

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for PROHOH\_25T

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

Equivalent concentration x path-length of composite spectrum:  $3.1329 \times 10^{-6}$  grams/liter-meter

### Sample Conditions-

- Chemical name and CAS number: propylene glycol, 1,2-propanediol, 1,2-dihydroxypropane, methylethylene glycol, PG-12, propane-1,2-diol, sirlene, trimethyl glycol,  $\text{CH}_3\text{CH}(\text{OH})\text{CH}_2\text{OH}$  : [57-55-6]
- Physical properties: M.W. 76.095 amu, F.P.  $-59^\circ\text{C}$ , B.P.  $187^\circ\text{C}$ , Density (20 C)  $1.036\text{ g/cm}^3$
- Supplier and stated purity: Aldrich, 99+%
- Sample class: I (PNNL scale).
- Temperature of White cell (815.76 cm optical path length)  $25 \pm 2\text{ C}$
- Diluent (high purity nitrogen) flowed at 25.20 liter/min ( $21.1^\circ\text{C}$ ), ambient atmospheric pressure  $760 \pm 5\text{ Torr}$ .
- Samples flowed at 1.000, 2.000, 4.000, 3.000, 1.500, 0.800, 5.000, 3.200, 1.800, 2.400, 4.200, 3.500, 6.000 and 4.500 microliters/minute
- Individual samples at equivalent pressures of 0.009831, 0.019666, 0.039291, 0.029492, 0.014746, 0.007863, 0.049133, 0.031441, 0.017681, 0.023568, 0.041250, 0.034370, 0.058905 and 0.044185 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:  $7,400$  to  $590\text{ cm}^{-1}$  (1.351 to 16.949 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:  $15798$  to  $0\text{ cm}^{-1}$

### 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  $\geq 1.6$  are given zero weight
- Calculated and estimated errors: Type A = 0.47%, Type B  $\leq 7\%$

- Frequency correction (already applied):  $V(\text{corrected})=V(\text{instrument})\cdot 0.9999987-4.24224\times 10^{-4}$
- Axis units: X=wavenumbers ( $\text{cm}^{-1}$ ), Y=Absorbance (base-10)
- Baseline correction via 7<sup>th</sup> order polynomial subtraction
- Trace water vapor features removed via spectral subtraction