

All data taken at Pacific Northwest National Laboratory (PNNL)

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

Version 1.0, December, 04

Composite spectrum for PROHOH_50T

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

Equivalent concentration x path-length of composite spectrum: 3.1329×10^{-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°C , B.P. 187°C , Density (20 C) 1.036 g/cm^3
- Supplier and stated purity: Aldrich, 99+%
- Sample class: I (PNNL scale).
- Temperature of White cell (815.76 cm optical path length) $50 \pm 2\text{ C}$
- Diluent (high purity nitrogen) flowed at 25.20 liter/min (21.1°C), ambient atmospheric pressure $760 \pm 5\text{ Torr}$.
- Samples flowed at 2.000, 1.000, 4.000, 1.500, 10.000, 2.500, 5.000, 12.000, 3.000, 8.000, 6.000, 18.000, 15.000, 7.000, 30.000 and 9.000 microliters/minute
- Individual samples at equivalent pressures of 0.019779, 0.009883, 0.039479, 0.014801, 0.098606, 0.024629, 0.049225, 0.118108, 0.029507, 0.078603, 0.058929, 0.176645, 0.147165, 0.068668, 0.294173 and 0.088252 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 cm^{-1} (1.351 to 16.949 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 ($\alpha=0.90$, $\epsilon=500$)
- Composite spectrum created from 16 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 = 3.55%, 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 (cm^{-1}), Y=Absorbance (base-10)
- Baseline correction via 7th order polynomial subtraction
- Trace water vapor features removed via spectral subtraction