

All data taken at Pacific Northwest National Laboratory (PNNL)

Operators: Steven W. Sharpe, Timothy J. Johnson and Robert L. Sams : sw.sharpe@pnl.gov

Version 1.0, January 18, 2006

Contaminated with water [1.21%] and corrected by rescaling and spectral subtraction.

Composite spectrum for FURFOH_50T

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

Equivalent concentration x path-length of composite spectrum: 4.0389×10^{-6} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: Furfuryl alcohol, FA, 2-furancarbinol, 2-furanmethanol, 2-hydroxymethylfuran, $C_5H_6O_2$: [98-00-1]
- Physical properties: MW=98.1012 g/mole, mp=-29° C, bp=170° C, Density (20 C) 1.135g/cm³
- Supplier and stated purity: Aldrich, 99%
- Sample class: I (PNNL scale).
- Temperature of White cell (796.0 cm optical path length) 50 ± 2 C
- Diluent (high purity nitrogen) flowed at 24.2 liter/min (21.1° C), ambient atmospheric pressure 760 ± 5 Torr.
- Samples flowed at 2.000, 9.000, 13.000, 7.000, 5.000, 19.000, 4.000, 1.000, 10.000, 6.000, 43.000, 25.000, 17.000, 41.000, 8.000 and 35.000 microliters/minute
- Individual samples at equivalent pressures of 0.017290, 0.077867, 0.112475, 0.060588, 0.043288, 0.164584, 0.034649, 0.008668, 0.086773, 0.052071, 0.373224, 0.217077, 0.147671, 0.356243, 0.069520 and 0.304312 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: 7,300 to 550 cm^{-1} (1.370 to 18.182 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 16 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 = 0.21%, Type B $\leq 7\%$

- Frequency correction (already applied): $V(\text{corrected})=V(\text{instrument})\cdot 0.99999959-3.45278\times 10^{-4}$
- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Trace carbon dioxide features removed by spectral subtraction
- Baseline correction via 7th order polynomial subtraction