

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for CHF₃_25T

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

Equivalent concentration x path-length of composite spectrum: 2.8852x10⁻⁶ grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: Trifluoromethane, fluoroform, carbon trifluoride, Freon-23, Halocarbon-23, R-23, CHF₃ : [75-46-7]
- Physical properties: fw=70.0141 g/mole, fp=-160° C, bp=-82.1° C
- Supplier and stated purity: Aldrich, 98+%
- Sample class: I (PNNL scale).
- Temperature of sample: 25.00 ± 0.02 C
- Diluent: Sample back filled with ultra high purity nitrogen to 760±5 Torr
- Individual samples at 1.1420, 0.73630, 6.0222, 0.58280, 14.06, 0.70940, 2.0120, 0.35080, 4.0040, 0.25670, 9.1052, 0.44300 and 25.50 Torr. Path length = 19.96 cm. Final data is a composite spectrum.
- Preparation: Multiple freeze-thaw cycles at 77 K to remove air.

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 to 600 cm⁻¹ (1.534 to 16.667 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 to 0 cm⁻¹

Post Processing and Related Parameters-

- Non-linearity detector correction (Bruker proprietary) applied to interferogram (=0.90, =500)
- Composite spectrum created from 13 individual absorbance (base-10) spectra via classical least squares fit: Intercept=0, slope is fitted, individual absorbance values weighted by T² (transmission squared), all absorbance values > 1.6 are given zero weight
- Calculated and estimated errors: Type A = 0.13%, Type B = 3%
- Frequency correction (already applied): V(corrected) = V(instrument)*0.999998+1.287x10⁻⁴
- Axis units: X=wavenumbers (cm⁻¹), Y=Absorbance (base-10)
- Trace carbon dioxide and chlorotrifluoromethane (CFC-13) features removed via spectral subtraction

- Baseline correction via 7th order polynomial subtraction