

All data taken at Pacific Northwest National Laboratory (PNNL)
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Composite spectrum for GERANOL_50T

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

Equivalent concentration x path-length of composite spectrum: 6.3505×10^{-6} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: Geraniol; 2,6-Octadien-1-ol, 3,7-dimethyl-, (E)-trans-; Geraniol; Guaniol; Lemonol; trans-3,7-Dimethyl-2,6-octadien-1-ol; Geraniol alcohol; Geraniol extra; Geranyl alcohol; 2,6-Dimethyl-trans-2,6-octadien-8-ol; 2,6-Octadien-1-ol, 3,7-dimethyl-, trans-; 3,7-Dimethyl-trans-2,6-octadien-1-ol; (E)-3,7-Dimethyl-2,6-octadien-1-ol; Meranol; trans-3,7-Dimethyl octa-2,6-dien-1-ol; (2E)-3,7-Dimethyl-2,6-octadien-1-ol; Nerol; Neryl Alcohol; (E)-3,7-dimethyl-2,6-octadien-1-ol (geraniol); (E)-geraniol; Geraniol (E); t-Geraniol; trans-3,7-dimethyl-2,6-octadien-1-ol (geraniol) $C_{10}H_{18}O$: [106-24-1]
- Physical properties: MW=154.2493 g/mole, mp= -15° C, bp=230° C, Density (25 C) = 0.879g/cm³
- Supplier and stated purity: Aldrich, 98%
- Sample class: I (PNNL scale).
- Temperature of White cell (805.0 cm optical path length) 50 ± 2 C
- Diluent (high purity nitrogen) flowed at 23.3 liter/min (21.1° C), ambient atmospheric pressure 760 ± 5 Torr.
- Samples flowed at microliters/minute 2.000, 4.000, 8.000, 3.000, 6.000, 12.000, 10.000, 7.000 and 5.000.
- Individual samples at equivalent pressures of 0.008856, 0.017712, 0.035419, 0.013265, 0.026529, 0.053037, 0.044186, 0.030930 and 0.022090 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 600 cm^{-1} (1.5385 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 ($\alpha=0.90$, $\varepsilon=500$)
- Composite spectrum created from 9 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 =1.91%, Type B $\leq 7\%$
- Frequency correction (already applied): $V(\text{corrected})=V(\text{instrument}) * 1.0000016 + 3.59033 \times 10^{-4}$
- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Trace carbon dioxide and 1% water features were removed via spectral subtraction and the composite spectrum was corrected by a rescaling of 1.01 %.
- Baseline correction via 7th order polynomial subtraction