

All data taken at Pacific Northwest National Laboratory (PNNL)
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Composite spectrum for 2PENFUR_25T

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

Equivalent concentration x path-length of composite spectrum: 5.6901×10^{-6} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: 2-Pentylfuran; Furan, 2-pentyl-; 2-n-Pentylfuran; 2-Amylfuran; 2-pentylfurane; Amyl furan (2-Pentyl furan); furane, 2-pentyl; $C_9H_{14}O$: [3777-69-3]
- Physical properties: MW=138.2069 g/mole, mp= n/a° C, bp=203° C, Density (25 C) = 0.886 g/cm³
- Supplier and stated purity: SAFC, 97%
- Sample class: I (PNNL scale).
- Temperature of White cell (797.3 cm optical path length) 25 ± 2 C
- Diluent (high purity nitrogen) flowed at 24.57 liter/min (21.1° C) ambient atmospheric pressure 760 ± 5 Torr.
- Samples flowed at microliters/minute 13.000, 18.000, 35.000, 45.000, 27.000, 20.000, 31.000, 50.000, 65.000, 40.000, 24.000 and 7.000.
- Individual samples at equivalent pressures of 0.061604, 0.085298, 0.165747, 0.212848, 0.127624, 0.094549, 0.146512, 0.236246, 0.307202, 0.188997, 0.113383 and 0.033061 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 18.18 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 11 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 =1.09%, Type B $\leq 7\%$
- Frequency correction (already applied): $V(\text{corrected})=V(\text{instrument}) * 1.00000566 + 2.6612 \times 10^{-4}$
- 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