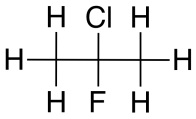
HCFC-271ba

Molecular Formula:	$CH_3CClFCH_3$
Name:	2-Chloro-2-fluoropropane
CAS number:	420-44-0
Molecular Weight:	96.53



Global Atmospheric Lifetime (years):	5.05
Tropospheric Atmospheric Lifetime (years):	5.37
Stratospheric Atmospheric Lifetime (years):	83.4
Ozone Depletion Potential (ODP):	0.028

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.115	0.106
Global Warming Potential (GWP_H):		
GWP_{20}	1327	1224
GWP_{100}	366	338
Global Temperature Potentials (GTP_H)		
GTP_{20}		675
GTP_{50}		72
GTP_{100}		47

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

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

OH Reactivity

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

$k_{SAR}(298\ K) = 1.09 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 0.697 \times 10^{-14}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 5.19$ years

$\tau^{OH}_{Trop} = 5.37$ years

$\tau^{OH}_{Strat} = 153.4$ years

Fractional Atmospheric Loss: 0.973

O(^{1}D) Reactivity

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

$k_{Est}(T) = 1.2 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 310$ years

Fractional Atmospheric Loss: 0.016

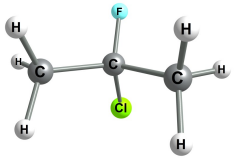
UV Photolysis

UV Spectrum: *No Recommendation*

$\tau_{hv} = 450$ years

Fractional Atmospheric Loss: 0.011

Molecular Structure and Infrared Spectrum (1 conformer)



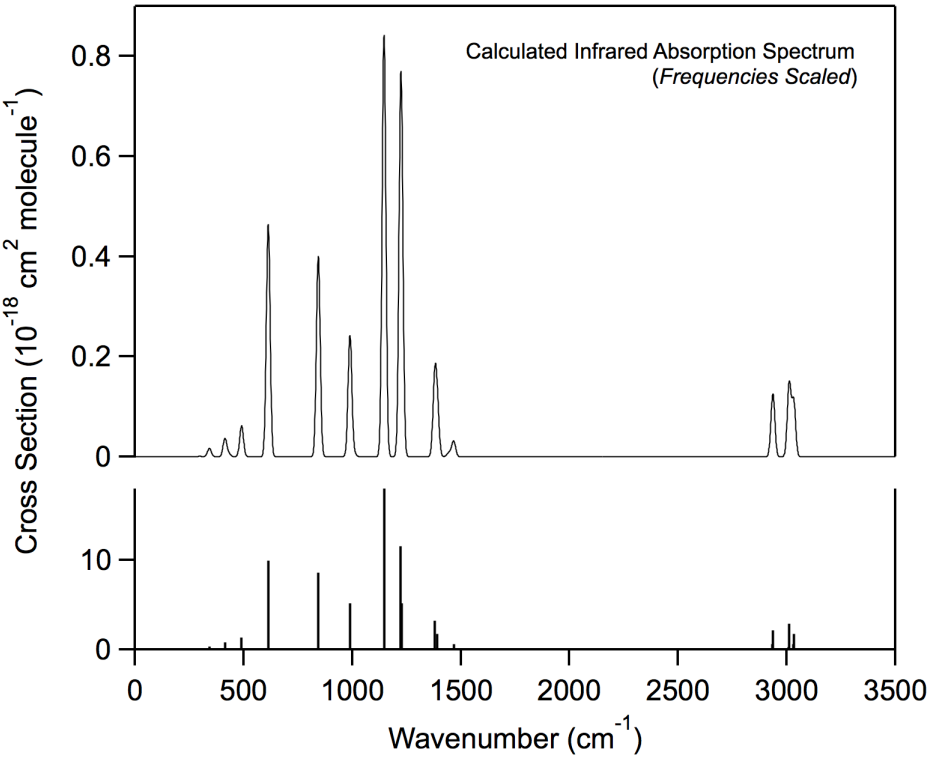
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	0.889850013700	1.282565509100	-0.576599187300
C	0.367096388900	-0.000023189600	0.043295453100
C	0.887751640200	-1.280344770200	-0.583019972800
Cl	-1.468635484100	0.001751247500	-0.064934519100
F	0.675434621500	-0.003605541100	1.372506725300
H	0.476017792900	2.146958519900	-0.054633885400
H	0.618784134800	1.338927973100	-1.632254158800
H	1.980813174600	1.300803113500	-0.485985428800
H	0.472502848600	-2.146662005200	-0.065387894800
H	0.616592611000	-1.330976043500	-1.638941363600
H	1.978683257700	-1.300822813400	-0.492507767600

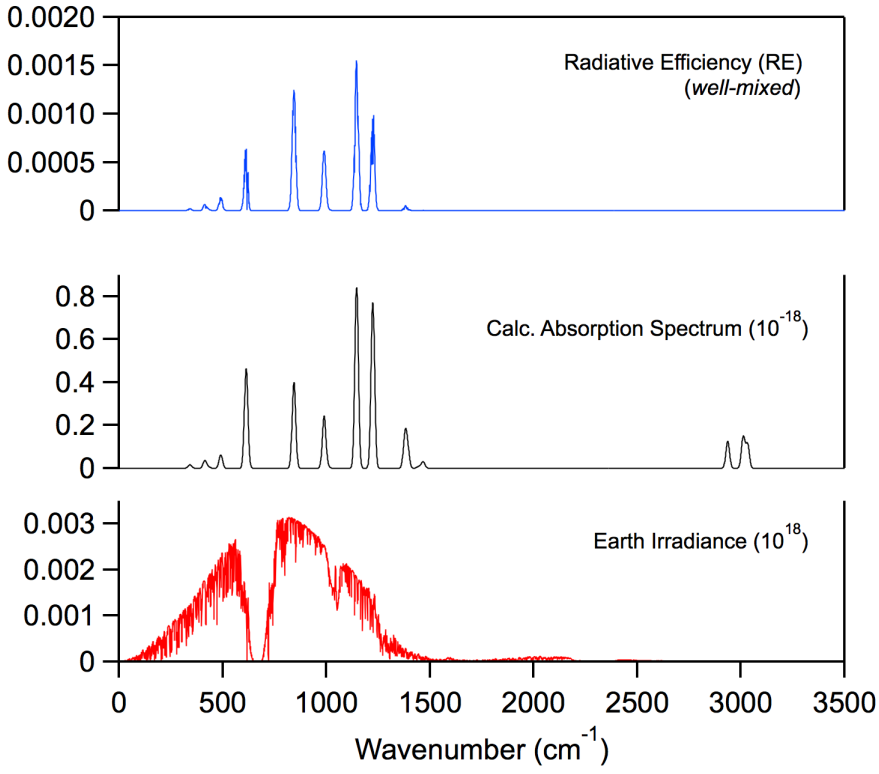
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
228.5754	0.00
259.0637	0.0168
294.4224	0.0132
306.0029	0.346
381.5410	0.773
400.5637	0.116
462.7252	1.32
592.4838	9.89
836.5717	8.54
936.4669	0.00649
990.9202	5.17
1013.1541	0.127
1156.8673	17.9
1238.5772	11.5
1241.9285	5.12
1404.4455	3.19
1417.3300	1.75
1471.9490	0.149
1474.1726	0.000
1486.7314	0.110
1497.1386	0.614
3048.6295	0.635
3053.5872	2.12
3127.1947	0.256
3132.1290	2.87
3151.8459	0.604
3154.6847	1.77

Infrared Spectrum

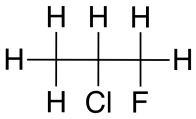


Radiative Efficiency



HCFC-271da

Molecular Formula:	$CH_3CHClCH_2F$
Name:	2-Chloro-1-fluoropropane
CAS number:	20372-78-5
Molecular Weight:	96.53



Global Atmospheric Lifetime (years):	0.273
Tropospheric Atmospheric Lifetime (years):	0.278
Stratospheric Atmospheric Lifetime (years):	20
Ozone Depletion Potential (ODP):	0.004

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.056	0.026
Global Warming Potential (GWP_H):		
GWP_{20}	36	17
GWP_{100}	10	5
Global Temperature Potentials (GTP_H)		
GTP_{20}		5
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*

$k_{SAR}(298\ K) = 2.11 \times 10^{-13}$; $k_{SAR}(272\ K) \approx 1.35 \times 10^{-13}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 0.274$ years

$\tau^{OH}_{Trop} = 0.278$ years

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

Fractional Atmospheric Loss: 0.998

$O(^1D)$ Reactivity

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

$k_{Est}(T) = 1.2 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 310$ years

Fractional Atmospheric Loss: 0.001

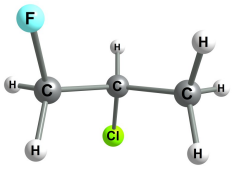
UV Photolysis

UV Spectrum: *No Recommendation*

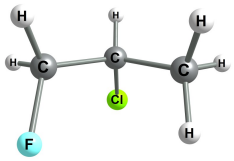
$\tau_{hv} = 450$ years

Fractional Atmospheric Loss: 0.001

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.662



$\Delta E = 0.73$ kcal mol^{-1}
Population = 0.193

Optimized Coordinates (Angstroms)

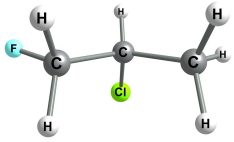
Atom	X	Y	Z
C	-0.948571614100	-0.807283974600	0.167895444700
C	0.033026947100	0.215637267600	-0.394108198500
C	-0.186312680700	1.617045297800	0.149091168200
H	-0.019620219500	0.207710144000	-1.484633286200
Cl	1.706600768400	-0.379963068900	0.006274836400
F	-2.228566628200	-0.410770332100	-0.167551968300
H	-0.866225761300	-0.857448999600	1.259938128100
H	-0.762420573600	-1.800429795000	-0.253004842900
H	0.509738374800	2.327475709000	-0.301321562000
H	-1.209801198200	1.925826041300	-0.084271224200
H	-0.054548414700	1.639163710600	1.234743504800

Atom	X	Y	Z
C	-1.224410704800	-0.294993933200	-0.605371818500
C	0.068326120100	0.503011648200	-0.556201934000
C	-0.013652293300	1.718197613900	0.356467915500
H	0.331377423400	0.790280479400	-1.577197449500
Cl	1.429791409100	-0.584776677000	-0.012905255400
F	-1.636182818100	-0.631874585700	0.662040659400
H	-1.097892079100	-1.210186603000	-1.192811062100
H	-2.002816467500	0.326435740900	-1.071375634200
H	0.937398708400	2.252633789300	0.381727055600
H	-0.787454945500	2.401223886600	-0.012981471800
H	-0.277958352800	1.411710640400	1.370091994900

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
127.1308	0.981
227.2564	1.34
250.1775	0.0591
302.1324	0.196
388.7223	0.521
421.2831	0.341
701.0705	5.90
896.4711	1.25
937.3632	0.398
1029.6810	3.91
1074.2130	16.4
1139.1835	0.575
1170.2022	0.267
1244.6696	2.52
1275.9546	0.636
1367.0777	0.458
1403.8764	0.929
1424.2196	1.20
1487.6380	1.02
1491.9273	0.634
1513.2623	0.312
3039.9657	3.63
3047.6960	1.29
3087.6208	1.12
3104.3443	3.29
3124.0145	2.87
3136.8164	2.13

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
108.8385	0.368
227.1676	0.225
244.7608	0.00523
335.4057	0.654
344.7178	0.467
585.4086	4.90
654.8567	1.74
880.2394	1.41
938.3096	0.648
1002.5814	3.88
1069.6934	4.32
1143.2388	2.73
1149.8791	4.75
1257.3736	1.43
1289.8915	4.59
1347.8911	0.191
1401.9622	1.02
1432.3628	1.39
1484.1243	1.24
1494.4556	0.167
1503.9048	0.870
3010.7456	5.08
3042.5581	2.68
3082.6835	3.59
3088.0971	2.41
3120.6734	2.32
3152.2285	1.34



$\Delta E = 0.90$ kcal mol^{-1}
Population = 0.146

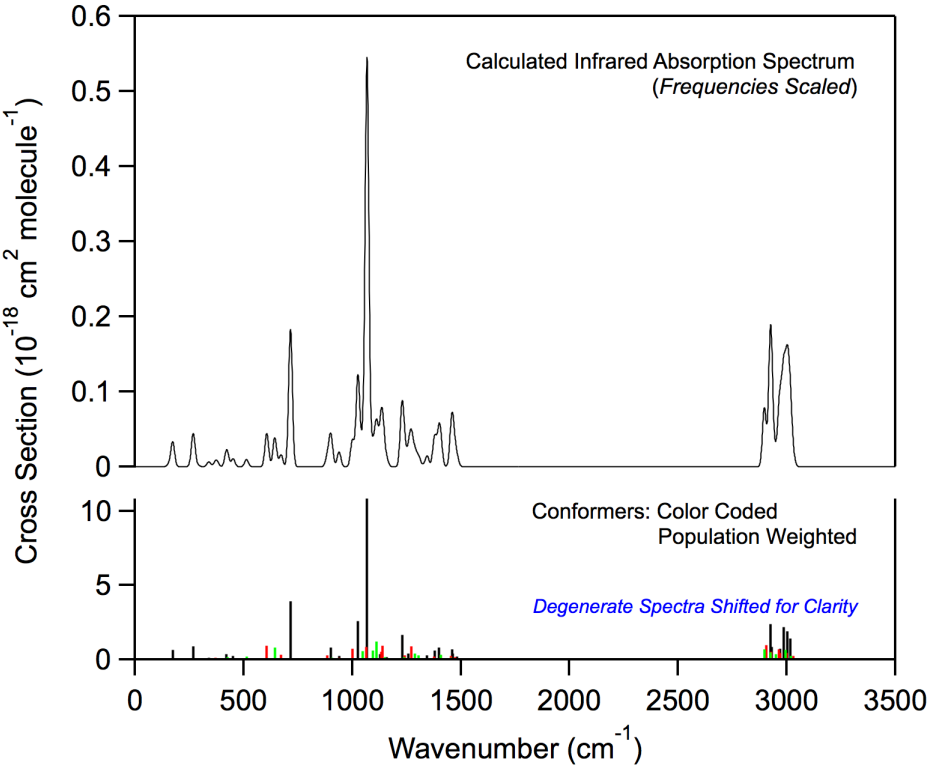
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-1.173681796200	0.541794285200	0.319058171100
C	0.179076420700	0.442704567700	-0.364039681200
C	1.109287174300	1.584067103900	0.020194537100
H	0.029959824500	0.400263909300	-1.444931624300
Cl	0.946603762900	-1.155684292700	0.055821348500
F	-2.022117008500	-0.435886664300	-0.134343175100
H	-1.613935370600	1.522520725500	0.089083700000
H	-1.063863376600	0.446817330900	1.405873176900
H	2.077344154900	1.473561808300	-0.471604663700
H	0.672578180300	2.540808114500	-0.288141884800
H	1.274659034400	1.609359111800	1.101045095500

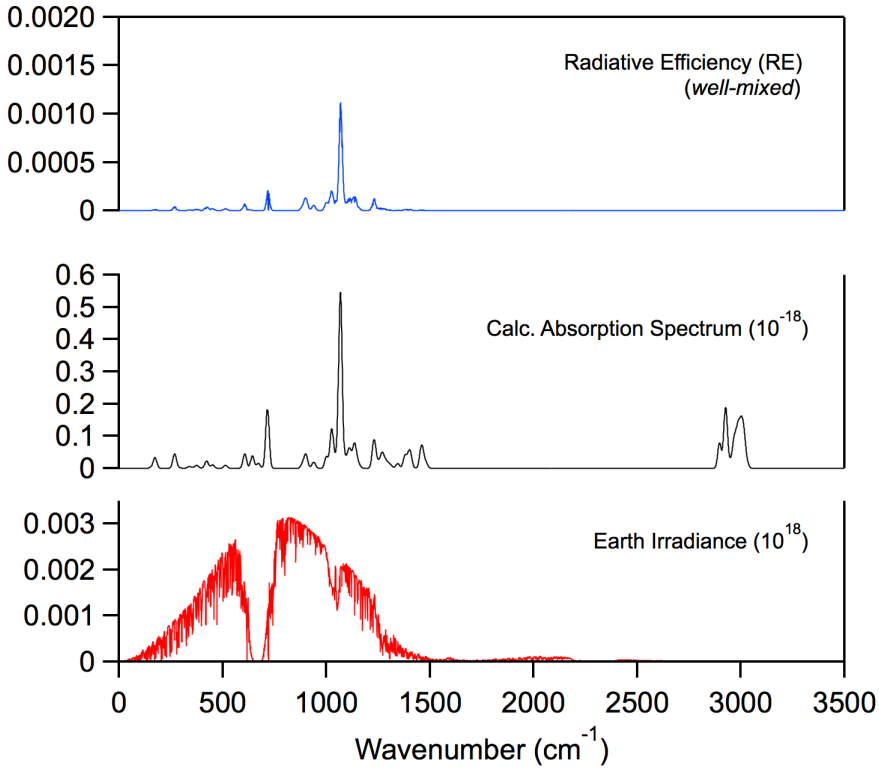
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
125.3829	0.381
215.3432	0.236
234.6854	0.0341
314.6043	0.0906
393.9715	1.08
486.4609	1.40
624.4260	5.66
904.6059	0.832
937.2169	0.212
1051.5957	3.81
1101.3416	4.21
1120.1604	8.45
1159.7928	1.01
1254.0398	1.16
1307.9725	2.91
1326.2820	1.85
1410.5673	0.275
1434.1096	2.13
1484.6110	0.791
1495.7963	0.613
1502.2148	0.680
3010.7529	4.74
3040.2650	3.23
3067.7068	2.50
3096.2640	0.581
3114.2112	4.41
3138.9488	1.75

Infrared Spectrum

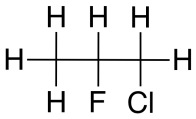


Radiative Efficiency



HCFC-271ea

Molecular Formula:	CH_3CHFCH_2Cl
Name:	1-Chloro-2-fluoropropane
CAS number:	430-46-6
Molecular Weight:	96.53



Global Atmospheric Lifetime (years):	0.297
Tropospheric Atmospheric Lifetime (years):	0.302
Stratospheric Atmospheric Lifetime (years):	20
Ozone Depletion Potential (ODP):	0.004

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.068	0.033
Global Warming Potential (GWP_H):		
GWP_{20}	47	23
GWP_{100}	13	6
Global Temperature Potentials (GTP_H)		
GTP_{20}		7
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) = 1.94×10^{-13}; k_{SAR}(272 K) ≈ 1.24×10^{-13} cm^3 $molecule^{-1}$ s^{-1}

τ^{OH}_{Global} = 0.298 years
τ^{OH}_{Trop} = 0.302 years
τ^{OH}_{Strat} = 20 years

Fractional Atmospheric Loss: 0.998

O(^{1}D) Reactivity

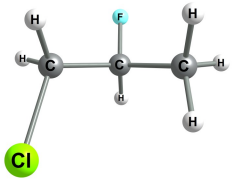
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 1.2 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)}$ = 310 years
Fractional Atmospheric Loss: 0.001

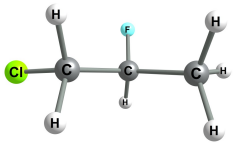
UV Photolysis

UV Spectrum: *No Recommendation*
τ_{hv} = 450 years
Fractional Atmospheric Loss: 0.001

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.448



$\Delta E = 0.19$ kcal mol^{-1}
Population = 0.326

Optimized Coordinates (Angstroms)

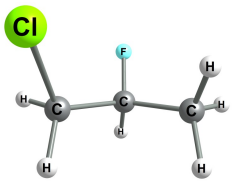
Atom	X	Y	Z
C	1.094842240100	-1.375584878300	0.162273167100
C	0.870701588100	0.026751655700	-0.371536681300
C	-0.303222402900	0.771627987900	0.260146835200
H	0.743491060700	0.012669548000	-1.460925517100
F	1.991451258100	0.800334802800	-0.089523935800
H	0.233685191400	-2.011173391800	-0.056650215600
H	1.247098211900	-1.349970198100	1.245934083300
H	1.981326680400	-1.813753631300	-0.303013870600
Cl	-1.882135069200	0.045739253800	-0.226114536000
H	-0.251850967500	0.737063862300	1.349388182700
H	-0.311096791100	1.808986988900	-0.073647511800

Atom	X	Y	Z
C	2.201229786000	-0.595861067800	-0.055785758300
C	0.851430443200	0.056771196900	-0.327246994200
C	-0.286361886000	-0.706028410400	0.331117343700
H	0.667748922800	0.126896723800	-1.406615597800
F	0.871219436100	1.344518562700	0.175297476500
H	2.996646141100	0.017156630500	-0.486633054800
H	2.250470156200	-1.592244566200	-0.504611058300
H	2.379559390900	-0.685472830100	1.020189229600
Cl	-1.896304048100	-0.004287120600	-0.082323354300
H	-0.297485203000	-1.745285519100	0.000332862400
H	-0.193748139200	-0.666908599500	1.417616905300

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
105.0143	0.812
204.7299	0.794
235.9133	0.255
360.1629	0.649
386.8295	0.486
458.0156	0.274
763.2389	7.52
843.0806	0.649
899.5091	0.657
948.7565	4.11
1077.0145	1.12
1110.6747	9.63
1155.8931	3.81
1226.0690	0.998
1276.1912	1.98
1375.7949	0.655
1388.7365	0.587
1414.1162	3.99
1478.1416	0.749
1487.2961	0.629
1500.8844	0.614
3041.7988	2.59
3048.3712	2.09
3090.5110	2.14
3123.2245	3.23
3137.2846	1.78
3156.9471	1.06

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
102.5765	0.227
199.6569	0.102
221.1397	0.0328
325.5822	0.0208
442.6488	1.66
462.0519	1.45
746.4492	5.31
844.9393	2.23
893.4338	0.134
947.8748	2.49
1074.6693	5.23
1109.4233	1.44
1166.5651	6.72
1226.7393	0.826
1284.5853	4.09
1369.0558	0.111
1396.7674	1.68
1408.4851	2.30
1462.2897	0.961
1484.9729	0.609
1498.3152	0.397
3039.9289	2.90
3044.9014	1.52
3086.1834	2.51
3119.6948	2.81
3128.8684	2.23
3151.0626	1.35



$\Delta E = 0.41$ kcal mol^{-1}
Population = 0.226

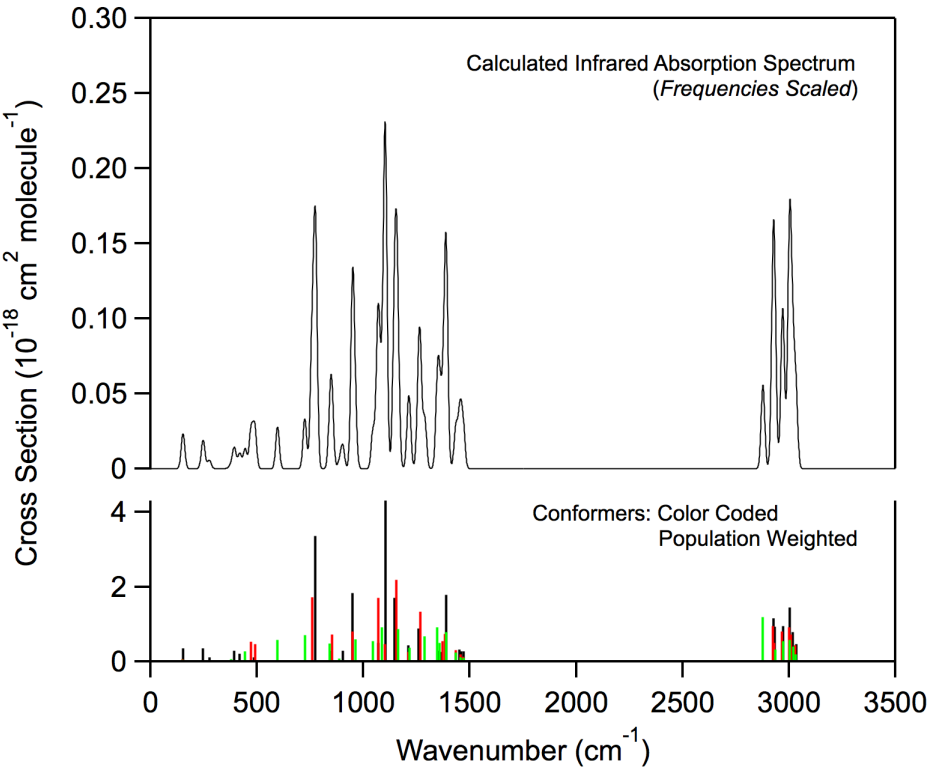
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	1.487207181900	-1.120791981000	0.261797010100
C	1.023480678600	0.160094911700	-0.410073118100
C	-0.392098474700	0.133665242000	-0.968631578600
H	1.679864246100	0.393427164200	-1.263428713700
F	1.128677140900	1.208107678100	0.485485170900
H	2.512977096100	-0.997891014100	0.617827109800
H	1.463342269000	-1.954730654200	-0.446438096900
H	0.845370799000	-1.363550589000	1.111196064600
Cl	-1.642645352100	-0.240933224300	0.280605018500
H	-0.651245955200	1.110852549100	-1.376439142700
H	-0.481305629600	-0.624277082500	-1.748387723800

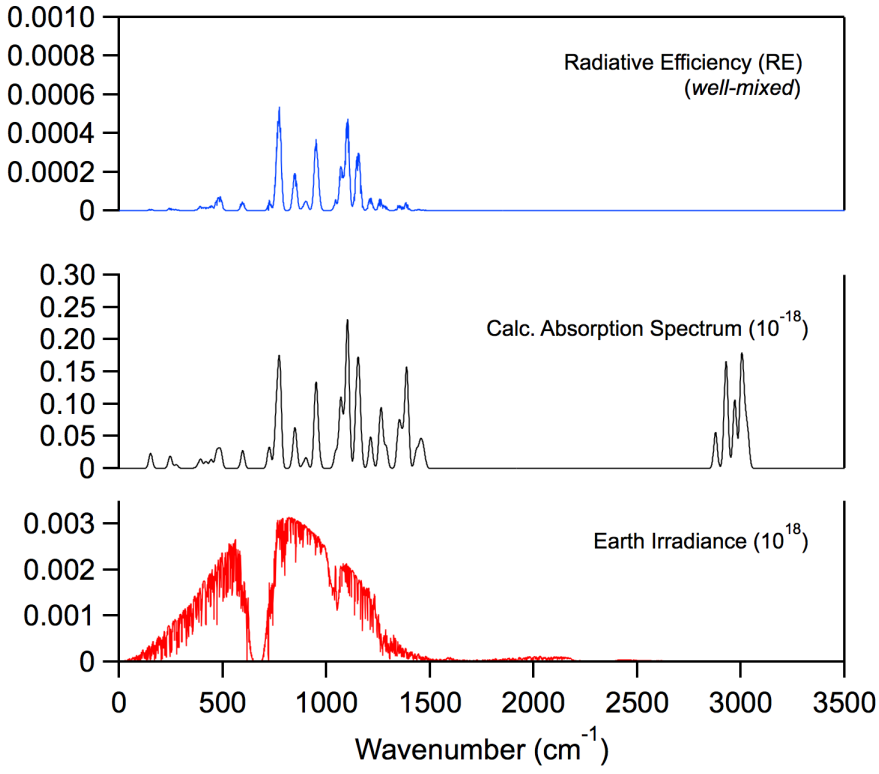
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
101.7452	0.267
202.6865	0.0815
228.0975	0.0282
344.8836	0.281
413.4209	1.26
574.7126	2.60
710.2491	3.12
834.9456	2.17
882.9271	0.418
961.9231	2.67
1049.8691	2.42
1092.9716	4.06
1174.5558	3.90
1232.2404	1.65
1307.5550	3.05
1370.0161	4.06
1381.4302	2.22
1413.9114	3.52
1461.0455	1.08
1484.6548	0.506
1499.1315	0.453
2990.2916	5.26
3051.4313	1.43
3089.5808	2.41
3123.9778	2.60
3142.5495	1.78
3152.6040	0.869

Infrared Spectrum

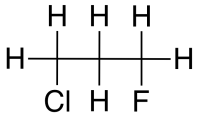


Radiative Efficiency



HCFC-271fa

Molecular Formula:	$CH_2ClCH_2CH_2F$
Name:	1-Chloro-3-fluoropropane
CAS number:	462-38-4
Molecular Weight:	96.53



Global Atmospheric Lifetime (years):	0.339
Tropospheric Atmospheric Lifetime (years):	0.345
Stratospheric Atmospheric Lifetime (years):	20
Ozone Depletion Potential (ODP):	0.004

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.055	0.028
Global Warming Potential (GWP_H):		
GWP_{20}	43	22
GWP_{100}	12	6
Global Temperature Potentials (GTP_H)		
GTP_{20}		7
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*

$k_{SAR}(298\ K) = 1.70 \times 10^{-13}$; $k_{SAR}(272\ K) \approx 1.08 \times 10^{-13}$ cm^3 $molecule^{-1}$ s^{-1}

τ^{OH}_{Global} = 0.339 years
τ^{OH}_{Trop} = 0.345 years
τ^{OH}_{Strat} = 20 years

Fractional Atmospheric Loss: 0.998

$O(^1D)$ Reactivity

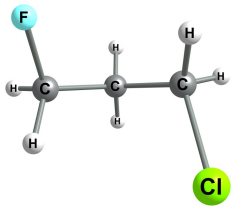
k_{Rec}(T), *No recommendation*

$k_{Est}(T) = 1.2 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}
$\tau_{O(^1D)}$ = 310 years
Fractional Atmospheric Loss: 0.001

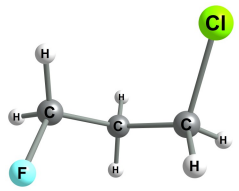
UV Photolysis

UV Spectrum: *No Recommendation*
τ_{hv} = 450 years
Fractional Atmospheric Loss: 0.001

Molecular Structure and Infrared Spectrum (7 conformers)



E = 0
Population = 0.323



E = 0
Population = 0.323

Optimized Coordinates (Angstroms)

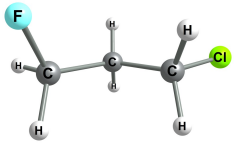
Atom	X	Y	Z
C	-0.592742601500	-0.772129362000	0.577731156400
C	0.599443316200	-1.045993559800	-0.328804105600
C	1.464769229300	0.179951895500	-0.574501068800
H	0.263351776900	-1.452014706100	-1.288735632700
H	1.212092470600	-1.816774482300	0.156913691700
Cl	-1.823214814500	0.300504107900	-0.219453399200
H	-0.281723752500	-0.256083024100	1.485629704100
H	-1.120601263300	-1.688703830800	0.838656210500
F	1.935782548500	0.657510729500	0.636510990300
H	2.325261313900	-0.072463709500	-1.205312233000
H	0.891777776400	0.978275941700	-1.059077313700

Atom	X	Y	Z
C	-0.569058127400	-0.723094128600	-0.608408348100
C	0.589070629900	-1.014649067700	0.335967567700
C	1.468386874800	0.196508609900	0.604278422000
H	1.202515111500	-1.798334845000	-0.127594652300
H	0.215859007100	-1.410597888000	1.286344956800
Cl	-1.804196531700	0.374782146500	0.146068166800
H	-1.105032292500	-1.631082601500	-0.882472558700
H	-0.220544959300	-0.216454158200	-1.507946823500
F	1.985560726800	0.660536820300	-0.593086763900
H	0.895116334000	1.007008218000	1.067858251400
H	2.304046226800	-0.068776105800	1.262593781700

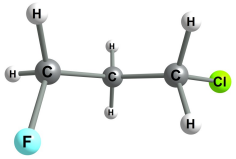
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
75.7342	0.399
178.4465	1.31
228.9658	0.562
376.6819	0.662
499.9198	0.415
657.8103	4.14
790.8782	1.33
882.9519	1.55
947.2163	2.78
1059.8029	3.31
1078.5020	5.38
1101.3602	4.22
1179.5607	1.27
1243.6714	1.06
1296.9133	0.580
1324.6329	4.50
1389.2374	0.186
1428.5259	1.80
1458.6289	0.871
1479.8433	0.929
1514.9995	0.668
3030.2847	2.12
3035.7797	5.03
3082.0064	3.33
3089.5937	3.40
3101.7578	3.46
3162.9515	0.630

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
75.7385	0.399
178.4450	1.31
228.9656	0.562
376.6819	0.662
499.9189	0.415
657.8016	4.14
790.8773	1.33
882.9533	1.55
947.2145	2.78
1059.8037	3.31
1078.4978	5.38
1101.3607	4.22
1179.5579	1.27
1243.6711	1.06
1296.9118	0.580
1324.6293	4.50
1389.2416	0.186
1428.5258	1.80
1458.6298	0.871
1479.8403	0.929
1514.9978	0.668
3030.2761	2.12
3035.7798	5.03
3082.0062	3.32
3089.5925	3.41
3101.7647	3.45
3162.9631	0.630



$\Delta E = 0.53$ kcal mol^{-1}
Population = 0.131



$\Delta E = 0.53$ kcal mol^{-1}
Population = 0.131

Optimized Coordinates (Angstroms)

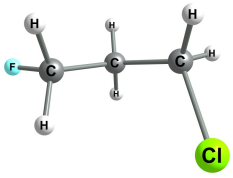
Atom	X	Y	Z
C	-0.456911273300	0.367747272400	-0.348399237800
C	0.460659190800	-0.725927949700	0.181268115900
C	1.908581662100	-0.477904217200	-0.219706369100
H	0.148797935900	-1.701969017400	-0.206192924700
H	0.389223121600	-0.769511143400	1.272696028400
Cl	-2.172665008400	0.095824938000	0.159520269600
H	-0.462594496300	0.400191457000	-1.439484253400
H	-0.167381645900	1.344855582200	0.036104204400
F	2.334867480700	0.736877820000	0.285996163600
H	2.559470675300	-1.266540151700	0.176074077600
H	2.021387357500	-0.450327590100	-1.311780074400

Atom	X	Y	Z
C	-0.457509851400	0.307813476100	0.424543463000
C	0.469241445300	-0.730431716600	-0.193338895400
C	1.919810850800	-0.482260701800	0.197867781600
H	0.378096667900	-0.702398937200	-1.283810098500
H	0.182109987000	-1.735907647800	0.133172202800
Cl	-2.177397648500	0.037857773300	-0.070257955700
H	-0.192677189400	1.313736758000	0.101443454200
H	-0.443247969200	0.267237497300	1.515279565200
F	2.314833368000	0.771446980300	-0.232614764500
H	2.052632267100	-0.525507311200	1.287178750400
H	2.577057072300	-1.230210170500	-0.261310503200

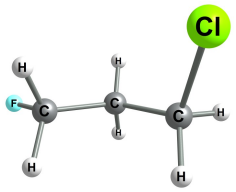
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
84.5251	0.658
134.2004	0.694
233.2111	0.198
293.3793	0.245
485.4025	2.54
731.8099	4.35
777.3706	0.892
898.6212	0.843
916.9174	2.05
1067.1535	0.450
1089.7850	10.9
1105.5882	1.98
1192.1029	1.33
1255.8461	0.782
1295.2957	2.80
1309.7839	0.726
1379.6842	1.73
1426.7754	2.88
1477.3274	0.571
1491.7242	0.454
1514.8147	0.283
3018.3603	6.47
3049.7885	0.417
3068.7203	6.52
3086.3993	2.06
3099.3258	3.38
3156.9948	1.10

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
84.5233	0.658
134.1966	0.694
233.2122	0.198
293.3803	0.245
485.4035	2.54
731.8139	4.35
777.3720	0.892
898.6237	0.843
916.9188	2.05
1067.1556	0.450
1089.7900	10.9
1105.5916	1.98
1192.1032	1.33
1255.8471	0.782
1295.2987	2.80
1309.7859	0.726
1379.6872	1.73
1426.7741	2.88
1477.3283	0.571
1491.7283	0.454
1514.8161	0.283
3018.3610	6.47
3049.7902	0.417
3068.7214	6.52
3086.3899	2.07
3099.3224	3.38
3156.9858	1.10



$\Delta E = 1.25$ kcal mol^{-1}
Population = 0.039



$\Delta E = 1.25$ kcal mol^{-1}
Population = 0.039

Optimized Coordinates (Angstroms)

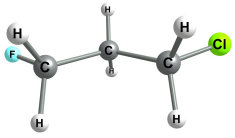
Atom	X	Y	Z
C	-0.850924177800	-0.957267762500	0.229059542800
C	0.570692791700	-0.798900787500	-0.286646779800
C	1.338214087500	0.348998057100	0.355429326400
H	0.564173552100	-0.668649075200	-1.373415625400
H	1.105243719900	-1.734212811800	-0.075146006900
Cl	-1.905262267900	0.460300069200	-0.197817153900
H	-0.887315908300	-1.039035332500	1.316999356800
H	-1.335963009700	-1.829548214000	-0.208108153200
F	2.632732665200	0.348433806300	-0.122345375400
H	0.878527639000	1.314724240700	0.120420916600
H	1.370445908400	0.235717810100	1.447653952000

Atom	X	Y	Z
C	-0.840185443500	-0.949067613400	-0.239985289100
C	0.567236470400	-0.773511855500	0.308084580600
C	1.363556204900	0.331784671800	-0.372516979000
H	1.099132974700	-1.722985918800	0.163621094300
H	0.530325321200	-0.584055183000	1.385497540800
Cl	-1.893478627700	0.497603098500	0.077911842000
H	-1.345673531300	-1.792497775600	0.229438659300
H	-0.845694781700	-1.089835974100	-1.322472405200
F	2.643565742600	0.347586925900	0.142620890300
H	1.426515889200	0.158759969800	-1.455533946800
H	0.906058781000	1.312339654400	-0.204067987200

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
92.4148	0.774
122.0347	0.408
245.5725	0.0646
311.7658	0.610
489.9867	1.63
656.7309	4.52
792.5725	0.935
857.3352	0.935
999.5570	1.73
1066.9303	1.69
1088.5705	15.4
1102.2555	0.816
1207.9865	0.417
1241.4453	0.862
1304.4305	1.57
1326.1419	4.13
1350.9174	0.154
1440.3119	1.78
1477.7699	0.672
1485.5532	0.526
1523.6710	0.204
3018.2441	5.43
3033.3286	2.20
3075.3425	2.34
3084.5275	0.414
3099.4470	6.65
3147.4717	1.28

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
92.4070	0.774
122.0355	0.408
245.5723	0.0646
311.7658	0.609
489.9864	1.63
656.7339	4.52
792.5720	0.935
857.3335	0.935
999.5562	1.73
1066.9288	1.69
1088.5769	15.4
1102.2546	0.818
1207.9848	0.417
1241.4476	0.862
1304.4325	1.57
1326.1427	4.13
1350.9160	0.154
1440.3125	1.78
1477.7706	0.672
1485.5539	0.526
1523.6716	0.204
3018.2397	5.44
3033.3324	2.20
3075.3429	2.34
3084.5255	0.414
3099.4470	6.65
3147.4690	1.28



$\Delta E = 1.86$ kcal mol^{-1}
Population = 0.014

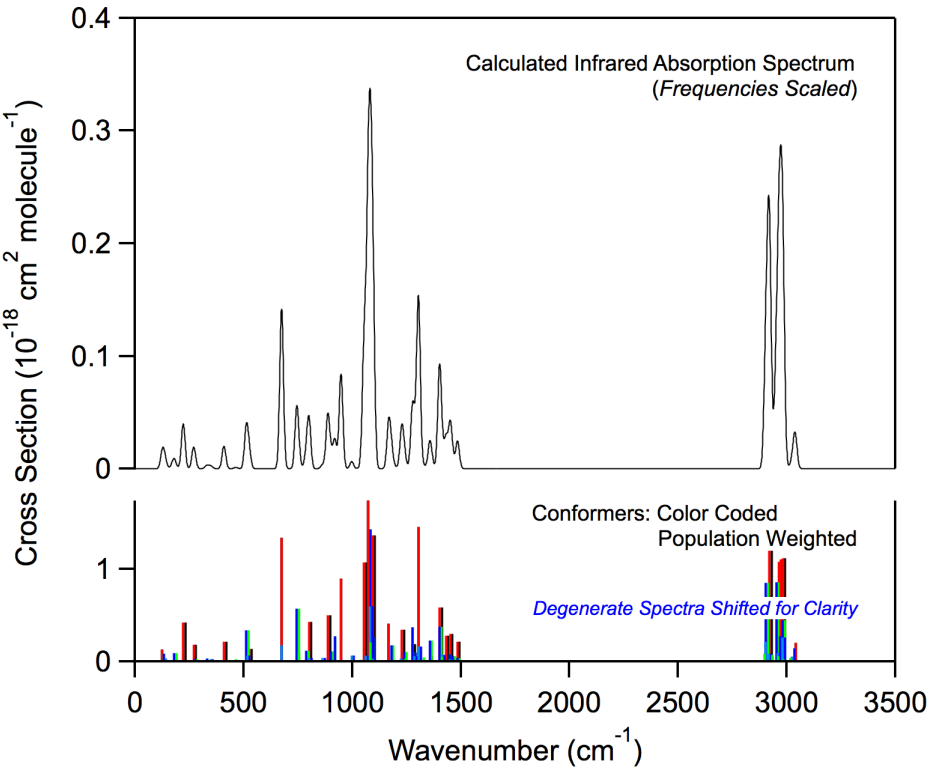
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-0.695660542000	0.666001718500	0.012478757700
C	0.486623182900	-0.292227784700	0.026094098600
C	1.814751323000	0.457383356200	-0.011429574300
H	0.431674343200	-0.964160755000	-0.835996176300
H	0.452734662900	-0.913175363900	0.926640469400
Cl	-2.269590320400	-0.226022742300	0.057090759900
H	-0.719040553700	1.275380536400	-0.892769487700
H	-0.697855055900	1.326760802200	0.881248082400
F	2.851180324900	-0.450642150300	0.002441967700
H	1.900703846900	1.068041959700	-0.920118754700
H	1.921890788200	1.119459423200	0.858166857300

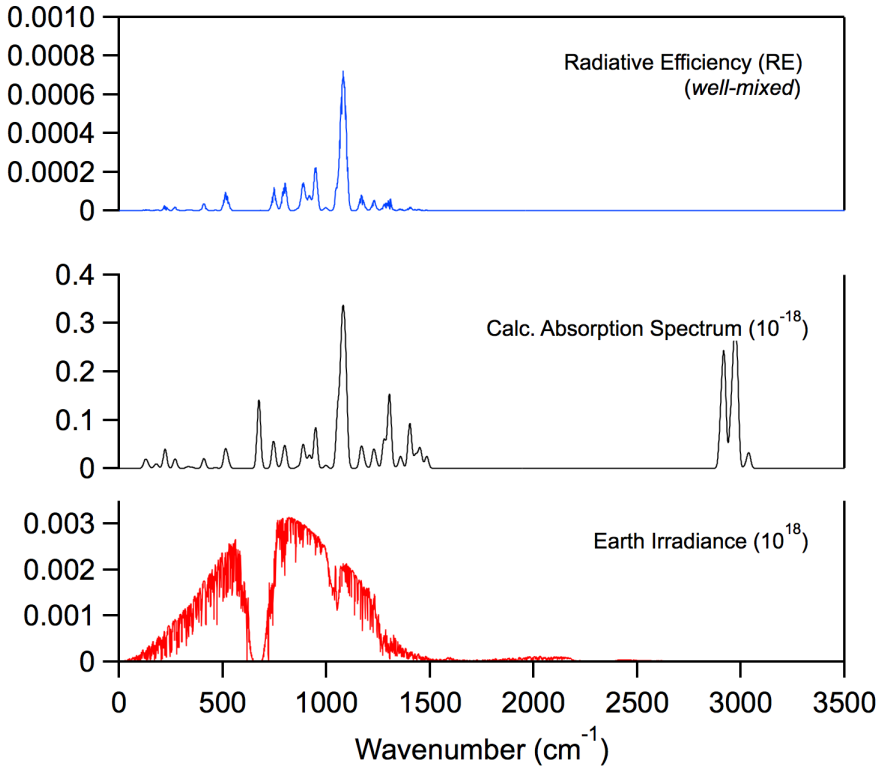
Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
100.1271	0.345
119.0708	0.109
159.6005	0.678
321.5555	0.547
435.0500	1.79
743.0621	7.60
763.2532	0.322
855.1226	0.110
1042.9618	1.31
1064.1343	0.932
1087.0702	0.00208
1092.3503	14.7
1221.9247	0.565
1260.4782	2.34
1296.1446	0.00935
1312.4353	0.0285
1350.8503	3.10
1440.6875	3.82
1487.2783	0.199
1499.0760	0.331
1525.2909	0.130
3010.8476	6.01
3050.9748	5.16
3057.6164	1.11
3079.1981	4.03
3103.4347	1.78
3138.6335	2.83

Infrared Spectrum

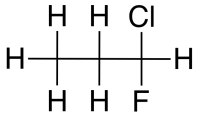


Radiative Efficiency



HCFC-271fb

Molecular Formula:	CH_3CH_2CHClF
Name:	1-Chloro-1-fluoropropane
CAS number:	430-55-7
Molecular Weight:	96.53



Global Atmospheric Lifetime (years):	0.492
Tropospheric Atmospheric Lifetime (years):	0.506
Stratospheric Atmospheric Lifetime (years):	20
Ozone Depletion Potential (ODP):	0.007

	Well-mixed	*Lifetime adjusted*
Radiative Efficiency (RE):	0.109	0.065
Global Warming Potential (GWP_H):		
GWP_{20}	125	75
GWP_{100}	34	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*

$k_{SAR}(298\ K) = 1.16 \times 10^{-13}$; $k_{SAR}(272\ K) \approx 0.739 \times 10^{-13}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau^{OH}_{Global} = 0.494$ years

$\tau^{OH}_{Trop} = 0.506$ years

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

Fractional Atmospheric Loss: 0.997

$O(^1D)$ Reactivity

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

$k_{Est}(T) = 1.2 \times 10^{-10}$ cm^3 $molecule^{-1}$ s^{-1}

$\tau_{O(^1D)} = 310$ years

Fractional Atmospheric Loss: 0.002

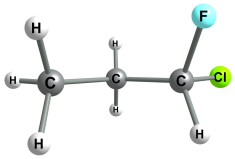
UV Photolysis

UV Spectrum: *No Recommendation*

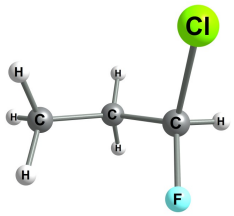
$\tau_{hv} = 450$ years

Fractional Atmospheric Loss: 0.001

Molecular Structure and Infrared Spectrum (3 conformers)



E = 0
Population = 0.469



$\Delta E = 0.33$ kcal mol^{-1}
Population = 0.268

Optimized Coordinates (Angstroms)

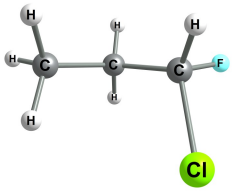
Atom	X	Y	Z
C	-2.381599446200	-0.253388006500	0.071184425800
C	-0.954755574100	-0.724547185300	-0.232831074200
C	0.078183481800	0.218361630500	0.352529219000
H	-0.786976386500	-0.782553032400	-1.313087120100
H	-0.775945575100	-1.722574524700	0.178119018200
H	-3.110717980000	-0.937967350100	-0.370041301500
H	-2.556807365300	0.744439071900	-0.338473347500
H	-2.569053048300	-0.215312071100	1.149689741600
Cl	1.762610175000	-0.353588469700	-0.013319889400
F	-0.068662536700	1.465328013200	-0.165405557000
H	0.029631255400	0.287444924300	1.442485884900

Atom	X	Y	Z
C	-1.796553070400	0.738357949300	0.491794443900
C	-1.160512483500	0.078078348500	-0.732704346200
C	0.170168017500	-0.596916623700	-0.452655929800
H	-1.010752578800	0.799642700500	-1.541702641100
H	-1.820881176900	-0.707780667700	-1.122392386100
H	-1.177253101100	1.557358200500	0.865721766300
H	-1.925153506000	0.012191927500	1.298258769900
H	-2.779154261200	1.142754331800	0.235324597300
Cl	1.455304965300	0.606067744400	0.014145910700
F	0.046078858000	-1.493683393000	0.558955972400
H	0.577806337100	-1.109685518100	-1.326487157300

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
110.0423	0.0923
213.0596	0.0177
224.8040	0.166
338.4198	1.04
387.3663	0.758
474.0213	0.775
744.1829	11.6
792.7938	4.03
903.0332	7.27
994.5058	4.73
1064.7451	3.37
1145.0612	2.08
1148.3953	12.6
1264.0840	4.55
1299.2665	0.904
1360.1640	1.50
1397.7171	1.43
1413.5839	0.577
1475.5158	0.234
1497.1505	0.929
1508.1853	1.10
3042.3824	2.98
3057.9680	1.28
3081.9314	2.36
3100.0037	0.413
3115.9224	5.27
3130.7127	3.43

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
108.5943	0.0149
206.6790	0.0295
238.0599	0.630
340.3868	0.131
371.8589	0.190
572.5013	4.14
704.6358	8.19
800.5338	1.84
878.5131	6.84
998.9868	6.40
1076.2958	0.858
1104.9919	4.69
1156.2676	11.6
1276.7468	2.11
1306.3925	5.33
1370.9823	2.04
1385.8060	0.688
1417.2263	1.26
1470.3748	0.397
1496.4851	0.644
1509.4948	1.12
3030.8035	2.30
3054.3811	2.62
3087.6543	1.14
3096.3633	4.04
3125.6561	3.22
3133.7809	2.94



$\Delta E = 0.34$ kcal mol^{-1}
Population = 0.264

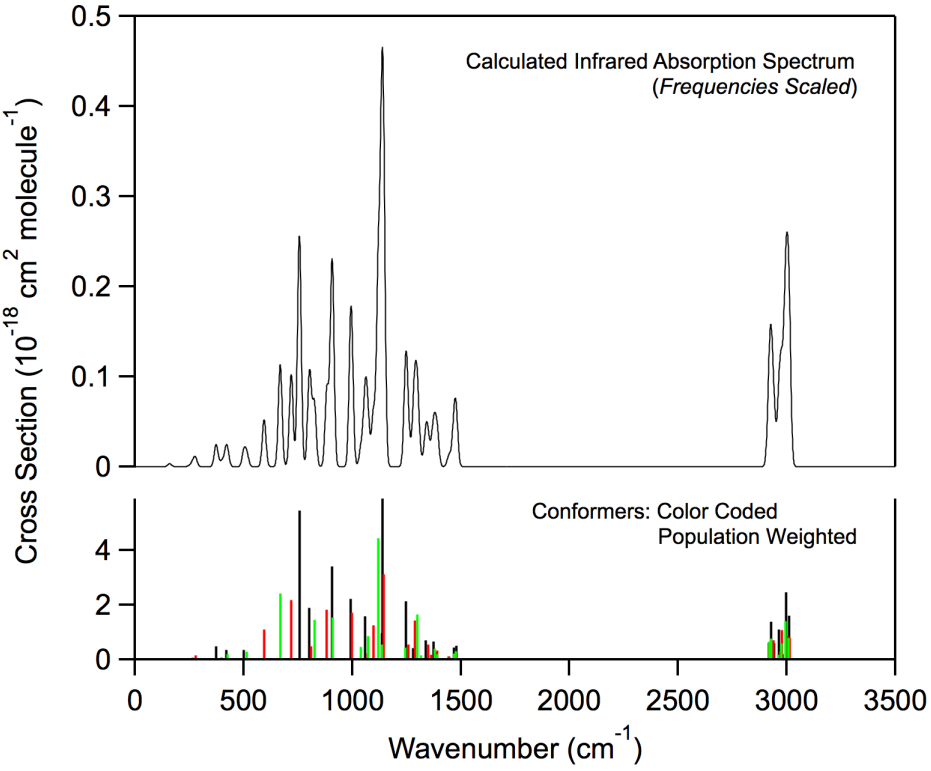
Optimized Coordinates (Angstroms)

Atom	X	Y	Z
C	-2.108290079500	-0.513556714400	0.111519777900
C	-1.132908104100	0.585675645200	-0.309401777500
C	0.225369913000	0.497510223400	0.359005006800
H	-1.531566499300	1.572228719300	-0.040840512600
H	-0.979638250900	0.585023561200	-1.393293434100
H	-3.082823797000	-0.353318107700	-0.357196430300
H	-2.258107448500	-0.520043746800	1.196597239100
H	-1.745712164600	-1.500563969100	-0.185606336000
Cl	1.127918017700	-0.998109524700	-0.148360505000
F	0.980068576000	1.573384224900	0.023658282900
H	0.165363837300	0.433581688600	1.448734688700

Infrared Absorption Spectrum (unscaled frequencies)

Band Center (cm^{-1})	Band Strength (10^{-18} cm^2 $molecule^{-1}$ cm^{-1})
115.5670	0.102
210.2410	0.0518
232.3105	0.177
363.5104	0.381
394.7058	0.790
488.5259	1.08
650.8282	9.17
817.6912	5.51
906.1087	5.87
1045.3456	1.74
1077.8989	3.29
1128.9348	16.9
1145.9682	2.11
1259.7193	1.68
1319.3069	6.24
1335.3644	0.571
1404.2664	1.49
1416.3324	0.740
1477.7868	0.261
1498.6252	0.811
1508.0315	1.19
3036.0501	2.51
3043.0531	2.90
3077.4422	0.683
3093.2338	2.26
3113.0520	5.38
3129.6842	2.99

Infrared Spectrum



Radiative Efficiency