

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for CADAVER_25T

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

Equivalent concentration x path-length of composite spectrum: 4.2068×10^{-6} grams/liter-meter

[Corrected composite spectrum for water contamination \[6.48%\] by rescaling and subtracting.](#)

Sample Conditions-

- Chemical name and CAS number: Cadaverine, 1,5-Diaminopentane, 1,5-Pentanediamine, Pentamethylene diamine, $\text{H}_2\text{N}(\text{CH}_2)_5\text{NH}_2$: [462-94-2]
- Physical properties: M.W. 102.179 amu, F.P. 9° C, B.P. 179° C, Density (20 C) 0.873 g/cm³
- Supplier and stated purity: Aldrich, 95+%
- Sample class: I (PNNL scale).
- Temperature of White cell (792.0 cm optical path length) 25 ± 2 C
- Diluent (high purity nitrogen) flowed at 24.90 liter/min (296 K), ambient atmospheric pressure 770 ± 5 Torr.
- Samples flowed at 1.000, 5.000, 12.000, 3.000, 7.000, 2.000, 4.000, 25.000, 6.000, 1.500, 34.000 and 8.000 microliters/minute
- Individual samples at equivalent pressures of 0.005915, 0.029570, 0.070959, 0.017740, 0.041387, 0.011823, 0.023643, 0.147752, 0.035456, 0.008863, 0.200862, and 0.047255 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: 7,000 to 550 cm^{-1} (1.429 to 18.1482 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 12 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 = 0.38%, 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 carbon dioxide and ammonia features removed from composite spectrum via spectral subtraction