

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for TRIDEC_50

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

Equivalent concentration x path-length of composite spectrum: 7.5904×10^{-6} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: Tridecane, n-tridecane, $\text{CH}_3(\text{CH}_2)_{11}\text{CH}_3$: [629-50-5]
- Physical properties: MW=184.3642 g/mole, mp=-5.5° C, bp=235.4° C, Density (20 C) 0.756 g/cm³
- Supplier and stated purity: Aldrich, 99+%
- Sample class: III (PNNL scale). Low vapor pressure sample.
- Temperature of White cell (796.0 cm optical path length) 50 ± 2 C
- Diluent (high purity nitrogen) flowed at 24.2 liter/min (21.1° C), ambient atmospheric pressure 760 ± 5 Torr.
- Samples flowed at 3.000, 6.000, 1.500, 8.000, 2.000, 10.000, 5.000, 17.000, 2.500, 4.000, 12.000, 1.000, 30.000, 7.000, 22.000, 9.000 and 15.000 microliters/minute
- Individual samples at equivalent pressures of 0.009169, 0.018337, 0.004583, 0.024443, 0.006109, 0.030534, 0.015265, 0.051893, 0.007635, 0.012215, 0.036640, 0.003053, 0.091564, 0.021365, 0.067147, 0.027477 and 0.04580 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 16.667 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 17 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 = 0.23%, Type B $\leq 7\%$
- Frequency correction (already applied): $V(\text{corrected})=V(\text{instrument}) * 0.99999959 - 3.45278 \times 10^{-4}$

- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Baseline correction via 7th order polynomial subtraction