

All data taken at Pacific Northwest National Laboratory (PNNL)  
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Composite spectrum for 2VPYRID\_50T

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

Equivalent concentration x path-length of composite spectrum:  $4.3286 \times 10^{-6}$  grams/liter-meter

#### Sample Conditions-

- Chemical name and CAS number: 2-Vinylpyridine; Pyridine, 2-ethenyl- Pyridine, 2-vinyl-; 2-Ethenylpyridine;  $\alpha$ -Vinylpyridine;  $C_7H_7N$ : [100-69-6]
- Physical properties: MW=105.1372 g/mole, mp= n/a° C, bp=159° C, Density (25 C) = 0.974 g/cm<sup>3</sup>
- Supplier and stated purity: Aldrich, 97%
- Sample class: I (PNNL scale).
- Temperature of White cell (797.3 cm optical path length)  $50 \pm 2$  C
- Diluent (high purity nitrogen) flowed at 24.57 liter/min (21.1° C) ambient atmospheric pressure  $760 \pm 5$  Torr.
- Samples flowed at microliters/minute 1.500, 2.500, 6.000, 4.000, 9.500, 8.000, 13.500, 11.500, 17.000, 15.000, 21.500, 19.500, 26.500, 30.000 and 40.000.
- Individual samples at equivalent pressures of 0.010374, 0.017288, 0.041481, 0.027651, 0.065662, 0.055272, 0.093137, 0.079318, 0.117190, 0.103362, 0.148172, 0.134300, 0.182438, 0.206424 and 0.275159 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: 7,300 to 540  $cm^{-1}$  (1.370 to 18.52 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 15 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 =2.98%, Type B  $\leq 7\%$
- Frequency correction (already applied):  $V(\text{corrected})=V(\text{instrument}) * 1.00000566 + 2.6612 \times 10^{-4}$
- Axis units: X=wavenumbers ( $\text{cm}^{-1}$ ), Y=Absorbance (base-10)
- Trace carbon dioxide and water features were removed via spectral subtraction.
- Baseline correction via 7<sup>th</sup> order polynomial subtraction