

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for HEXOH_50

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

Equivalent concentration x path-length of composite spectrum: 4.2066×10^{-6} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: n-Hexanol, 1-hexanol, hexyl alcohol, hexan-1-ol, caproic alcohol, amyl carbinol, $\text{CH}_3(\text{CH}_2)_5\text{OH}$: [111-27-3]
- Physical properties: MW=102.176 g/mole, mp=-52° C, bp=156.5° C, Density (20 C) 0.819 g/cm³
- Supplier and stated purity: Aldrich, 99%
- 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, 5.000, 0.800, 15.000, 4.000, 12.000, 6.000, 22.000, 8.000, 11.000, 44.000, 3.000, 35.000 and 13.000 microliters/minute
- Individual samples at equivalent pressures of 0.012319, 0.030802, 0.004923, 0.092251, 0.024594, 0.073782, 0.036886, 0.135214, 0.049175, 0.067607, 0.270357, 0.018436, 0.215029 and 0.079847 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 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 = 0.16%, Type B $\leq 7\%$

- Frequency correction (already applied): $V(\text{corrected})=V(\text{instrument})\cdot 0.99999959-3.45278\times 10^{-4}$
- 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