

All data taken at Pacific Northwest National Laboratory (PNNL)

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Water contamination (0.11%) corrected for by rescaling composite spectrum.

Composite spectrum for ISOAMOH_25T

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

Equivalent concentration x path-length of composite spectrum: 3.6292×10^{-6} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: Isoamyl alcohol, 3-methyl-1-butanol, 3-methylbutanol, isobutylcarbinol, fermentation amyl alcohol, 1-hydroxy-3-methylbutane, $(\text{CH}_3)_2\text{CHCH}_2\text{CH}_2\text{OH}$: [123-51-3]
- Physical properties: M.W. 88.1492 amu, F.P. -117°C , B.P. 130°C , Density (20 C) 0.809 g/cm^3
- Supplier and stated purity: Aldrich, 99+%
- Sample class: I (PNNL scale).
- Temperature of White cell (792.0 cm optical path length) $25 \pm 2 \text{ C}$
- Diluent (high purity nitrogen) flowed at 24.90 liter/min (296 K), ambient atmospheric pressure $770 \pm 5 \text{ Torr}$.
- Samples flowed at 5.000, 25.000, 2.000, 10.000, 50.000, 15.000, 7.000, 100.000, 37.500 and 3.000 microliters/minute
- Individual samples at equivalent pressures of 0.033724, 0.168489, 0.013477, 0.067351, 0.336711, 0.100987, 0.047108, 0.672977, 0.252233 and 0.020179 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: $7,300$ to 600 cm^{-1} (1.370 to 16.667 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 ($\alpha=0.90$, $\beta=500$)
- Composite spectrum created from 10 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 = 0.34%, Type B = 7%
- Frequency correction (already applied): $V(\text{corrected}) = V(\text{instrument}) * 0.999998 + 1.566836e-04$
- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Baseline correction via 7th order polynomial subtraction
- Trace water vapor features removed via spectral subtraction.