

All data taken at Pacific Northwest National Laboratory (PNNL)
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Composite spectrum for C16H34_50T

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

Equivalent concentration x path-length of composite spectrum: 9.3227×10^{-6} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: Hexadecane; n-Cetane; n-Hexadecane; Cetane $C_{16}H_{34}$: [544-76-3]
- Physical properties: MW=226.4412g/mole, mp=18° C, bp=281° C, Density (25 C) = 0.773 g/cm³
- Supplier and stated purity: Sigma Aldrich, 99%
- Sample class: I (PNNL scale).
- Temperature of White cell (805.0 cm optical path length) 50 ± 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 0.500, 0.750, 1.250, 1.750, 1.000, 1.500, 2.000, 3.000 and 2.500.
- Individual samples at equivalent pressures of 0.001333, 0.001995, 0.003327, 0.004665, 0.002665, 0.003994, 0.005331, 0.007989 and 0.006652 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: 6,500 to 550 cm⁻¹ (1.538 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 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 =3.32%, Type B \leq 7%
- Frequency correction (already applied): $V(\text{corrected})=V(\text{instrument})\cdot 0.9999996+6.17682\times 10^{-4}$
- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Trace water vapor and carbon dioxide were removed by spectral subtraction
- Baseline correction via 11th order polynomial subtraction