

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for PACETATE_50T

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

Equivalent concentration x path-length of composite spectrum: 4.2049×10^{-6} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: Propyl acetate, 1-acetoxypropane, 1-propyl acetate, acetic acid propyl ester, $\text{CH}_3\text{CO}_2\text{CH}_2\text{CH}_2\text{CH}_3$: [109-60-4]
- Physical properties: fw=102.1328 g/mole, mp=-96° C, bp=102° C
- Supplier and stated purity: Aldrich, 99%
- Sample class: I (PNNL scale).
- Temperature of sample: 49.97 ± 0.02 C
- Diluent: Sample back filled with ultra high purity nitrogen to 760 ± 5 Torr
- Individual samples at 1.0464, 0.53991, 2.1130, 7.1300, 4.8303 and 10.6035 Torr. Path length = 19.96 cm. Final data is a composite spectrum.
- Preparation: Multiple freeze-thaw cycles at 77° K to remove air.

Instrument Parameters-

- Bruker-66V FTIR, temperature controlled environment, evacuated optics bench
- Modified to include second aperture, between interferometer output and sample cell. This substantially reduces both “ghosting” and warm aperture effects.
- Spectral range: 6,500 to 560 cm^{-1} (1.534 to 17.857 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 ($\alpha=0.85$, $\epsilon=530$)
- Composite spectrum created from 6 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 = 0.83%, Type B $\leq 3\%$
- Frequency correction (already applied): $V(\text{corrected}) = V(\text{instrument}) * 0.99999896 + 8.812 \times 10^{-4}$
- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Trace water vapor and carbon dioxide features removed via spectral subtraction
- Baseline correction via 7th order polynomial subtraction