

All data taken at Pacific Northwest National Laboratory (PNNL)
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Composite spectrum for BENZENE_5T

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

Equivalent concentration x path-length of composite spectrum: 3.216×10^{-6} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: Benzene, C₆H₆ : [71-43-2]
- Physical properties: M.W. 78.11 amu, F.P. -5.5 C, B.P. 80.1 C
- Supplier and stated purity: Aldrich, 99.99%
- 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 0.16947, 2.1605, 0.29825, 4.1685, 0.11213, 10.0360, 1.00796, 22.43 and 0.69987 Torr. Path length = 19.94 cm. Final data is a composite spectrum.
- Preparation: Multiple freeze-thaw cycles at 77K 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 600 cm⁻¹ (1.534 to 16.667 microns)
- Instrumental resolution based on maximum interferometer displacement is 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: 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 9 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 = 0.40%, Type B = 3%
- Frequency correction (already applied): $V(\text{corrected}) = V(\text{instrument}) * 0.999998 + 2.164 \times 10^{-5}$
- Axis units: X=wavenumbers (cm⁻¹), Y=Absorbance (base-10)
- Baseline correction via 7th order polynomial