All data taken at Pacific Northwest National Laboratory (PNNL)
Operator: Steven W. Sharpe and Robert L. Sams, sw.sharpe@pnl.gov
Version 1.0, March, 2000

Composite spectrum for F125_50T
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_2HF_5 : [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: 50.04 ± 0.02 C
- Diluent: Sample back filled with ultra high purity nitrogen to 760±5 Torr
- Individual samples at 1.13935, 2.2559, 1.6238, 9.6748, 1.5508, 0.88020 and 46.42 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 550 cm^{-1} (1.534 to 18.18 microns)
- Instrumental resolution (interferogram): 0.112 cm^{-1}
- Spectral intervals after FFT: 0.06 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 cm^{-1}

Post Processing and Related Parameters-

- Non-linearity detector correction (Bruker proprietary) applied to interferogram (α=0.85, ε=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^2 (transmission squared), all absorbance values ≥ 1.6 are given zero weight
- Calculated and estimated errors: Type A = 0.32%, Type B ≤ 3%
- Frequency correction: V(corrected) = V(instrument)*0.9999984669+0.005187
- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Baeline corrected via 4^{th} order polynomial.