

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for WINTGREN_50T

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

Equivalent concentration x path-length of composite spectrum: 6.2641×10^{-6} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: Methyl salicylate, wintergreen oil, 2-carbomethoxyphenol, o-hydroxybenzoic acid methyl ester, analgit, betula oil, panalgesic, sweet birch oil, teaberry oil, $(\text{OH})\text{C}_6\text{H}_4\text{CO}_2\text{CH}_3$: [119-36-8]
- Physical properties: MW=152.1494 g/mole, mp=-8° C, bp=222° C, Density (20 C) 1.174 g/cm³
- Supplier and stated purity: Aldrich, 99+%
- Sample class: I (PNNL scale).
- Temperature of White cell (815.76 cm optical path length) 50 ± 2 C
- Diluent (high purity nitrogen) flowed at 25.20 liter/min (21.1° C), ambient atmospheric pressure 760 ± 5 Torr.
- Samples flowed at 3.000, 1.000, 5.000, 2.000, 4.000, 7.000, 10.000, 15.000, 20.000 and 30.000 microliters/minute
- Individual samples at equivalent pressures of 0.016907, 0.005636, 0.028164, 0.011264, 0.022523, 0.039415, 0.056292, 0.084427, 0.112539 and 0.168742 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 550 cm⁻¹ (1.538 to 18.182 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 10 individual absorbance (base-10) spectra via classical least squares fit: Intercept=0, slope is fitted, individual absorbance values weighted by T² (transmission squared), all absorbance values ≥ 1.6 are given zero weight
- Calculated and estimated errors: Type A = 0.45%, Type B $\leq 7\%$

- Frequency correction (already applied): $V(\text{corrected})=V(\text{instrument})*0.9999987-4.24224\times 10^{-4}$
- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Baseline correction via 6th order polynomial subtraction