

All data taken at Pacific Northwest National Laboratory (PNNL)
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Composite spectrum for C15H32_25T

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

Equivalent concentration x path-length of composite spectrum: 8.7452×10^{-6} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: Pentadecane; n-Pentadecane; $\text{CH}_3(\text{CH}_2)_{13}\text{CH}_3$; $\text{C}_{15}\text{H}_{32}$: [629-62-9]
- Physical properties: MW=212.4146 g/mole, mp=10° C, bp=267° C, Density (25 C) = 0.769 g/cm³
- Supplier and stated purity: Sigma 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, 1.200, 0.400, 0.350, 0.550, 0.800, 0.500, 0.900, 0.450, 1.100 and 1.400
- Individual samples at equivalent pressures of 0.002848, 0.003415, 0.001137, 0.000993, 0.001560, 0.002269, 0.001418, 0.002551, 0.001275, 0.003116 and 0.003964 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 600 cm^{-1} (1.538 to 6.67 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 ≥ 1.6 are given zero weight

- Calculated and estimated errors: Type A =8.70%, Type B \leq 7%
- Frequency correction (already applied): $V(\text{corrected})=V(\text{instrument})*0.9999996+6.17682 \times 10^{-4}$
- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Trace water vapor was removed by spectral subtraction
- Baseline correction via 7th order polynomial subtraction