All data taken at Pacific Northwest National Laboratory (PNNL)
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Version 1.0, March 11, 2010.

Composite spectrum for VYNLTOL_50T
Effective burden of composite spectrum: 1 part-per-million-meter (ppm-meter) at 296 K
Equivalent concentration x path-length of composite spectrum: 4.8654 x10^{-6} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: meta- and para-Vinyltoluene; Styrene, m-methyl-; m-Methylstyrene; 1-Methyl-3-vinylbenzene; 3-Methylstyrene; 3-Vinyltoluene; 1-Methyl-4-vinylbenzene; 4-Methylstyrene C_9H_{10} [100-80-1] and [622-97-9]
- Physical properties: MW=118.1757 g/mole, mp=-86° C, bp=171° C, Density (25 C) = 0.896 g/cm^3
- Supplier and stated purity: Sigma Aldrich, 60% meta, 40% para
- Sample class: I (PNNL scale).
- Temperature of White cell (805.0 cm optical path length) 50 ± 2 C
- Diluent (high purity nitrogen) flowed at 23.3 liter/min (21.1° C), ambient atmospheric pressure 760 ± 5 Torr.
- Samples flowed at microliters/minute 1.000, 5.000, 15.000, 10.000, 25.000, 35.000, 7.500, 45.000, 12.500, 30.000, 60.000, 20.000, 40.000 and 50.000.
- Individual samples at equivalent pressures of: 0.005908, 0.029535, 0.088616, 0.059085, 0.147712, 0.206770, 0.044314, 0.265953, 0.073866, 0.177302, 0.354651, 0.118233, 0.236654 and 0.295857 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 (α=0.90, ε=500)

- Composite spectrum created from 14 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 =0.85%, Type B $\leq$ 7%
- Frequency correction (already applied): V(corrected)=V(instrument)*0.9999996+6.17682x10^{-4}
- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Trace water vapor was removed by spectral subtraction
- Baseline correction via 7^{th} order polynomial subtraction