

All data taken at Pacific Northwest National Laboratory (PNNL)
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Composite spectrum for FURALD_25T

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

Equivalent concentration x path-length of composite spectrum: 3.9557×10^{-6} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: Furfural; 2-Furaldehyde; α -Furole; Artificial ant oil; Fural; Furaldehyde; Furale; Furancarbal; Furfuraldehyde; Furfurole; Furfurylaldehyde; Furole; Pyromucic aldehyde; 2-Formylfuran; 2-Furalaldehyde; 2-Furancarbal; 2-Furfural; 2-Furfuraldehyde; 2-Furylaldehyde; Furol; 2-Furylmethanal; Artificial oil of ants; Furfurale; Furfurol; Nci-C56177; 2-Furil-metanale; 2-Furankarbaldehyd; Furfuralu; ; 2-Furylaldehyde xypropane; 2-Furylcarboxaldehyde; Cyclic aldehyde; Qo furfural; 2-Furancarboxaldehyde (furfural); 2-furancarboxyaldehyde; furan-2-aldehyde; furan-2-carbaldehyde; furancarboxaldehyde $C_5H_4O_2$: [98-01-1]
- Physical properties: MW=96.0841 g/mole, mp= -38.7° C, bp=161.6° C, Density (25 C) = 1.159 g/cm³
- Supplier and stated purity: Sigma Aldrich, 99%
- Sample class: I (PNNL scale).
- Temperature of White cell (805.0 cm optical path length) 25 ± 2 C
- Diluent (high purity nitrogen) flowed at 23.30 liter/min (21.1° C) ambient atmospheric pressure 760 ± 5 Torr.
- Samples flowed at microliters/minute 2.000, 1.000, 3.000, 0.500, 3.500, 1.500, 4.000, 2.500, 5.000, 0.250, 0.750, 7.500, 1.250, 4.500 and 1.000.
- Individual samples at equivalent pressures of 0.018693, 0.009348, 0.028047, 0.004676, 0.032740, 0.014029, 0.037412, 0.023379, 0.046752, 0.002338, 0.007017, 0.070156, 0.011693, 0.042099 and 0.009357 Torr.
- Final data is a composite spectrum.
- Preparation: None

Instrument Parameters-

- Bruker-66V FTIR, evacuated optics bench.
- Modified to include second aperture, between interferometer output and White 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 15 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 =1.49%, Type B $\leq 7\%$
- Frequency correction (already applied): $V(\text{corrected})=V(\text{instrument}) * 0.99999959 + 6.1768 \times 10^{-4}$
- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Trace carbon dioxide and water features were removed via spectral subtraction.
- Baseline correction via 7th order polynomial subtraction