

All data taken at Pacific Northwest National Laboratory (PNNL)

Operators: Steven W. Sharpe, Timothy J. Johnson and Robert L. Sams : [sw.sharpe@pnl.gov](mailto:sw.sharpe@pnl.gov)

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Composite spectrum for TEXANOL\_50T

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

Equivalent concentration x path-length of composite spectrum:  $8.906 \times 10^{-6}$  grams/liter-meter

#### Sample Conditions-

- Chemical name and CAS number: Texanol, 2,2,4-Trimethyl-1,3-pentanediol monoisobutyrate, 2,2,4-Trimethyl-1,3-pentanediol isobutyrate,  $(\text{CH}_3)_2\text{CHCH}[\text{OHR}]\text{C}(\text{CH}_3)_2\text{CH}_2\text{OR}(\text{H})$  R=-COCHCH<sub>3</sub>)<sub>2</sub> : [25265-77-4]
- Physical properties: M.W. 216.3198 amu, F.P. -50° C, B.P. 244° C, Density (20 C) 0.950 g/cm<sup>3</sup>
- Supplier and stated purity: Aldrich, 99%
- Sample class: I (PNNL scale).
- Temperature of White cell (792.0 cm optical path length)  $50 \pm 2$  C
- Diluent (high purity nitrogen) flowed at 24.90 liter/min (296 K), ambient atmospheric pressure  $770 \pm 5$  Torr.
- Samples flowed at 4.000, 1.000, 2.500, 5.000, 0.700, 3.141, 1.500, 2.000, 0.600, 6.000 and 4.500 microliters/minute
- Individual samples at equivalent pressures of 0.012661, 0.003164, 0.007910, 0.015818, 0.002214, 0.009936, 0.004744, 0.006326, 0.001897, 0.018969 and 0.014223 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 600 cm<sup>-1</sup> (1.538 to 16.667 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 ( $\eta=0.90$ ,  $\xi=500$ )
- 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<sup>2</sup> (transmission squared), all absorbance values  $\geq 1.6$  are given zero weight
- Calculated and estimated errors: Type A = 0.40%, Type B  $\leq 7\%$

- Frequency correction (already applied):  $V(\text{corrected}) = V(\text{instrument}) * 0.999998 + 1.566836e-04$
- Axis units: X=wavenumbers ( $\text{cm}^{-1}$ ), Y=Absorbance (base-10)
- Baseline correction via 7<sup>th</sup> order polynomial subtraction