

All data taken at Pacific Northwest National Laboratory (PNNL)
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Composite spectrum for 4M1PENT_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: 4-Methyl-1-pentanol; Isohexyl alcohol; Isohexanol; 2-Methyl-5-pentanol; 4-Methyl-1-pentanol; 4-methylpentanol; Pentanol, 4-methyl-; 4-Methylpentan-1-ol $C_6H_{14}O$: [626-89-1]
- Physical properties: MW=102.1748 g/mole, mp=-70° C, bp=152° C, Density (25 C) = 0.814 g/cm³
- Supplier and stated purity: Sigma Aldrich, 97%
- 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 5.000, 1.500, 9.000, 3.000, 13.000, 7.000, 19.000, 16.000, 29.000, 22.000, 26.000, 43.000, 31.000, 36.000 and 50.000
- Individual samples at equivalent pressures of: 0.031203, 0.009362, 0.056187, 0.018754, 0.081258, 0.043760, 0.118827, 0.100010, 0.181269, 0.137514, 0.162429, 0.268633, 0.193613, 0.224841 and 0.312321Torr. 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 15 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 =2.23%, 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