

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 STYRENE\_25T

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

Equivalent concentration x path-length of composite spectrum:  $4.288 \times 10^{-6}$  grams/liter-meter

#### Sample Conditions-

- Chemical name and CAS number: Styrene, ethenylbenzene, phenethylene, vinyl benzene, styrol, cinnamene, annamene,  $C_6H_5CH=CH_2$  : [100-42-5]
- Physical properties: M.W. 104.1512 amu, F.P.  $-31^\circ C$ , B.P.  $145^\circ C$ , Density (20 C)  $0.906 \text{ g/cm}^3$
- Supplier and stated purity: Aldrich, 99+%, inhibited with 12 ppm of t-butylcatechol
- 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 ( $21.1^\circ C$ ), ambient atmospheric pressure  $760 \pm 5$  Torr.
- Samples flowed at 3.000, 6.000, 10.000, 15.000, 20.000, 30.000, 40.000, 50.000 and 65.000 microliters/minute
- Individual samples at equivalent pressures of 0.018833, 0.037672, 0.062786, 0.094167, 0.125573, 0.188359, 0.251046, 0.313807 and 0.406334 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  $600 \text{ cm}^{-1}$  (1.538 to 16.667 microns)
- Instrumental resolution based on maximum interferometer displacement is  $0.112 \text{ cm}^{-1}$
- Spectral interval after 2X zero-filling interferogram and FFT:  $0.06 \text{ cm}^{-1}$
- 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  $0 \text{ cm}^{-1}$

#### Post Processing and Related Parameters-

- Non-linearity detector correction (Bruker proprietary) applied to interferogram ( $\alpha=0.90$ ,  $\epsilon=500$ )
- Composite spectrum created from 9 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  $\geq 1.6$  are given zero weight
- Calculated and estimated errors: Type A = 0.90%, 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  $\text{CO}_2$  features removed via spectral subtraction
- Baseline correction via 4<sup>th</sup> order polynomial subtraction