

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for 2NONNY\_50T

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

Equivalent concentration x path-length of composite spectrum:  $5.8560 \times 10^{-6}$  grams/liter-meter

### Sample Conditions-

- Chemical name and CAS number: 2-Nonanone; Heptyl methyl ketone; Methyl heptyl ketone; Methyl n-heptyl ketone; Nonan-2-one; n-C<sub>7</sub>H<sub>15</sub>COCH<sub>3</sub>;  $\beta$ -Nonanone; Ketone, heptyl methyl; NONANONE-2 C<sub>9</sub>H<sub>18</sub>O : [821-55-6]
- Physical properties: MW=142.2386 g/mole, mp= -21° C, bp=195° C, Density (25 C) = 0.8167g/cm<sup>3</sup>
- Supplier and stated purity: Aldrich, 99+%
- Sample class: I (PNNL scale).
- Temperature of White cell (805.0 cm optical path length)  $50 \pm 2$  C
- Diluent (high purity nitrogen) flowed at 23.3 liter/min (21.1° C), ambient atmospheric pressure  $760 \pm 5$  Torr.
- Samples flowed at microliters/minute 2.000, 8.000, 12.000, 7.000, 5.000, 42.000, 6.000 and 18.000.
- Individual samples at equivalent pressures of 0.009091, 0.036365, 0.054476, 0.031765, 0.022674, 0.190341, 0.027188 and 0.081553 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: 6500 to 550 cm<sup>-1</sup> (1.5385 to 18.18 microns)
- Instrumental resolution based on maximum interferometer displacement is 0.112 cm<sup>-1</sup>
- Spectral interval after 2X zero-filling interferogram and FFT: 0.06 cm<sup>-1</sup>
- 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<sup>-1</sup>

### Post Processing and Related Parameters-

- Non-linearity detector correction (Bruker proprietary) applied to interferogram ( $\alpha=0.90$ ,  $\epsilon=500$ )
- Composite spectrum created from 8 individual absorbance (base-10) spectra via classical least squares fit: Intercept=0, slope is fitted, individual absorbance values weighted by T<sup>2</sup> (transmission squared), all absorbance values  $\geq 1.6$  are given zero weight

- Calculated and estimated errors: Type A =5.72%, Type B  $\leq$  7%
- Frequency correction (already applied):  $V(\text{corrected})=V(\text{instrument})\cdot 1.0000016+3.59034\times 10^{-4}$
- Axis units: X=wavenumbers ( $\text{cm}^{-1}$ ), Y=Absorbance (base-10)
- Trace water and carbon dioxide features were removed via spectral subtraction.
- Baseline correction via 7<sup>th</sup> order polynomial subtraction