

All data taken at Pacific Northwest National Laboratory (PNNL)

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Trace water contamination removed from composite spectrum via spectral subtraction and corrected by rescaling composite (0.28%).

Composite spectrum for NBUTOH_25T

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

Equivalent concentration x path-length of composite spectrum: 3.0517×10^{-6} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: n-Butanol, 1-butanol, butyl alcohol, propylcarbinol, butan-1-ol, $\text{CH}_3(\text{CH}_2)_3\text{OH}$: [7732-18-5]
- Physical properties: M.W. 74.1224 amu, F.P. -89.5°C , B.P. 118°C , Density (20 C) 0.81 g/cm^3
- Supplier and stated purity: Aldrich, 99.8+%
- Sample class: I (PNNL scale).
- Temperature of White cell (792.0 cm optical path length) $25 \pm 2 \text{ C}$
- Diluent (high purity nitrogen) flowed at 24.90 liter/min (296 K), ambient atmospheric pressure $770 \pm 5 \text{ Torr}$.
- Samples flowed at 1.000, 2.000, 8.000, 1.200, 4.000, 3.000, 0.800, 10.000, 5.000, 15.000, 5.000, 30.000, 10.000, 60.000, 7.500, 40.000, 15.000, 25.000 and 50.000 microliters/minute
- Individual samples at equivalent pressures of 0.008014, 0.016022, 0.064062, 0.009608, 0.031989, 0.023979, 0.006394, 0.079898, 0.039949, 0.119815, 0.039843, 0.238995, 0.079623, 0.477546, 0.059685, 0.318111, 0.119307, 0.198846 and 0.397691 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: $7,300$ to 600 cm^{-1} (1.370 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 (=0.90 , =500)

- Composite spectrum created from 19 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 = 0.28%, Type B = 7%
- Frequency correction (already applied): $V(\text{corrected}) = V(\text{instrument}) * 0.999998 + 1.566836e-04$
- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Baseline correction via 7th order polynomial subtraction