

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for 2MEFURN\_25T

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

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

#### Sample Conditions-

- Chemical name and CAS number: 2-Methyl furan;  $\alpha$ -Methylfuran; Silvan; Sylvan; 2-Methylfuran; 5-Methylfuran; Methylfuran; UN 2301; 2-methylfurane C<sub>5</sub>H<sub>6</sub>O: [534-22-5]
- Physical properties: MW=82.1005 g/mole, mp= -92.28. C, bp=64.86° C, Density (25 C) = 0.9093 g/cm<sup>3</sup>.
- Supplier and stated purity: Aldrich 99 %
- Sample class: I (PNNL scale).
- Temperature of sample:  $25.01 \pm 0.02$  C
- Diluent: Sample back filled with ultra high purity nitrogen to  $760 \pm 5$  Torr.
- Individual samples at 1.17100, 2.0551, 2.9660, 0.51850, 1.5725, 96.02, 49.22, 24.66, 12.17 and 6.3300 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<sup>-1</sup> (1.538 to 18.18 microns)
- Instrumental resolution based on maximum interferometer displacement is 0.112 cm<sup>-1</sup>
- Spectral interval after 2X zero-filling interferogram and FFT: 0.06 cm<sup>-1</sup>
- 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<sup>-1</sup>

#### Post Processing and Related Parameters-

- Non-linearity detector correction (Bruker proprietary) applied to interferogram ( $\alpha=0.90$ ,  $\epsilon=500$ )
- Composite spectrum created from 10 individual absorbance (base-10) spectra via classical least squares fit: Intercept=0, slope is fitted, individual absorbance values weighted by T<sup>2</sup> (transmission squared), all absorbance values  $\geq 1.6$  are given zero weight
- Calculated and estimated errors: Type A =0.36%, Type B  $\leq 3\%$
- Frequency correction (already applied):  $V(\text{corrected})=V(\text{instrument}) * 1.00000135 + 8.5741 \times 10^{-4}$
- Axis units: X=wavenumbers (cm<sup>-1</sup>), Y=Absorbance (base-10)
- Trace carbon dioxide features were removed via spectral subtraction.
- Baseline correction via 8<sup>th</sup> order polynomial subtraction.