

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for ET4TOL_25T

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

Equivalent concentration x path-length of composite spectrum: 4.9485×10^{-6} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: 4-Ethyltoluene, p-ethyltoluene, 1-ethyl-4-ethylbenzene, $(C_2H_5)C_6H_4(CH_3)$: [622-96-8]
- Physical properties: M.W. 120.1938 amu, F.P. -62° C, B.P. 162° C, Density (20 C) 0.861 g/cm³
- Supplier and stated purity: Aldrich, 90+%
- Sample class: I (PNNL scale).
- Temperature of White cell (815.76 cm optical path length) 25 ± 2 C
- Diluent (high purity nitrogen) flowed at 25.20 liter/min (21.1° C), ambient atmospheric pressure 760 ± 5 Torr.
- Samples flowed at 4.000, 1.000, 6.000, 3.000, 10.000, 2.000, 1.500, 15.000, 0.800, 22.000, 5.000, 2.000, 33.000 and 8.000 microliters/minute
- Individual samples at equivalent pressures of 0.020739, 0.005183, 0.031080, 0.015534, 0.051793, 0.010356, 0.007762, 0.077618, 0.004140, 0.113764, 0.025852, 0.010339, 0.170555 and 0.041347 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 14 individual absorbance (base-10) spectra via classical least squares fit: Intercept=0, slope is fitted, individual absorbance values weighted by T² (transmission squared), all absorbance values ≥ 1.6 are given zero weight
- Calculated and estimated errors: Type A = 0.60%, Type B $\leq 7\%$
- Frequency correction (already applied): $V(\text{corrected}) = V(\text{instrument}) * 0.9999965 + 2.87506e-3$

- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Baseline correction via 7th order polynomial subtraction
- Trace water vapor and CO features removed via spectral subtraction