

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for H2O_50T

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

Equivalent concentration x path-length of composite spectrum: 7.417×10^{-7} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: Water, hydrogen oxide, dihydrogen oxide, aqua, H₂O : [7732-18-5]
- Physical properties: M.W. 18.0152 amu, F.P. 0 C, B.P. 100 C, Density (20 C) 0.998 g/cm³
- Supplier and stated purity: Aldrich, 99+%
- Sample class: I (PNNL scale).
- Temperature of White cell (792.0 cm optical path length) 50 ± 2 C
- Diluent (high purity nitrogen) flowed at 24.90 liter/min (296 K), ambient atmospheric pressure 770 ± 5 Torr.
- Samples flowed at 5.000, 2.500, 10.000, 1.000, 15.000, 0.500, 20.000, 0.250, 50.000 and 100.000 microliters/minute
- Individual samples at equivalent pressures of 0.206547, 0.103300, 0.413147, 0.041315, 0.619559, 0.020649, 0.825972, 0.010325, 2.065198 and 4.131469 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: 7,500 to 550 cm⁻¹ (1.333 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 ($\alpha=0.90$, $\beta=500$)
- 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 T² (transmission squared), all absorbance values > 1.6 are given zero weight
- Calculated and estimated errors: Type A = 0.74%, Type B = 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