All data taken at Pacific Northwest National Laboratory (PNNL)
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Corrected for acetic acid dimer [11.72%] by scaling composite spectrum and subtracting dimer spectrum.

Composite spectrum for AACID_25T
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) 25 ± 2 C
- Diluent (high purity nitrogen) flowed at 24.90 liter/min (296 K), ambient atmospheric pressure 770 ± 5 Torr.
- Samples flowed at 2.000, 0.500, 1.000, 0.100, 0.250, 5.000, 1.000, 0.700, 0.350, 1.400, 1.100, 2.200, 0.800, 1.600, 0.500 and 0.250 microliters/minute
- Individual samples at equivalent pressures of 0.025748, 0.006437, 0.012871, 0.001287, 0.003218, 0.064362, 0.012801, 0.008960, 0.004479, 0.017917, 0.014080, 0.028163, 0.010242, 0.020490, 0.006405 and 0.003202 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 16 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 = 2.64%, 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