

All data taken at Pacific Northwest National Laboratory (PNNL)  
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Composite spectrum for HEXACE\_50T

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

Equivalent concentration x path-length of composite spectrum:  $5.9459 \times 10^{-6}$  grams/liter-meter

#### Sample Conditions-

- Chemical name and CAS number: Hexyl acetate; Hexyl ethanoate; Acetic acid, hexyl ester; n-Hexyl acetate; 1-Hexyl acetate; Acetic acid n-hexyl ester; n-Hexyl ethanoate; Hexyl alcohol, acetate; Methylamyl acetate; l-Hexyl acetate; Hexyl ester of acetic acid  $C_8H_{16}O_2$ : [142-92-7]
- Physical properties: MW=144.2114 g/mole, mp=-61° C, bp=170° C, Density (25 C) = 0.868 g/cm<sup>3</sup>
- Supplier and stated purity: Aldrich, 99%
- Sample class: I (PNNL scale).
- Temperature of White cell (805.0 cm optical path length)  $50 \pm 2$  C
- Diluent (high purity nitrogen) flowed at 23.3 liter/min (21.1° C), ambient atmospheric pressure  $760 \pm 5$  Torr.
- Samples flowed at microliters/minute 3.000, 6.000, 12.000, 5.000, 10.000, 4.000, 11.000, 7.000, 9.000, 15.000, 8.000, 13.000, 2.000, 16.000 and 7.500.
- Individual samples at equivalent pressures 0.014114, 0.028214, 0.056428, 0.023505, 0.047011, 0.018799, 0.051691, 0.032890, 0.042282, 0.070469, 0.037574, 0.061033, 0.009388, 0.075087 and 0.035202 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 580 cm<sup>-1</sup> (1.538 to 17.24 microns)
- Instrumental resolution based on maximum interferometer displacement is 0.112 cm<sup>-1</sup>
- Spectral interval after 2X zero-filling interferogram and FFT: 0.06 cm<sup>-1</sup>
- 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<sup>-1</sup>

#### Post Processing and Related Parameters-

- Non-linearity detector correction (Bruker proprietary) applied to interferogram ( $\alpha=0.90$ ,  $\epsilon=500$ )

- Composite spectrum created from 15 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 =1.06%, 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 ( $\text{cm}^{-1}$ ), Y=Absorbance (base-10)
- 1.29% water vapor was removed by spectral subtraction and the composite spectrum was rescaled by multiplying by 1.0130
- Baseline correction via 7<sup>th</sup> order polynomial subtraction