

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for VALERAL\_5T

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

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

### Sample Conditions-

- Chemical name and CAS number: Valeraldehyde; n-Pentanal; n-Valeraldehyde; Valeral; Valerianic aldehyde; Valeric acid aldehyde; Valeric aldehyde; Valeryl aldehyde; n-C<sub>4</sub>H<sub>9</sub>CHO; Amyl aldehyde; Butyl formal; UN 2058; n-Valeric aldehyde; 1-pentanal; pentan-1-al; Pentanal C<sub>5</sub>H<sub>10</sub>O: [110-62-3]
- Physical properties: MW=86.1323 g/mole, mp=-85.2. C, bp=102.85° C, Density (25 C) = 0.81 g/cm<sup>3</sup>
- Supplier and stated purity: Aldrich 97 %
- Sample class: I (PNNL scale).
- Temperature of sample:  $5.01 \pm 0.02$  C
- Diluent: Sample back filled with ultra high purity nitrogen to  $760 \pm 5$  Torr.
- Individual samples at 1.21800, 8.1030, 4.1858, 2.1584, 9.3000 and 6.0733 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 600 cm<sup>-1</sup> (1.538 to 16.67 microns)
- Instrumental resolution based on maximum interferometer displacement is 0.112 cm<sup>-1</sup>
- Spectral interval after 2X zero-filling interferogram and FFT: 0.06 cm<sup>-1</sup>
- 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<sup>-1</sup>

### Post Processing and Related Parameters-

- Non-linearity detector correction (Bruker proprietary) applied to interferogram ( $\alpha=0.90$ ,  $\epsilon=500$ )
- Composite spectrum created from 6 individual absorbance (base-10) spectra via classical least squares fit: Intercept=0, slope is fitted, individual absorbance values weighted by T<sup>2</sup> (transmission squared), all absorbance values  $\geq 1.6$  are given zero weight
- Calculated and estimated errors: Type A =1.44%, Type B  $\leq 3\%$
- Frequency correction (already applied):  $V(\text{corrected})=V(\text{instrument})*1.00000135+8.5741 \times 10^{-4}$

- Axis units: X=wavenumbers ( $\text{cm}^{-1}$ ), Y=Absorbance (base-10)
- Trace carbon dioxide and water were removed by spectral subtraction
- Baseline correction via 9<sup>th</sup> order polynomial subtraction