

All data taken at Pacific Northwest National Laboratory (PNNL)

Operators: Steven W. Sharpe, Timothy J. Johnson and Robert L. Sams : sw.sharpe@pnl.gov

Version 1.0, March, 02

Composite spectrum for MEACRL_50T

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

Equivalent concentration x path-length of composite spectrum: 3.5444×10^{-6} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: Methyl acrylate, methyl propenoate, methoxycarbonylethylene, acrylic acid methyl ester, 2-propenoic acid methyl ester, curithane-103, $\text{CH}_2=\text{CHCOOCH}_3$: [96-33-3]
- Physical properties: fw=86.0902 g/mole, fp=-76.5° C, bp=80.5° C
- Supplier and stated purity: Aldrich, 99%
- Sample class: I (PNNL scale).
- Temperature of sample: 50.05 ± 0.02 C
- Diluent: Sample back filled with ultra high purity nitrogen to 760 ± 5 Torr
- Individual samples at 1.1400, 4.0693, 0.75522, 9.1010, 2.0588, 6.0960 and 0.51970 Torr. Path length = 19.96 cm. Final data is a composite spectrum.
- Preparation: Sample placed over CaSO_4 to remove water and pumped on at -65 C to remove air.

Instrument Parameters-

- Bruker-66V FTIR, temperature controlled environment, evacuated optics bench
- Modified to include second aperture, between interferometer output and sample cell. This substantially reduces both “ghosting” and warm aperture effects.
- Spectral range: $6,500$ to 580 cm^{-1} (1.534 to 17.241 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 ($\tau = 0.90$, $\nu = 500$)
- Composite spectrum created from 7 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 = 0.26%, Type B = 3%
- Frequency correction (already applied): $V(\text{corrected}) = V(\text{instrument}) * 0.999998 + 1.287 \times 10^{-4}$
- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Trace carbon dioxide features removed via spectral subtraction
- Baseline correction via 7th order polynomial subtraction