

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for CH₂BR₂_25T

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

Equivalent concentration x path-length of composite spectrum: 3.668x10⁻⁶ grams/liter-meter

Observed 1.6% CH₂BrCl. Might be due to residual material adsorbed onto manifold from prior sample. Composite spectrum corrected for contamination by rescaling (x 1.016).

Sample Conditions-

- Chemical name and CAS number: Dibromomethane, methylene bromide, methylene dibromide, CH₂Br₂ : [74-95-3]
- Physical properties: fw=173.8348 g/mole, fp=-53° C, bp=97° C
- Supplier and stated purity: Aldrich, 99+%
- Sample class: I (PNNL scale).
- Temperature of sample: 25.00 ± 0.02 C
- Diluent: Sample back filled with ultra high purity nitrogen to 760±5 Torr
- Individual samples at 2.0300, 8.0666, 2.0910, 1.1340, 0.64190, 12.13, 4.0733, 25.25, 6.0707, 21.05, 10.0790 and 16.31 Torr. Path length = 19.94 cm. Final data is a composite spectrum.
- Preparation: Sample placed over CaSO₄ to remove dissolved CO₂. Multiple freeze-thaw cycles at -60 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: 7,100 to 540 cm⁻¹ (1.408 to 18.519 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 (=0.85, =530)
- Composite spectrum created from 12 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 = 1.08%, Type B = 3%
- Frequency correction (already applied): V(corrected) = V(instrument)* 0.99999896+8.812x10⁻⁴
- Axis units: X=wavenumbers (cm⁻¹), Y=Absorbance (base-10)

- Trace carbon dioxide features removed via spectral subtraction. Contaminant CH₂BrCl features removed via spectral subtraction.
- Baseline correction via 7th order polynomial subtraction