

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, January, 04

Composite spectrum for CH3BR_5T

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

Equivalent concentration x path-length of composite spectrum: 3.9087×10^{-6} grams/liter-meter

Contaminated and corrected for dimethyl ether [0.10%].

Sample Conditions-

- Chemical name and CAS number: Methyl bromide, bromomethane, MB, MBX, MeBr, Metafume, brom-o-gaz, celfume, terabol, zytox, CH₃Br : [74-83-9]
- Physical properties: fw=94.9387 g/mole, fp=-94° C, bp=4° C
- Supplier and stated purity: Aldrich, 99.5+%
- Sample class: I (PNNL scale).
- Temperature of sample: 5.03 ± 0.02 C
- Diluent: Sample back filled with ultra high purity nitrogen to 760 ± 5 Torr
- Individual samples at 1.05155, 16.03, 8.3397, 2.1008, 4.4880, 32.90 and 65.88 Torr. Path length = 19.96 cm. Final data is a composite spectrum.
- Preparation: Multiple freeze-thaw cycles at 77 K 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: 6,500 to 550 cm⁻¹ (1.534 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 ($\alpha=0.85$, $\epsilon=530$)
- 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 = 0.64%, Type B $\leq 3\%$
- Frequency correction (already applied): $V(\text{corrected}) = V(\text{instrument}) * 0.99999896 + 8.812 \times 10^{-4}$
- Axis units: X=wavenumbers (cm⁻¹), Y=Absorbance (base-10)
- Baseline correction via 7th order polynomial subtraction