

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for HEPTOH_50T

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

Equivalent concentration x path-length of composite spectrum: 4.7841×10^{-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/cm³
- Supplier and stated purity: Aldrich, 98%
- 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 8.000, 1.000, 11.000, 16.000, 4.000, 5.000, 2.000, 26.000, 12.000, 3.000, 20.000, 14.000, 24.000, 7.000, 10.000 and 42.00 microliters/minute
- Individual samples at equivalent pressures of 0.043281, 0.005409, 0.059480, 0.086516, 0.021626, 0.027033, 0.010812, 0.140497, 0.064853, 0.016211, 0.108089, 0.075652, 0.129673, 0.037816, 0.054016 and 0.226838 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 cm^{-1} (1.370 to 16.667 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 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 ≥ 1.6 are given zero weight
- Calculated and estimated errors: Type A = 0.35%, 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)
- Trace water vapor features removed by spectral subtraction
- Baseline correction via 7th order polynomial subtraction