

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for BNZYLBR_50T

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

Equivalent concentration x path-length of composite spectrum: 7.0417×10^{-6} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: Benzyl bromide, \square -bromophenylmethane, \square -bromotoluene, bromomethylbenzene, $C_5H_5(CH_2Br)$: [100-39-0]
- Physical properties: M.W. 171.0363 amu, F.P. $-3^\circ C$, B.P. $197^\circ C$, Density (20 C) 1.438 g/cm^3
- Supplier and stated purity: Aldrich, 98+%
- Sample class: I (PNNL scale).
- Temperature of White cell (792.0 cm optical path length) $50 \pm 2 C$
- Diluent (high purity nitrogen) flowed at 24.90 liter/min (296 K), ambient atmospheric pressure 760 ± 5 Torr.
- Samples flowed at 5.000, 2.500, 30.000, 15.000, 20.000, 8.000, 25.000, 12.000, 40.000, 4.000, 55.000, 17.000 and 35.000 microliters/minute
- Individual samples at equivalent pressures of 0.030504, 0.015248, 0.182826, 0.091376, 0.121786, 0.048695, 0.152151, 0.073033, 0.243377, 0.024328, 0.334509, 0.103366 and 0.212983 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 ($\square=0.90$, $\square=500$)
- 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 = 1.61%, Type B $\leq 7\%$
- Frequency correction (already applied): $V(\text{corrected}) = V(\text{instrument}) * 0.999998 + 1.566836e-04$

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