All data taken at Pacific Northwest National Laboratory (PNNL)
Operator: Steven W. Sharpe and Robert L. Sams, sw.sharpe@pnl.gov
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Composite spectrum for NITROPROP_25T
Effective burden of composite spectrum: 1 part-per-million-meter (ppm-meter) at 296 K
Equivalent concentration x path-length of composite spectrum: 3.668×10^{-6} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: 1-Nitropropane, $CH_3(CH_2)_2NO_2$: [108-03-2]
- Physical properties: M.W. 89.09 amu, F.P. –108 C, B.P. 131 C
- Supplier and stated purity: Aldrich, 98%
- Sample class: I (PNNL scale).
- Temperature of sample: 25.00 ± 0.02 C
- Diluent: Sample back filled with ultra high purity nitrogen to 760±5 Torr
- Individual samples at 2.7610, 5.6000, 3.2780, 4.1650, 7.3800, 1.07519, 0.75930, 6.3750, 3.5930 and 1.9157 Torr. Path length = 19.94 cm. Final data is a composite spectrum.
- Preparation: Multiple freeze-thaw cycles at 0 C to remove air.

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 600 cm^{-1} (1.534 to 16.667 microns)
- Instrumental resolution based on maximum interferometer displacement is 0.112 cm^{-1}
- Spectral intervals after 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 (α=0.85, ε=530)
- Composite spectrum created from 10 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 = 0.62%, Type B ≤ 3%
- Frequency correction (already applied): V(corrected) = V(instrument)*0.999998+2.164×10^{-5}
- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Trace water vapor features removed via spectral subtraction
- Baseline correction via 5^{th} order polynomial subtraction