

All data taken at Pacific Northwest National Laboratory (PNNL)

Operators: Steven W. Sharpe, Timothy J. Johnson and Robert L. Sams : sw.sharpe@pnl.gov

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Composite spectrum for PARGOH_25T

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

Equivalent concentration x path-length of composite spectrum: 2.3082×10^{-6} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: Propargyl alcohol, 1-propyne-3-ol, ethynylcarbinol, propiolic alcohol, propyn-1-ol, HC::CCH₂OH : [107-19-7]
- Physical properties: fw=56.064 g/mole, mp=-53° C, bp=113.6° C
- Supplier and stated purity: Aldrich, 99%
- Sample class: I (PNNL scale).
- Temperature of sample: 25.05 ± 0.02 C
- Diluent: Sample back filled with ultra high purity nitrogen to 760±5 Torr
- Individual samples at 1.04250, 2.1330, 4.0900, 7.9000, 1.5100, 2.9645, 5.3000, 6.3000, 5.9500 and 4.5800 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: 7,300 to 530 cm⁻¹ (1.370 to 18.868 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 ($\alpha=0.85$, $\epsilon=530$)
- Composite spectrum created from 10 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 = 0.77%, Type B $\leq 3\%$
- Frequency correction (already applied): $V(\text{corrected}) = V(\text{instrument}) * 0.999996 + 2.2203 \times 10^{-3}$
- Axis units: X=wavenumbers (cm⁻¹), Y=Absorbance (base-10)
- Trace water vapor features removed via spectral subtraction
- Baseline correction via 7th order polynomial subtraction