

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for HEXACID\_50T

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

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

Corrected for water contamination [1.81%] 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.  $-3^\circ \text{C}$ , B.P.  $202.5^\circ \text{C}$ , Density (20 C)  $0.927 \text{ g/cm}^3$
- Supplier and stated purity: Aldrich, 99%
- Sample class: I (PNNL scale).
- Temperature of White cell (792.0 cm optical path length)  $50 \pm 2 \text{ C}$
- 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, 2.000, 10.000, 1.000, 7.000, 1.500, 0.800, 1.200, 3.000, 0.600, 2.500, 1.700, 1.300 and 0.700 microliters/minute
- Individual samples at equivalent pressures of 0.028760, 0.011502, 0.057497, 0.005749, 0.040216, 0.008615, 0.004594, 0.006890, 0.017224, 0.003444, 0.014351, 0.009756, 0.007460 and 0.004016 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  $550 \text{ cm}^{-1}$  (1.408 to 18.182 microns)
- Instrumental resolution based on maximum interferometer displacement is  $0.112 \text{ cm}^{-1}$
- Spectral interval after 2X zero-filling interferogram and FFT:  $0.06 \text{ cm}^{-1}$
- 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  $0 \text{ cm}^{-1}$

### Post Processing and Related Parameters-

- Non-linearity detector correction (Bruker proprietary) applied to interferogram ( $\beta=0.90$ ,  $\alpha=500$ )
- Composite spectrum created from 14 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  $\geq 1.6$  are given zero weight

- Calculated and estimated errors: Type A = 1.04%, Type B  $\leq$  7%
- Frequency correction (already applied):  $V(\text{corrected}) = V(\text{instrument}) * 0.999998 + 1.566836e-04$
- Axis units: X=wavenumbers ( $\text{cm}^{-1}$ ), Y=Absorbance (base-10)
- Baseline correction via 7<sup>th</sup> order polynomial subtraction