

All data taken at Pacific Northwest National Laboratory (PNNL)
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Composite spectrum for DLIMONE_25T

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

Equivalent concentration x path-length of composite spectrum: 5.6088×10^{-6} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: D-Limonene; Cyclohexene, 1-methyl-4-(1-methylethenyl)-, (R)-; p-Mentha-1,8-diene, (R)-(+)-; (+)-(R)-Limonene; (+)-(4R)-Limonene; (+)-p-Mentha-1,8-diene; (R)-(+)-Limonene; Carvene; D-(+)-Limonene; Dipentene; Limonene; Limonene, (+)-; (R)-1-methyl-4-(1-methylethenyl)cyclohexene; Dextro-limonene; (γ)-Carvene; (R)-4-Isopropenyl-1-methyl-1-cyclohexene; p-Mentha-1,8-diene; R(γ)-Limonene; 4-Isopropenyl-1-methyl-1-cyclohexene; (R)-limonene C₁₀H₁₆: [5989-27-5]
- Physical properties: MW=136.2340 g/mole, mp=-74.5° C, bp=176.5° C, Density (25 C) = 0.839 g/cm³
- Supplier and stated purity: Fluka Analytical, 99%
- Sample class: I (PNNL scale).
- Temperature of White cell (805.0 cm optical path length) 25 ± 2 C
- Diluent (high purity nitrogen) flowed at 22.77 liter/min (21.1° C), ambient atmospheric pressure 760 ± 5 Torr.
- Samples flowed at microliters/minute 6.000, 9.000, 15.000, 11.000, 23.000, 32.000 and 18.000
- Individual samples at equivalent pressures of: 0.029540, 0.044340, 0.073890, 0.054193, 0.113373, 0.157694 and 0.088703 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: 6,500 to 520 cm⁻¹ (1.538 to 19.23 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 7 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 ≥ 1.6 are given zero weight
- Calculated and estimated errors: Type A =4.08%, Type B $\leq 7\%$
- Frequency correction (already applied): $V(\text{corrected})=V(\text{instrument}) * 1.00000160 + 3.5903 \times 10^{-4}$
- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Trace water vapor and carbon dioxide were removed by spectral subtraction
- Baseline correction via 7th order polynomial subtraction