

All data taken at Pacific Northwest National Laboratory (PNNL)
Operators: Steven W. Sharpe, Timothy J. Johnson and Robert L. Sams : sw.sharpe@pnl.gov
Version 1.0, January, 02

Composite spectrum for APINENE_25T

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

Equivalent concentration x path-length of composite spectrum: 5.6089×10^{-6} grams/liter-meter

Note that the (1S)(-)- α -pinene and its enantiomer, (1R)(+)- α -pinene are chiral and will differ in their spectrum only under circularly polarized light conditions. Consequently, the (+) and (-) forms for α -pinene will have identical infrared spectra when observed under normal (unpolarized) conditions. See for instance CAS 80-56-8 and 7785-26-4

Sample Conditions-

- Chemical name and CAS number: (1S)(-)- α -Pinene, 2,6,6-trimethylbicyclo[3.1.1]hept-2-ene, 2-pinene, acitene A, C₁₀ H₁₆ : [7785-26-4]
- Physical properties: fw=132.236 g/mole, fp=-64° C, bp=155° C
- Supplier and stated purity: Aldrich, 99%
- Sample class: I (PNNL scale).
- Temperature of sample: 25.02 \pm 0.02 C
- Diluent: Sample back filled with ultra high purity nitrogen to 760 \pm 5 Torr
- Individual samples at 1.06400, 2.0860, 2.6200, 3.1770, 0.76890, 1.5500, 3.5337, 0.53335, 2.8660 and 1.8010 Torr. Path length = 19.94 cm. Final data is a composite spectrum.
- Preparation: Multiple freeze-thaw cycles at 0 C 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 600 cm⁻¹ (1.534 to 16.667 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 ($\alpha = 0.85$, $\beta = 530$)
- 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 = 0.98%, Type B = 3%
- Frequency correction (already applied): $V(\text{corrected}) = V(\text{instrument}) * 0.99999896 + 8.812 \times 10^{-4}$

- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Trace water vapor and carbon dioxide features removed via spectral subtraction
- Baseline correction via 7th order polynomial subtraction