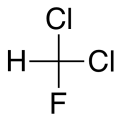
# HCFC-21

| | |
|---|---|
| Molecular Formula: | $CHFCl_2$ |
| Name: | Dichlorofluoromethane |
| CAS number: | 75-43-4 |
| Molecular Weight: | 102.92 |




| | | | |
|---|---|---|---|
| Global Atmospheric Lifetime (years): | 2.66 | | 1.7 # |
| Tropospheric Atmospheric Lifetime (years): | 2.87 | | 1.8 # |
| Stratospheric Atmospheric Lifetime (years): | 36.4 | | ~35 # |
| Ozone Depletion Potential (ODP): | 0.053 | | |
| | *Well-mixed* | *Lifetime adjusted* | |
| Radiative Efficiency (RE): | 0.212 | 0.185 | 0.15 # |
| Global Warming Potential ($GWP_H$): | | | |
| $GWP_{20}$ | 1235 | 1078 | 543 # |
| $GWP_{100}$ | 335 | 292 | 148 # |
| Global Temperature Potentials ($GTP_H$) | | | |
| $GTP_{20}$ | | 438 | 192 # |
| $GTP_{50}$ | | 53 | 26 # |
| $GTP_{100}$ | | 41 | 20 # |

* RE units: W $m^2$ $ppb^{-1}$
* GWP and GTP: Relative to $CO_2$
# Value taken from WMO (2014)

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

### OH Reactivity

$k_{Rec}(T) = 1.52 \times 10^{-12} \exp(-1170/T)$; $k_{Rec}(272\ K) = 2.06 \times 10^{-14}$ $cm^3$ $molecule^{-1}$ $s^{-1}$

$k_{SAR}(298\ K) = 2.04 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 1.30 \times 10^{-14}$ $cm^3$ $molecule^{-1}$ $s^{-1}$

$\tau^{OH}_{Global} = 2.78$ years

$\tau^{OH}_{Trop} = 2.87$ years

$\tau^{OH}_{Strat} = 87.2$ years

Fractional Atmospheric Loss: 0.957

### O($^1$D) Reactivity

$k_{Rec}(T) = 0.80 \times 1.9 \times 10^{-10}$ $cm^3$ $molecule^{-1}$ $s^{-1}$

$k_{Est}(T) = 1.3 \times 10^{-10}$ $cm^3$ $molecule^{-1}$ $s^{-1}$

$\tau_{O(^1D)} = 285$ years

Fractional Atmospheric Loss: 0.009

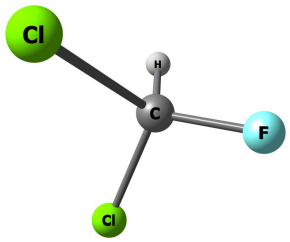
### UV Photolysis

UV Spectrum: *Recommendation Available*

$\tau_{hv} = 80$ years

Fractional Atmospheric Loss: 0.033

## **Molecular Structure and Infrared Spectrum** (1 conformer)



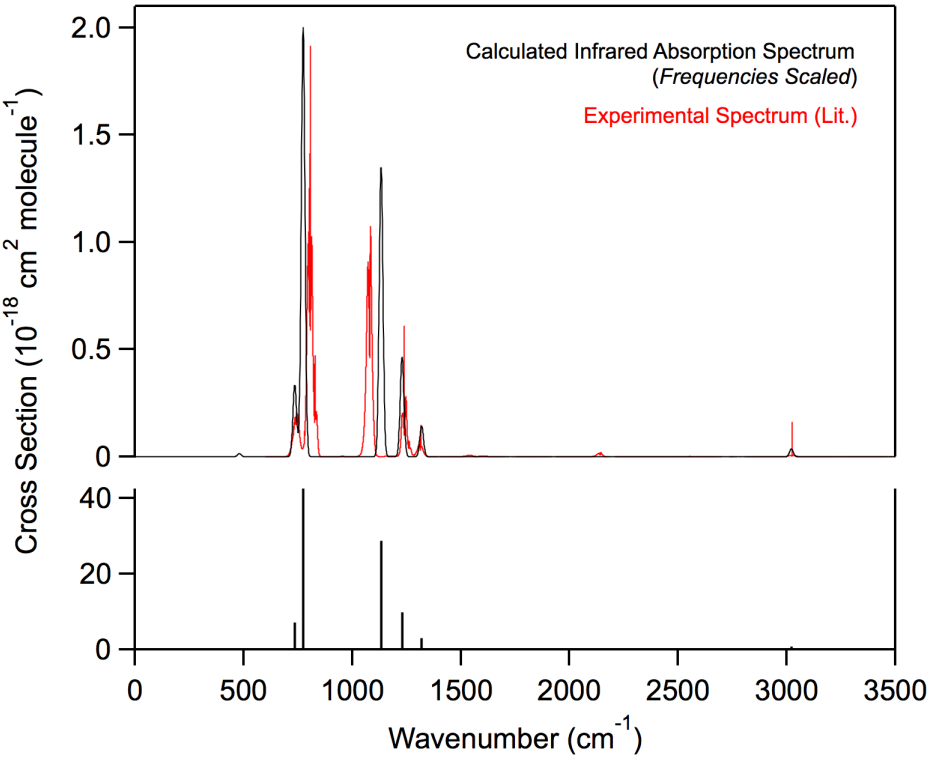

Optimized Coordinates (Angstroms)

| Atom | X | Y | Z |
|---|---|---|---|
| Cl | 1.475551675463 | -0.738751307670 | 0.110037971949 |
| Cl | -1.475617908874 | -0.738582646955 | 0.110122475911 |
| F | 0.000087927183 | 1.352992186257 | 0.162625846251 |
| C | 0.000002789951 | 0.138240773815 | -0.386148046469 |
| H | -0.000024476708 | 0.205400993154 | -1.472438247789 |

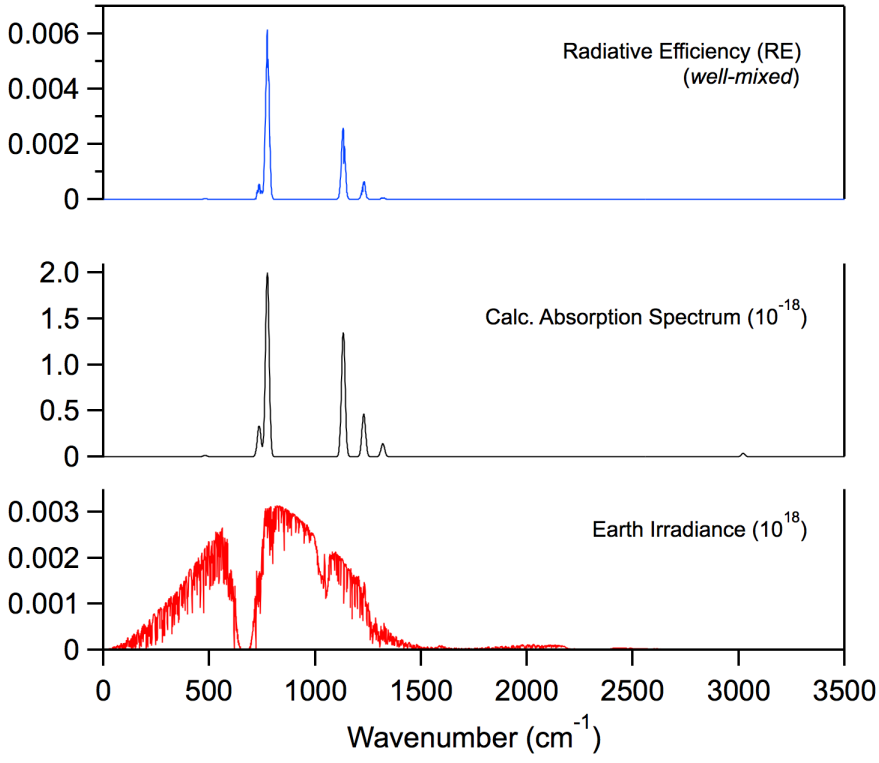
Infrared Absorption Spectrum (unscaled frequencies)

| Band Center ($cm^{-1}$) | Band Strength ($10^{-18}$ $cm^2$ $molecule^{-1}$ $cm^{-1}$) |
|---|---|
| 268.6921 | 0.0211 |
| 362.5257 | 0.0273 |
| 451.3936 | 0.311 |
| 721.8254 | 7.11 |
| 762.7758 | 42.6 |
| 1142.6109 | 28.7 |
| 1245.0392 | 9.90 |
| 1340.2790 | 3.05 |
| 3142.6198 | 0.776 |

## Infrared Spectrum

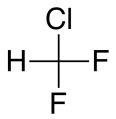



## Radiative Efficiency



# HCFC-22

| | |
|---|---|
| Molecular Formula: | $CHF_2Cl$ |
| Name: | Difluorochloromethane |
| CAS number: | 75-45-6 |
| Molecular Weight: | 86.47 |




| | | | |
|---|---|---|---|
| Global Atmospheric Lifetime (years): | 8.09 | | 11.9 # |
| Tropospheric Atmospheric Lifetime (years): | 8.67 | | 13.0 # |
| Stratospheric Atmospheric Lifetime (years): | 119.8 | | 161 # |
| Ozone Depletion Potential (ODP): | 0.032 | | |
| | *Well-mixed* | *Lifetime adjusted* | |
| Radiative Efficiency (RE): | 0.211 | 0.200 | 0.21 # |
| Global Warming Potential ($GWP_H$): | | | |
| $GWP_{20}$ | 4066 | 3847 | 5280 # |
| $GWP_{100}$ | 1203 | 1138 | 1760 # |
| Global Temperature Potentials ($GTP_H$) | | | |
| $GTP_{20}$ | | 2661 | 4200 # |
| $GTP_{50}$ | | 344 | 832 # |
| $GTP_{100}$ | | 162 | 262 # |

* RE units: W $m^2$ $ppb^{-1}$
* GWP and GTP: Relative to $CO_2$
\# Value taken from WMO (2014)

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

### OH Reactivity

$k_{Rec}(T) = 9.2 \times 10^{-13} \exp(-1560/T)$; $k_{Rec}(272\ K) = 2.97 \times 10^{-15}$ $cm^3$ $molecule^{-1}$ $s^{-1}$

$k_{SAR}(298\ K) = 6.76 \times 10^{-15}$; $k_{SAR}(272\ K) \approx 4.32 \times 10^{-15}$ $cm^3$ $molecule^{-1}$ $s^{-1}$

$\tau^{OH}_{Global} = 8.37$ years

$\tau^{OH}_{Trop} = 8.67$ years

$\tau^{OH}_{Strat} = 236.2$ years

Fractional Atmospheric Loss: 0.967

### O($^1$D) Reactivity

$k_{Rec}(T) = 0.75 \times 1.02 \times 10^{-10}$ $cm^3$ $molecule^{-1}$ $s^{-1}$

$k_{Est}(T) = 0.7 \times 10^{-10}$ $cm^3$ $molecule^{-1}$ $s^{-1}$

$\tau_{O(^1D)} = 529$ years

Fractional Atmospheric Loss: 0.015

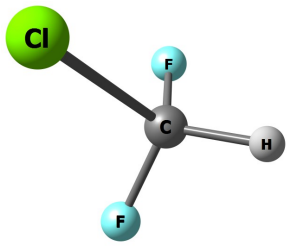
### UV Photolysis

UV Spectrum: *Recommendation Available*

$\tau_{hv} = 450$ years

Fractional Atmospheric Loss: 0.018

## **Molecular Structure and Infrared Spectrum** (1 conformer)



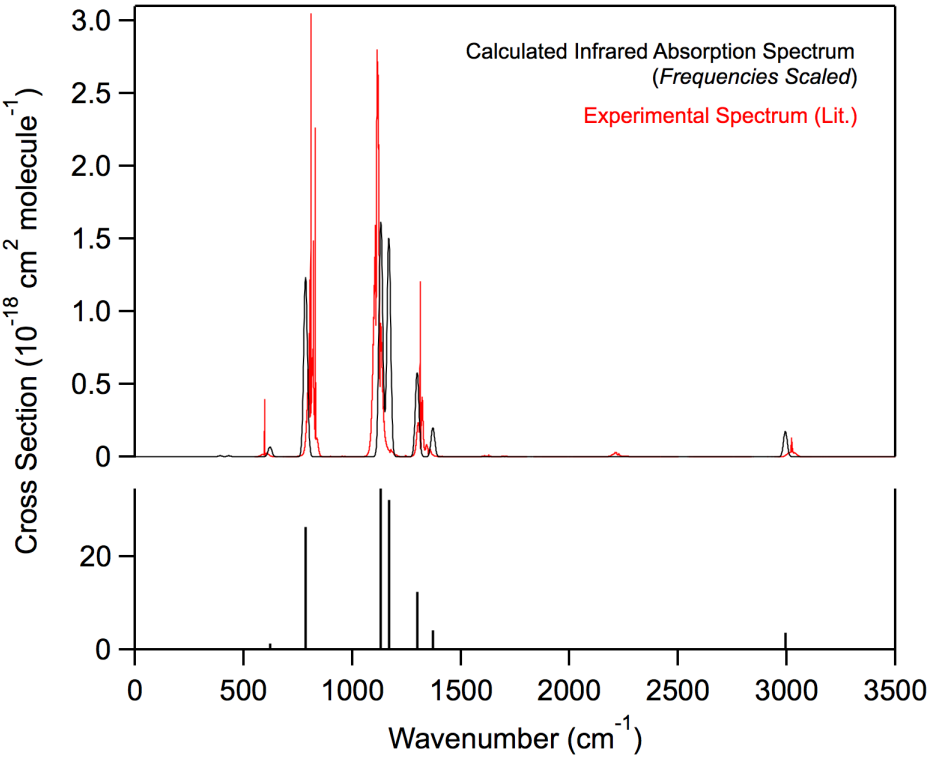

Optimized Coordinates (Angstroms)

| Atom | X | Y | Z |
|---|---|---|---|
| Cl | -1.595187201568 | -0.000093523658 | 0.099829127582 |
| F | 0.730919033948 | 1.083257949134 | 0.132729883802 |
| F | 0.731013340305 | -1.083242786826 | 0.132717225556 |
| C | 0.141394919762 | -0.000015163329 | -0.367429843329 |
| H | 0.195459907553 | -0.000006481704 | -1.458046393612 |

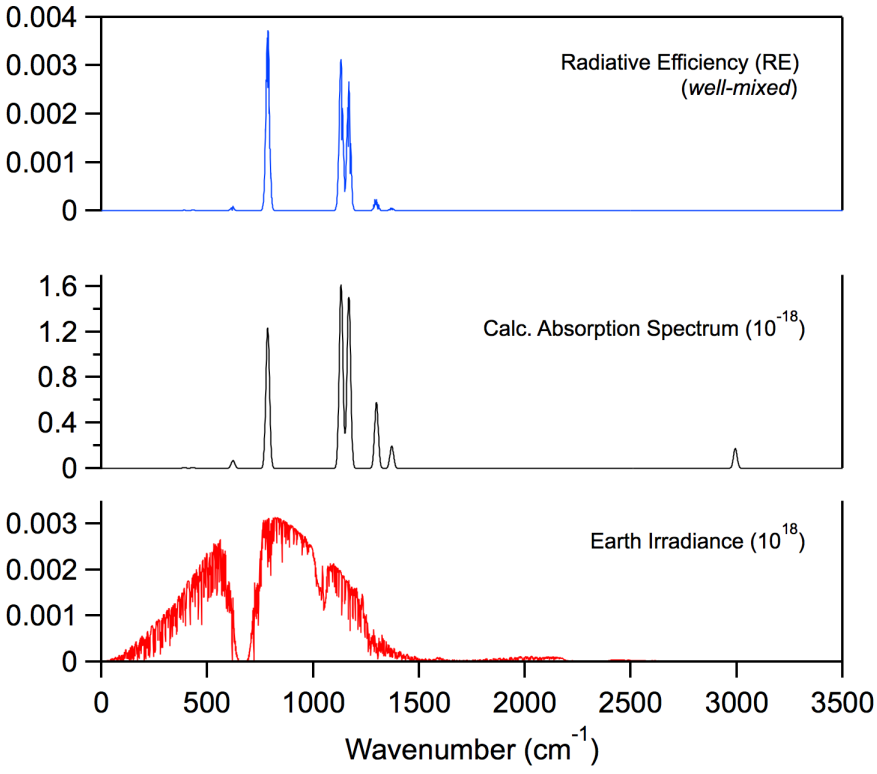
Infrared Absorption Spectrum (unscaled frequencies)

| Band Center ($cm^{-1}$) | Band Strength ($10^{-18}$ $cm^2$ $molecule^{-1}$ $cm^{-1}$) |
|---|---|
| 358.5470 | 0.144 |
| 400.0331 | 0.141 |
| 601.1112 | 1.45 |
| 774.5755 | 26.3 |
| 1141.5492 | 34.4 |
| 1180.3622 | 32.0 |
| 1318.4344 | 12.4 |
| 1395.1002 | 4.21 |
| 3113.1987 | 3.71 |

## Infrared Spectrum

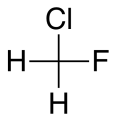



## Radiative Efficiency



# HCFC-31

| | |
|---|---|
| Molecular Formula: | $CH_2FCl$ |
| Name: | Chlorofluoromethane |
| CAS number: | 593-70-4 |
| Molecular Weight: | 68.48 |




| | | |
|---|---|---|
| Global Atmospheric Lifetime (years): | 0.897 | 1.2 # |
| Tropospheric Atmospheric Lifetime (years): | 0.927 | 1.3 # |
| Stratospheric Atmospheric Lifetime (years): | 27.7 | ~35 # |
| Ozone Depletion Potential (ODP): | 0.015 | |

| | *Well-mixed* | *Lifetime adjusted* |
|---|---|---|
| Radiative Efficiency (RE): | 0.081 | 0.059 |
| Global Warming Potential ($GWP_H$): | | |
| $GWP_{20}$ | 240 | 173 |
| $GWP_{100}$ | 65 | 47 |
| Global Temperature Potentials ($GTP_H$) | | |
| $GTP_{20}$ | | 55 |
| $GTP_{50}$ | | 8 |
| $GTP_{100}$ | | 7 |

* RE units: W $m^2$ $ppb^{-1}$
* GWP and GTP: Relative to $CO_2$
\# Value taken from WMO (2014)

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

### OH Reactivity

$k_{Rec}(T) = 2.4 \times 10^{-12} \exp(-1210/T)$; $k_{Rec}(272\ K) = 2.8 \times 10^{-14}$ $cm^3$ $molecule^{-1}$ $s^{-1}$

$k_{SAR}(298\ K) = 6.32 \times 10^{-14}$; $k_{SAR}(272\ K) \approx 4.04 \times 10^{-14}$ $cm^3$ $molecule^{-1}$ $s^{-1}$

$\tau^{OH}_{Global} = 0.90$ years

$\tau^{OH}_{Trop} = 0.927$ years

$\tau^{OH}_{Strat} = 31.5$ years

Fractional Atmospheric Loss: 0.996

### $O(^1D)$ Reactivity

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

$k_{Est}(T) = 0.8 \times 10^{-10}$ $cm^3$ $molecule^{-1}$ $s^{-1}$

$\tau_{O(^1D)} = 463$ years

Fractional Atmospheric Loss: 0.002

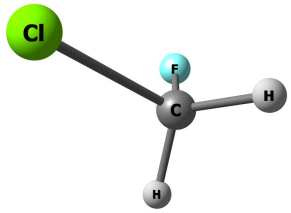
### UV Photolysis

UV Spectrum: *Recommendation Available*

$\tau_{hv} = 450$ years

Fractional Atmospheric Loss: 0.002

## **Molecular Structure and Infrared Spectrum** (1 conformer)



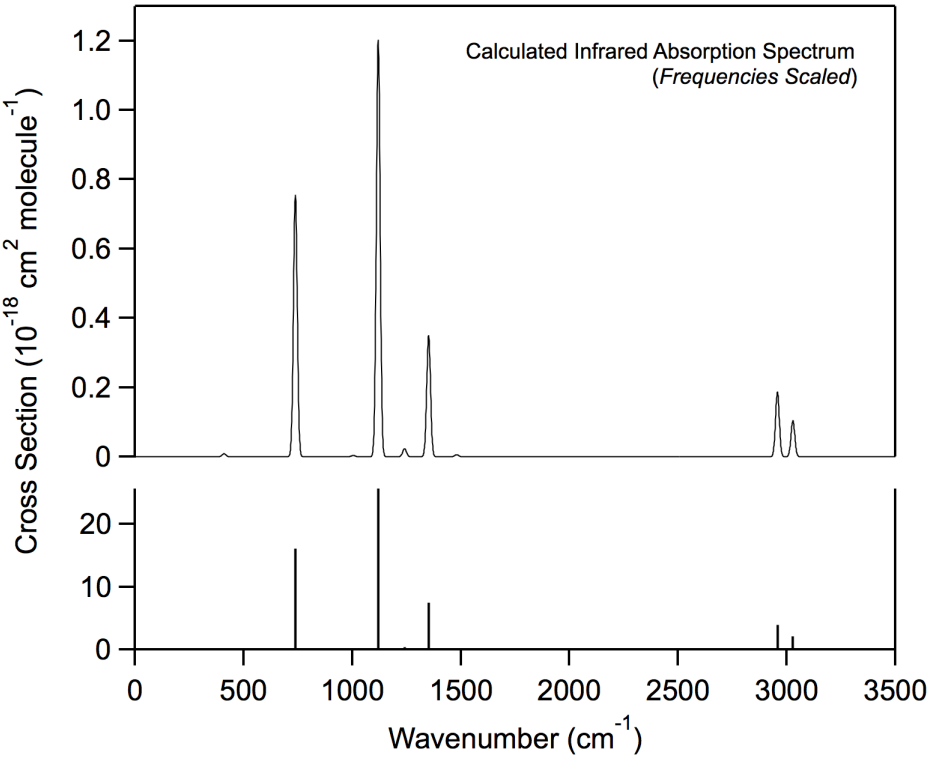

Optimized Coordinates (Angstroms)

| Atom | X | Y | Z |
|---|---|---|---|
| Cl | -1.570835418981 | -0.053480890868 | 0.107386629930 |
| F | 0.773140057913 | 1.061952857705 | 0.143720172579 |
| H | 0.618479723889 | -0.936636277406 | 0.077573295505 |
| C | 0.170335388395 | -0.037862507820 | -0.349233423145 |
| H | 0.212480248785 | -0.034073181612 | -1.439646674868 |

Infrared Absorption Spectrum (unscaled frequencies)

| Band Center ($cm^{-1}$) | Band Strength ($10^{-18}$ $cm^2$ $molecule^{-1}$ $cm^{-1}$) |
|---|---|
| 377.2034 | 0.181 |
| 724.8467 | 16.1 |
| 1006.7713 | 0.0799 |
| 1128.7369 | 25.6 |
| 1256.9509 | 0.490 |
| 1374.3528 | 7.48 |
| 1511.1938 | 0.126 |
| 3074.5677 | 3.97 |
| 3150.0099 | 2.21 |

## Infrared Spectrum




## Radiative Efficiency