

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for BENZOH_50T

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

Equivalent concentration x path-length of composite spectrum: 4.4522×10^{-6} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: Benzyl alcohol, alpha-hydroxytoluene, alpha-toluenol, benzenecarbinol, benzenemethanol, phenylcarbinol, phenylmethanol, $C_6H_5CH_2OH$: [100-51-6]
- Physical properties: M.W. 108.1396 amu, F.P. $-15.3^\circ C$, B.P. $205^\circ C$, Density (20 C) 1.045 g/cm^3
- Supplier and stated purity: Aldrich, 99.8+%
- Sample class: I (PNNL scale).
- Temperature of White cell (815.76 cm optical path length) $50 \pm 2 C$
- Diluent (high purity nitrogen) flowed at 25.20 liter/min ($21.1^\circ C$), ambient atmospheric pressure 760 ± 5 Torr.
- Samples flowed at 4.000, 2.000, 1.000, 10.000, 5.000, 2.500, 15.000, 8.000, 1.500, 12.000, 3.000, 22.000, 6.000 and 18.000 microliters/minute
- Individual samples at equivalent pressures of 0.027966, 0.013981, 0.006990, 0.069878, 0.034939, 0.017472, 0.104817, 0.055895, 0.010479, 0.083831, 0.020955, 0.153670, 0.041905 and 0.125714 Torr. Final data is a composite spectrum.
- Preparation: None

Instrument Parameters-

- Bruker-66V FTIR, evacuated optics bench.
- Modified to include second aperture, between interferometer output and White cell. This substantially reduces both "ghosting" and warm aperture effects.
- Spectral range: 6,500 to 600 cm^{-1} (1.538 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 ($\alpha=0.90$, $\epsilon=500$)
- Composite spectrum created from 14 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 = 0.33%, Type B $\leq 7\%$

- Frequency correction (already applied): $V(\text{corrected})=V(\text{instrument})*0.9999987-4.24224\times 10^{-4}$
- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Trace water vapor features removed via spectral subtraction
- Baseline correction via 8th order polynomial subtraction