

All data taken at Pacific Northwest National Laboratory (PNNL)
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Version 1.0, June 3, 2009

Composite spectrum for 2VPYRID_25T

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

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

Sample Conditions-

- Chemical name and CAS number: 2-Vinylpyridine; Pyridine, 2-ethenyl- Pyridine, 2-vinyl-; 2-Ethenylpyridine; α -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/cm³
- Supplier and stated purity: Aldrich, 97%
- Sample class: I (PNNL scale).
- Temperature of White cell (797.3 cm optical path length) 25 ± 2 C
- Diluent (high purity nitrogen) flowed at 24.57 liter/min (21.1° C) ambient atmospheric pressure 760 ± 5 Torr.
- Samples flowed at microliters/minute 4.000, 7.000, 3.500, 5.250, 9.000, 11.500, 10.000, 13.000, 16.000, 18.500 and 23.000.
- Individual samples at equivalent pressures of 0.027767, 0.048586, 0.024296, 0.036440, 0.062476, 0.079820, 0.069391, 0.090208, 0.111010, 0.128339 and 0.159431 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 11 individual absorbance (base-10) spectra via classical least squares fit: Intercept=0, slope is fitted, individual absorbance values weighted by T² (transmission squared), all absorbance values ≥ 1.6 are given zero weight

- Calculated and estimated errors: Type A =2.60%, Type B \leq 7%
- Frequency correction (already applied): $V(\text{corrected})=V(\text{instrument})\cdot 1.00000566+2.6612\times 10^{-4}$
- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Trace carbon dioxide and water features were removed via spectral subtraction.
- Baseline correction via 7th order polynomial subtraction