All data taken at Pacific Northwest National Laboratory (PNNL)
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Composite spectrum for DLIMENE_50T
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

Sample Conditions-

- Chemical name and CAS number: d(+)-Limonene, (+)-1,8-para-methanediene, (+)-4-isopropenyl-1-methylcyclohexene, (+)-carvene, hemo-sol, $C_{10}H_{16}$: [5989-27-5]
- Physical properties: M.W. 136.2364 amu, F.P. –74.3° C, B.P. 176° C, Density (20 C) 0.8411 g/cm^3
- Supplier and stated purity: Aldrich, 97+%
- Sample class: I (PNNL scale).
- Temperature of White cell (792.0 cm optical path length) 50 ± 2 C
- Diluent (high purity nitrogen) flowed at 24.90 liter/min (296 K), ambient atmospheric pressure 745 ± 5 Torr.
- Samples flowed at 5.000, 10.000, 1.000, 2.500, 7.500, 3.000, 25.000, 50.000, 75.000 and 15.000 microliters/minute
- Individual samples at equivalent pressures of 0.021634, 0.043257, 0.004326, 0.010820, 0.032452, 0.012979, 0.108158, 0.216316, 0.324430 and 0.064877 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 550 cm^{-1} (1.538 to 18.182 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 (α=0.90, ε=500)
- 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 T^2 (transmission squared), all absorbance values ≥ 1.6 are given zero weight
- Calculated and estimated errors: Type A = 0.44%, Type B ≤ 7%

- Frequency correction (already applied): V(corrected) = V(instrument)*0.999998+1.566836e-04
- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Trace water vapor features removed via spectral subtraction
- Baseline correction via 7^{th} order polynomial subtraction