All data taken at Pacific Northwest National Laboratory (PNNL)
Operator: Steven W. Sharpe, sw.sharpe@pnl.gov
Version 1.0, September, 1999

Composite spectrum for F113_25T
Effective burden of composite spectrum: 1 part-per-million-meter (ppm-meter) at 296 K

Sample Conditions-

- Chemical name and CAS number: Freon-113, 1,1,2-Trichlorortrifluoroethane, Trifluorotrichloroethane, Fluorocarbon-113, CCl_2FCClF_2: [76-13-1]
- Physical properties: M.W. 187 AMU, F.P. –35C, B.P. 47.5C
- Supplier and stated purity: Aldrich, 99+%
- Sample class: I (PNNL scale)
- Temperature of sample 25.00 ± 0.02C
- Diluent: Sample back filled with ultra high purity nitrogen to 760±5 Torr
- Individual samples 1.0397, 2.0202, 3.0157, 4.0570, 11.4506, 1.5156, 2.5128 and 3.5006 Torr. Path length = 19.96 cm. Final data is a composite spectrum.
- Preparation: Multiple freeze-thaw cycles at 77K to remove N_2 and O_2. Sample passed through Ascarite-II for CO_2 removal.
- **Instrument Parameters-**
- Bruker-120HR FTIR, evacuated optics bench
- Spectral range: 5,000 to 620 cm^{-1} (1.54 to 16.67 microns)
- Instrumental resolution (interferogram): 0.1 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 8 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)*1+ 0
- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Trace water features removed from composite spectrum. Baseline straightened between 5000 and 3500 cm^{-1}.