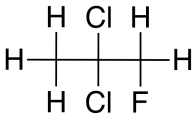
HCFC-261aa

Molecular Formula:	$CH_3CCl_2CH_2F$
Name:	2,2-Dichloro-1-fluoropropane
CAS number:	–
Molecular Weight:	130.98



Global Atmospheric Lifetime (years):	1.06
Tropospheric Atmospheric Lifetime (years):	1.11
Stratospheric Atmospheric Lifetime (years):	22.7
Ozone Depletion Potential (ODP):	0.020

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.097	0.073
Global Warming Potential (GWP_H):		
GWP_{20}	176	132
GWP_{100}	48	36
Global Temperature Potentials (GTP_H)		
GTP_{20}		43
GTP_{50}		6
GTP_{100}		5

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

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

OH Reactivity

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

k_{SAR}(298 K) = 5.27×10^{-14}; k_{SAR}(272 K) ≈ 3.37×10^{-14} cm^3 $molecule^{-1}$ s^{-1}

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

Fractional Atmospheric Loss: 0.982

O(^{1}D) Reactivity

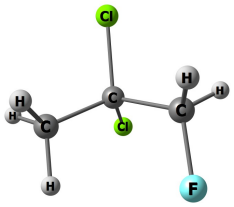
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 1.7 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)}$ = 220 years
Fractional Atmospheric Loss: 0.005

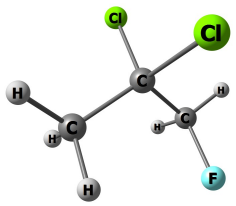
UV Photolysis

UV Spectrum: *No Recommendation*
τ_{hv} = 80 years
Fractional Atmospheric Loss: 0.013

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.479



E = 0
Population = 0.479

Optimized Coordinates (Angstroms)

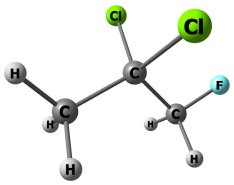
Atom	X	Y	Z
C	-0.049949711500	-0.327103334000	1.690051518900
C	0.094230863800	-0.103030783200	0.194636566200
C	-0.807856816100	-1.011804301700	-0.643120638900
Cl	1.791566992600	-0.456510258800	-0.331094422100
Cl	-0.298273201400	1.619865915800	-0.193180278700
H	0.592541466400	0.356220605000	2.245878394300
H	0.226426986600	-1.356625220700	1.934819938000
H	-1.091537498700	-0.159105693600	1.972447597100
H	-0.699740090800	-0.779245591800	-1.705836124600
H	-0.523539985500	-2.054685522300	-0.460457910100
F	-2.113720005400	-0.830253814800	-0.262125640100

Atom	X	Y	Z
C	-0.045230182600	0.331385022500	1.690039309500
C	0.097049128400	0.106485926900	0.194567079000
C	-0.811440949300	1.009703267800	-0.642276040200
Cl	-0.287375606000	-1.618824864700	-0.190639950300
Cl	1.791451444700	0.468148699400	-0.335022776300
H	0.601889052200	-0.348051015500	2.245262092200
H	-1.085365747900	0.158344845300	1.974738496800
H	0.226364220300	1.362566368900	1.933169503500
H	-0.532128937100	2.054229048700	-0.461282898500
H	-0.704290322200	0.776586649500	-1.704967151300
F	-2.115563100400	0.821816051300	-0.258415664400

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
125.4385	0.519
198.3695	0.629
249.7659	0.235
268.3208	0.0684
304.3150	0.151
352.1155	0.466
363.3772	0.330
430.1314	1.48
593.4925	7.23
717.0600	14.0
915.7298	1.57
965.4878	1.37
1089.4297	15.4
1099.4105	6.38
1151.0706	3.02
1206.1943	1.29
1282.4802	1.67
1399.9576	0.987
1421.2606	1.10
1479.4244	0.384
1482.8588	1.04
1499.4558	0.525
3044.8516	2.50
3056.8748	0.963
3113.1448	2.10
3135.0424	1.06
3157.9492	0.469

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
125.4417	0.519
198.3702	0.629
249.7658	0.235
268.3254	0.0684
304.3166	0.151
352.1157	0.466
363.3766	0.330
430.1333	1.48
593.4851	7.23
717.0662	14.0
915.7335	1.57
965.4892	1.37
1089.4343	15.4
1099.4212	6.39
1151.0711	3.02
1206.1979	1.29
1282.4855	1.67
1399.9595	0.987
1421.2640	1.10
1479.4258	0.384
1482.8594	1.04
1499.4576	0.525
3044.8363	2.50
3056.8723	0.963
3113.1382	2.10
3135.0387	1.06
3157.9491	0.469



$\Delta E = 1.43$ kcal mol^{-1}
Population = 0.043

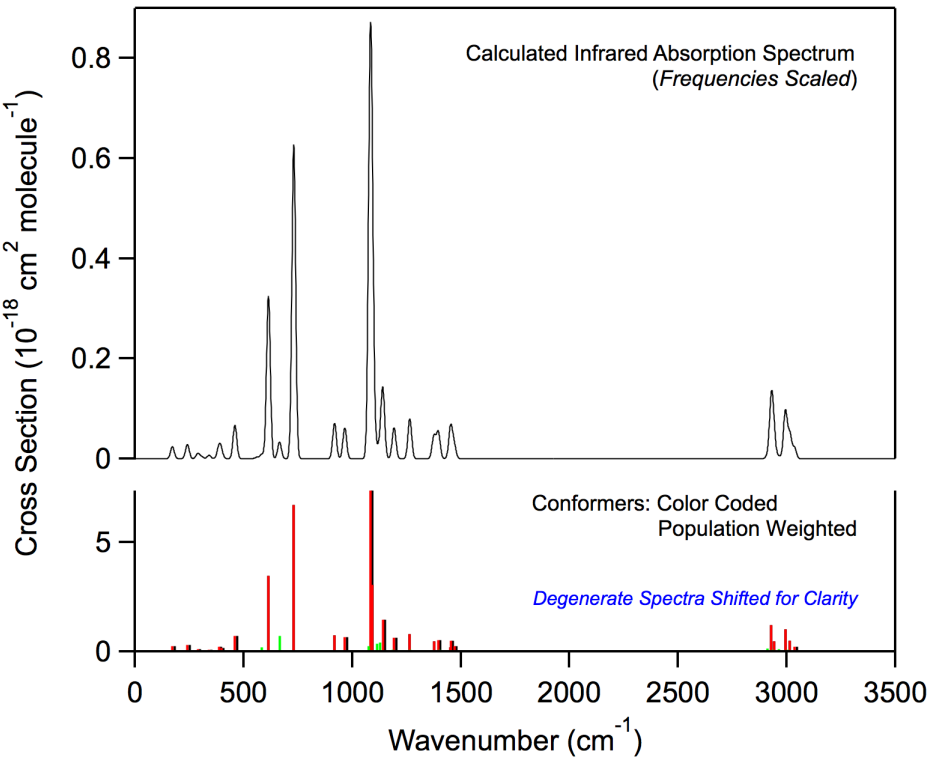
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.129851894800	0.545394740600	1.467370469800
C	0.204048566200	0.100403944100	0.346089768000
C	-1.081853656100	-0.525860572800	0.882483778900
Cl	1.051353071800	-1.119225806200	-0.689376313400
Cl	-0.233148434000	1.527101781000	-0.679066703000
H	1.406382181800	-0.314410509600	2.084189604400
H	0.627303450300	1.290660339600	2.090458626700
H	2.036835478300	0.987282426700	1.053773812000
H	-0.816810009700	-1.396019132900	1.495372068000
H	-1.599647205500	0.216797547700	1.501680581000
F	-1.905926337900	-0.921894758100	-0.128263692300

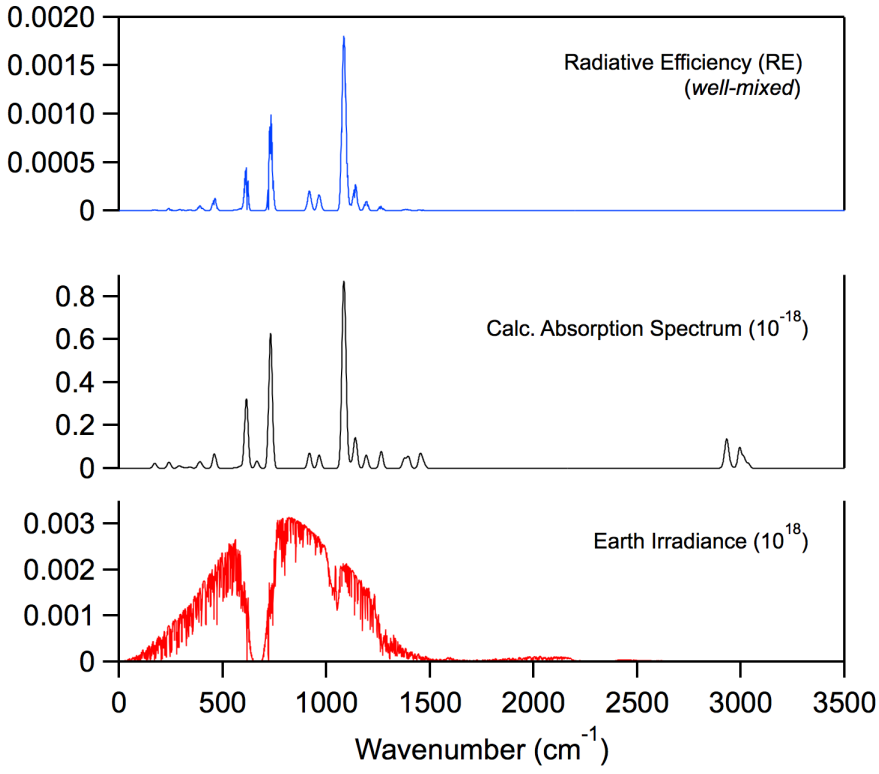
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
117.9232	0.236
188.8038	0.0124
257.1440	0.0005
270.6884	0.275
287.4705	0.00948
345.6140	0.0239
354.5189	0.614
537.6114	1.54
561.8881	4.52
647.7197	16.5
914.3641	0.0773
1013.6906	0.0589
1081.9315	5.47
1122.5829	8.38
1138.7292	9.41
1200.2270	2.06
1285.4366	2.04
1408.6094	0.408
1426.5439	1.83
1476.5143	0.597
1485.6739	0.416
1494.7950	0.900
3027.0528	3.06
3051.3769	1.72
3080.8110	2.55
3125.5632	1.76
3152.8727	0.504

Infrared Spectrum

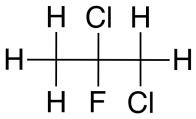


Radiative Efficiency



HCFC-261ba

Molecular Formula:	$CH_3CClFCH_2Cl$
Name:	1,2-Dichloro-2-fluoropropane
CAS number:	420-97-3
Molecular Weight:	130.98



Global Atmospheric Lifetime (years):	2.19
Tropospheric Atmospheric Lifetime (years):	2.31
Stratospheric Atmospheric Lifetime (years):	43.5
Ozone Depletion Potential (ODP):	0.031

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.097	0.083
Global Warming Potential (GWP_H):		
GWP_{20}	365	312
GWP_{100}	99	84
Global Temperature Potentials (GTP_H)		
GTP_{20}		118
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*

$k_{SAR}(298\ K) = 2.54 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 1.62 \times 10^{-14}$ 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: 0.980

O(^{1}D) Reactivity

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

$k_{Est}(T) = 1.7 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 220$ years

Fractional Atmospheric Loss: 0.010

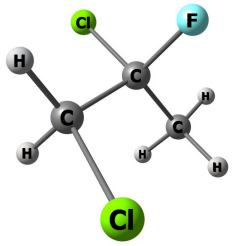
UV Photolysis

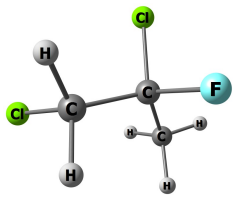
UV Spectrum: *No Recommendation*

$\tau_{hv} = 225$ years

Fractional Atmospheric Loss: 0.010

Molecular Structure and Infrared Spectrum (2 conformers)





E = 0
Population = 0.911

$\Delta E = 1.57$ kcal mol^{-1}
Population = 0.064

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-0.387407204800	1.527995890300	-0.712023339600
C	-0.420803312100	0.246643686400	0.095303670300
C	0.612140614000	-0.816032940400	-0.270152099300
Cl	-2.045617842400	-0.577105365000	-0.147423110600
F	-0.314979332100	0.534991186600	1.415584365100
H	-1.187498715400	2.189158624600	-0.375621116400
H	-0.520233058200	1.316811359800	-1.774550578200
H	0.575931134900	2.020655794400	-0.559681403600
H	0.492344600100	-1.682731868200	0.377439591600
H	0.508324778200	-1.107780312600	-1.313550793800
Cl	2.296074337900	-0.209355056000	-0.037769185600

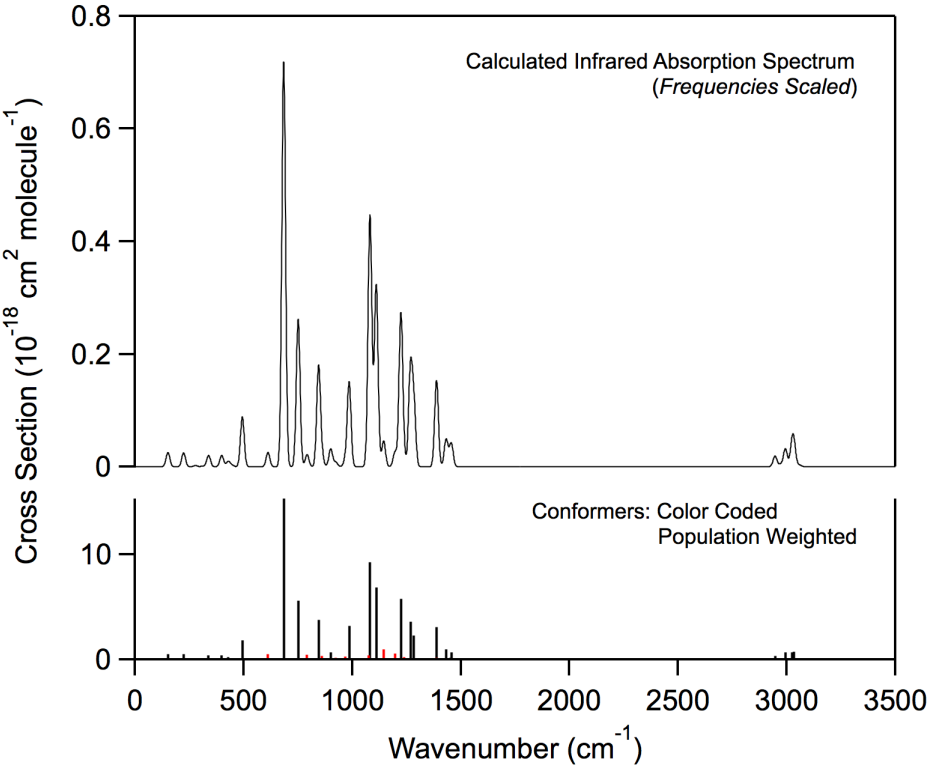
Atom	X	Y	Z
C	-0.683525794000	1.017802310000	-1.337259818000
C	-0.613146512300	0.400287493200	0.043947084800
C	0.716910809200	0.559431112300	0.784493719400
Cl	-1.058864383300	-1.361046924100	-0.045405536500
F	-1.536934678800	1.002565222000	0.853949962200
H	-1.694682564100	0.907650180100	-1.732173279000
H	0.024115382700	0.536348903400	-2.011905096800
H	-0.442460672000	2.083208988400	-1.264296887400
H	0.893394428500	1.625307789300	0.939590197900
H	0.664841220500	0.049943075700	1.745336088000
Cl	2.127630763600	-0.091525150200	-0.109507434600

Infrared Absorption Spectrum (unscaled frequencies)

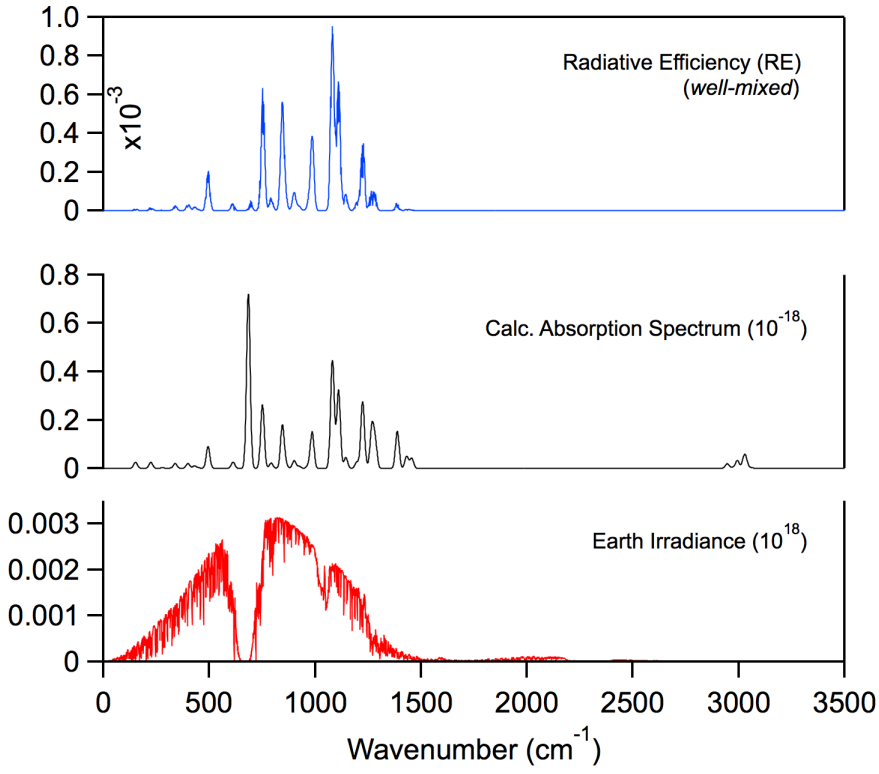
Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
103.9790	0.572
179.9824	0.548
238.4288	0.0471
273.3949	0.0223
301.5514	0.425
365.4534	0.455
398.1506	0.223
466.0808	2.02
667.9519	16.8
738.4592	6.13
837.9913	4.17
897.1505	0.740
987.0116	3.50
1088.5924	10.2
1118.8912	7.55
1239.2552	6.35
1285.6958	3.98
1302.4177	2.52
1412.8394	3.38
1459.2487	1.10
1480.4647	0.190
1485.7575	0.752
3064.1856	0.395
3113.2574	0.749
3145.9173	0.734
3154.9249	0.790
3183.3955	0.0647

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
95.6115	0.359
180.5638	0.413
237.1683	0.0325
301.9763	0.308
307.0401	0.315
376.7782	0.360
416.2320	0.800
472.0653	1.000
591.2584	8.41
781.9279	7.11
854.7613	5.37
922.0132	2.64
968.5990	4.11
1080.7384	6.25
1155.0614	15.0
1210.2364	8.53
1254.0686	3.48
1306.6913	0.321
1411.8112	3.01
1464.7197	0.815
1480.8567	0.377
1486.1356	0.565
3055.1826	1.06
3091.1600	1.46
3136.1749	1.09
3164.6677	0.211
3167.2529	0.455

Infrared Spectrum

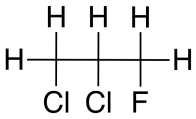


Radiative Efficiency



HCFC-261da

Molecular Formula:	$CH_2ClCHClCH_2F$
Name:	1,2-Dichloro-3-fluoropropane
CAS number:	453-01-0
Molecular Weight:	130.98



Global Atmospheric Lifetime (years):	0.450
Tropospheric Atmospheric Lifetime (years):	0.462
Stratospheric Atmospheric Lifetime (years):	20
Ozone Depletion Potential (ODP):	0.009

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.058	0.034
Global Warming Potential (GWP_H):		
GWP_{20}	45	26
GWP_{100}	12	7
Global Temperature Potentials (GTP_H)		
GTP_{20}		8
GTP_{50}		1
GTP_{100}		1

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 1.27 \times 10^{-13}$; $k_{SAR}(272\ K) \approx 0.81 \times 10^{-13}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 0.452$ years

$\tau^{OH}_{Trop} = 0.462$ years

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

Fractional Atmospheric Loss: 0.996

$O(^1D)$ Reactivity

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

$k_{Est}(T) = 1.7 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 220$ years

Fractional Atmospheric Loss: 0.002

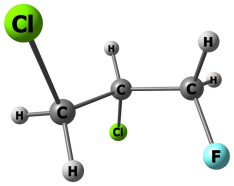
UV Photolysis

UV Spectrum: *No Recommendation*

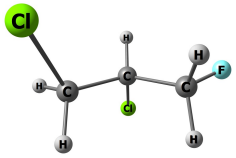
$\tau_{hv} = 225$ years

Fractional Atmospheric Loss: 0.002

Molecular Structure and Infrared Spectrum (4 conformers)



E = 0
Population = 0.662



$\Delta E = 1.01$ kcal mol^{-1}
Population = 0.120

Optimized Coordinates (Angstroms)

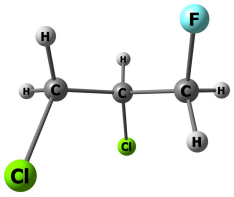
Atom	X	Y	Z
C	0.699330922500	-0.755213659600	-0.450866427700
C	-0.311055234300	-0.222854898100	0.557937978900
C	-0.435953022100	1.292069157400	0.558240463600
H	-0.072684877900	-0.568479572000	1.565256592500
Cl	-1.916938706600	-0.968936731000	0.136590797100
H	0.519736677100	-0.327795245500	-1.435764208100
H	0.673424744000	-1.841503116500	-0.497815468400
Cl	2.381508790100	-0.293218276100	0.037563853600
H	-1.246518813200	1.607205763800	1.222724330100
H	0.509788068200	1.728029975600	0.901651889800
F	-0.695250547900	1.743789602000	-0.714195801300

Atom	X	Y	Z
C	0.911875032700	-0.873101098500	-0.187325365000
C	-0.291096661700	-0.084614096300	0.312805308000
C	-0.527533665400	1.219414520500	-0.432359397900
H	-0.207095356500	0.110951617900	1.382758332900
Cl	-1.743669319000	-1.161983285600	0.123611174100
H	0.872566282200	-1.025301333400	-1.266452130900
H	0.974200409200	-1.836941067700	0.313711457000
Cl	2.457186206000	0.001514836700	0.172849254900
H	0.370067295300	1.843867758800	-0.355916669500
H	-0.743358893200	1.022016327200	-1.489274505700
F	-1.585155329700	1.889700820500	0.126423542200

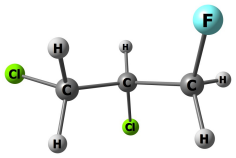
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
78.1957	0.392
133.6779	0.524
200.0557	0.996
233.5404	1.47
287.6904	0.251
362.4588	0.560
596.5087	2.57
681.4592	11.2
737.3814	3.40
871.4420	0.208
944.6801	2.16
1009.3885	2.38
1089.5415	3.73
1136.3652	6.21
1185.3733	1.04
1226.0894	2.40
1277.8996	2.63
1307.1021	0.140
1365.0956	0.139
1423.1764	1.35
1475.8389	0.871
1499.9361	1.54
3042.1894	2.92
3097.4531	2.89
3109.2213	0.449
3118.2549	0.929
3187.7407	0.0291

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
97.1307	1.19
110.7492	0.471
189.4843	0.647
215.7087	0.199
294.1210	0.0497
382.6606	0.571
491.9657	2.39
672.5292	11.2
733.4300	5.18
856.2481	0.467
1001.9673	2.00
1052.3425	0.0437
1100.9881	4.36
1121.3523	9.13
1184.0897	1.60
1235.7686	1.31
1285.4199	2.78
1314.9479	0.193
1341.3484	0.975
1433.6662	1.17
1482.3501	1.01
1503.7970	0.580
3033.1268	3.38
3084.9444	2.10
3100.8343	0.460
3118.3587	1.43
3171.9226	0.163



E = 1.18 kcal mol^{-1}
Population = 0.090



E = 1.21 kcal mol^{-1}
Population = 0.086

Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	0.774676725400	-0.044832827000	0.965516882800
C	-0.672862510700	0.144362938100	0.540361249800
C	-0.876970441300	1.231610578500	-0.509606874200
H	-1.237079676900	0.405490726600	1.440471137000
Cl	-1.411927276700	-1.385489301400	-0.074274403000
H	0.861380247400	-0.828132909000	1.716975407300
H	1.139612432500	0.901641287100	1.367088362600
Cl	1.880851282000	-0.491604307500	-0.386359340900
H	-0.343690997700	0.984031928100	-1.431834101100
H	-1.942620440600	1.357746237500	-0.722881270600
F	-0.374255343500	2.411503649000	0.002939950300

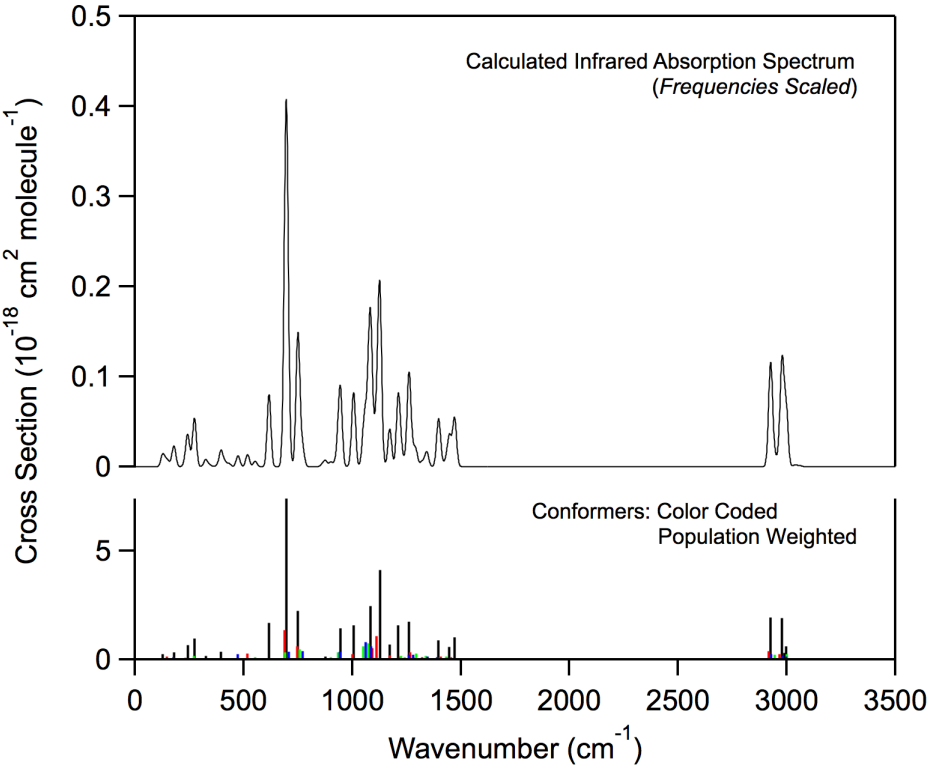
Atom	X	Y	Z
C	0.512280154900	0.771353016600	-0.459436109100
C	-0.453511524700	-0.099787696700	0.325303270300
C	-1.904687756700	0.222317692300	-0.033239954800
H	-0.297071299400	0.033056307300	1.396776648000
Cl	-0.193882468000	-1.857332824000	-0.010375071300
H	0.207235877600	1.812654426400	-0.348316569600
H	0.522187499000	0.499964150600	-1.515592996100
Cl	2.203600512700	0.649517752000	0.140648436800
H	-2.085194596000	0.060802337400	-1.102228761700
H	-2.585392226000	-0.409589495500	0.544834843500
F	-2.148471173600	1.546627333600	0.269474263900

Infrared Absorption Spectrum (unscaled frequencies)

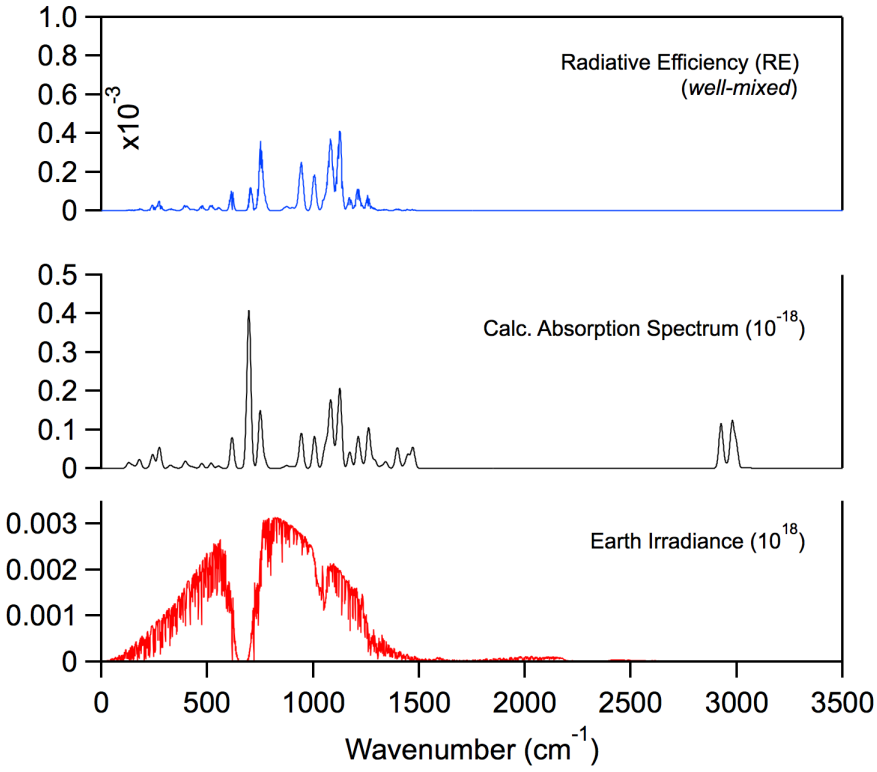
Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
74.9515	0.231
136.3376	0.444
195.1429	0.460
229.9326	2.05
308.2851	0.437
402.1246	0.775
528.8565	1.42
674.6487	3.71
744.5066	5.24
896.8418	1.15
931.4249	3.89
1056.9292	6.92
1080.0504	8.38
1113.3501	1.08
1204.7401	0.149
1240.4031	1.83
1258.5763	1.29
1313.0104	3.02
1361.0004	1.79
1421.0967	0.908
1459.1070	1.46
1509.6826	0.783
3060.0778	2.56
3074.9042	0.569
3097.5099	1.36
3119.7848	2.81
3163.0681	0.146

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
85.8301	0.286
129.2701	1.33
182.8501	0.192
210.2913	0.481
345.9358	0.363
378.6324	0.526
445.2627	3.02
692.6880	4.25
760.6657	4.68
915.1292	0.628
940.8966	4.38
1067.4241	9.37
1092.5037	7.16
1110.1391	0.0874
1174.1463	0.313
1241.8135	0.684
1278.6557	2.63
1297.7739	2.64
1368.8715	1.52
1415.3314	1.48
1467.8188	0.975
1510.7113	0.387
3044.4551	3.08
3089.8656	1.11
3099.3654	2.04
3117.7055	1.67
3156.0899	0.248

Infrared Spectrum

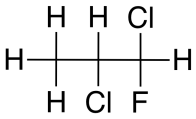


Radiative Efficiency



HCFC-261db

Molecular Formula:	$CH_3CHClCHClF$
Name:	1,2-Dichloro-1-fluoropropane
CAS number:	7799-55-5
Molecular Weight:	130.98



Global Atmospheric Lifetime (years):	0.465
Tropospheric Atmospheric Lifetime (years):	0.478
Stratospheric Atmospheric Lifetime (years):	20
Ozone Depletion Potential (ODP):	0.009

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.106	0.062
Global Warming Potential (GWP_H):		
GWP_{20}	85	50
GWP_{100}	23	14
Global Temperature Potentials (GTP_H)		
GTP_{20}		15
GTP_{50}		2
GTP_{100}		2

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 1.23 \times 10^{-13}$; $k_{SAR}(272\ K) \approx 0.783 \times 10^{-13}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 0.467$ years
$\tau^{OH}_{Trop} = 0.478$ years
$\tau^{OH}_{Strat} = 20$ years

Fractional Atmospheric Loss: 0.996

O(^{1}D) Reactivity

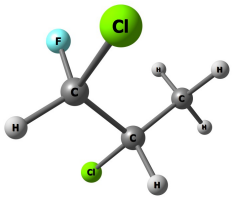
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 1.7 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)} = 220$ years
Fractional Atmospheric Loss: 0.002

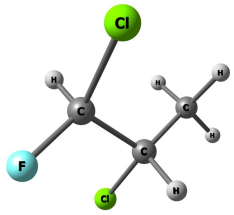
UV Photolysis

UV Spectrum: *No Recommendation*
$\tau_{hv} = 225$ years
Fractional Atmospheric Loss: 0.002

Molecular Structure and Infrared Spectrum (5 conformers)



E = 0
Population = 0.596



$\Delta E = 0.57$ kcal mol^{-1}
Population = 0.228

Optimized Coordinates (Angstroms)

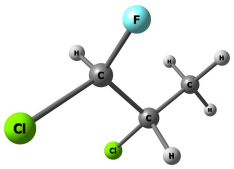
Atom	X	Y	Z
C	0.489918439645	1.620353414655	-0.650345293421
C	0.513090761401	0.505204149927	0.382727402080
C	-0.520649780363	-0.591484518644	0.140656179558
H	1.273924575109	2.347635096864	-0.433982737015
H	0.646499232497	1.216302007058	-1.651902390614
H	-0.478680401401	2.127523060582	-0.621382000087
H	0.381327797556	0.883875941787	1.396166039755
Cl	2.145093939786	-0.311047669314	0.387139883784
F	-0.484929586932	-1.014236293188	-1.140107238435
H	-0.387144106001	-1.442506184559	0.809156615619
Cl	-2.182199871295	0.054217994835	0.492973538776

Atom	X	Y	Z
C	-0.539296097673	1.874185651334	0.055468489456
C	-0.527348396390	0.413934417501	-0.368537393239
C	0.519158343514	-0.441778659626	0.339600922868
H	-1.364409180495	2.393813613056	-0.434826796741
H	-0.670068882681	1.966324659163	1.137395130505
H	0.398968393232	2.356138817120	-0.228960147497
H	-0.392788795485	0.302409775365	-1.445611057473
Cl	-2.145817599218	-0.339408349311	-0.001283697020
H	0.417061942824	-0.409127513432	1.426461769397
F	0.458062750554	-1.719506447362	-0.084693885063
Cl	2.181497521818	0.186871036192	-0.032519335192

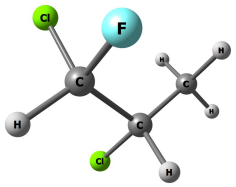
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
80.1209	0.356
191.8012	0.566
235.6100	0.0237
254.3830	0.364
267.9958	0.391
348.2604	0.606
386.0201	0.294
641.5733	1.90
670.7733	13.8
756.6380	12.4
879.1723	2.26
998.2886	5.04
1058.6468	5.87
1110.4149	5.00
1173.1797	10.6
1247.0030	3.80
1279.9029	0.442
1342.3407	0.182
1388.9440	1.38
1416.0984	1.78
1488.1951	1.09
1494.1630	0.653
3060.3187	1.01
3117.7409	0.594
3124.9170	0.794
3136.6639	1.38
3155.1314	0.971

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
73.2496	0.226
186.0005	0.279
229.3347	0.119
272.0769	0.180
340.0207	0.0312
345.2209	1.23
382.0241	0.532
504.7722	1.02
674.7885	15.5
754.2993	10.5
904.5901	2.09
1020.4475	5.33
1102.7276	2.70
1140.4375	12.0
1150.5030	2.52
1218.4667	7.24
1280.4480	0.515
1325.7169	0.742
1401.1808	1.04
1414.1025	1.61
1488.9074	1.31
1492.8631	0.810
3055.5871	1.09
3099.5313	0.676
3113.5974	0.724
3135.1285	2.01
3143.3428	1.14



$\Delta E = 1.29$ kcal mol^{-1}
Population = 0.068



$\Delta E = 1.29$ kcal mol^{-1}
Population = 0.067

Optimized Coordinates (Angstroms)

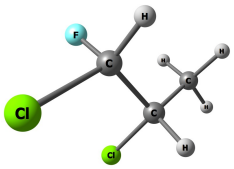
Atom	X	Y	Z
C	1.635627960405	1.508136059685	0.033929735569
C	0.714878948830	0.334986963786	0.348701112676
C	-0.628143393310	0.462151120173	-0.374064729447
H	1.169951196496	2.437778169044	0.370079094847
H	2.589720666479	1.381516673380	0.548715307734
H	1.829266985981	1.578924500217	-1.040108721481
H	0.534994061318	0.248634829594	1.421214883834
Cl	1.494532664393	-1.220351531609	-0.152266271466
F	-1.129289916079	1.704009727606	-0.140939788966
H	-0.530328189203	0.307463548484	-1.450663945670
Cl	-1.829113985312	-0.744563060361	0.209925322370

Atom	X	Y	Z
C	-0.646727654149	1.342960988310	1.160618185253
C	-0.660193757655	0.677612940042	-0.204843805079
C	0.698198466547	0.150992436020	-0.672299268111
H	-1.617724357945	1.796717288939	1.367194320125
H	-0.417937093137	0.621396901112	1.946520992400
H	0.117954177776	2.125704061702	1.166109937315
H	-0.973226425927	1.388223304946	-0.974580651075
Cl	-1.874007756123	-0.662385327342	-0.281425833495
H	0.623488866830	-0.380837407878	-1.621860747150
F	1.525485828303	1.220274539541	-0.817542009777
Cl	1.455901705480	-1.004419725392	0.483335879593

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
73.4202	0.198
167.2246	0.116
236.8144	0.0642
304.8235	0.498
321.5049	0.674
371.2726	0.883
401.8404	1.20
445.1889	0.877
723.0142	5.15
765.7166	12.3
920.8072	6.24
1027.1498	4.02
1086.7878	9.54
1097.7230	9.63
1146.6747	1.70
1228.2076	4.60
1286.0235	3.77
1336.0842	1.73
1380.9894	0.524
1409.2736	0.684
1488.5740	1.47
1492.4501	0.516
3053.8867	1.35
3099.8706	0.678
3112.7979	0.618
3134.1664	2.22
3142.8810	1.00

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
83.5649	0.280
176.6144	0.134
233.5870	0.554
248.5838	0.414
301.8627	0.228
361.8949	0.414
432.8620	0.487
540.0088	3.21
719.7607	5.00
737.4681	9.97
905.9512	5.50
1026.3905	3.81
1076.5380	1.24
1094.0265	21.0
1145.9695	1.95
1251.5633	1.80
1288.9460	3.75
1358.1209	0.693
1362.7952	3.34
1410.8201	1.53
1485.9460	0.980
1493.2935	0.836
3056.5366	1.10
3080.8717	0.829
3114.8179	1.61
3132.7882	1.10
3152.3536	1.11



$\Delta E = 1.97$ kcal mol^{-1}
Population = 0.021

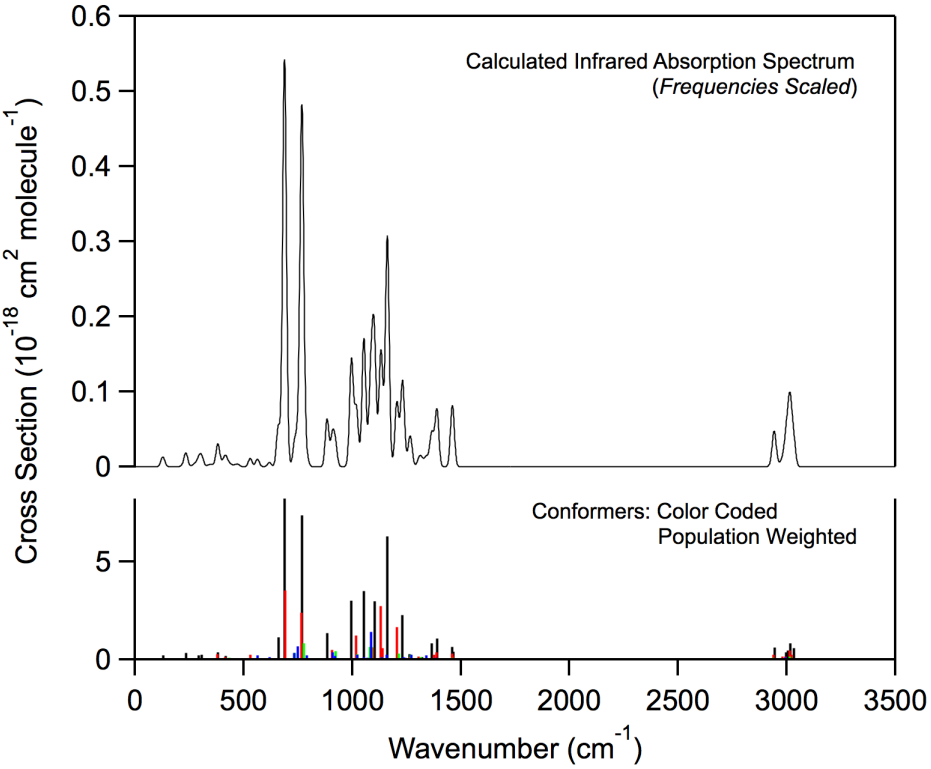
Optimized Coordinates (Angstroms)

z	X	Y	Z
C	-1.8514088826021	1.214295608143	-0.477589848429
C	-0.730215136876	0.186447546720	-0.598838219350
C	0.586766551145	0.757615213766	-0.079620044537
H	-1.608938869266	2.104166438084	-1.069518527797
H	-2.788084678093	0.796719564828	-0.850195101255
H	-1.986060054818	1.511288193699	0.564440476728
H	-0.582842566793	-0.120764296903	-1.635047351415
Cl	-1.172811409759	-1.315631018711	0.305757306578
H	0.831691241112	1.672257659654	-0.628705208695
F	0.498498290276	1.047402042857	1.237588670749
Cl	1.980302459094	-0.350150952137	-0.351339152579

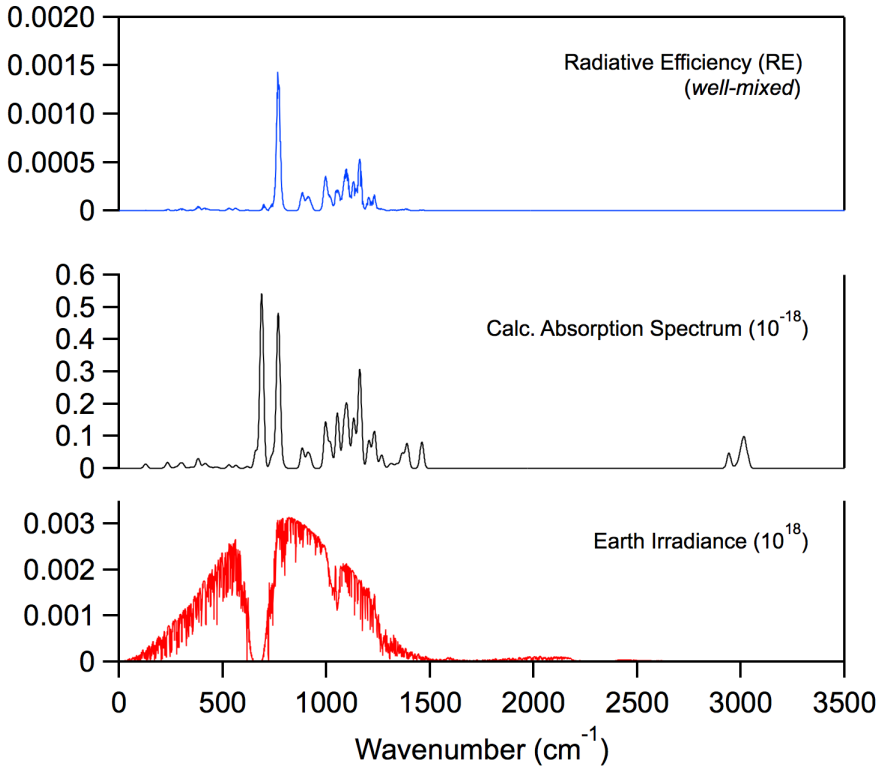
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
79.8900	0.00477
173.1982	0.0701
223.9107	0.0391
249.0422	0.00227
298.8749	0.154
372.5055	0.671
419.0892	1.58
598.1892	5.56
684.8637	1.85
781.9357	10.1
917.7453	8.78
983.4272	2.72
1058.8891	5.98
1095.5768	0.607
1168.6443	11.9
1259.6599	4.28
1285.5696	2.83
1337.0166	1.12
1376.8516	3.34
1410.1924	0.472
1486.1811	1.23
1495.1332	0.474
3043.3436	1.74
3070.9203	2.68
3109.9186	0.155
3123.5483	2.34
3151.7981	0.970

Infrared Spectrum

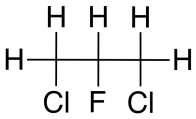


Radiative Efficiency



HCFC-261ea

Molecular Formula: $CH_2ClCHFCH_2Cl$
Name: 1,3-Dichloro-2-fluoropropane
CAS number: 816-38-6
Molecular Weight: 130.98



Global Atmospheric Lifetime (years): 0.536
  Tropospheric Atmospheric Lifetime (years): 0.554
  Stratospheric Atmospheric Lifetime (years): 20
Ozone Depletion Potential (ODP): 0.011

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.080	0.049
Global Warming Potential (GWP_H):		
GWP_{20}	73	45
GWP_{100}	20	12
Global Temperature Potentials (GTP_H)		
GTP_{20}		14
GTP_{50}		2
GTP_{100}		2

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 1.06 \times 10^{-13}$; $k_{SAR}(272\ K) \approx 0.676 \times 10^{-13}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 0.539$ years
$\tau^{OH}_{Trop} = 0.554$ years
$\tau^{OH}_{Strat} = 20$ years

Fractional Atmospheric Loss: 0.995

O(^{1}D) Reactivity

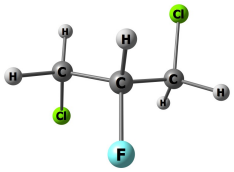
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 1.7 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)} = 220$ years
Fractional Atmospheric Loss: 0.002

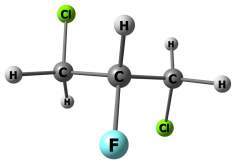
UV Photolysis

UV Spectrum: *No Recommendation*
$\tau_{hv} = 225$ years
Fractional Atmospheric Loss: 0.002

Molecular Structure and Infrared Spectrum (7 conformers)



E = 0
Population = 0.285



E = 0
Population = 0.285

Optimized Coordinates (Angstroms)

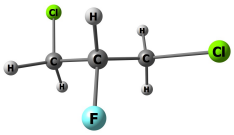
Atom	X	Y	Z
C	-1.063587497700	0.617226830900	-0.590998199400
C	-0.033574088300	0.924103351500	0.491609864200
C	0.848996366700	-0.238647978100	0.914218010700
H	-0.550253678000	1.285313128400	1.391758269100
F	0.756378076900	1.947733555600	0.008664146800
H	-0.600905627800	0.145975954100	-1.457022057100
H	-1.564409772600	1.537674171500	-0.888669993500
Cl	-2.328239437400	-0.507372209700	0.031488389000
H	1.571654973900	0.098621942500	1.657021784900
H	0.244208827200	-1.047393458700	1.323461311200
Cl	1.802202857200	-0.917653287900	-0.459723525800

Atom	X	Y	Z
C	-0.858511765900	-0.216601485500	0.916558500900
C	0.024649530400	0.943768816300	0.488673362300
C	1.065118733900	0.627562424500	-0.581176008400
H	0.532288136000	1.316583651300	1.389234015300
F	-0.763724402600	1.959651176900	-0.012854946000
H	-1.588686977200	0.127018589700	1.649029233100
H	-0.255218502900	-1.018966159900	1.340310260200
Cl	-1.797564982700	-0.913774478700	-0.458029910000
H	0.611468078300	0.145252065400	-1.445888072300
H	1.566088629900	1.545986540800	-0.884789116500
Cl	2.327197522800	-0.486373140800	0.065247681400

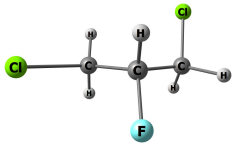
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
58.8199	0.283
143.9705	0.717
201.1459	0.336
213.1033	1.53
366.1893	1.03
388.8315	0.338
565.1014	2.33
707.6780	2.34
770.6670	8.70
839.4002	1.93
896.2982	0.830
986.1214	0.480
1068.8052	8.19
1128.7400	4.18
1150.7992	0.313
1232.8877	2.00
1278.1832	2.19
1315.7017	2.72
1373.3709	1.91
1389.8914	2.40
1460.3084	2.27
1481.1740	1.81
3025.1599	2.50
3101.6642	1.61
3106.2498	1.10
3165.8788	0.245
3173.6961	0.179

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
58.8198	0.283
143.9704	0.717
201.1459	0.336
213.1033	1.53
366.1894	1.03
388.8314	0.338
565.1016	2.33
707.6783	2.34
770.6663	8.70
839.4002	1.93
896.2983	0.830
986.1215	0.480
1068.8049	8.19
1128.7398	4.18
1150.7993	0.313
1232.8880	2.00
1278.1829	2.19
1315.7023	2.72
1373.3706	1.91
1389.8917	2.40
1460.3087	2.27
1481.1740	1.81
3025.1605	2.50
3101.6638	1.61
3106.2502	1.10
3165.8783	0.245
3173.6967	0.179



$\Delta E = 0.46$ kcal mol^{-1}
Population = 0.132



$\Delta E = 0.46$ kcal mol^{-1}
Population = 0.132

Optimized Coordinates (Angstroms)

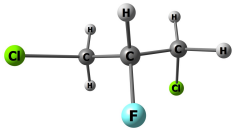
Atom	X	Y	Z
C	0.758617227000	0.382018966300	-0.540655146600
C	0.012947163400	-0.619866861400	0.322522868800
C	-1.454231608800	-0.776397441500	-0.080801273400
H	0.083160439500	-0.338600110900	1.378781606900
F	0.583860009600	-1.867765378100	0.165120715200
H	0.277795152200	1.358582043000	-0.499859798500
H	0.805325720800	0.032485093500	-1.573544382200
Cl	2.455939445900	0.592344647800	0.022765673400
H	-1.556109419200	-0.961452088000	-1.151177356300
H	-1.893738830800	-1.604553273600	0.474344659300
Cl	-2.409454299600	0.701098402900	0.308613433400

Atom	X	Y	Z
C	-1.454939108400	0.776623762300	-0.092572400800
C	0.010970861100	0.621297824800	0.315798207200
C	0.766073118800	-0.363477997600	-0.558795383900
H	0.077304031500	0.324226444500	1.367972659600
F	0.576300540400	1.874313925700	0.180432827600
H	-1.552375684100	0.977543264500	-1.160498668200
H	-1.901449742700	1.593958259800	0.472925641800
Cl	-2.404562717900	-0.711444053700	0.269310902200
H	0.290031417400	-1.342951050300	-0.535422486100
H	0.816204636600	0.002092938600	-1.585956660800
Cl	2.461584647200	-0.573908318600	0.010013361500

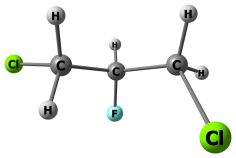
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
76.3295	0.407
103.7235	1.16
194.9759	0.502
200.5184	0.0557
356.7415	0.234
416.1586	1.91
459.6407	1.65
747.8797	4.50
766.4853	7.36
850.0118	2.19
888.3728	1.68
1032.9527	0.829
1068.4797	7.71
1108.7953	3.34
1160.8164	3.14
1233.4397	0.673
1274.3672	2.94
1296.0081	1.98
1374.1570	0.0141
1397.4910	0.944
1463.7986	1.36
1483.9294	1.03
3065.6550	1.13
3090.1502	1.08
3093.9665	2.72
3158.5479	0.374
3162.7127	0.409

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
76.3291	0.407
103.7241	1.16
194.9764	0.502
200.5190	0.0557
356.7410	0.234
416.1586	1.91
459.6404	1.65
747.8791	4.50
766.4844	7.36
850.0110	2.19
888.3725	1.68
1032.9524	0.829
1068.4789	7.71
1108.7933	3.34
1160.8158	3.14
1233.4390	0.673
1274.3663	2.94
1296.0078	1.98
1374.1567	0.0141
1397.4894	0.944
1463.7976	1.36
1483.9293	1.03
3065.6586	1.13
3090.1509	1.08
3093.9674	2.72
3158.5490	0.374
3162.7137	0.409



$\Delta E = 0.84$ kcal mol^{-1}
Population = 0.068



$\Delta E = 0.84$ kcal mol^{-1}
Population = 0.068

Optimized Coordinates (Angstroms)

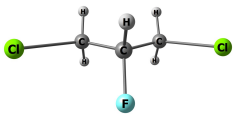
Atom	X	Y	Z
C	-1.349878897800	0.129239333500	0.958220557900
C	0.072264077400	0.494325367000	0.550945128700
C	0.874005030300	-0.680683080000	0.014255514400
H	0.567815546300	0.895487275800	1.446842614100
F	0.032487982200	1.491579935000	-0.393498656400
H	-1.883656009900	1.031114133300	1.257834855500
H	-1.344086280200	-0.583797631500	1.783885030400
Cl	-2.303418237500	-0.612599676700	-0.383351171100
H	0.845318021900	-1.518905914900	0.711760906300
H	0.492913925900	-0.995698901200	-0.955757908100
Cl	2.604944841500	-0.233525840200	-0.210244871700

Atom	X	Y	Z
C	-0.879448344600	-0.687186390100	0.017438059300
C	-0.071098470500	0.476570239200	0.568537323000
C	1.350041782500	0.099210139600	0.968045873200
H	-0.563049582000	0.867827801500	1.470777070000
F	-0.028324372100	1.486410623900	-0.362304832600
H	-0.853453655800	-1.534976113200	0.703390722400
H	-0.501688724000	-0.990744648700	-0.957519481600
Cl	-2.608651780900	-0.228793043100	-0.197578858000
H	1.888685275600	0.994368021000	1.278884346200
H	1.342389544600	-0.624983257200	1.783927124800
Cl	2.297508327200	-0.628794372900	-0.385356346600

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
78.0239	0.619
94.8206	0.452
159.6564	0.102
227.2552	0.115
327.4842	0.133
439.0792	2.07
577.3381	5.40
687.8805	2.59
783.3637	4.56
855.0903	1.18
889.8445	2.39
955.5800	0.307
1076.8519	0.558
1094.7889	8.84
1218.3032	2.09
1224.1395	0.994
1268.8960	1.72
1307.5971	6.11
1368.5408	1.22
1397.1468	2.00
1460.7431	1.48
1466.0749	0.756
3018.5674	2.32
3091.1040	1.96
3097.3907	1.69
3155.0886	0.347
3169.1062	0.260

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
78.0238	0.619
94.8210	0.452
159.6565	0.102
227.2560	0.115
327.4848	0.133
439.0793	2.07
577.3384	5.40
687.8794	2.59
783.3646	4.56
855.0903	1.18
889.8450	2.39
955.5806	0.307
1076.8529	0.558
1094.7878	8.84
1218.3037	2.09
1224.1390	0.994
1268.8961	1.72
1307.5974	6.11
1368.5418	1.22
1397.1466	2.00
1460.7437	1.48
1466.0756	0.756
3018.5654	2.32
3091.1044	1.96
3097.3904	1.69
3155.0890	0.347
3169.1038	0.260



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

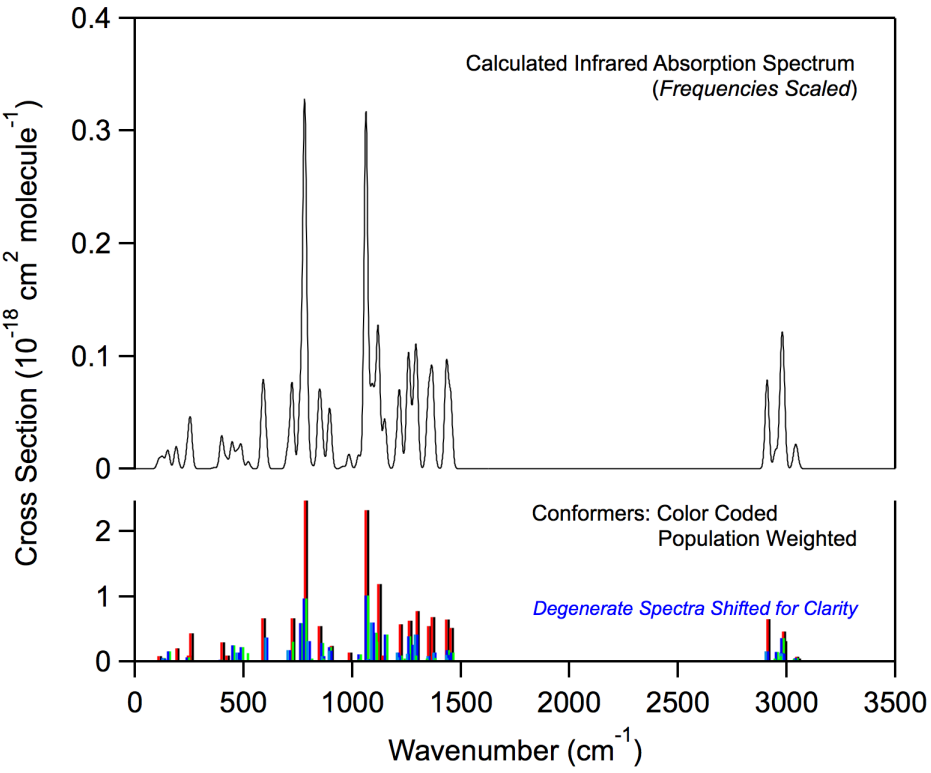
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.249037375400	-0.647913016600	-0.469761956100
C	0.001047200400	0.042811167000	0.062717936100
C	1.253064784600	-0.638749391000	-0.476979047900
H	0.004284660500	0.021567382500	1.158382074600
F	-0.004926433000	1.355588018200	-0.341915858700
H	-1.249912889300	-1.707466563100	-0.210592597800
H	-1.320414647800	-0.533009813900	-1.552481679500
Cl	-2.741644671900	0.069983035100	0.234413848500
H	1.263189935300	-1.698266677500	-0.217857849000
H	1.317358392400	-0.523332151900	-1.560087767600
Cl	2.744411044100	0.090057011100	0.218609897400

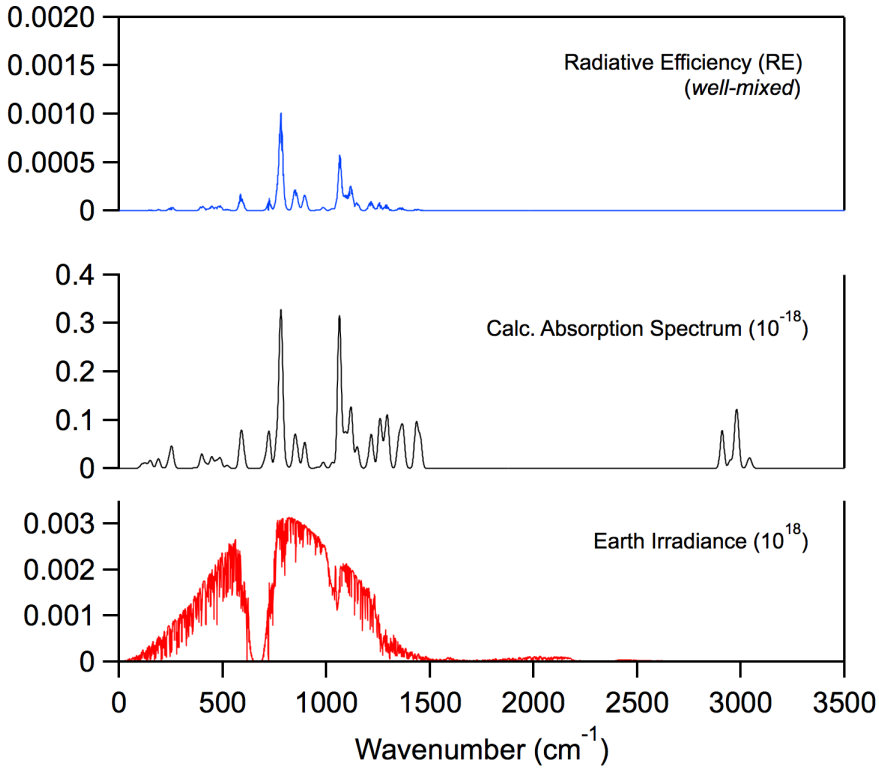
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
71.7075	0.405
102.9922	0.0773
133.2695	0.515
255.2414	0.00357
287.6439	0.111
446.8938	0.887
495.0157	4.23
712.1309	9.69
806.7087	1.61
862.4229	1.63
863.0623	0.344
1034.3315	1.20
1049.7404	0.168
1121.8819	9.81
1174.6038	0.726
1246.5917	0.490
1257.0111	1.60
1314.7048	2.95
1365.7470	1.34
1406.1659	1.83
1458.7828	0.836
1468.7262	0.628
3059.9632	1.45
3081.1891	1.18
3089.1169	2.82
3144.5982	0.0104
3154.0848	1.30

Infrared Spectrum

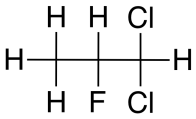


Radiative Efficiency



HCFC-261eb

Molecular Formula:	$CH_3CHFCHCl_2$
Name:	1,1-Dichloro-2-fluoropropane
CAS number:	53074-31-0
Molecular Weight:	130.98



Global Atmospheric Lifetime (years): 0.309
- Tropospheric Atmospheric Lifetime (years): 0.315
- Stratospheric Atmospheric Lifetime (years): 20

Ozone Depletion Potential (ODP): 0.006

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.125	0.062
Global Warming Potential (GWP_H):		
GWP_{20}	66	33
GWP_{100}	18	9
Global Temperature Potentials (GTP_H)		
GTP_{20}		10
GTP_{50}		2
GTP_{100}		1

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 1.86 \times 10^{-13}$; $k_{SAR}(272\ K) \approx 1.19 \times 10^{-13}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 0.310$ years

$\tau^{OH}_{Trop} = 0.315$ years

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

Fractional Atmospheric Loss: 0.995

O(^{1}D) Reactivity

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

$k_{Est}(T) = 1.7 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 220$ years

Fractional Atmospheric Loss: 0.001

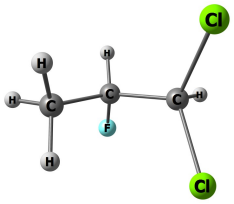
UV Photolysis

UV Spectrum: *No Recommendation*

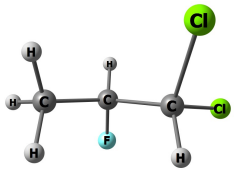
$\tau_{hv} = 80$ years

Fractional Atmospheric Loss: 0.004

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.498



$\Delta E = 0.22$ kcal mol^{-1}
Population = 0.344

Optimized Coordinates (Angstroms)

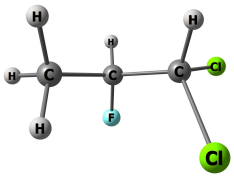
Atom	X	Y	Z
C	1.331040170700	-0.966901404100	1.169081483900
C	0.987909386200	-0.689611990600	-0.281489202700
C	-0.305907650100	0.094881715700	-0.537991290500
H	0.889692993600	-1.628176121200	-0.842952752100
F	2.003192275800	0.043864506800	-0.866114435800
H	2.272286450900	-1.520072297500	1.211648017900
H	0.550403238500	-1.567646811900	1.640899382300
H	1.446086438500	-0.033055860800	1.722942090700
H	-0.400539659500	0.314336820600	-1.598915520400
Cl	-1.733765449800	-0.896448280900	-0.087388050900
Cl	-0.321012194800	1.679763724000	0.297793277600

Atom	X	Y	Z
C	2.181763883400	0.768227373300	-0.091284133400
C	1.087982465200	-0.202042069800	0.328012266000
C	-0.249750240300	0.034304111600	-0.384642305100
H	0.916926269800	-0.169259376800	1.410134489500
F	1.489651201700	-1.480998193000	-0.006427548200
H	3.120254368800	0.458578042300	0.375056788800
H	1.951228005900	1.786717364800	0.224077803800
H	2.315025085300	0.753036002300	-1.177350461900
H	-0.134006496600	-0.008283412900	-1.466186871700
Cl	-1.434997783100	-1.234906684600	0.054384251600
Cl	-0.894344760100	1.662229842700	0.012193720600

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
85.7847	0.336
189.0755	0.207
211.6235	0.0810
225.6615	0.458
270.0336	0.125
368.5605	0.841
429.5578	0.695
564.9358	3.70
699.3071	3.87
776.4223	19.2
858.6946	1.70
957.9064	3.94
1071.7540	1.58
1115.6037	8.51
1168.6325	3.49
1227.5036	1.71
1277.1828	1.78
1364.7043	3.35
1378.5615	0.520
1415.9651	3.99
1485.8420	0.641
1495.3548	0.321
3032.3317	3.04
3061.9429	0.801
3138.3759	1.63
3147.5116	0.458
3148.3659	1.13

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
72.9093	0.232
184.2812	0.151
215.6407	0.0704
254.5033	0.172
330.5511	0.731
349.9416	0.0858
391.8342	1.66
469.9546	1.63
742.2301	4.75
774.5146	20.3
882.2444	1.68
951.6432	4.88
1108.5606	3.42
1110.8313	2.52
1151.2312	7.02
1222.8703	2.31
1256.4067	2.31
1364.4940	0.211
1382.6544	1.20
1409.3966	1.86
1487.9485	0.758
1493.4932	0.561
3052.3774	0.598
3057.5388	2.57
3126.5318	2.21
3138.7521	0.666
3151.2527	1.35



$\Delta E = 0.68$ kcal mol^{-1}
Population = 0.158

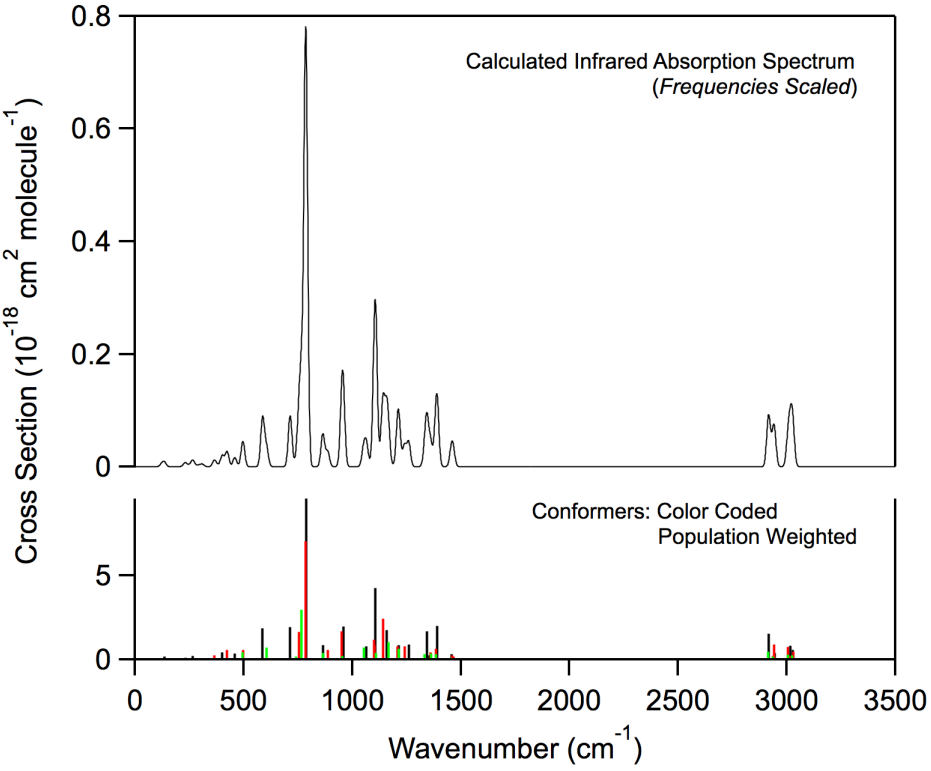
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	2.277243891800	-0.123149289400	0.542903406600
C	0.942806279600	-0.761186882500	0.189075669600
C	-0.266749371800	0.104192305000	0.553827199100
H	0.816426808500	-1.706809585900	0.733541105100
F	0.908542541500	-1.041464763300	-1.155410195900
H	2.337312646900	0.079910029400	1.616420331500
H	2.417886530900	0.811337064700	-0.003726028000
H	3.082524532000	-0.812246953300	0.277108336700
H	-0.253970294200	0.351535316900	1.613559060500
Cl	-0.274127562800	1.659102797900	-0.340149760400
Cl	-1.792197002200	-0.794840039400	0.257235875300

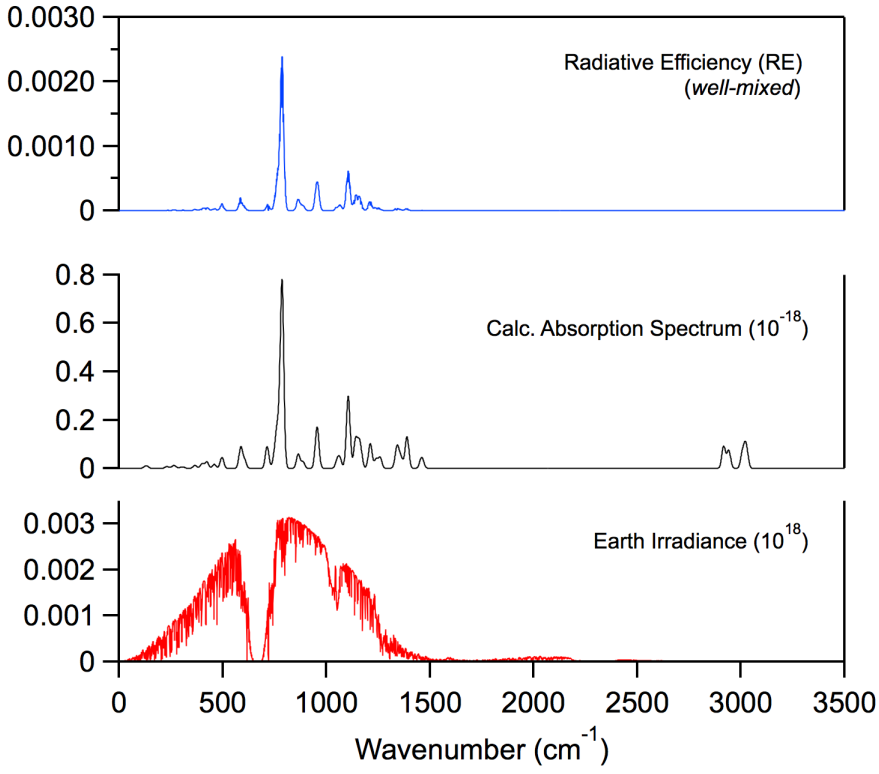
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
77.4203	0.0933
196.3484	0.0447
206.6519	0.0115
223.3944	0.0010
273.7448	0.206
339.2626	0.0529
467.6452	2.59
584.1052	4.54
729.2358	1.24
754.7650	18.6
858.2001	2.48
952.9904	1.45
1057.6729	4.43
1116.0309	2.47
1178.6230	6.54
1229.6644	4.09
1273.9969	0.271
1354.2762	1.97
1386.8915	2.15
1409.7361	1.94
1482.8726	0.592
1497.2030	0.455
3028.2102	2.87
3052.7885	1.20
3125.6557	1.86
3138.3532	0.549
3145.9850	1.53

Infrared Spectrum

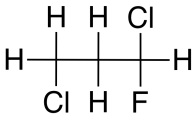


Radiative Efficiency



HCFC-261fa

Molecular Formula:	CH_2ClCH_2CHClF
Name:	1,3-Dichloro-1-fluoropropane
CAS number:	83124-60-1
Molecular Weight:	130.98



Global Atmospheric Lifetime (years):	0.572
Tropospheric Atmospheric Lifetime (years):	0.591
Stratospheric Atmospheric Lifetime (years):	20
Ozone Depletion Potential (ODP):	0.011

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.118	0.075
Global Warming Potential (GWP_H):		
GWP_{20}	116	73
GWP_{100}	31	20
Global Temperature Potentials (GTP_H)		
GTP_{20}		23
GTP_{50}		3
GTP_{100}		3

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 9.93 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 6.33 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 0.575$ years

$\tau^{OH}_{Trop} = 0.591$ years

$\tau^{OH}_{Strat} = 21.0$ years

Fractional Atmospheric Loss: 0.995

$O(^1D)$ Reactivity

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

$k_{Est}(T) = 1.7 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 220$ years

Fractional Atmospheric Loss: 0.002

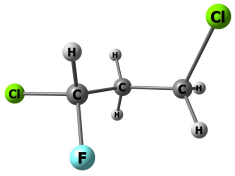
UV Photolysis

UV Spectrum: *No Recommendation*

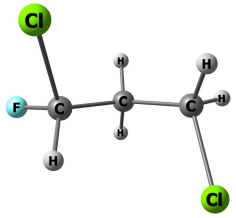
$\tau_{hv} = 225$ years

Fractional Atmospheric Loss: 0.003

Molecular Structure and Infrared Spectrum (5 conformers)



E = 0
Population = 0.480



$\Delta E = 0.40$ kcal mol^{-1}
Population = 0.245

Optimized Coordinates (Angstroms)

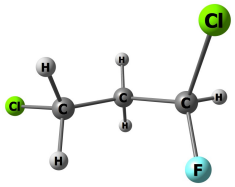
Atom	X	Y	Z
C	-1.468701096800	-0.398694672500	0.823351163300
C	-0.077402474700	0.218404100100	0.906917483100
C	0.788304253700	-0.136482899200	-0.289341654600
H	0.413945453200	-0.164592840000	1.808879251900
H	-0.141563765400	1.305418897800	0.995133280000
H	-2.032780499100	-0.211748760000	1.736383561500
H	-1.417871552900	-1.471054360700	0.637846836200
Cl	-2.447493326600	0.310203259300	-0.529524256600
H	0.404064693000	0.256539906500	-1.231443983300
Cl	2.444272118300	0.567443149500	-0.098577340200
F	0.901037197200	-1.487218780900	-0.391955341300

Atom	X	Y	Z
C	-1.313417242200	-0.177302580400	0.959702616500
C	-0.072908650100	-1.006956217900	0.671092542100
C	0.891704662800	-0.398261870900	-0.332408839100
H	-0.361331550000	-1.988228190900	0.278567540800
H	0.467354167500	-1.169222641700	1.610739483200
H	-1.062473539500	0.833406852200	1.279977094800
H	-1.929582863700	-0.657323553600	1.719170406400
Cl	-2.368451240300	-0.002573464800	-0.506503482800
H	0.419653340000	-0.133339490200	-1.279328069000
Cl	1.607442078300	1.147528057300	0.298059799200
F	1.903161837000	-1.269762899000	-0.563918092200

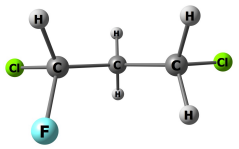
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
60.4528	0.438
104.2533	0.552
211.0034	0.119
261.6423	0.688
371.1991	0.522
431.9116	2.96
478.6713	0.996
666.3426	4.45
731.9303	6.10
847.5280	14.6
950.2059	2.76
986.3180	3.21
1078.6303	4.46
1120.7108	9.82
1186.4555	5.00
1219.2647	0.837
1287.8663	6.12
1324.4091	2.47
1371.3139	1.87
1402.0762	1.92
1459.5284	0.928
1479.2414	0.745
3054.0603	0.459
3100.8021	1.56
3113.3925	0.468
3125.5895	1.64
3165.3024	0.381

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
55.6579	0.389
117.4764	0.633
198.7460	0.353
313.5389	0.483
371.0334	0.575
408.0940	1.07
515.8580	1.50
642.3288	9.08
674.5593	3.80
839.5759	8.94
964.4770	3.96
1029.1391	1.59
1096.2814	3.61
1117.6745	16.0
1166.4490	4.30
1227.3547	1.29
1300.7790	9.22
1334.7604	2.61
1343.0516	0.815
1410.6891	1.73
1463.4014	0.809
1480.6467	1.32
3046.4532	0.950
3090.8916	0.218
3104.0442	1.63
3121.6966	1.67
3163.8436	0.427



$\Delta E = 0.82$ kcal mol^{-1}
Population = 0.120



$\Delta E = 0.95$ kcal mol^{-1}
Population = 0.096

Optimized Coordinates (Angstroms)

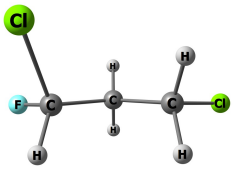
Atom	X	Y	Z
C	-1.024671500900	0.087030594600	-0.487019975000
C	-0.200025118700	0.447209702700	0.743370711400
C	1.284237130500	0.581766016000	0.443621364600
H	-0.337261569500	-0.296114021100	1.532604553400
H	-0.533596142800	1.414214327000	1.136872746300
H	-0.780721215500	-0.905202276900	-0.863436382400
H	-0.890866674000	0.819049255100	-1.282246767900
Cl	-2.785703391600	0.070010017900	-0.082100693600
H	1.857842297600	0.887300282000	1.320800511200
Cl	2.017600354100	-0.999028660900	-0.070850838500
F	1.485073830800	1.485983763600	-0.549209229400

Atom	X	Y	Z
C	-1.379157357400	-0.458040715300	-0.411052630400
C	-0.164222811400	0.399028042500	-0.063151496500
C	1.121805995600	-0.337237858400	-0.400445454400
H	-0.164295350000	0.638219645700	1.003630961400
H	-0.189410649500	1.339992131900	-0.618082669200
H	-1.390334694200	-1.383690826500	0.162866494600
H	-1.420172798800	-0.696034749400	-1.475564315000
Cl	-2.910648649900	0.416889819200	-0.024784002200
H	1.231985470600	-0.548496294700	-1.467275317300
Cl	2.562531408500	0.660872013200	0.044370332800
F	1.181000436600	-1.512703208000	0.279584096100

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
69.0884	0.563
105.9277	0.102
166.0929	0.860
250.8959	0.477
342.8416	0.211
377.7049	0.238
582.1261	7.88
675.1417	7.04
778.9672	0.508
799.0068	7.01
916.6932	6.60
1012.2261	1.54
1070.6289	4.03
1120.9342	8.96
1180.9095	7.46
1260.9649	0.832
1288.2428	6.46
1313.1597	4.29
1367.7732	4.42
1392.8871	0.231
1471.6594	0.727
1492.2991	0.540
3053.4511	0.575
3102.1178	2.76
3107.2317	1.20
3113.6104	0.836
3171.8061	0.372

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
81.1533	0.735
108.0770	0.107
129.2897	0.563
258.0383	0.151
342.0928	1.35
384.0100	0.346
495.1558	2.35
703.0271	16.4
780.0189	0.919
814.7751	5.09
928.2848	6.12
1043.3125	0.623
1064.2583	2.02
1125.9689	14.6
1178.6905	4.13
1245.7772	1.98
1299.3255	2.50
1308.4908	0.991
1364.6239	5.51
1394.5951	3.22
1475.6327	0.481
1492.0426	0.377
3073.7832	0.228
3084.2608	0.880
3089.7018	3.65
3125.3598	0.582
3158.7834	0.902



$\Delta E = 1.34$ kcal mol^{-1}
Population = 0.050

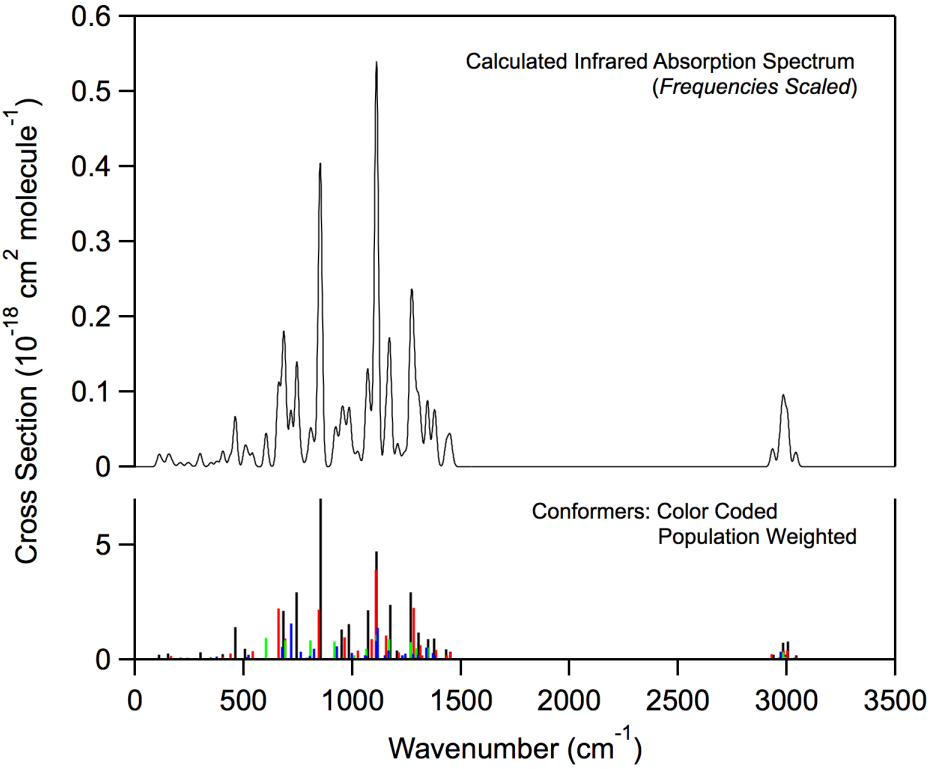
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.161539073300	0.435089320400	-0.329851380100
C	-0.209870460700	-0.636692503800	0.184448873100
C	1.205249493400	-0.486850531800	-0.349593001000
H	-0.559224482500	-1.625869000500	-0.131737059100
H	-0.176402690200	-0.629784000800	1.277209170200
H	-1.195948004900	0.461836448100	-1.420557884600
H	-0.899458545200	1.423992242900	0.043220946000
Cl	-2.849605695900	0.103197851400	0.223715546800
H	1.254572467600	-0.449607196300	-1.440944447700
Cl	1.970491402700	1.061737307300	0.210959818600
F	1.964828589000	-1.518095937000	0.089106417800

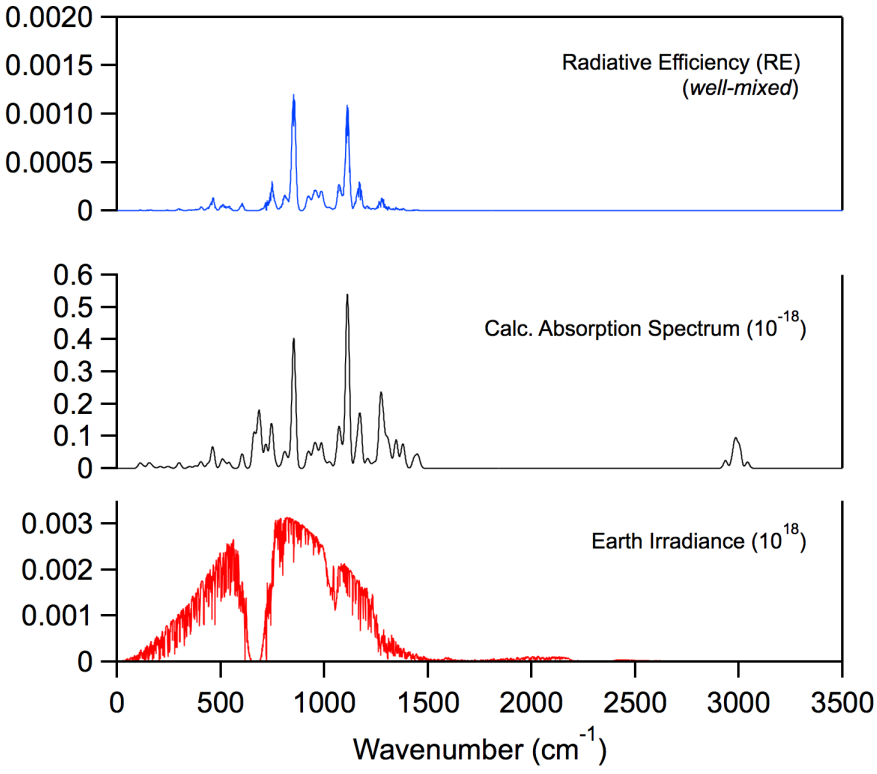
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
75.4594	0.733
109.8437	0.170
153.5397	0.599
243.7201	0.155
364.1257	0.515
406.6214	0.855
487.9694	2.38
660.0077	11.0
750.2552	6.72
794.0828	3.36
999.6102	5.91
1060.8144	0.479
1070.3681	3.47
1118.9023	16.2
1161.9016	3.59
1260.8606	5.15
1285.6136	1.65
1321.5642	4.54
1348.9422	1.46
1405.4382	4.04
1478.3671	0.443
1492.2175	0.420
3055.9194	0.754
3083.8091	1.57
3088.3203	2.37
3114.5721	1.34
3159.7542	0.663

Infrared Spectrum

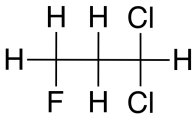


Radiative Efficiency



HCFC-261fb

Molecular Formula: $CH_2FCH_2CHCl_2$
Name: 1,1-Dichloro-3-fluoropropane
CAS number: 53074-30-9
Molecular Weight: 130.98



Global Atmospheric Lifetime (years): 0.332
  Tropospheric Atmospheric Lifetime (years): 0.339
  Stratospheric Atmospheric Lifetime (years): 20
Ozone Depletion Potential (ODP): 0.006

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.109	0.056
Global Warming Potential (GWP_H):		
GWP_{20}	62	32
GWP_{100}	17	9
Global Temperature Potentials (GTP_H)		
GTP_{20}		10
GTP_{50}		1
GTP_{100}		1

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 1.73 \times 10^{-13}$; $k_{SAR}(272\ K) \approx 1.10 \times 10^{-13}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 0.333$ years
$\tau^{OH}_{Trop} = 0.339$ years
$\tau^{OH}_{Strat} = 20$ years

Fractional Atmospheric Loss: 0.994

O(^{1}D) Reactivity

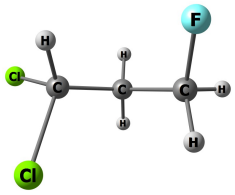
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 1.7 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)} = 220$ years
Fractional Atmospheric Loss: 0.002

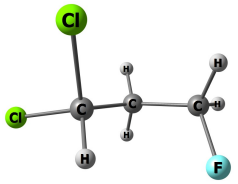
UV Photolysis

UV Spectrum: *No Recommendation*
$\tau_{hv} = 80$ years
Fractional Atmospheric Loss: 0.004

Molecular Structure and Infrared Spectrum (5 conformers)



E = 0
Population = 0.451



E = 0
Population = 0.451

Optimized Coordinates (Angstroms)

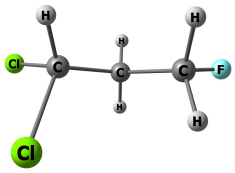
Atom	X	Y	Z
C	-2.052833697700	-0.278052766600	-0.486845108300
C	-0.631199049400	-0.792328964500	-0.667273506000
C	0.361638775000	-0.103370579800	0.258890156200
H	-0.317055827400	-0.666841436700	-1.707689015000
H	-0.607292735000	-1.862309200100	-0.435646058800
F	-2.442564565600	-0.467612242800	0.826811037200
H	-2.738173374300	-0.832490486600	-1.138352372700
H	-2.127131768800	0.789530384700	-0.718774785200
H	0.032355104000	-0.132181870100	1.293978858300
Cl	1.958182683700	-0.927753723800	0.203503596400
Cl	0.550332455400	1.641404886300	-0.153637802100

Atom	X	Y	Z
C	-2.056543936100	-0.188256736200	0.486937690900
C	-0.649172685600	-0.733439275300	0.687331170500
C	0.359680980600	-0.113477097700	-0.269765092700
H	-0.655545875100	-1.812774449100	0.502737352300
H	-0.328681826700	-0.571352998300	1.720729883000
F	-2.455173319200	-0.424168894400	-0.816500532700
H	-2.100595540900	0.890096779800	0.672032859700
H	-2.755078840200	-0.694432144300	1.163242319700
H	0.026745697900	-0.178360314500	-1.302049625700
Cl	0.597786787200	1.641750637300	0.065656955200
Cl	1.932946558100	-0.978681507200	-0.180995980200

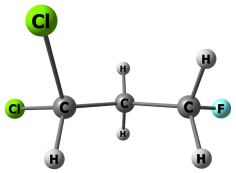
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
64.9439	0.425
122.6533	0.709
208.8227	0.294
261.1509	0.499
319.2658	0.117
392.8368	0.630
494.0873	3.77
639.3774	4.84
751.9229	16.3
866.2743	1.73
912.2267	1.56
1074.8598	7.30
1089.8462	1.77
1097.3922	7.99
1208.4109	1.07
1239.7704	3.22
1269.3412	1.89
1317.1907	1.74
1376.9719	0.892
1425.2612	2.27
1460.1679	0.838
1513.7501	0.723
3039.6470	5.21
3057.2694	0.422
3091.3781	3.83
3110.8892	1.52
3162.5788	0.0819

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
64.9425	0.425
122.6500	0.709
208.8198	0.294
261.1511	0.499
319.2654	0.117
392.8362	0.630
494.0876	3.77
639.3773	4.84
751.9239	16.3
866.2748	1.73
912.2267	1.56
1074.8618	7.30
1089.8459	1.77
1097.3970	7.99
1208.4118	1.07
1239.7703	3.22
1269.3438	1.89
1317.1914	1.74
1376.9736	0.892
1425.2636	2.27
1460.1679	0.838
1513.7496	0.723
3039.6467	5.21
3057.2684	0.422
3091.3738	3.83
3110.8854	1.52
3162.5756	0.0819



$\Delta E = 1.73$ kcal mol^{-1}
Population = 0.024



$\Delta E = 1.73$ kcal mol^{-1}
Population = 0.024

Optimized Coordinates (Angstroms)

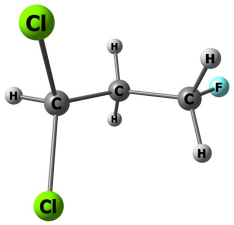
Atom	X	Y	Z
C	-2.003365231000	0.152006037800	0.282170984700
C	-0.763280804400	-0.624966049200	-0.156141434900
C	0.529430784200	-0.073104536000	0.419611241600
H	-0.700345788600	-0.642574895500	-1.247669703900
H	-0.864319797600	-1.659840390300	0.187634702800
F	-3.117332191300	-0.516156564100	-0.177311074200
H	-2.007187995900	1.166775205700	-0.127846670500
H	-2.061924086500	0.216854130400	1.376989491400
H	0.518098570500	-0.022218312500	1.506682339100
Cl	1.917229345500	-1.133768081800	-0.009526559500
Cl	0.842231195000	1.613011455400	-0.140609316700

Atom	X	Y	Z
C	-2.002948036000	0.117588383900	-0.319593879000
C	-0.757139130100	-0.634960869700	0.144340658200
C	0.532985433200	-0.082446336300	-0.436554457600
H	-0.844642856800	-1.678707216300	-0.175494983700
H	-0.700820177500	-0.626162327900	1.236336774700
F	-3.112328110600	-0.551975067400	0.148868664700
H	-2.055392507800	0.156008931400	-1.415968007000
H	-2.020515820500	1.141617455600	0.066336039400
H	0.527872685000	-0.057330588800	-1.524572425200
Cl	0.823730732200	1.619782058100	0.085506560800
Cl	1.929662789100	-1.117186422600	0.025815054700

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
88.2674	0.816
111.2343	0.133
152.7439	0.564
243.9914	0.106
331.5746	0.759
348.6659	0.824
473.1028	1.64
654.3429	8.44
747.6593	14.9
814.0185	1.96
1026.5242	2.28
1053.9170	3.35
1092.4952	15.9
1110.6963	0.696
1229.8221	1.77
1236.3193	3.11
1283.6691	2.09
1310.9767	0.474
1347.7143	1.20
1437.8658	3.11
1479.0325	0.501
1523.3636	0.132
3021.4648	5.46
3058.8889	0.751
3085.1514	2.77
3113.6673	1.43
3138.0183	1.08

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
88.2798	0.816
111.2298	0.133
152.7442	0.564
243.9895	0.106
331.5739	0.759
348.6650	0.824
473.1037	1.64
654.3488	8.44
747.6474	14.9
814.0205	1.96
1026.5309	2.28
1053.9210	3.35
1092.4855	15.9
1110.7008	0.694
1229.8228	1.77
1236.3166	3.12
1283.6735	2.09
1310.9762	0.474
1347.7179	1.20
1437.8666	3.11
1479.0341	0.501
1523.3653	0.132
3021.4636	5.46
3058.8825	0.751
3085.1477	2.77
3113.6639	1.43
3138.0227	1.08



$\Delta E = 1.76$ kcal mol^{-1}
Population = 0.023

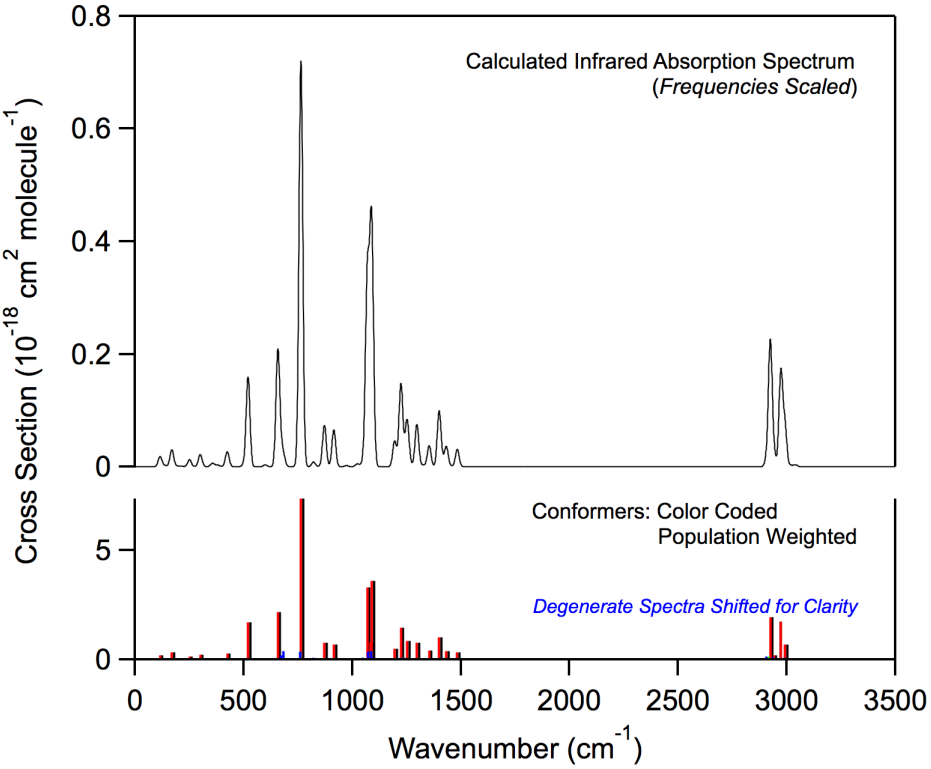
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.666459547100	-0.037212305200	-0.475260342300
C	-0.852212112000	-0.015391268900	0.814617035500
C	0.658252229700	-0.001134571600	0.646274721600
H	-1.111214727900	-0.896057435300	1.412529542500
H	-1.129897295800	0.871673489000	1.394419318000
F	-3.003170487600	-0.047811842000	-0.133029126500
H	-1.448338744800	-0.931690243500	-1.067592891000
H	-1.467156273600	0.849326667700	-1.085876755800
H	1.165070030200	0.014062179800	1.607473191200
Cl	1.256608852000	-1.484218600200	-0.189420811700
Cl	1.225341076900	1.476640930200	-0.219879881600

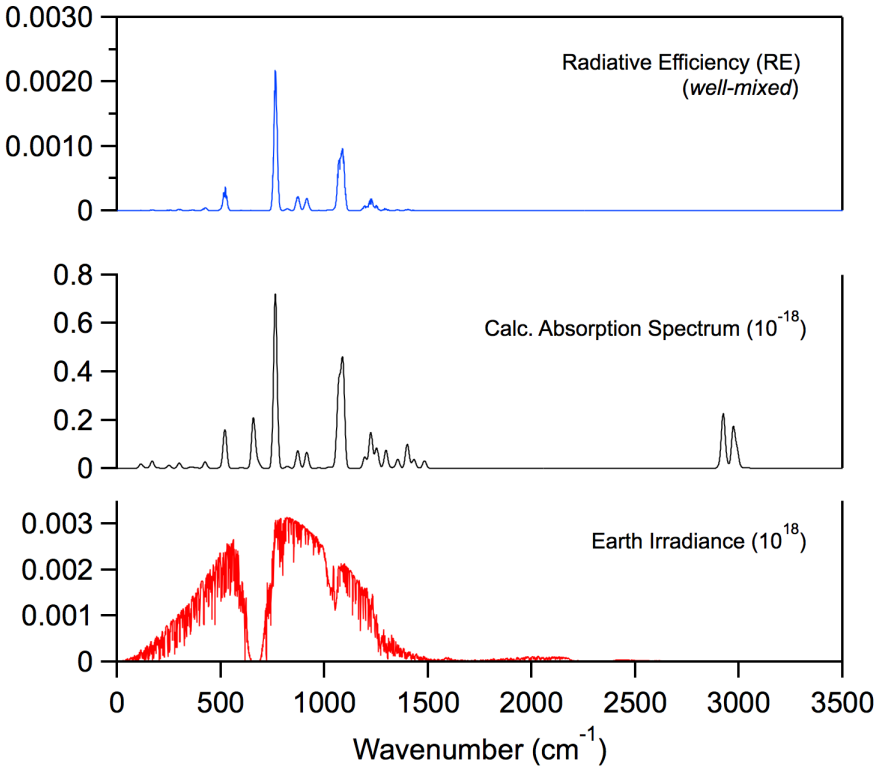
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
76.9611	0.696
106.8399	0.0463
170.9605	0.616
262.5945	0.377
315.9820	0.298
343.1795	0.682
577.7097	3.02
666.5942	17.0
671.8929	0.911
812.5274	3.74
974.0565	1.84
1078.6257	15.4
1099.0750	4.31
1099.7131	3.86
1233.1295	2.31
1256.2482	3.18
1259.9613	2.07
1316.3424	0.658
1346.5715	0.414
1439.8579	1.29
1471.7271	0.647
1525.6246	0.296
3045.1612	0.144
3052.5109	4.40
3086.9015	0.150
3108.9207	4.21
3150.5782	0.330

Infrared Spectrum

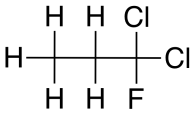


Radiative Efficiency



HCFC-261fc

Molecular Formula:	$CH_3CH_2CCl_2F$
Name:	1,1-Dichloro-1-fluoropropane
CAS number:	7799-56-6
Molecular Weight:	130.98



Global Atmospheric Lifetime (years):	0.614
Tropospheric Atmospheric Lifetime (years):	0.638
Stratospheric Atmospheric Lifetime (years):	20
Ozone Depletion Potential (ODP):	0.013

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.212	0.137
Global Warming Potential (GWP_H):		
GWP_{20}	224	145
GWP_{100}	61	39
Global Temperature Potentials (GTP_H)		
GTP_{20}		45
GTP_{50}		7
GTP_{100}		5

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 9.19 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 5.86 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 0.621$ years

$\tau^{OH}_{Trop} = 0.638$ years

$\tau^{OH}_{Strat} = 22.5$ years

Fractional Atmospheric Loss: 0.990

$O(^1D)$ Reactivity

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

$k_{Est}(T) = 1.7 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 220$ years

Fractional Atmospheric Loss: 0.002

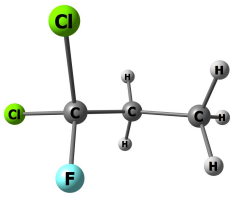
UV Photolysis

UV Spectrum: *No Recommendation*

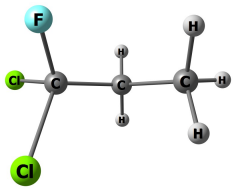
$\tau_{hv} = 80$ years

Fractional Atmospheric Loss: 0.008

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.378



E = 0
Population = 0.378

Optimized Coordinates (Angstroms)

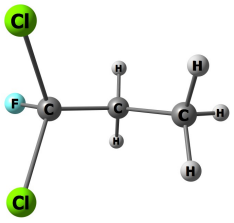
Atom	X	Y	Z
C	-2.370035827900	-0.636969014900	0.173816180000
C	-0.926230119700	-0.958286696400	0.568193929000
C	0.102567084200	-0.115698732900	-0.174371144700
H	-0.689142420900	-2.000845693000	0.330755820300
H	-0.762702001400	-0.821801165000	1.639563908000
H	-2.517555225500	-0.759806707000	-0.901881216200
H	-2.640779302300	0.386136346100	0.444675530900
H	-3.049821770700	-1.318482538100	0.691801279500
F	-0.057166197300	-0.230488860400	-1.501813240600
Cl	-0.038342592500	1.638128596000	0.238144110500
Cl	1.776421373900	-0.665550534300	0.222396843200

Atom	X	Y	Z
C	-2.371943222200	-0.630057448500	-0.178065032200
C	-0.928828549300	-0.949023590600	-0.576854693500
C	0.101978640800	-0.122426086300	0.180742644400
H	-0.764066175700	-0.794743233500	-1.645617588400
H	-0.695116450500	-1.996214668600	-0.357112165000
H	-3.053417878000	-1.300529694500	-0.708100508800
H	-2.639349729200	0.398353715700	-0.431591075300
H	-2.520654974700	-0.770804648900	0.895271441300
F	-0.059113437600	-0.259414038900	1.505913446700
Cl	1.774443254700	-0.670551096800	-0.224190006200
Cl	-0.033248478500	1.638625790800	-0.201807462900

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
109.5910	0.00709
197.3728	0.0264
215.5905	0.00520
252.7432	0.0587
331.7869	0.366
368.6352	0.848
389.2513	0.931
435.9968	0.545
594.4921	5.25
764.7174	18.4
817.7437	16.5
934.6668	13.2
1000.9029	8.42
1088.7039	4.63
1131.1930	5.43
1195.2262	11.6
1304.1062	2.60
1362.5001	0.432
1411.0108	0.334
1469.8711	0.339
1494.9443	0.871
1508.0996	1.12
3055.4972	2.18
3060.0430	1.27
3113.1594	0.107
3128.1099	2.41
3139.5007	2.56

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
109.5899	0.00709
197.3726	0.0264
215.5900	0.00520
252.7434	0.0587
331.7871	0.366
368.6348	0.848
389.2514	0.931
435.9970	0.545
594.4917	5.25
764.7177	18.4
817.7435	16.5
934.6673	13.2
1000.9029	8.42
1088.7045	4.63
1131.1930	5.43
1195.2260	11.6
1304.1067	2.60
1362.5008	0.432
1411.0114	0.334
1469.8716	0.339
1494.9446	0.871
1508.0999	1.12
3055.4970	2.18
3060.0413	1.27
3113.1592	0.107
3128.1093	2.41
3139.5006	2.56



$\Delta E = 0.26$ kcal mol^{-1}
Population = 0.245

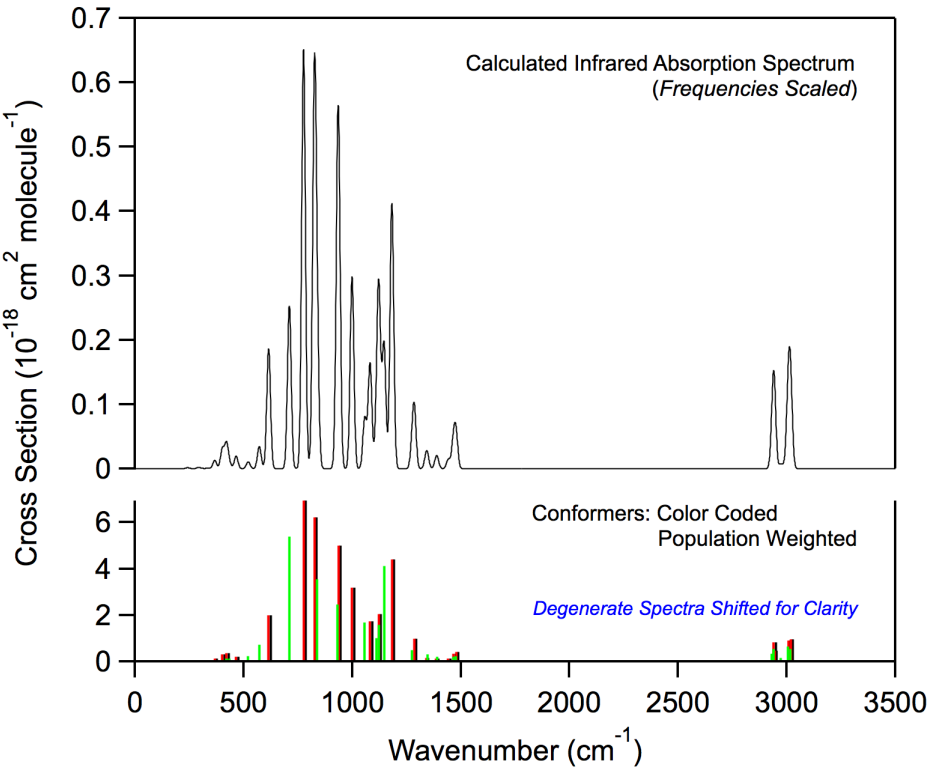
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-2.276584540900	-0.014517474400	-0.350982249100
C	-1.264866695800	-0.012722433100	0.791754445700
C	0.203265957100	0.004184804700	0.387471690100
H	-1.386497920200	-0.900703693700	1.421686985500
H	-1.403453484600	0.863933122900	1.433929495000
H	-3.289333428000	-0.027103843900	0.060593942600
H	-2.157265597100	-0.895356540200	-0.986235127700
H	-2.174299650000	0.877181420700	-0.973936685200
F	0.971228022200	0.003925413800	1.488009481100
Cl	0.652025781200	-1.454727378300	-0.578446123500
Cl	0.623806556000	1.484677601300	-0.558064854500

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
110.7550	0.00
201.8694	0.0485
207.7013	0.00130
273.0611	0.0341
300.3288	0.106
388.0685	0.496
404.2989	0.558
494.9680	0.933
548.9258	3.00
695.3437	22.0
831.0849	14.5
928.6241	10.1
1062.8622	6.83
1120.9809	4.14
1131.9389	6.44
1156.8815	16.8
1293.0837	1.99
1367.9063	1.25
1416.7116	0.838
1470.3724	0.209
1496.1976	0.882
1507.4603	0.979
3047.6135	1.37
3055.9391	2.18
3091.6628	0.634
3126.3942	2.65
3137.9006	2.21

Infrared Spectrum



Radiative Efficiency