

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for AMYLNO3_50T

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

Equivalent concentration x path-length of composite spectrum: 5.4817×10^{-6} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: Amyl nitrate, 1-pentyl nitrate, n-amyl nitrate, aspirols, $\text{CH}_3(\text{CH}_2)_4\text{ONO}_2$: [1002-16-0]
- Physical properties: M.W. 133.1468 amu, F.P. n° C, B.P. 157° C, Density (20 C) 0.996 g/cm^3
- Supplier and stated purity: TCI America, 99+%
- Sample class: I (PNNL scale).
- Temperature of White cell (815.76 cm optical path length) 50 ± 2 C
- Diluent (high purity nitrogen) flowed at 25.20 liter/min (21.1° C), ambient atmospheric pressure 760 ± 5 Torr.
- Samples flowed at 2.000, 5.000, 10.000, 3.000, 15.000, 7.000, 0.500, 8.000, 4.000, 20.000, 2.500, 30.000, 6.000 and 45.000 microliters/minute
- Individual samples at equivalent pressures of 0.010735, 0.026842, 0.053684, 0.016103, 0.080494, 0.037569, 0.002682, 0.042884, 0.021439, 0.107182, 0.013391, 0.160514, 0.032099 and 0.240707 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 540 cm^{-1} (1.538 to 18.519 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 ($\alpha=0.90$, $\epsilon=500$)
- Composite spectrum created from 14 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 = 0.85%, Type B $\leq 7\%$
- Frequency correction (already applied): $V(\text{corrected})=V(\text{instrument}) * 0.9999987 - 4.24224 \times 10^{-4}$

- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Trace water vapor and CO_2 features removed from composite via spectral subtraction
- Baseline correction via 7th order polynomial subtraction