

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for ETOHOH\_25T

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

Equivalent concentration x path-length of composite spectrum:  $2.5554 \times 10^{-6}$  grams/liter-meter

### Sample Conditions-

- Chemical name and CAS number: Ethylene glycol, 1,2-dihydroxyethane, 1,2-ethanediol, dowtherm-4000, dowtherm-SR-1, fridex, lutrol-9, M.E.G., tescol, ucar-17,  $\text{HOCH}_2\text{CH}_2\text{CH}_2\text{OH}$  : [107-21-1]
- Physical properties: M.W. 62.0682 amu, F.P.  $-13^\circ\text{C}$ , B.P.  $195^\circ\text{C}$ , Density (20 C)  $0.11155\text{ g/cm}^3$
- Supplier and stated purity: Aldrich, 99.8%
- Sample class: I (PNNL scale).
- Temperature of White cell (792.0 cm optical path length)  $50 \pm 2\text{ C}$
- Diluent (high purity nitrogen) flowed at 24.90 liter/min (296 K), ambient atmospheric pressure  $770 \pm 5\text{ Torr}$ .
- Samples flowed at 5.000, 2.500, 7.000, 10.000, 1.000, 12.500, 3.000, 15.000, 9.000, 6.000, 4.000, 2.000, 1.500 and 11.000 microliters/minute
- Individual samples at equivalent pressures of 0.065902, 0.032951, 0.092263, 0.131804, 0.013173, 0.164602, 0.039499, 0.197497, 0.118420, 0.078821, 0.052526, 0.026260, 0.019671, and 0.144198 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:  $7,500\text{ to }550\text{ cm}^{-1}$  (1.333 to 18.182 microns)
- Instrumental resolution based on maximum interferometer displacement is  $0.112\text{ cm}^{-1}$
- Spectral interval after 2X zero-filling interferogram and FFT:  $0.06\text{ cm}^{-1}$
- 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:  $15798\text{ to }0\text{ cm}^{-1}$

### Post Processing and Related Parameters-

- Non-linearity detector correction (Bruker proprietary) applied to interferogram ( $\alpha=0.90$ ,  $\beta=500$ )
- Composite spectrum created from 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  $\geq 1.6$  are given zero weight

- Calculated and estimated errors: Type A = 1.48%, Type B  $\leq$  7%
- Frequency correction (already applied):  $V(\text{corrected}) = V(\text{instrument}) * 0.999998 + 1.566836e-04$
- Axis units: X=wavenumbers ( $\text{cm}^{-1}$ ), Y=Absorbance (base-10)
- Baseline correction via 6<sup>th</sup> order polynomial subtraction