

All data taken at Pacific Northwest National Laboratory (PNNL)
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Composite spectrum for NONAN5OL_25T

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

Equivalent concentration x path-length of composite spectrum: 5.939×10^{-6} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: 5-Nonanol; Dibutylcarbinol; Nonanol-(5); Nonan-5-ol
 $C_9H_{20}O$: [623-93-8]
- Physical properties: MW=144.2545 g/mole, mp=5.6 °C, bp=195 °C, Density (25 °C) = 0.822 g/cm³
- Supplier and stated purity: Fluka; 95%
- Sample class: I (PNNL scale).
- Temperature of White cell (805.0 cm optical path length) 25 ± 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 1.000, 2.000, 3.000, 0.500, 1.500, 2.500, 3.500, 4.000 and 4.500
- Individual samples at equivalent pressures of: 0.004497, 0.008992, 0.013487, 0.002247, 0.006739, 0.011231, 0.015737, 0.017990 and 0.020241 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 580 cm⁻¹ (1.3699 to 17.241 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 9 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 =2.70 %, Type B \leq 7%
- Frequency correction (already applied): $V(\text{corrected})=V(\text{instrument})\cdot 1.00000160+3.5903\times 10^{-4}$
- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- 2.85 % water was removed by spectral subtraction and the composite spectrum was rescaled by multiplying by 1.02941.
- Baseline correction via 7th order polynomial subtraction