All data taken at Pacific Northwest National Laboratory (PNNL)
Operators: Steven W. Sharpe, Timothy J. Johnson and Robert L. Sams : sw.sharpe@pnl.gov
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Composite spectrum for HCHO_50T
Effective burden of composite spectrum: 1 part-per-million-meter (ppm-meter) at 296 K
Equivalent concentration x path-length of composite spectrum: 1.2362×10^{-6} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: Formaldehyde, methylene oxide, methyl aldehyde, methanal, formic aldehyde, oxomethane, formalin, morbicid, veracur, methylene glycol, formalin-40, FYDE, karasan, HCHO, HOCH : [50-00-0]
- Physical properties: fw=30.026 g/mole, fp=–118° C, bp=-19° C
- Supplier and stated purity: Synthesized from paraformaldehyde by heating gently and condensing vapors at liquid nitrogen temperature. Condensate was then cooled to –120 C and pumped on to remove air and CO_2. Sample kept at –50 C to reduce polymerization, minimize polymers and minimize water vapor. Small batches were made as needed to prevent bulk from converting back to paraformaldehyde. No methanol was observed.
- Sample class: III (PNNL scale). Extremely unstable due to rapid polymerization.
- Temperature of sample: 49.99 ± 0.02 C
- Diluent: Sample back filled with ultra high purity nitrogen to 760±5 Torr
- Individual samples at 1.0202, 0.545, 2.1017, 1.5317, 2.8074, 9.710, 0.254 and 5.0524 Torr. Path length = 19.94 cm. Final data is a composite spectrum.
- Preparation: Multiple freeze-thaw cycles at -120 C to remove air and CO_2.

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=0.85, ε=530)
- Composite spectrum created from 8 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 = 0.50%, Type B ≤ 10%

- Frequency correction (already applied): V(corrected) = V(instrument)* $0.99999896+8.812x10^{-4}$
- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Trace water vapor and carbon dioxide features removed via spectral subtraction. Some residual still observed.
- Baseline correction via 7^{th} order polynomial subtraction