

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for HEXACID_25T

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

Equivalent concentration x path-length of composite spectrum: 4.7824×10^{-6} grams/liter-meter

Corrected for water contamination [1.33%] by rescaling and subtracting composite spectrum. Some hexanoic acid dimer observed, but not removed.

Sample Conditions-

- Chemical name and CAS number: Hexanoic acid, 1-hexanoic acid, 1-pentanecarboxylic acid, butylacetic acid, caproic acid, pentiformic acid $\text{CH}_3(\text{CH}_2)_4\text{COOH}$: [142-62-1]
- Physical properties: M.W. 116.1596 amu, F.P. -3°C , B.P. 202.5°C , Density (20 C) 0.927 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 2.000, 1.000, 0.700, 1.800, 0.600, 0.400, 1.200, 0.500, 1.500, 0.300, 0.250 and 0.800 microliters/minute
- Individual samples at equivalent pressures of 0.011492, 0.005744, 0.004018, 0.010464, 0.003442, 0.002294, 0.006881, 0.002866, 0.008595, 0.001719, 0.001431 and 0.004579 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: $7,100$ to 550 cm^{-1} (1.408 to 18.182 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 12 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 = 1.32%, Type B \leq 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