

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 CF₃SF₅_50T

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

Equivalent concentration x path-length of composite spectrum: 8.0718x10⁻⁶ grams/liter-meter

Contamination consisted of 0.53% SF₆, and 0.02 % CS₂ (P/P). Fitted spectrum is corrected for these contaminants by adjusting partial pressure of CF₃SF₅ of individual absorbance spectra.

Sample Conditions-

- Chemical name and CAS number: Trifluoromethylsulfur pentafluoride, sulfur-pentafluoro(trifluoromethyl), CF₃SF₅ : [373-80-8]
- Physical properties: fw=196.0582 g/mole, fp=-87° C, bp=-9.8° C
- Supplier and stated purity: Oakwood Products, unavailable, lots of CO₂
- Sample class: I (PNNL scale).
- Temperature of sample: 50.03 ± 0.02 C
- Diluent: Sample back filled with ultra high purity nitrogen to 760±5 Torr
- Individual samples at 0.284598, 2.233927, 0.545689, 4.555180, 0.397307, 32.983850, 0.759834, 16.140249 and 8.435237 Torr. Path length = 19.94 cm. Final data is a composite spectrum.
- Preparation: Multiple freeze-thaw cycles at -80 C to remove any air. Subsequent distillations at -50 C. Sample finally placed over lithium hydroxide to scavenge CO₂.

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 520 cm⁻¹ (1.534 to 19.231 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 (=0.85, =530)
- Composite spectrum created from 9 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 = 0.38%, Type B = 3%
- Frequency correction (already applied): V(corrected) = V(instrument)* 0.99999896+8.812x10⁻⁴

- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Trace water vapor, carbon disulfide, carbon dioxide and SF_6 features removed via spectral subtraction. Residual SF_6 features still observed in composite spectrum.
- Baseline correction via 7th order polynomial subtraction