

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for IBSH_50T

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

Equivalent concentration x path-length of composite spectrum: 7.417×10^{-6} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: 2-Methyl-1-propanethiol, isobutyl mercaptan, $(\text{CH}_3)_2\text{CH}_2\text{CH}_2\text{SH}$: [513-44-0]
- Physical properties: MW=90.183 g/mole, mp=-145° C, bp=88° C, Density (20 C) 0.831 g/cm³
- Supplier and stated purity: Aldrich, 92%
- Sample class: I (PNNL scale).
- Temperature of White cell (796.0 cm optical path length) 50 ± 2 C
- Diluent (high purity nitrogen) flowed at 24.2 liter/min (21.1° C), ambient atmospheric pressure 760 ± 5 Torr.
- Samples flowed at 2.000, 10.000, 0.800, 5.000, 4.000, 15.000, 1.000, 22.000, 11.000, 6.000, 42.000, 7.000, 35.000 and 14.000 microliters/minute
- Individual samples at equivalent pressures of 0.013807, 0.069009, 0.005519, 0.034472, 0.027578, 0.103403, 0.006892, 0.151597, 0.075778, 0.041317, 0.289103, 0.048177, 0.240791 and 0.096303 Torr. Final data is a composite spectrum.
- Preparation: None

Instrument Parameters-

- Bruker-66V FTIR, evacuated optics bench.
- Modified to include second aperture, between interferometer output and White cell. This substantially reduces both “ghosting” and warm aperture effects.
- Spectral range: 6,500 to 550 cm^{-1} (1.538 to 18.182 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 ($\alpha=0.90$, $\epsilon=500$)
- Composite spectrum created from 14 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 = 0.38%, Type B $\leq 7\%$
- Frequency correction (already applied): $V(\text{corrected})=V(\text{instrument}) * 0.99999959 - 3.45278 \times 10^{-4}$

- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Baseline correction via 7th order polynomial subtraction
- Trace water vapor features removed by spectral subtraction