

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for C₂H₆_50T

Effective burden of composite spectrum: 1 part-per-million-meter (ppm-meter) at 296 K

Equivalent concentration x path-length of composite spectrum: 1.238x10⁻⁶ grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: Ethane, dimethyl, methylmethane CH₃CH₃: [74-84-0]
- Physical properties: F.W. 30.07 amu, F.P. -183.2 C, B.P. -88.6 C
- Supplier and stated purity: Matheson, 99%, 0.063% (P/P) of CO₂ observed and corrected.
- Sample class: I (PNNL scale).
- Temperature of sample: 50.01 ± 0.02 C
- Diluent: Sample back filled with ultra high purity nitrogen to 760±5 Torr
- Individual samples at 1.02133, 0.71595, 4.8261, 17.50, 33.99, 1.4935, 2.0488, 52.48 and 8.2474 Torr. Path length = 19.94 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 (=0.85, =530)
- Composite spectrum created from 9 individual absorbance (base-10) spectra via classical least squares fit: Intercept=0, slope is fitted, individual absorbance values weighted by T² (transmission squared), all absorbance values 1.6 are given zero weight
- Calculated and estimated errors: Type A = 0.54%, Type B 3%
- Frequency correction (already applied): V(corrected) = V(instrument)*0.999997+5.18x10⁻⁴
- Axis units: X=wavenumbers (cm⁻¹), Y=Absorbance (base-10)
- Trace CO₂ vapor features removed via spectral subtraction. Some residuals of subtraction observed.