

All data taken at Pacific Northwest National Laboratory (PNNL)
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Version 1.0, March, 02

Composite spectrum for NCCN_5T

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

Equivalent concentration x path-length of composite spectrum: 2.142×10^{-6} grams/liter-meter.

Unknown trace impurity (probably an organic nitrile) observed at 2188-2242 cm^{-1} .

Sample Conditions-

- Chemical name and CAS number: Cyanogen, oxalonitrile, dicyan, dicyanogen, ethanedinitrile, N::C-C::N : [460-19-5]
- Physical properties: fw=89.09 g/mole, fp=-28° C, bp=-21° C
- Supplier and stated purity: Atomergic Corp., 98.5% (In their dreams). Badly contaminated with nitrogen and CO₂
- Sample class: II (PNNL scale). Readily hydrolyzes and polymerizes.
- Temperature of sample: 4.98 ± 0.02 C
- Diluent: Sample back filled with ultra high purity nitrogen to 760±5 Torr
- Individual samples at 11.17, 1.5333, 108.35, 6.000, 312.22, 20.69, 213.71 and 65.22 Torr. Path length = 19.94 cm. Final data is a composite spectrum.
- Preparation: Multiple freeze-thaw cycles at liquid nitrogen temperature to remove air. Subsequent multiple freeze-thaws from -78 C slush bath to remove CO₂.

Instrument Parameters-

- Bruker-66V FTIR, temperature controlled environment, evacuated optics bench
- Modified to include second aperture, between interferometer output and sample cell. This substantially reduces both “ghosting” and warm aperture effects.
- Spectral range: 6,500 to 575 cm^{-1} (1.534 to 17.391 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 (=0.85, =530)
- Composite spectrum created from 8 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 = 0.65%, Type B = 5%
- Frequency correction (already applied): $V(\text{corrected}) = V(\text{instrument}) * 0.99999896 + 8.812 \times 10^{-4}$
- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)

- Trace water vapor, carbon dioxide and hydrogen cyanide features removed via spectral subtraction. Some residuals still observed.