

All data taken at Pacific Northwest National Laboratory (PNNL)
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Composite spectrum for PXYLENE_50T

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

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

Sample Conditions-

- Chemical name and CAS number: p-Xylene; 1,4-dimethylbenzene; 1,4-xylene; $(\text{CH}_3)_2\text{C}_6\text{H}_4$: [106-42-3]
- Physical properties: M.W. 106.167 amu, F.P. 13° C, B.P. 138° C, Density (20 C) 0.866 g/cm³
- Supplier and stated purity: Aldrich, 99+%
- Sample class: I (PNNL scale).
- Temperature of White cell (815.76 cm optical path length) 50 ± 2 C
- Diluent (high purity nitrogen) flowed at 25.20 liter/min (21.1° C), ambient atmospheric pressure 760 ± 5 Torr.
- Samples flowed at 3.000, 6.000, 0.700, 20.000, 4.000, 10.000, 5.000, 15.000, 1.500, 24.000, 50.000, 8.000 and 68.000 microliters/minute
- Individual samples at equivalent pressures of 0.017843, 0.035686, 0.004163, 0.119016, 0.023797, 0.059485, 0.029734, 0.089203, 0.008922, 0.142650, 0.297110, 0.047531 and 0.403910 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^{-1} (1.538 to 17.241 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 13 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 = 0.70%, 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 (cm^{-1}), Y=Absorbance (base-10)

- Trace water vapor feature removed by spectral subtraction
- Baseline correction via 6th order polynomial subtraction