

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for TRIDEC\_25T

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

Equivalent concentration x path-length of composite spectrum:  $7.5904 \times 10^{-6}$  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/cm<sup>3</sup>
- 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)  $25 \pm 2$  C
- Diluent (high purity nitrogen) flowed at 24.2 liter/min (21.1° C), ambient atmospheric pressure  $760 \pm 5$  Torr.
- Samples flowed at 2.000, 4.000, 8.000, 1.500, 3.000, 5.000, 10.000, 1.000, 2.500, 3.500, 4.200, 2.700, 1.250 and 3.200 microliters/minute
- Individual samples at equivalent pressures of 0.006189, 0.012379, 0.024751, 0.004635, 0.009268, 0.015455, 0.030906, 0.003089, 0.007720, 0.010808, 0.012967, 0.008334, 0.003857 and 0.009869 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  $\text{cm}^{-1}$  (1.538 to 16.667 microns)
- Instrumental resolution based on maximum interferometer displacement is 0.112  $\text{cm}^{-1}$
- Spectral interval after 2X zero-filling interferogram and FFT: 0.06  $\text{cm}^{-1}$
- 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  $\text{cm}^{-1}$

#### Post Processing and Related Parameters-

- Non-linearity detector correction (Bruker proprietary) applied to interferogram ( $\alpha=0.90$ ,  $\epsilon=500$ )
- Composite spectrum created from 14 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  $\geq 1.6$  are given zero weight
- Calculated and estimated errors: Type A = 1.83%, 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 ( $\text{cm}^{-1}$ ), Y=Absorbance (base-10)
- Baseline correction via 6<sup>th</sup> order polynomial subtraction