

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for TMB5\_25T

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

Equivalent concentration x path-length of composite spectrum:  $5.5259 \times 10^{-6}$  grams/liter-meter

### Sample Conditions-

- Chemical name and CAS number: 1,2,3,5-Tetramethylbenzene, isodurene,  $C_6H_2(CH_3)_4$  : [527-53-7]
- Physical properties: MW=134.2206 g/mole, mp=-24° C, bp=198° C, Density (20 C) 0.891g/cm<sup>3</sup>
- Supplier and stated purity: TCI America, 70+% (ugh)
- Sample class: I (PNNL scale).
- Temperature of White cell (796.0 cm optical path length)  $25 \pm 2$  C
- Diluent (high purity nitrogen) flowed at 24.2 liter/min (21.1° C), ambient atmospheric pressure  $760 \pm 5$  Torr.
- Samples flowed at 50.000, 25.000, 12.500, 37.500, 19.000, 15.000, 10.000, 7.000, 5.000, 4.000 and 3.000 microliters/minute
- Individual samples at equivalent pressures of 0.249568, 0.124800, 0.062392, 0.187176, 0.094760, 0.074811, 0.049874, 0.034907, 0.024934, 0.019947 and 0.014958 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  $cm^{-1}$  (1.538 to 16.667 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 11 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 = 0.15%, Type B  $\leq 7\%$
- Frequency correction (already applied):  $V(\text{corrected})=V(\text{instrument})*0.99999959-3.45278 \times 10^{-4}$

- Axis units: X=wavenumbers ( $\text{cm}^{-1}$ ), Y=Absorbance (base-10)
- Trace water vapor features removed from composite spectrum by spectral subtraction
- Baseline correction via 7<sup>th</sup> order polynomial subtraction