All data taken at Pacific Northwest National Laboratory (PNNL)
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Composite spectrum for CH4_25T
Effective burden of composite spectrum: 1 part-per-million-meter (ppm-meter) at 296 K
Equivalent concentration x path-length of composite spectrum: 6.605×10^{-7} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: Methane, natural gas, methyl hydride, marsh gas, biogas, fire damp, CH_4: [74-82-8]
- Physical properties: fw=16.0426 g/mole, fp=–182.5° C, bp=-161.5° C
- Supplier and stated purity: Matheson, 99%
- Sample class: I (PNNL scale).
- Temperature of sample: 25.01 ± 0.02 C
- Diluent: Sample back filled with ultra high purity nitrogen to 760±5 Torr
- Individual samples at 2.4528, 0.91451, 5.6150, 0.65690, 1.6592, 9.2340, 0.79330, 6.7259, 0.90108, 4.1602, 8.1280, 53.73 and 147.54, 23.95 Torr. Path length = 19.96 cm. Final data is a composite spectrum.
- Preparation: 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: 6,500 to 600 cm^{-1} (1.534 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=0.90, ε=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 = 0.95%, Type B ≤ 3%
- Frequency correction (already applied): V(corrected) = V(instrument)* 0.999998-2.75000e-6
- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Trace carbon dioxide features removed via spectral subtraction
- Baseline correction via 7^{th} order polynomial subtraction