

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for GLYOXAL_25T

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

Equivalent concentration x path-length of composite spectrum: 2.3894×10^{-6} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: Glyoxal; Biformal; Biformyl; Diformyl; Ethanedione; Glyoxal aldehyde; Glyoxylaldehyde; Oxal; Oxalaldehyde; 1,2-Ethanedione; (CHO)₂; Diformal; Ethane-1,2-dione; Ethandial; Aerotex glyoxal 40; ODIX; Protectol GL 40 C₂H₂O₂: [107-22-2]
- Physical properties: MW=58.0361 g/mole, mp= 15. C, bp=50.45° C, Density (25 C) = 1.14 g/cm³
- Supplier and stated purity: Synthesized in house. See Cole, A. R. H. and Osborne, G. A. "Spectra of glyoxal, monodeuteroglyoxal and dideuteroglyoxal", Spectrochimica Acta **27A** pg 2461 (1971).
- 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 1.0330, 2.1064, 3.8708, 3.0437, 10.3900, 5.5030, 30.14, 25.94, 14.12 8.0187, 7.0310 and 6.0810 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 600 cm⁻¹ (1.538 to 16.67 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 12 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 =1.13%, Type B $\leq 3\%$

- Frequency correction (already applied): $V(\text{corrected})=V(\text{instrument})\cdot 1.00000135+8.5741\times 10^{-4}$
- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Trace carbon dioxide and carbon monoxide were removed by spectral subtraction
- Baseline correction via 7th order polynomial subtraction