

All data taken at Pacific Northwest National Laboratory (PNNL)
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Composite spectrum for 2CARENE_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: 2-Carene; (+)-2-Carene; 3,7,7-Trimethylbicyclo[4.1.0]hept-2-ene; δ -2-Carene; δ -4-carene; 4- δ -carene; Bicyclo[4.1.0]hept-2-ene, 3,7,7-trimethyl-; $C_{10}H_{16}$: [554-61-0]
- Physical properties: MW=136.2340 g/mole, mp= 25° C, bp=167.6° C, Density (25 C) = 0.862 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 12.000, 3.500, 8.000, 5.500, 2.000, 7.000, 13.500, 9.000, 4.000, 11.000 and 3.000.
- Individual samples at equivalent pressures of 0.057104, 0.016653, 0.038064, 0.026155, 0.009507, 0.033263, 0.064133, 0.042749, 0.018995, 0.052229 and 0.014239 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 600 cm⁻¹ (1.370 to 16.67 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 T^2 (transmission squared), all absorbance values ≥ 1.6 are given zero weight
- Calculated and estimated errors: Type A =1.43%, Type B $\leq 7\%$
- Frequency correction (already applied): $V(\text{corrected})=V(\text{instrument}) * 1.00000566 + 2.6612 \times 10^{-4}$
- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Trace water features were removed via spectral subtraction.
- Baseline correction via 7th order polynomial subtraction