

All data taken at Pacific Northwest National Laboratory (PNNL)

Operators: Steven W. Sharpe, Timothy J. Johnson and Robert L. Sams : sw.sharpe@pnl.gov

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Composite spectrum for F13B1_25T

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

Equivalent concentration x path-length of composite spectrum: 6.1307×10^{-6} grams/liter-meter

Trace unidentified impurity observed at 1150 cm^{-1} .

Sample Conditions-

- Chemical name and CAS number: Bromotrifluoromethane, Freon-13B1, Halon-1301, trifluorobromomethane, CBrF_3 : [75-63-8]
- Physical properties: fw=148.9102 g/mole, fp=-168° C, bp=-57.8° C
- Supplier and stated purity: SynQuest Labs, 99%
- Sample class: II (PNNL scale). Extremely strong absorber requiring small partial pressures of sample.
- Temperature of sample: $25.00 \pm 0.02 \text{ C}$
- Diluent: Sample back filled with ultra high purity nitrogen to $760 \pm 5 \text{ Torr}$
- Individual samples at 1.04155, 0.51286, 0.21044, 0.12407, 0.40448, 0.10344, 3.9686, 33.18, 17.08, 8.5711, 0.31914 and 67.20 Torr. Path length = 19.96 cm. Final data is a composite spectrum.
- Preparation: Multiple freeze-thaw cycles at 77 K to remove air. Bulk sample kept at -55 C during transfer to sample cell to avoid water vapor contamination.

Instrument Parameters-

- Bruker-66V FTIR, temperature controlled environment, evacuated optics bench
- Modified to include second aperture, between interferometer output and sample cell. This substantially reduces both “ghosting” and warm aperture effects.
- Spectral range: $6,500 \text{ to } 510 \text{ cm}^{-1}$ (1.534 to 19.608 microns)
- Instrumental resolution based on maximum interferometer displacement is 0.112 cm^{-1}
- Spectral interval after 2X zero-filling interferogram and 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: 60KHz (HeNe crossing frequency)
- Number of interferograms averaged per single channel spectra: 256
- Detector: Mid-band HgCdTe, photoconductive, 77K operation
- Folding limits: $15798 \text{ to } 0 \text{ cm}^{-1}$

Post Processing and Related Parameters-

- Non-linearity detector correction (Bruker proprietary) applied to interferogram ($\alpha=0.85$, $\epsilon=530$)
- Composite spectrum created from 12 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 = 1.77%, Type B $\leq 5\%$
- Frequency correction (already applied): $V(\text{corrected}) = V(\text{instrument}) * 0.99999896 + 8.812 \times 10^{-4}$

- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Trace carbon dioxide features removed via spectral subtraction
- Baseline correction via 7th order polynomial subtraction