

All data taken at Pacific Northwest National Laboratory (PNNL)
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Version 1.0, May 1, 2009

Composite spectrum for 3CARENE_50T

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

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

Sample Conditions-

- Chemical name and CAS number: 3-Carene; 3,7,7-Trimethylbicyclo[4.1.0]hept-3-ene; (+)-3-Carene; Bicyclo[4.1.0]hept-3-ene, 3,7,7-trimethyl-, (1S)-; $C_{10}H_{16}$: [13466-78-9]
- Physical properties: MW=136.2340 g/mole, mp= 25° C, bp=171° C, Density (25 C) = 0.864 g/cm³
- Supplier and stated purity: Aldrich, 98.5%
- Sample class: I (PNNL scale).
- Temperature of White cell (797.3 cm optical path length) 50 ± 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 10.000, 6.000, 2.000, 4.000, 13.000, 9.000, 15.000, 9.000, 26.000, 34.000 and 16.000.
- Individual samples at equivalent pressures of 0.047267, 0.028353, 0.009451, 0.018897, 0.061431, 0.042518, 0.070788, 0.089641, 0.122667, 0.160368 and 0.075457 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 =1.48%, 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