

All data taken at Pacific Northwest National Laboratory (PNNL)  
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Composite spectrum for 4M1PENT\_25T

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

Equivalent concentration x path-length of composite spectrum:  $4.2066 \times 10^{-6}$  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/cm<sup>3</sup>
- Supplier and stated purity: Sigma Aldrich, 97%
- Sample class: I (PNNL scale).
- Temperature of White cell (805.0 cm optical path length)  $25 \pm 2$  C
- Diluent (high purity nitrogen) flowed at 22.77 liter/min (21.1° C), ambient atmospheric pressure  $760 \pm 5$  Torr.
- Samples flowed at microliters/minute 6.000, 2.000, 4.500, 10.000, 7.500, 14.000, 12.000, 21.000, 15.000, 28.000, 26.000, 34.000, 30.000, 36.000 and 40.000
- Individual samples at equivalent pressures of: 0.038198, 0.012736, 0.028656, 0.063689, 0.047767, 0.089177, 0.076437, 0.133801, 0.095572, 0.178448, 0.165702, 0.216716, 0.191270, 0.229525 and 0.255061Torr. 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  $\geq 1.6$  are given zero weight
- Calculated and estimated errors: Type A =0.84%, 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 ( $\text{cm}^{-1}$ ), Y=Absorbance (base-10)
- Trace water vapor was removed by spectral subtraction
- Baseline correction via 7<sup>th</sup> order polynomial subtraction