

All data taken at Pacific Northwest National Laboratory (PNNL)
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Composite spectrum for ISPNTAC_50T

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

Equivalent concentration x path-length of composite spectrum: 5.3598×10^{-6} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: Isopentyl acetate; 1-Butanol, 3-methyl-,acetate; Isopentyl alcohol, acetate; Acetic acid, 3-methylbutyl ester; Banana oil; Isoamyl acetate; Isoamyl ethanoate; Pear oil; 3-Methyl-1-butyl acetate; 3-Methylbutyl acetate; $\text{CH}_3\text{C}(\text{O})\text{O}(\text{CH}_2)_2\text{CH}(\text{CH}_3)_2$; Isopentyl ethanoate; 3-Methyl-1-butanol acetate; 3-Methylbutyl ethanoate; Acetic acid, isopentyl ester; 2-Methylbutyl ethanoate; Isoamylester kyseliny octove; i-Amyl acetate; 3-Methylbutyl ester of acetic acid; β -Methyl butyl acetate; 3-Methyl butyl ester acetic acid; Amyl acetate ester; Amyl acetate, common; Isopentyl alcohol, acetate pear oil; Isopentyl ester acetic acid; Acetic acid, isoamyl ester; 3-Methyl-1-butanyl acetate; 3-methyl-but-1-yl acetate; 3-methyl-1-butyl acetate (isoamyl acetate) $\text{C}_7\text{H}_{14}\text{O}_2$: [123-92-2]
- Physical properties: MW=130.1849 g/mole, mp=79° C, bp=141° C, Density (25 C) = 0.871 g/cm³
- Supplier and stated purity: Sigma Aldrich, 99%
- Sample class: I (PNNL scale).
- Temperature of White cell (805.0 cm optical path length) 50 ± 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 5.000, 1.000, 8.000, 12.000, 2.000, 6.000, 18.000, 4.000, 0.500, 10.000, 15.000, 25.000, 3.000, 7.000, 21.000 and 9.000.
- Individual samples at equivalent pressures of 0.026079, 0.005216, 0.041727, 0.062591, 0.010433, 0.031299, 0.093886, 0.020864, 0.002608, 0.052145, 0.078207, 0.130345, 0.015641, 0.036487, 0.109446 and 0.046905 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 550 cm^{-1} (1.538 to 18.18 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 16 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 =0.51%, 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)
- Trace water vapor and carbon monoxide were removed by spectral subtraction
- Baseline correction via 7th order polynomial subtraction