

All data taken at Pacific Northwest National Laboratory (PNNL)

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Version 1.0, January, 02

Composite spectrum for PRTHIOL2_5T

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

Equivalent concentration x path-length of composite spectrum: 3.1354×10^{-6} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: 2-Propanethiol, isopropyl mercaptan, $(\text{CH}_3)_2\text{CH}(\text{HS})$: [75-33-2]
- Physical properties: fw=76.156 g/mole, fp=-131° C, bp=58° C
- Supplier and stated purity: Aldrich, 97%
- 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 2.1288, 8.0270, 1.2480, 20.13, 4.0820 and 12.51Torr. Path length = 19.96 cm. Final data is a composite spectrum.
- Preparation: Place sample over CaSO_3 to remove water. Multiple freeze-thaw cycles at 77 K 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 580 cm^{-1} (1.534 to 17.241 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 ($\alpha = 0.90$, $\beta = 500$)
- 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^2 (transmission squared), all absorbance values > 1.6 are given zero weight
- Calculated and estimated errors: Type A = 0.50%, Type B = 3%
- Frequency correction (already applied): $V(\text{corrected}) = V(\text{instrument}) * 0.999998 + 1.287 \times 10^{-4}$
- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Baseline correction via 7th order polynomial subtraction