

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for HONO_25T

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

Equivalent concentration x path-length of composite spectrum: 1.936×10^{-6} grams/liter-meter

Spectrum is NOT a composite fit to individual spectra and the intensity is scaled to agree with literatures value. See R. H. Kagnan and A. G. Maki, *J. Quant. Spectrosc. Radiat. Transfer* Vol. 30, No. 1, pp. 37-44 (1983). Considerable contamination: NO₂, NO, N₂O, NOCl, CO₂ and H₂O.

Sample Conditions-

- Chemical name and CAS number: Nitrous acid, HONO : [7782-77-6]
- Physical properties: M.W. 47.0134 amu, F.P. ?° C, B.P. ?° C
- Supplier and stated purity: Nitrous acid synthesized *in situ*. via HCl + NaNO₂
- Sample class: III (PNNL scale).
- Temperature of White cell (815.76 cm optical path length) 25 ± 2 C
- Diluent (high purity nitrogen, ambient atmospheric pressure 760 ± 5 Torr).
- Preparation: Synthesized *in situ*.

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 550 cm⁻¹ (1.538 to 18.182 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 ($\alpha=0.90$, $\epsilon=500$)
- Calculated and estimated errors: Type A = ?, Type B $\leq 10\%$
- 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)
- Baseline correction via 7th order polynomial subtraction