

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for VALERIC_67T

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

Equivalent concentration x path-length of composite spectrum: 4.2048×10^{-6} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: Valeric acid; n-Pentanoic acid; n-Valeric acid; Propylacetic acid; Valerianic acid; 1-Butanecarboxylic acid; n-C₄H₉COOH; Butanecarboxylic acid; Valeric acid, n-; Valeric acid, normal; 1-pentanoic acid C₅H₁₀O₂ : [109-52-4]
- Physical properties: MW=102.1317 g/mole, mp= -34° C, bp=186° C, Density (25 C) = 0.893g/cm³
- Supplier and stated purity: Aldrich, 99+%
- Sample class: I (PNNL scale).
- Temperature of White cell (805.0 cm optical path length) 67 ± 2 C
- Diluent (high purity nitrogen) flowed at 23.3 liter/min (21.1° C), ambient atmospheric pressure 760 ± 5 Torr.
- Samples flowed at microliters/minute 4.000, 8.000, 3.000, 5.000, 2.000, 1.000, 6.000, 7.000, 12.000, 10.000 and 9.000.
- Individual samples at equivalent pressures of 0.028693, 0.057372, 0.021517, 0.035862, 0.014350, 0.007176, 0.043069, 0.050247, 0.086160, 0.071781 and 0.064620 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: 7,100 to 520 cm⁻¹ (1.4085 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 11 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): $V(\text{corrected})=V(\text{instrument}) * 1.0000016 + 3.59033 \times 10^{-4}$
- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Trace water and carbon dioxide features were removed via spectral subtraction small amount of the dimer can be seen in the following regions: $3400\text{-}2386 \text{ cm}^{-1}$, 1726.77 cm^{-1} , 1419.5 cm^{-1} and 942.5 cm^{-1} .
- Baseline correction via 7th order polynomial subtraction