

All data taken at Pacific Northwest National Laboratory (PNNL)  
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Composite spectrum for 3CARENE\_25T

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

Equivalent concentration x path-length of composite spectrum:  $5.6088 \times 10^{-6}$  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/cm<sup>3</sup>
- Supplier and stated purity: Aldrich, 98.5%
- Sample class: I (PNNL scale).
- Temperature of White cell (797.3 cm optical path length)  $25 \pm 2$  C
- Diluent (high purity nitrogen) flowed at 24.57 liter/min (21.1° C) ambient atmospheric pressure  $760 \pm 5$  Torr.
- Samples flowed at microliters/minute 8.000, 17.000, 9.500, 3.000, 5.000, 32.000, 12.000, 29.000, 15.500, 22.000, 18.000 and 6.500.
- Individual samples at equivalent pressures of 0.037574, 0.079845, 0.044619, 0.014090, 0.023484, 0.150257, 0.056339, 0.135989, 0.072626, 0.103013, 0.084261 and 0.030428 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  $\geq 1.6$  are given zero weight

- Calculated and estimated errors: Type A =2.43%, 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 ( $\text{cm}^{-1}$ ), Y=Absorbance (base-10)
- Trace water features were removed via spectral subtraction.
- Baseline correction via 7<sup>th</sup> order polynomial subtraction