

All data taken at Pacific Northwest National Laboratory (PNNL)
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Composite spectrum for HEX2OL_50T

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

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

Sample Conditions-

- Chemical name and CAS number: 2-Hexanol; n-C₄H₉CH(OH)CH₃; n-Butylmethylcarbinol; Hexanol-(2); sec-Hexyl alcohol; n-Hexan-2-ol; Hexan-2-ol; 2-Hexyl alcohol C₆H₁₄O : [626-93-7]
- Physical properties: MW=102.1748 g /mole, mp=-50° C, bp=138° C, Density (25 C) = 0.8103 g/cm³
- Supplier and stated purity: Sigma Aldrich, 99 %
- Sample class: I (PNNL scale).
- Temperature of White cell (805.0 cm optical path length) 50 ± 2 C
- Diluent (high purity nitrogen) flowed at 22.77 liter/min (21.1° C), ambient atmospheric pressure 760 ± 5 Torr.
- Samples flowed at microliters/minute 4.000, 1.500, 9.000, 6.500, 15.000, 11.000, 18.000, 13.000, 23.000, 29.000, 42.000, 31.000, 36.000 and 40.000
- Individual samples at equivalent pressures of: 0.025195, 0.009449, 0.056696, 0.040947, 0.094494, 0.069296, 0.113378, 0.081840, 0.144794, 0.182542, 0.264372, 0.195105, 0.226634 and 0.251816 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: 7,250 to 520 cm⁻¹ (1.379 to 19.23 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 13 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 =1.48%, Type B $\leq 7\%$
- Frequency correction (already applied): $V(\text{corrected})=V(\text{instrument}) * 1.00000160 + 3.5903 \times 10^{-4}$
- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Trace water vapor was removed by spectral subtraction
- Baseline correction via 7th order polynomial subtraction