

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for CF4\_25T

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

Equivalent concentration x path-length of composite spectrum:  $3.6232 \times 10^{-6}$  grams/liter-meter

### Sample Conditions-

- Chemical name and CAS number: Tetrafluoromethane, carbon tetrafluoride, R-14, FC-14, halocarbon-14, Freon-14, CF<sub>4</sub>: [75-73-0]
- Physical properties: fw=88.0046 g/mole, fp=-184° C, bp=-128° C
- Supplier and stated purity: Spectra Gases, 99+%
- Sample class: I (PNNL scale).
- Temperature of sample: 25.02 ± 0.02 C
- Diluent: Sample back filled with ultra high purity nitrogen to 760±5 Torr
- Individual samples at 0.08500, 0.03454, 0.03130, 0.02356, 0.06472, 14.81, 1.03437, 2.2706, 4.3532, 8.7388, 34.48 and 65.09 Torr. Path length = 19.96 cm. Final data is a composite spectrum.
- Preparation: Multiple freeze-thaw cycles at 77 K to remove air with pumping.

### 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 570 cm<sup>-1</sup> (1.534 to 17.544 microns)
- Instrumental resolution based on maximum interferometer displacement is 0.112 cm<sup>-1</sup>
- Spectral interval after 2X zero-filling interferogram and 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: 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<sup>-1</sup>

### Post Processing and Related Parameters-

- Non-linearity detector correction (Bruker proprietary) applied to interferogram ( =0.85, =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<sup>2</sup> (transmission squared), all absorbance values > 1.6 are given zero weight
- Calculated and estimated errors: Type A = 0.74%, Type B = 3%
- Frequency correction (already applied): V(corrected) = V(instrument)\* 0.99999896+8.812x10<sup>-4</sup>
- Axis units: X=wavenumbers (cm<sup>-1</sup>), Y=Absorbance (base-10)
- Trace water vapor features removed via spectral subtraction
- Baseline correction via 7<sup>th</sup> order polynomial subtraction