

All data taken at Pacific Northwest National Laboratory (PNNL)
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Composite spectrum for ACRACID_50T

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

Equivalent concentration x path-length of composite spectrum: 2.9669×10^{-6} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: Acrylic acid; 2-Propenoic acid; Acroleic acid; Ethylenecarboxylic acid; Propenoic acid; Vinylformic acid; $\text{CH}_2=\text{CHCOOH}$; Propene acid; Kyselina akrylova; Acrylate; Glacial acrylic acid $\text{C}_3\text{H}_4\text{O}_2$: [79-10-7]
- Physical properties: MW=72.0627 g/mole, mp=12.9° C, bp=140° C, Density (25 C) = 0.807 g/cm³
- Supplier and stated purity: Aldrich, 99%
- 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, 6.000, 5.000, 1.000 and 4.500.
- Individual samples at equivalent pressures of 0.023242, 0.046484, 0.069698, 0.058082, 0.011607 and 0.052233 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 525 cm^{-1} (1.538 to 19.05 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 6 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 =3.21%, Type B $\leq 7\%$

- Frequency correction (already applied): $V(\text{corrected})=V(\text{instrument})\cdot 0.9999996+6.17682\times 10^{-4}$
- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Trace dimer features identified in the deviation vector between 2400 and 3400 cm^{-1} were removed by spectral subtraction. Other dimer features that were identified in the deviation vector and not removed were located at 1060, 1185, 1246, 1269, 1296, 1407, 1437 and 1725 cm^{-1} .
- Baseline correction via 7th order polynomial subtraction