

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for TBUTBZ_50T

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

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

Sample Conditions-

- Chemical name and CAS number: tert-Butylbenzene, (1,1-dimethylethyl)benzene, 2-methyl-2-phenylpropane, $C_6H_5C_4H_9$: [7732-18-5]
- Physical properties: MW=18.0152 g/mole, mp=-58 C, bp=169° C, Density (20 C) 0.867 g/cm³
- Supplier and stated purity: Aldrich, 99+%
- Sample class: I (PNNL scale).
- Temperature of White cell (796.0 cm optical path length) 50 ± 2 C
- Diluent (high purity nitrogen) flowed at 24.2 liter/min (21.1° C), ambient atmospheric pressure 760 ± 5 Torr.
- Samples flowed at 2.000, 5.000, 9.000, 4.000, 1.500, 13.000, 3.500, 7.000, 1.000, 22.000, 6.000, 18.000, 24.000, 44.000 and 4.500 microliters/minute
- Individual samples at equivalent pressures of 0.009727, 0.024314, 0.043747, 0.019441, 0.007288, 0.063140, 0.016995, 0.033980, 0.004854, 0.106753, 0.029107, 0.087308, 0.116396, 0.213364 and 0.021813 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 520 cm^{-1} (1.538 to 19.231 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 15 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 = 0.92%, 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 (cm^{-1}), Y=Absorbance (base-10)
- Trace water vapor features removed by spectral subtraction
- Baseline correction via 7th order polynomial subtraction