

All data taken at Pacific Northwest National Laboratory (PNNL)
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Composite spectrum for MMAM_5T

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

Sample Conditions-

- Chemical name and CAS number: Monomethylamine, methylamine, aminomethane, CH_3NH_2 : [74-89-5]
- Physical properties: M.W. 31 amu, F.P. -92.5C , B.P. -6.8C
- Supplier and stated purity: Matheson., CP Grade, 99.5%
- Sample class: I (PNNL scale).
- Temperature of sample: $4.95 \pm 0.02\text{ C}$
- Diluent: Sample back filled with ultra high purity nitrogen to 760 ± 5 Torr
- Individual samples 2.2360, 30.57, 4.2420, 17.75, 7.7580 and 61.70 Torr. Path length = 19.96 cm. Final data is a composite spectrum.
- Preparation: Multiple freeze-thaw cycles at 77K to remove air. Sample used at -40C to minimize volatiles.

Instrument Parameters-

- Bruker-66V FTIR, temperature controlled environment, evacuated optics bench
- Spectral range: $6,750$ to 600 cm^{-1} (1.48 to 16.667 microns)
- Instrumental resolution (interferogram): 0.112 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 ($\alpha=0.85$, $\beta=530$)
- 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 = 0.31%, Type B = 3%
- Frequency correction: $V(\text{corrected}) = V(\text{instrument}) * 0.9999984669 + 0.005187$
- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Trace ammonia (0.5%) removed and compensated for in composite spectrum via spectral subtraction and re-scaling. Baseline corrected via quadratic function.