

All data taken at Pacific Northwest National Laboratory (PNNL)  
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Composite spectrum for F12\_50T

Effective burden of composite spectrum: 1 part-per-million-meter (ppm-meter) at 296 K

#### **Sample Conditions-**

- Chemical name and CAS number: Dichlorodifluoromethane, Fluorocarbon-12, Arcton-6, Gentrion-12, CFC-12, CF-12, Freon-12, Frigen-12,  $\text{CCl}_2\text{F}_2$  : [75-71-8]
- Physical properties: M.W. 120 AMU, F.P.  $-158$  C, B.P.  $-29.8$  C
- Supplier and stated purity: Dupont, 98%
- Sample class: I (PNNL scale)
- Temperature of sample  $49.97$  C  $\pm 0.02$  C
- Diluent: Sample back filled with ultra high purity nitrogen to  $755 \pm 5$  Torr
- Concentration: Composite spectrum
- Preparation: Multiple freeze-thaw cycles.

#### **Instrument Parameters-**

- Bruker-120HR FTIR, evacuated optics bench
- Instrumental resolution (interferogram):  $0.1$   $\text{cm}^{-1}$
- Spectral intervals after FFT:  $0.06$   $\text{cm}^{-1}$
- Interferogram zero-fill: 2X
- Apodization: Boxcar
- Phase correction: Mertz
- Beam splitter: Potassium bromide (KBr)
- IR source: Carbide glowbar (22 V)
- Scanner velocity: 9 (Bruker arbitrary)
- Number of interferograms averaged per single channel spectra: 256
- Detector: Mid-band HgCdTe, photoconductive, 77K operation
- Folding limits: 15798 to  $0$   $\text{cm}^{-1}$

#### **Post Processing and Related Parameters-**

- Non-linearity detector correction (Bruker proprietary) applied to interferogram
- Composite spectrum created from 5 individual absorbance (base-10) spectra via classical least squares fit: Intercept=0, slope is fitted, individual absorbance values weighted by  $T^2$  (transmission squared), all absorbance values  $> 1.6$  are given zero weight
- Calculated and estimated errors: Type A = 0.54%, Type B = 3%
- Frequency correction:  $V(\text{corrected}) = V(\text{instrument}) * 1 + 0$
- Axis units: X=wavenumbers ( $\text{cm}^{-1}$ ), Y=Absorbance (base-10)