

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for PRTHIOL2\_50T

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

Equivalent concentration x path-length of composite spectrum:  $3.1354 \times 10^{-6}$  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:  $50.03 \pm 0.02$  C
- Diluent: Sample back filled with ultra high purity nitrogen to  $760 \pm 5$  Torr
- Individual samples at 2.0404, 9.1776, 1.1741, 18.32, 4.6543, 13.33 and 50.40 Torr. Path length = 19.96 cm. Final data is a composite spectrum.
- Preparation: Place sample over  $\text{CaSO}_3$  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  $580 \text{ cm}^{-1}$  (1.534 to 17.241 microns)
- Instrumental resolution based on maximum interferometer displacement is  $0.112 \text{ cm}^{-1}$
- Spectral interval after 2X zero-filling interferogram and FFT:  $0.06 \text{ cm}^{-1}$
- 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  $0 \text{ cm}^{-1}$

### Post Processing and Related Parameters-

- Non-linearity detector correction (Bruker proprietary) applied to interferogram ( $\alpha = 0.90$ ,  $\beta = 500$ )
- Composite spectrum created from 7 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 = 0.15%, Type B = 3%
- Frequency correction (already applied):  $V(\text{corrected}) = V(\text{instrument}) * 0.999998 + 1.287 \times 10^{-4}$
- Axis units: X=wavenumbers ( $\text{cm}^{-1}$ ), Y=Absorbance (base-10)
- Baseline correction via 7<sup>th</sup> order polynomial subtraction