

All data taken at Pacific Northwest National Laboratory (PNNL)

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Version 1.0, January, 04

Composite spectrum for MEACRLCL_5T

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

Equivalent concentration x path-length of composite spectrum: 4.3038×10^{-6} grams/liter-meter

Sample contaminated and corrected for SO₂ [1.30%] and HCl [0.32%]. Unidentified trace contaminations peaks noted at 1680 and 782 cm⁻¹.

Sample Conditions-

- Chemical name and CAS number: Methacryloyl chloride, 2-methyl-2-propenoyl, H₂C=C(CH₃)COCl : [920-46-7]
- Physical properties: fw=104.5359 g/mole, fp=-60° C, bp=96° C
- Supplier and stated purity: Aldrich, 98+%, stabilized with monomethyl ether hydroquinone
- Sample class: II (PNNL scale). Sample hydrolyses easily.
- Temperature of sample: 4.96 ± 0.02 C
- Diluent: Sample back filled with ultra high purity nitrogen to 760±5 Torr
- Individual samples at 1.0339, 2.1695, 4.0808, 7.0409, 5.8749 and 3.5546 Torr. Path length = 19.96 cm. Final data is a composite spectrum.
- Preparation: Multiple freeze-thaw cycles at 77 K 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 530 cm⁻¹ (1.534 to 18.868 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 ($\alpha=0.85$, $\epsilon=530$)
- Composite spectrum created from 6 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 = 1.17%, Type B ≤ 5%
- Frequency correction (already applied): $V(\text{corrected}) = V(\text{instrument}) * 0.99999896 + 8.812 \times 10^{-4}$
- Axis units: X=wavenumbers (cm⁻¹), Y=Absorbance (base-10)
- Trace CO₂ and CO features removed via spectral subtraction

- Baseline correction via 6th order polynomial subtraction