

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, 08

Composite spectrum for FACID_50T

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

Equivalent concentration x path-length of composite spectrum: 1.8949×10^{-6} grams/liter-meter

Corrected for water contamination [4.70%] by rescaling and spectral subtraction. Dimer features present at 3400-2500, 1736, 1365, 1221 and 926 cm^{-1} .

Sample Conditions-

- Chemical name and CAS number: Formic acid, methanoic acid, aminic acid, hydrogencarboxylic acid, HC(O)OH : [64-18-6]
- Physical properties: M.W. 42.0254 amu, F.P. 8.3° C , B.P. 100.7° C , Density (20 C) 1.215 g/cm^3
- Supplier and stated purity: Aldrich, 96+% (Stabilized with ~4% water)
- Sample class: II (PNNL scale).
- Temperature of White cell (815.76 cm optical path length) $50 \pm 2 \text{ C}$
- Diluent (high purity nitrogen) flowed at 25.20 liter/min (21.1° C), ambient atmospheric pressure $760 \pm 5 \text{ Torr}$.
- Samples flowed at 3.000, 1.000, 0.500, 1.200, 2.400, 0.700, 1.600, 4.000, 2.000, 0.400, 7.000, 1.400, 3.500 and 5.000 microliters/minute
- Individual samples at equivalent pressures of 0.054940, 0.018313, 0.009155, 0.021976, 0.043946, 0.012818, 0.029298, 0.073244, 0.036617, 0.007324, 0.128160, 0.025632, 0.064071 and 0.091518 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: $7,200$ to 540 cm^{-1} (1.390 to 18.519 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 14 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 = 1.22%, 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 7th order polynomial subtraction