

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for 2NONNY_25T

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

Equivalent concentration x path-length of composite spectrum: 5.8560×10^{-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-C₇H₁₅COCH₃; β-Nonanone; Ketone, heptyl methyl; NONANONE-2 C₉H₁₈O : [821-55-6]
- Physical properties: MW=142.2386 g/mole, mp= -21° C, bp=195° C, Density (25 C) = 0.8167g/cm³
- Supplier and stated purity: Aldrich, 99+%
- Sample class: I (PNNL scale).
- Temperature of White cell (805.0 cm optical path length) 25 ± 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 1.000, 6.000, 7.000, 11.000, 3.000, 21.000, 5.000, 13.000, 41.000, 4.000, 36.000, 4.500 and 43.000.
- Individual samples at equivalent pressures of 0.004570, 0.027418, 0.031972, 0.050241, 0.013700, 0.095902, 0.022837, 0.059383, 0.187262, 0.018274, 0.164446, 0.020561 and 0.196448 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⁻¹ (1.5385 to 18.18 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 13 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 =1.46%, Type B $\leq 7\%$
- Frequency correction (already applied): $V(\text{corrected})=V(\text{instrument}) * 1.0000016 + 3.59034 \times 10^{-4}$
- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Trace water and carbon dioxide features were removed via spectral subtraction.
- Baseline correction via 7th order polynomial subtraction