

All data taken at Pacific Northwest National Laboratory (PNNL)

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Version 1.0, December, 04

Composite spectrum for MPK_5T

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

Equivalent concentration x path-length of composite spectrum: 3.5462×10^{-6} grams/liter-meter

[Impurity from previous run identified as cis-1,2-Dichloroethene \[0.66%\] and removed via spectral subtraction. Composite spectrum rescaled to reflect this impurity.](#)

Sample Conditions-

- Chemical name and CAS number: Methyl propyl ketone, MPK, 2-pentanone, ethyl acetone, pentan-2-one, $\text{CH}_3\text{CH}_2\text{CH}_2\text{COCH}_3$; [107-87-9]
- Physical properties: fw=86.1334 g/mole, mp=-78° C, bp=100-110° C
- Supplier and stated purity: Aldrich, 99.5%
- Sample class: I (PNNL scale).
- Temperature of sample: 5.04 ± 0.02 C
- Diluent: Sample back filled with ultra high purity nitrogen to 760 ± 5 Torr
- Individual samples at 1.08650, 2.0810, 4.1620, 7.48, 6.1140 and 5.0550Torr. 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 520 cm^{-1} (1.534 to 19.231 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 = 0.63%, Type B $\leq 3\%$
- Frequency correction (already applied): $V(\text{corrected}) = V(\text{instrument}) * 1.00004 + 1.17713 \times 10^{-3}$
- 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