

All data taken at Pacific Northwest National Laboratory (PNNL)

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Trace water vapor in sample (0.24%) subtracted and corrected for by rescaling composite spectrum.

Composite spectrum for BTXETOH_50T

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

Equivalent concentration x path-length of composite spectrum: 4.8654×10^{-6} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: 2-butoxy-1-ethanol, 2-Butoxy ethanol, o-butyl ethylene glycol, 2-n-Butoxy-1-ethanol, 2-n-Butoxyethanol, 3-oxa-1-heptanol, Beta-butoxyethanol, BUCS, butoxyethanol, Butyl cellosolve, butyl glycol, Butyl oxitol, Dowanol EB, Ektasolve EB, Ektasolve EB solvent, Ethylene glycol butyl ether, Ethylene glycol mono butyl ether, Ethylene glycol monobutyl ether (EGBE) (2-Butoxyet , Ethylene Glycol Mono-n-butyl Ether, Ethylene glycol n-butyl ether, gafcol eb, glycol butyl ether, glycol ether eb, glycol ether eb acetate, Jeffersol EB, monobutyl ether of ethylene glycol, monobutyl glycol ether, n-butoxyethanol, n-Butyl Cellosolve, poly-solv eb, $\text{CH}_3(\text{CH}_2)_3\text{OCH}_2\text{CH}_2\text{OH}$: [111-76-2]
- Physical properties: M.W. 118.1754 amu, F.P. -75°C , B.P. 171°C , Density (20 C) 0.903 g/cm^3
- Supplier and stated purity: Aldrich, 99+%
- Sample class: I (PNNL scale).
- Temperature of White cell (792.0 cm optical path length) $50 \pm 2 \text{ C}$
- Diluent (high purity nitrogen) flowed at 24.90 liter/min (296 K), ambient atmospheric pressure $750 \pm 5 \text{ Torr}$.
- Samples flowed at 4.000, 2.000, 10.000, 8.000, 20.000, 5.000, 15.000, 40.000, 6.000, 12.000, 1.000 and 70.000 microliters/minute
- Individual samples at equivalent pressures of 0.022288, 0.011143, 0.055698, 0.044558, 0.111381, 0.027842, 0.083514, 0.222644, 0.033392, 0.066784, 0.005565 and 0.389471 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 ($\tau = 0.90$, $\tau = 500$)
- 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 T^2 (transmission squared), all absorbance values > 1.6 are given zero weight
- Calculated and estimated errors: Type A = 0.29%, 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