557855437
C	-0.697772964320	-0.546042356790	-1.047294248530
C	0.562182222400	0.002771559761	-0.385313106953
F	-2.498449742883	0.266461667956	0.300071225461
H	-2.603674604553	-1.465380821987	-0.715823479495
H	-1.558650715355	-1.466468288131	0.724929416018
H	-1.009241951539	0.188988888596	-1.796545518530
H	-0.388919113021	-1.454685791829	-1.575131375466
Cl	0.288975104908	1.571626709687	0.440304232132
Cl	1.246609750285	-1.180163891406	0.800341686982
F	1.495258158094	0.199668221743	-1.331698976182

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
51.1253	0.399
132.9419	0.321
200.2567	0.271
241.0378	0.142
281.0367	0.183
357.2653	0.0339
389.3281	0.497
432.2700	1.09
526.2284	2.99
559.0626	2.42
716.3033	27.5
901.1110	1.96
915.8887	8.18
1079.8105	6.81
1105.6732	18.5
1124.0266	10.4
1147.3550	18.5
1248.1389	1.04
1298.0243	0.744
1379.9227	2.01
1434.4215	1.87
1452.2574	0.491
1512.8821	0.803
3035.3786	4.90
3054.9055	0.511
3087.1272	3.59
3108.3023	1.10

Infrared Spectrum



Radiative Efficiency