

All data taken at Pacific Northwest National Laboratory (PNNL)

Operators: Steven W. Sharpe, Timothy J. Johnson and Robert L. Sams : [sw.sharpe@pnl.gov](mailto:sw.sharpe@pnl.gov)

Version 1.0, July, 05

Composite spectrum for IBSH\_25T

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

Equivalent concentration x path-length of composite spectrum:  $7.417 \times 10^{-6}$  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/cm<sup>3</sup>
- Supplier and stated purity: Aldrich, 92%
- Sample class: I (PNNL scale).
- Temperature of White cell (796.0 cm optical path length)  $25 \pm 2$  C
- Diluent (high purity nitrogen) flowed at 24.2 liter/min (21.1° C), ambient atmospheric pressure  $760 \pm 5$  Torr.
- Samples flowed at 4.000, 8.000, 0.800, 5.000, 15.000, 3.000, 7.000, 12.000, 2.000, 9.000, 1.000, 37.000, 6.000, 47.000, 14.000 and 31.000 microliters/minute
- Individual samples at equivalent pressures of 0.027563, 0.055133, 0.005515, 0.034449, 0.103334, 0.020664, 0.048216, 0.082634, 0.013772, 0.061951, 0.006882, 0.254618, 0.041289, 0.323390, 0.096329 and 0.213272 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  $\text{cm}^{-1}$  (1.538 to 18.182 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 ( $\alpha=0.90$ ,  $\epsilon=500$ )
- Composite spectrum created from 16 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  $\geq 1.6$  are given zero weight
- Calculated and estimated errors: Type A = 0.29%, 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 ( $\text{cm}^{-1}$ ), Y=Absorbance (base-10)
- Baseline correction via 7<sup>th</sup> order polynomial subtraction
- Trace water vapor features removed by spectral subtraction