All data taken at Pacific Northwest National Laboratory (PNNL)
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Composite spectrum for ACETONE_25T
Effective burden of composite spectrum: 1 part-per-million-meter (ppm-meter) at 296 K
Equivalent concentration x path-length of composite spectrum: 2.3912×10^{-6} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: Acetone, 2-propanone, dimethyl formaldehyde, dimethylketal, beta-ketopropane, methyl ketone, pyroacetic acid, pyroacetic ether, $CH_3C(O)CH_3$: [67-64-1]
- Physical properties: fw=58.0798 g/mole, fp=–94.3° C, bp=56.2° C
- Supplier and stated purity: Aldrich, 99.9+%
- Sample class: I (PNNL scale).
- Temperature of sample: 25.00 ± 0.02 C
- Diluent: Sample back filled with ultra high purity nitrogen to 760±5 Torr
- Individual samples at 1.07161, 16.79, 8.4113, 4.1380, 2.2727, 64.42, 33.11, 6.3050, 25.30 and 46.12 Torr. Path length = 19.96 cm. Final data is a composite spectrum.
- Preparation: Multiple freeze-thaw cycles at 77 K to remove air. Place sample over $CaSO_4$ to remove water.

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: 6,500 to 510 cm^{-1} (1.534 to 19.608 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, ε=530)
- Composite spectrum created from 10 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 = 0.24%, 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