

All data taken at Pacific Northwest National Laboratory (PNNL)
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Composite spectrum for FURAN3M_5T

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

Equivalent concentration x path-length of composite spectrum: 3.3801×10^{-6} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: 3-Methylfuran; 3-Methylfurane; Furan, 3-methyl- C_5H_6O : [930-27-8]
- Physical properties: MW=82.1005 g/mole, mp= -90.71. °C, bp=65.5 °C, Density (25 C) = 0.9024 g/cm³
- Supplier and stated purity: Acros Organics, 98 %
- Sample class: I (PNNL scale).
- Temperature of sample: 5.01 ± 0.02 C
- Diluent: Sample back filled with ultra high purity nitrogen to 760 ± 5 Torr.
- Individual samples at 0.406, 0.812, 1.218, 11.42 and 7.987 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 5 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 =2.98 %, Type B $\leq 3\%$
- Frequency correction (already applied): $V(\text{corrected})=V(\text{instrument}) * 1.00000566 + 2.0343 \times 10^{-4}$
- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Trace carbon dioxide was removed by spectral subtraction

- Baseline correction via 7th order polynomial subtraction