

All data taken at Pacific Northwest National Laboratory (PNNL)

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Version 1.0, May, 03

Composite spectrum for BZCN_50T

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

Equivalent concentration x path-length of composite spectrum: 4.2456×10^{-6} grams/liter-meter

[Water contamination \[0.57%\] corrected for by rescaling composite spectrum.](#)

Sample Conditions-

- Chemical name and CAS number: Benzonitrile, benzenenitrile, cyanobenzene, phenyl cyanide, benzoic acid nitrile, BN, C_6H_5CN : [100-47-0]
- Physical properties: M.W. 103.1232 amu, F.P. $-13^\circ C$, B.P. $190.7^\circ C$, Density (20 C) 1.010 g/cm^3
- Supplier and stated purity: Aldrich, 99.9%
- 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 770 ± 5 Torr.
- Samples flowed at 5.000, 10.000, 15.000, 7.000, 22.000, 3.000, 12.000, 9.000, 52.000, 4.000, 32.000, 62.000 and 82.000 microliters/minute
- Individual samples at equivalent pressures of 0.035577, 0.071135, 0.106688, 0.049781, 0.156455, 0.021329, 0.085305, 0.063953, 0.369506, 0.028420, 0.227327, 0.440329 and 0.582371 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 ($\alpha=0.90$, $\beta=500$)
- 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 = 1.96%, Type B = 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 vapor features removed via spectral subtraction