All data taken at Pacific Northwest National Laboratory (PNNL)
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Some acetic acid dimer present in composite spectrum. Concentration unknown.

Composite spectrum for AACID_50T
Effective burden of composite spectrum: 1 part-per-million-meter (ppm-meter) at 296 K
Equivalent concentration x path-length of composite spectrum: 2.4724×10^{-6} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: Acetic acid, methanecarboxylic acid, vinegar acid, ethylic acid, glacial acetic acid, : [64-19-7]
- Physical properties: M.W. 18.0152 amu, F.P. 16.6° C, B.P. 117.9° C, Density (20 C) 1.0492 g/cm^3
- Supplier and stated purity: Aldrich, 99.99+%
- Sample class: I (PNNL scale).
- Temperature of White cell (792.0 cm optical path length) 50 ± 2 C
- Diluent (high purity nitrogen) flowed at 24.90 liter/min (296 K), ambient atmospheric pressure 770 ± 5 Torr.
- Samples flowed at 1.000, 0.500, 0.750, 1.300, 0.300, 1.500, 0.600, 1.700, 0.400, 2.000, 0.250, 1.000, 0.500, 0.750, 1.300, 0.300, 1.500, 0.600, 1.700, 0.400, 2.000 and 0.250 microliters/minute
- Individual samples at equivalent pressures of 0.012901, 0.006450, 0.009675, 0.016765, 0.003868, 0.019344, 0.007737, 0.021915, 0.005156, 0.025782, 0.003223, 0.012839, 0.006422, 0.009637, 0.016706, 0.003856, 0.019281, 0.007712, 0.021849, 0.005141, 0.025704 and 0.003214 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: 7,100 to 550 cm^{-1} (1.409 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 (α=0.90, ε=500)

- Composite spectrum created from 22 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 = 0.94%, Type B ≤ 7%
- Frequency correction (already applied): V(corrected) = V(instrument)*0.999998+1.566836e-04
- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Baseline correction via 7^{th} order polynomial subtraction