

All data taken at Pacific Northwest National Laboratory (PNNL)

Operators: Steven W. Sharpe, Timothy J. Johnson and Robert L. Sams : sw.sharpe@pnl.gov

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Trace water vapor in sample (0.89%) subtracted and corrected for by rescaling composite spectrum.

Composite spectrum for EEACET_50T

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

Equivalent concentration x path-length of composite spectrum: 5.4411×10^{-6} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: 2-Ethoxyethyl acetate, 2EEA, 2-Ethoxyethanol acetate, 2-ethoxyethanol, ester with acetic acid, beta-ethoxyethyl acetate, Cellosolve acetate, CSAC, ektasolve ee acetate solvent, Ethoxyethanol acetate, Ethoxyethyl acetate, Ethyl acetyl glycolate, Ethyl Cellosolve Acetate, ethylene glycol ethyl ether acetate, Ethylene glycol monethyl ether acetate, Ethylene glycol monoethylether acetate, Ethylglycol acetate, glycol ether ee acetate, Glycol, monoethyl ether acetate, oxytol acetate, poly-solv ee acetate, $\text{CH}_3\text{CO}_2\text{CH}_2\text{CH}_2\text{OC}_2\text{H}_5$: [111-15-9]
- Physical properties: M.W. 132.159 amu, F.P. -61.7°C , B.P. 156°C , Density (20 C) 0.975 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 $755 \pm 5\text{ Torr}$.
- Samples flowed at 4.000, 2.000, 10.000, 3.000, 20.000, 5.000, 12.500, 1.500, 6.000, 15.000, 30.000, 7.000 and 50.000 microliters/minute
- Individual samples at equivalent pressures of 0.021633, 0.010815, 0.054019, 0.016201, 0.107981, 0.026988, 0.067452, 0.008092, 0.032351, 0.080857, 0.161327, 0.037628 and 0.268700 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: $7,100$ 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 ($\alpha=0.90$, $\beta=500$)
- Composite spectrum created from 11 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 = 0.31%, Type B $\leq 7\%$
- 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