

All data taken at Pacific Northwest National Laboratory (PNNL)  
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Composite spectrum for F125\_5T\_

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

#### Sample Conditions-

- Chemical name and CAS number: Freon-125, halocarbon-125, pentafluoroethane, C<sub>2</sub>HF<sub>5</sub> : [354-33-6]
- Physical properties: M.W. 120 amu, F.P. -103C, B.P. -49C
- Supplier and stated purity: Scott Specialty Gases, 99.0%
- Sample class: I (PNNL scale).
- Temperature of sample:  $4.96 \pm 0.02$  C
- Diluent: Sample back filled with ultra high purity nitrogen to  $760 \pm 5$  Torr
- Individual samples at 0.76675, 3.0733, 0.19700, 0.50049, 1.5427, 11.1012 and 32.27 Torr. Path length = 19.96 cm. Final data is a composite spectrum.
- Preparation: Multiple freeze-thaw cycles at 77K to remove air. Use sample at -90C to minimize water.

#### Instrument Parameters-

- Bruker-66V FTIR, temperature controlled environment, evacuated optics bench
- Spectral range: 6,500 to 600 cm<sup>-1</sup> (1.534 to 16.67 microns)
- Instrumental resolution (interferogram): 0.112 cm<sup>-1</sup>
- Spectral intervals after FFT: 0.06 cm<sup>-1</sup>
- 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 cm<sup>-1</sup>

#### Post Processing and Related Parameters-

- Non-linearity detector correction (Bruker proprietary) applied to interferogram ( $\alpha=0.85$ ,  $\beta=530$ )
- Composite spectrum created from 7 individual absorbance (base-10) spectra via classical least squares fit: Intercept=0, slope is fitted, individual absorbance values weighted by T<sup>2</sup> (transmission squared), all absorbance values  $> 1.6$  are given zero weight
- Calculated and estimated errors: Type A = 0.64%, Type B = 3%
- Frequency correction:  $V(\text{corrected}) = V(\text{instrument}) * 0.9999984669 + 0.005187$
- Axis units: X=wavenumbers (cm<sup>-1</sup>), Y=Absorbance (base-10)
- Baseline corrected via 3rd order polynomial.