

All data taken at Pacific Northwest National Laboratory (PNNL)  
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Composite spectrum for NONAN5OL\_50T

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

Equivalent concentration x path-length of composite spectrum:  $5.939 \times 10^{-6}$  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/cm<sup>3</sup>
- Supplier and stated purity: Fluka; 95%
- 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 3.250, 5.400, 7.100, 6.300, 8.200, 13.900, 11.000, 29.600, 23.700, 26.000 and 32.000
- Individual samples at equivalent pressures of: 0.014719, 0.024456, 0.032155, 0.028532, 0.037137, 0.062952, 0.049818, 0.134055, 0.107335, 0.117751 and 0.144925 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 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  $\geq 1.6$  are given zero weight

- Calculated and estimated errors: Type A =12.7 %, 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 and carbon dioxide were removed by spectral subtraction.
- Baseline correction via 7<sup>th</sup> order polynomial subtraction