

All data taken at Pacific Northwest National Laboratory (PNNL)
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Composite spectrum for MYRCENE_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: Myrcene; β -Myrcene; 1,6-Octadiene, 7-methyl-3-methylene-; 7-Methyl-3-methylene-1,6-octadiene; 7-Methyl-3-methyleneoctadiene-(1,6); 2-Methyl-6-methylene-2,7-octadiene; 3-Methylene-7-methyl-1,6-octadiene; b-Geraniolene; b-Myrcene; 7-Methyl-3-methylene-octa-1,6-diene; β -mircene; 7-methyl-3-methylene-1,6-octadiene (myrcene); 7-methyl-3-methylene-1,6-octadiene (β -myrcene) $C_{10}H_{16}$: [123-35-3]
- Physical properties: MW=136.2340 g/mole, mp= na ° C, bp=167° C, Density (25 C) = 0.8013 g/cm³
- Supplier and stated purity: Fluka Analytical, $\geq 95\%$
- 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 5.000, 2.000, 14.000, 8.000, 12.000, 19.000, 30.000 and 21.000
- Individual samples at equivalent pressures of: 0.023246, 0.009299, 0.065114, 0.037208, 0.055827, 0.088404, 0.139642 and 0.097762 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 8 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 =3.35%, 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 was removed by spectral subtraction
- Baseline correction via 7th order polynomial subtraction