

All data taken at Pacific Northwest National Laboratory (PNNL)
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Composite spectrum for DMHYDRZ_50T

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

Equivalent concentration x path-length of composite spectrum: 2.474×10^{-6} grams/liter-meter

Extremely difficult sample to handle and analyze due to extreme reactivity with many common materials.

Sample Conditions-

- Chemical name and CAS number: 1,1-Dimethylhydrazine, $(\text{CH}_3)_2\text{NNH}_2$: [57-14-7]
- Physical properties: M.W. 60.10 amu, F.P. -58 C, B.P. 63 C
- Supplier and stated purity: Aldrich, 98%
- Sample class: III (PNNL scale). Sample is extremely reactive and undergoes spontaneous degradation with many materials to form NH_3 and ammonium compounds.
- Temperature of sample: 50.04 ± 0.02 C
- Diluent: Sample back filled with ultra high purity nitrogen to 760 ± 5 Torr
- Individual samples at 1.1682, 5.1100, 2.0580, 7.5080, 3.5090 and 16.34 Torr. Path length = 19.96 cm. Final data is a composite spectrum.
- Preparation: Multiple freeze-thaw cycles at -35 C to remove air.
- Replaced (standard) KCl, wedged windows on sample cell with plane ZnSe windows to prevent reaction of hydrazine with salt windows.

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: 6,700 to 600 cm^{-1} (1.493 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 ($\alpha = 0.85$, $\beta = 530$)
- 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 = 2.11%, Type B = 10%
- Frequency correction (already applied): $V(\text{corrected}) = V(\text{instrument}) * 0.999998 + 1.287 \times 10^{-4}$

- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Trace water vapor features removed via spectral subtraction
- Baseline correction via 5th order polynomial subtraction
- Composite spectrum rescaled by dividing through with 1.118. This was necessary since the two plane ZnSe windows on the sample cell acted as an optical cavity, increasing the effective optical path length. Correction based on ratio of ethene spectra with standard KCl versus ZnSe windows.