

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for COF<sub>2</sub>\_5T

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

Equivalent concentration x path-length of composite spectrum: 2.718x10<sup>-6</sup> grams/liter-meter

### Sample Conditions-

- Chemical name and CAS number: Carbonyl fluoride, fluoroformyl fluoride, carbon oxyfluoride, COF<sub>2</sub>: [353-50-4]
- Physical properties: M.W. 66.00 amu, F.P. -114 C, B.P. -83 C
- Supplier and stated purity: Scott specialty gasses, 97% (Yah, right. No way!)
- Sample class: II (PNNL scale).
- Temperature of sample: 5.04 ± 0.02 C
- Diluent: Sample back filled with ultra high purity nitrogen to 760±5 Torr
- Individual samples at 2.0751, 0.26985, 0.47681, 1.16911, 4.8315 and 10.1804 Torr. Path length = 19.94 cm. Final data is a composite spectrum. [Serious CO<sub>2</sub> contamination \(~12%\), and similar vapor pressure curves for COF<sub>2</sub> and CO<sub>2</sub> did not allow distillation separation. Pressure values for individual absorbance spectra were corrected for CO<sub>2</sub> contamination.](#)
- Preparation: Multiple freeze-thaw cycles at 77 K to remove air. Samples drawn from solid COF<sub>2</sub> (-120 C) to minimize HF 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 to 600 cm<sup>-1</sup> (1.534 to 16.667 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 (  $\alpha=0.85$ ,  $\beta=530$ )
- Composite spectrum created from 6 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 = 0.35%, Type B = 5%
- Frequency correction (already applied):  $V(\text{corrected}) = V(\text{instrument}) * 0.999997 + 5.18 \times 10^{-4}$
- Axis units: X=wavenumbers (cm<sup>-1</sup>), Y=Absorbance (base-10)

- Trace HF, HCl and SiF<sub>4</sub> features removed via spectral subtraction. Carbon dioxide removed via spectral subtraction.
- Baseline correction via 9<sup>th</sup> order polynomial subtraction