

All data taken at Pacific Northwest National Laboratory (PNNL)

Operators: Steven W. Sharpe, Timothy J. Johnson and Robert L. Sams : sw.sharpe@pnl.gov

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Composite spectrum for ETHEXOH_50T

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

Equivalent concentration x path-length of composite spectrum: 5.3616×10^{-6} grams/liter-meter

[Corrected composite spectrum for water contamination \[0.21%\] by rescaling and subtracting water features.](#)

Sample Conditions-

- Chemical name and CAS number: 2-Ethyl-2-hexanol, 2-ethylhexan-1-ol, 2-ethylhexanol, $\text{CH}_3(\text{CH}_2)_3\text{CH}(\text{C}_2\text{H}_5)\text{CH}_2\text{OH}$: [104-76-7]
- Physical properties: M.W. 130.2296 amu, F.P. -76°C , B.P. 183°C , Density (20 C) 0.833 g/cm^3
- Supplier and stated purity: Aldrich, 99+%
- Sample class: I (PNNL scale).
- Temperature of White cell (792.0 cm optical path length) $50 \pm 2\text{ C}$
- Diluent (high purity nitrogen) flowed at 24.90 liter/min (296 K), ambient atmospheric pressure $770 \pm 5\text{ Torr}$.
- Samples flowed at 4.000, 2.000, 12.000, 5.000, 18.000, 3.000, 7.000, 10.000, 6.000, 25.000, 8.000, 1.000 and 20.000 microliters/minute
- Individual samples at equivalent pressures of 0.018692, 0.009346, 0.056083, 0.023371, 0.084136, 0.014026, 0.032715, 0.046742, 0.028045, 0.116825, 0.037384, 0.004672, and 0.093447 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 550 cm^{-1} (1.370 to 18.182 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 ($\alpha=0.90$, $\beta=500$)
- 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 = 0.74%, Type B \leq 7%
- Frequency correction (already applied): $V(\text{corrected}) = V(\text{instrument}) * 0.999998 + 1.566836e-04$
- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Baseline correction via 7th order polynomial subtraction