All data taken at Pacific Northwest National Laboratory (PNNL)
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Composite spectrum for ETOH_5T
Effective burden of composite spectrum: 1 part-per-million-meter (ppm-meter) at 296 K
Equivalent concentration x path-length of composite spectrum: 1.89678×10^{-6} grams/liter-meter
Windows (KCl) appear to adsorb with ethyl alcohol and produce broad, featureless "bumps" in the 3300 cm^{-1} region. These bumps have been fitted with a polynomial baseline and subtracted from the composite spectrum.

Sample Conditions-

- Chemical name and CAS number: Ethyl alcohol, ethanol, anhydro, ethyl hydrate, ethyl hydroxide, grain alcohol, jaysol, methylcarbinol, tecsol, CH_3CH_2OH : [64-17-5]
- Physical properties: fw=46.0688 g/mole, fp=–114° C, bp=78° C
- Supplier and stated purity: Aldrich, 99.5%
- Sample class: I (PNNL scale).
- Temperature of sample: 4.93 ± 0.02 C
- Diluent: Sample back filled with ultra high purity nitrogen to 760±5 Torr
- Individual samples at 1.08503, 2.0685, 8.3110, 4.0750, 3.0190 and 6.0500 Torr. Path length = 19.96 cm. Final data is a composite spectrum.
- Preparation: Place sample of $CaSO_4$ to remove water. 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: 7,500 to 600 cm^{-1} (1.333 to 16.667 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=0.85, β=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 T^2 (transmission squared), all absorbance values ≥ 1.6 are given zero weight
- Calculated and estimated errors: Type A = 3.39%, Type B ≤ 3%
- Frequency correction (already applied): V(corrected) = V(instrument)* $0.99999896+8.812 \times 10^{-4}$

- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Trace water vapor and carbon dioxide features removed via spectral subtraction
- Baseline correction via 7^{th} order polynomial subtraction