

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for PETA3OL_50T

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

Equivalent concentration x path-length of composite spectrum: 3.6291×10^{-6} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: 3-Pentanol; Diethyl carbinol; 3-Pentyl alcohol; (C₂H₅)₂CHOH; Pentan-3-ol; Pentanol-3; C₅H₁₂O:[584-02-1]
- Physical properties: MW=88.1482 g/mole, mp= -70° C, bp=114.9° C, Density (25 C) = 0.807 g/cm³
- Supplier and stated purity: Fluka, 99.5%
- Sample class: I (PNNL scale).
- Temperature of sample 49.92 ± 0.02 C
- Diluent: Sample back filled with ultra high purity nitrogen to 760 ± 5 Torr.
- Individual samples at 1.17500, 4.1800, 7.2000, 6.0000, 5.0000, 3.0000 and 2.1300 Torr. Path length=19.96 cm. Final data is a composite spectrum.
- Preparation: Multiple freeze-thaw cycles at 77K to remove air.

Instrument Parameters-

- Bruker-66V FTIR, evacuated optics bench.
- Modified to include second aperture, between interferometer output and sample cell. This substantially reduces both “ghosting” and warm aperture effects.
- Spectral range: 7,250 to 570 cm⁻¹ (1.379 to 17.54 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 10 individual absorbance (base-10) spectra via classical least squares fit: Intercept=0, slope is fitted, individual absorbance values weighted by T² (transmission squared), all absorbance values ≥ 1.6 are given zero weight
- Calculated and estimated errors: Type A =0.51%, Type B $\leq 3\%$
- Frequency correction (already applied): $V(\text{corrected})=V(\text{instrument}) * 1.00000135 + 8.5741 \times 10^{-4}$
- Axis units: X=wavenumbers (cm⁻¹), Y=Absorbance (base-10)
- Trace carbon dioxide and water features were removed via spectral subtraction.

- Baseline correction via 7th order polynomial subtraction