

All data taken at Pacific Northwest National Laboratory (PNNL)

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Sample contaminated with 8.9% methanol and 0.38% water. Contaminant features removed from composite spectrum via spectral subtraction followed by rescaling of composite spectrum to reflect partial pressure of contaminants.

Composite spectrum for CYHEXOH\_50T

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

Equivalent concentration x path-length of composite spectrum:  $4.124 \times 10^{-6}$  grams/liter-meter

### Sample Conditions-

- Chemical name and CAS number: Cyclohexanol, hexalin, hydralin, hydroxycyclohexane, hexahydrophenol, 1-cyclohexanol, cyclohexyl alcohol, adronal, ANOL, hydrophenol, naxol,  $C_6H_{11}OH$  : [108-93-0]
- Physical properties: M.W. 100.1602 amu, F.P. 23° C, B.P. 161° C, Density (20 C) 0.962 g/cm<sup>3</sup>
- Supplier and stated purity: Aldrich, 99%
- Sample class: I (PNNL scale).
- Temperature of White cell (792.0 cm optical path length)  $50 \pm 2$  C
- Diluent (high purity nitrogen) flowed at 24.90 liter/min (296 K), ambient atmospheric pressure  $770 \pm 5$  Torr.
- Samples flowed at 1.000, 2.000, 6.000, 0.600, 5.000, 0.800, 9.000, 3.000, 4.000, 1.500, 14.00, 5.000, 20.00, 7.000, 30.00, 10.00, 60.00, 25.00, 40.00 and 15.00 microliters/minute
- Individual samples at equivalent pressures of 0.021240, 0.028320, 0.010619, 0.099095, 0.035247, 0.140969, 0.049333, 0.211314, 0.070410, 0.422461, 0.176025, 0.281603 and 0.105587 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: 7,200 to 600  $cm^{-1}$  (1.389 to 16.667 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 20 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 = 0.67%, Type B = 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 7<sup>th</sup> order polynomial subtraction