

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for ISOBYIC_67T

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

Equivalent concentration x path-length of composite spectrum: 3.6273×10^{-6} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: Isobutyric acid; α -Methylpropanoic acid; α -Methylpropionic acid; Dimethylacetic acid; Isobutanoic acid; Isopropylformic acid; 2-Methylpropanoic acid; 2-Methylpropionic acid; iso-C₃H₇COOH; Acetic acid, dimethyl-; Cenex RP b2; Propionic acid, 2-methyl-; Tenox EBP 2; Kyselina isomaselna; UN 2529; Methylpropanoic acid; Methylpropionic acid C₄H₈O₂: [79-31-2]
- Physical properties: MW=88.1051 g/mole, mp= -46.2 C, bp=153.8° C, Density (25 C) 0.9485 g/cm³
- Supplier and stated purity: Aldrich, 99 %
- Sample class: I (PNNL scale).
- Temperature of White cell (805.0 cm optical path length) 67.2 ± 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 2.000, 4.000, 8.000, 1.000, 3.000, 6.000, 10.000, 16.000 5.000
- Individual samples at equivalent pressures of 0.016822, 0.033635, 0.067270, 0.008408, 0.025223, 0.050446, 0.084020, 0.134415, 0.041988 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: 7,250 to 530 cm⁻¹ (1.379 to 18.87 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 9 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 =1.94%, Type B $\leq 7\%$
- Frequency correction (already applied): $V(\text{corrected})=V(\text{instrument})\cdot 0.9999996+6.17682\times 10^{-4}$
- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Trace water vapor and carbon dioxide were removed by spectral subtraction
- Baseline correction via 7th order polynomial subtraction