

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for DPGME\_25T

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

Equivalent concentration x path-length of composite spectrum:  $6.1015 \times 10^{-6}$  grams/liter-meter

This compound is a mixture of the following isomers 2-(2-Hydroxypropoxy)-1-propanol, 1,1'-Oxydi-2-propanol and 2,2'-Oxydi-1-propanol.

### Sample Conditions-

- Chemical name and CAS number: Dipropylene glycol methyl ether, bis-(2-methoxypropyl) ether, Dowanol-50b,  $C_7H_{16}O_3$  : [34590-94-8]
- Physical properties: MW=148.2016 g/mole, mp=-83° C, bp=190 C, Density (20 C) 0.951 g/cm<sup>3</sup>
- Supplier and stated purity: Aldrich, 99+%
- Sample class: I (PNNL scale).
- Temperature of White cell (815.76 cm optical path length)  $25 \pm 2$  C
- Diluent (high purity nitrogen) flowed at 25.20 liter/min (21.1° C), ambient atmospheric pressure  $760 \pm 5$  Torr.
- Samples flowed at 2.000, 0.600, 5.000, 3.000, 1.000, 10.000, 6.000, 12.000, 22.000, 16.000, 8.000, 27.000 and 4.000 microliters/minute
- Individual samples at equivalent pressures of 0.009209, 0.002762, 0.023010, 0.013804, 0.004601, 0.046021, 0.027609, 0.055210, 0.101219, 0.073613, 0.036802, 0.124206 and 0.018398 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: 7,250 to 530  $cm^{-1}$  (1.379 to 18.686 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 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  $\geq 1.6$  are given zero weight

- Calculated and estimated errors: Type A = 0.33%, 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)
- Trace water vapor and carbon dioxide features removed by spectral subtraction.
- Baseline correction via 7<sup>th</sup> order polynomial subtraction