

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for PXYLENE\_25T

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

Equivalent concentration x path-length of composite spectrum:  $4.371 \times 10^{-6}$  grams/liter-meter

#### **Sample Conditions-**

- Chemical name and CAS number: p-Xylene; 1,4-dimethylbenzene; 1,4-xylene;  $(\text{CH}_3)_2\text{C}_6\text{H}_4$  : [108-38-3]
- Physical properties: M.W. 106.167 amu, F.P. 13° C, B.P. 138° C, Density (20 C) 0.866 g/cm<sup>3</sup>
- Supplier and stated purity: Aldrich, 99+%
- Sample class: I (PNNL scale).
- Temperature of White cell (815.76 cm optical path length)  $25 \pm 2$  C
- Diluent (high purity nitrogen) flowed at 25.20 liter/min (21.1° C), ambient atmospheric pressure  $760 \pm 5$  Torr.
- Samples flowed at 2.000, 5.000, 10.000, 0.500, 12.000, 3.000, 20.000, 7.000, 30.000, 4.000, 8.000, 1.500 and 50.000 microliters/minute
- Individual samples at equivalent pressures of 0.012022, 0.030055, 0.060102, 0.003005, 0.072085, 0.018019, 0.120110, 0.042033, 0.180165, 0.024019, 0.048007, 0.009004 and 0.300080 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 580 cm<sup>-1</sup> (1.538 to 17.241 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 13 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 = 0.12%, Type B  $\leq 7\%$
- Frequency correction (already applied):  $V(\text{corrected})=V(\text{instrument}) * 0.9999987 - 4.24224 \times 10^{-4}$

- Axis units: X=wavenumbers ( $\text{cm}^{-1}$ ), Y=Absorbance (base-10)
- Trace water vapor and carbon monoxide feature removed by spectral subtraction
- Baseline correction via 6<sup>th</sup> order polynomial subtraction