

All data taken at Pacific Northwest National Laboratory (PNNL)
Operators: Steven W. Sharpe, Timothy J. Johnson and Robert L. Sams : sw.sharpe@pnl.gov
Version 1.0, July, 01

Composite spectrum for HI_5T

Effective burden of composite spectrum: 1 part-per-million-meter (ppm-meter) at 296 K
Equivalent concentration x path-length of composite spectrum: 5.2662×10^{-6} grams/liter-meter
Note that some of the higher J-lines for the fundamental band of HI exhibit “ringing”. This ringing is due to the fact that these lines do not pressure broaden significantly and act as a delta function, resulting in the instrumental response function (SINC²) characteristic of a Fourier transform spectrometer. In an effort to preserve the integrity of the data, we have resisted applying an apodization function that would “cut the feet off” of the SINC² response.

Sample Conditions-

- Chemical name and CAS number: Hydrogen iodide, HI : [10034-85-2]
- Physical properties: fw=127.912 g/mole, fp=-51° C, bp=-35° C
- Supplier and stated purity: Matheson Air Products, 98%(?)
- Sample class: II (PNNL scale). Considerable impurities found in sample including HCl, HBr, Benzene, carbon dioxide and Formic acid
- Temperature of sample: 5.03 ± 0.02 C
- Diluent: Sample back filled with ultra high purity nitrogen to 760 ± 5 Torr
- Individual samples at 57.87, 28.19, 15.57, 7.3920, 41.23 and 20.39 Torr. Path length = 19.94 cm. Final data is a composite spectrum.
- Preparation: Multiple freeze-thaw cycles at -100 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: 6,550 to 600 cm^{-1} (1.527 to 16.667 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 ($\tau = 0.85$, $\nu = 530$)
- Composite spectrum created from 6 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 = 7.8%, Type B = 5%

- Frequency correction (already applied): $V(\text{corrected}) = V(\text{instrument}) * 0.999997 + 5.18 \times 10^{-4}$
- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Trace water vapor, carbon dioxide, HCl, HBr, benzene and formic acid features removed via spectral subtraction
- Baseline correction via 7th order polynomial subtraction