

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for CSI_5T

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

Equivalent concentration x path-length of composite spectrum: 5.827×10^{-6} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: Chlorosulfonyl isocyanate, CSI, ClSO₂NCO : [1189-71-5]
- Physical properties: fw=141.529 g/mole, fp=-44° C, bp=107° C
- Supplier and stated purity: Fluka, 99%
- Sample class: II (PNNL scale). Sample undergoes hydrolysis.
- Temperature of sample: 5.09 ± 0.02 C
- Diluent: Sample back filled with ultra high purity nitrogen to 760 ± 5 Torr
- Individual samples at 0.58405, 2.5990, 0.15754, 0.99050, 0.38083 and 1.8785 Torr. Path length = 19.94 cm. Final data is a composite spectrum.
- Preparation: Multiple freeze-thaw cycles at -35 C 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 550 cm⁻¹ (1.534 to 18.183 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 ($\alpha=0.85$, $\beta=530$)
- 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 T² (transmission squared), all absorbance values > 1.6 are given zero weight
- Calculated and estimated errors: Type A = 0.87%, 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⁻¹), Y=Absorbance (base-10)
- Trace carbon dioxide and hydrogen chloride features removed via spectral subtraction. Residual CO₂ features observed in composite spectrum after subtraction.
- Baseline correction via 7th order polynomial subtraction