

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for METHGLY_25T

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

Equivalent concentration x path-length of composite spectrum: 2.9669×10^{-6} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: Methyl glyoxal; Propanal, 2-oxo-; Pyruvaldehyde; α -Ketopropionaldehyde; Acetylformaldehyde; Acetylformyl; Pyroracemic aldehyde; Pyruvic aldehyde; 2-Ketopropionaldehyde; 2-Oxopropanal; 1,2-Propanedione; CH₃COCHO; Glyoxal, methyl; Propanedione; Propanolone; Propionaldehyde, 2-keto; Propionaldehyde, 2-oxo-; C₃H₄O₂: [78-98-8]
- Physical properties: MW=72.0627 g/mole, mp= 25 C, bp=71.9° C, Density (25 C) = 1.14 g/cm³
- Supplier and stated purity: Synthesized in house see Dyllick-Brenzinger, C. E. and Bauder, A. Chem. Phys. 30, 147 (1978).
- Sample class: I (PNNL scale).
- Temperature of sample: 25.02 ± 0.02 C
- Diluent: Sample back filled with ultra high purity nitrogen to 760 ± 5 Torr.
- Individual samples at 1.07000, 4.6800, 2.0560, 6.0400, 7.3400, 4.0500, 3.0820, 2.5236, 1.5000 and 11.3000 Torr. Path length= 19.96 cm. Final data is a composite spectrum.
- Preparation: Multiple freeze-thaw cycles at 77K to remove air.

Instrument Parameters-

- Bruker-66V FTIR, 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 550 cm⁻¹ (1.538 to 18.18 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 ($\alpha=0.90$, $\epsilon=500$)
- 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 T² (transmission squared), all absorbance values ≥ 1.6 are given zero weight

- Calculated and estimated errors: Type A =2.33%, Type B \leq 3%
- Frequency correction (already applied): $V(\text{corrected})=V(\text{instrument})\cdot 1.00000566+2.0343\times 10^{-3}$
- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Trace hydrogen cyanide, carbon monoxide, acetic acid, 2.0% of formaldehyde, 0.7% of carbon dioxide and 0.46% of hydrogen chloride were removed by spectral subtraction and the composite spectrum was corrected by a rescaling of 3.561%. Five additional unknown bands as determined from the deviation spectrum are at 887, 952, 1109, 1170 and 1252 cm^{-1} .
- Baseline correction via 7th order polynomial subtraction