

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for ISOVAL_25T

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

Equivalent concentration x path-length of composite spectrum: 3.5461×10^{-6} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: Isovaleraldehyde; β -Methylbutanal; Isopentanal; Isovaleral; Isovaleric aldehyde; Isovalerylaldehyde; 3-Methylbutan-1-al; 3-Methylbutanal; 3-Methylbutyraldehyde; iso-C₄H₉CHO; Butyraldehyde, 3-methyl-; Isoamylaldehyde; Isopentaldehyde; 1-Butanal, 3-methyl-; 2-Methylbutanal-4; 3-Methyl-1-butanal C₅H₁₀O: [590-86-3]
- Physical properties: MW=86.1323 g/mole, mp= -51 C, bp=92.2° C, Density (25 C) = 0.803 g/cm³
- Supplier and stated purity: Aldrich 97 %
- Sample class: I (PNNL scale).
- Temperature of sample: 25.02 \pm 0.02 C
- Diluent: Sample back filled with ultra high purity nitrogen to 760 \pm 5 Torr.
- Individual samples at 1.02000, 2.3120, 7.2345, 4.0840, 5.4030, 17.48, 38.20, 27.90, 11.5300 and 22.22 Torr. Path length= 19.96 cm. Final data is a composite spectrum.
- Preparation: Multiple freeze-thaw cycles at 77K to remove air.

Instrument Parameters-

- Bruker-66V FTIR, 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 500 cm⁻¹ (1.538 to 20.00 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 10 individual absorbance (base-10) spectra via classical least squares fit: Intercept=0, slope is fitted, individual absorbance values weighted by T² (transmission squared), all absorbance values ≥ 1.6 are given zero weight
- Calculated and estimated errors: Type A =0.50%, Type B \leq 3%

- Frequency correction (already applied): $V(\text{corrected})=V(\text{instrument})\cdot 1.00000135+8.5741\times 10^{-4}$
- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Trace carbon dioxide, water and a small unknown feature at 3576 cm^{-1} were removed by spectral subtraction
- Baseline correction via 7th order polynomial subtraction