

All data taken at Pacific Northwest National Laboratory (PNNL)
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Composite spectrum for HEXACE_25T

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

Equivalent concentration x path-length of composite spectrum: 5.9459×10^{-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/cm³
- Supplier and stated purity: 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 3.000, 6.000, 12.000, 5.000, 10.000, 15.000, 7.000, 4.000, 2.000, 8.000, 11.000, 9.000, 2.500, 7.500 and 13.000.
- Individual samples at equivalent pressures 0.014292, 0.028584, 0.057154, 0.023814, 0.047622, 0.071433, 0.033331, 0.019044, 0.009522, 0.038088, 0.052357, 0.042832, 0.011898, 0.035684 and 0.061844 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⁻¹ (1.538 to 17.24 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 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 ≥ 1.6 are given zero weight
- Calculated and estimated errors: Type A =0.41%, 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)
- 1.09% water vapor was removed by spectral subtraction and the composite spectrum was rescaled by multiplying by 1.01105
- Baseline correction via 7th order polynomial subtraction