

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for SO<sub>2</sub>F<sub>2</sub>\_50T

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

Equivalent concentration x path-length of composite spectrum: 4.202x10<sup>-6</sup> grams/liter-meter

### Sample Conditions-

- Chemical name and CAS number: Sulfuryl fluoride, sulfuric oxyfluoride, Vikane, SO<sub>2</sub>F<sub>2</sub> : [2699-79-8]
- Physical properties: M.W. 102.062 amu, F.P. -137 C, B.P. -55 C
- Supplier and stated purity: Aldrich, DowElanco, 99+%
- Sample class: I (PNNL scale).
- Temperature of sample: 4.99 ± 0.02 C
- Diluent: Sample back filled with ultra high purity nitrogen to 760±5 Torr
- Individual samples at 1.00645, 0.13065, 10.4955, 0.51978, 2.2266, 23.08, 5.1871, 0.75840, 7.2282 and 105.28 Torr. Path length = 19.94 cm. Final data is a composite spectrum.
- Preparation: Multiple freeze-thaw cycles at 77 °K to remove air. Sample maintained at -85 °C to reduce water and other lower volatility contaminants.

### 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 500 cm<sup>-1</sup> (1.534 to 20.000 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 10 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)\*0.999997+5.18x10<sup>-4</sup>
- Axis units: X=wavenumbers (cm<sup>-1</sup>), Y=Absorbance (base-10)
- Trace carbon dioxide vapor features removed via spectral subtraction (less than 0.1% P/P).
- Baseline correction via 7<sup>th</sup> order polynomial subtraction