

All data taken at Pacific Northwest National Laboratory (PNNL)
Operator: Steven W. Sharpe, sw.sharpe@pnl.gov
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Composite spectrum for NO_5T

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

Sample Conditions-

- Chemical name and CAS number: Nitric Oxide, Nitrogen monoxide, NO : [10102-43-9]
- Physical properties: M.W. 30 AMU, F.P. -163.6 C, B.P. -151.7 C
- Supplier and stated purity: Matheson, 99% (doubtful)
- Sample class: II (PNNL scale)
- Temperature of sample 4.97 C \pm 0.02 C
- Diluent: Sample back filled with ultra high purity nitrogen to 755 \pm 5 Torr
- Concentration: Composite spectrum
- Preparation: Multiple freeze-thaw cycles.

Instrument Parameters-

- Bruker-120HR FTIR, evacuated optics bench
- Instrumental resolution (interferogram): 0.1 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: 9 (Bruker arbitrary)
- 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
- Composite spectrum created from 4 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 \leq 1.6 are given zero weight
- Calculated and estimated errors: Type A = 0.76%, Type B = 5%
- Frequency correction: V(corrected) = V(instrument)*1+ 0
- Axis units: X=wavenumbers (cm⁻¹), Y=Absorbance (base-10)
- Trace water vapor, carbon dioxide and nitrogen dioxide observed.