

All data taken at Pacific Northwest National Laboratory (PNNL)

Operators: Steven W. Sharpe, Timothy J. Johnson and Robert L. Sams : [sw.sharpe@pnl.gov](mailto:sw.sharpe@pnl.gov)

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Composite spectrum for BZCN\_25T

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

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

[Water contamination \[0.237%\] 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)  $1.010 \text{ g/cm}^3$
- Supplier and stated purity: Aldrich, 99.9%
- Sample class: I (PNNL scale).
- Temperature of White cell (792.0 cm optical path length)  $25 \pm 2 C$
- Diluent (high purity nitrogen) flowed at 24.90 liter/min (296 K), ambient atmospheric pressure  $770 \pm 5$  Torr.
- Samples flowed at 8.000, 6.000, 10.000, 1.000, 22.000, 12.000, 32.000, 5.000, 50.000, 3.000, 15.000, 4.000 and 20.000 microliters/minute
- Individual samples at equivalent pressures of 0.056991, 0.042738, 0.071135, 0.007112, 0.156288, 0.085236, 0.227236, 0.035496, 0.354914, 0.021292, 0.106446, 0.028382 and 0.141890 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  $520 \text{ cm}^{-1}$  (1.538 to 19.231 microns)
- Instrumental resolution based on maximum interferometer displacement is  $0.112 \text{ cm}^{-1}$
- Spectral interval after 2X zero-filling interferogram and FFT:  $0.06 \text{ cm}^{-1}$
- 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  $0 \text{ cm}^{-1}$

### 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 = 1.16%, Type B = 7%
- Frequency correction (already applied):  $V(\text{corrected}) = V(\text{instrument}) * 0.999998 + 1.566836e-04$
- Axis units: X=wavenumbers ( $\text{cm}^{-1}$ ), Y=Absorbance (base-10)
- Baseline correction via 7<sup>th</sup> order polynomial subtraction
- Trace water vapor features removed via spectral subtraction