

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for HEPTOH\_25T

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

Equivalent concentration x path-length of composite spectrum:  $4.7841 \times 10^{-6}$  grams/liter-meter

### Sample Conditions-

- Chemical name and CAS number: 1-Heptanol, n-heptanol, heptyl alcohol, enanthic alcohol, hydroxyheptane,  $\text{CH}_3(\text{CH}_2)_6\text{OH}$ : [111-70-6]
- Physical properties: MW=116.2026 g/mole, mp=-36° C, bp=175° C, Density (20 C) 0.756 g/cm<sup>3</sup>
- Supplier and stated purity: Aldrich, 98%
- 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 3.000, 11.000, 7.000, 15.000, 8.000, 27.000, 1.000, 4.000, 9.000, 19.000, 6.000 and 17.000 microliters/minute
- Individual samples at equivalent pressures of 0.016245, 0.059565, 0.037910, 0.081226, 0.043320, 0.146187, 0.005414, 0.021657, 0.048723, 0.102845, 0.032477 and 0.092020 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 7,300 to 600  $\text{cm}^{-1}$  (1.370 to 16.667 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 12 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 = 0.21%, 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)
- Trace water vapor features removed by spectral subtraction
- Baseline correction via 7<sup>th</sup> order polynomial subtraction