

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for PROPANAL\_5T

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

Equivalent concentration x path-length of composite spectrum:  $2.3912 \times 10^{-6}$  grams/liter-meter

Unidentified contamination features at 1122 to 1200  $\text{cm}^{-1}$ . Subtracted contaminant feature based on deviation vector.

### Sample Conditions-

- Chemical name and CAS number: Propanal, propionaldehyde, methylacetaldehyde, propyl aldehyde,  $\text{CH}_3\text{CH}_2\text{C}(\text{O})\text{H}$  : [123-38-6]
- Physical properties: fw=58.0798 g/mole, fp=-81° C, bp=49° C
- Supplier and stated purity: Avocado, 98%
- Sample class: I (PNNL scale).
- Temperature of sample:  $5.13 \pm 0.02$  C
- Diluent: Sample back filled with ultra high purity nitrogen to  $760 \pm 5$  Torr
- Individual samples at 1.16309, 4.1230, 2.0921, 19.00, 8.0500 and 35.00 Torr. Path length = 19.96 cm. Final data is a composite spectrum.
- Preparation: Multiple freeze-thaw cycles at 77 K to remove air.

### Instrument Parameters-

- Bruker-66V FTIR, temperature controlled environment, 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 520  $\text{cm}^{-1}$  (1.534 to 19.231 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 ( $\alpha=0.85$ ,  $\epsilon=530$ )
- 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  $T^2$  (transmission squared), all absorbance values  $\geq 1.6$  are given zero weight
- Calculated and estimated errors: Type A = 0.96%, Type B  $\leq 3\%$
- Frequency correction (already applied):  $V(\text{corrected}) = V(\text{instrument}) * 0.99999896 + 8.812 \times 10^{-4}$
- Axis units: X=wavenumbers ( $\text{cm}^{-1}$ ), Y=Absorbance (base-10)
- Trace water vapor and  $\text{CO}_2$  features removed via spectral subtraction

- Baseline correction via 5<sup>th</sup> order polynomial subtraction