

All data taken at Pacific Northwest National Laboratory (PNNL)  
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Composite spectrum for DMOPHENOL\_50T

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

Equivalent concentration x path-length of composite spectrum:  $6.3470 \times 10^{-6}$  grams/liter-meter

### Sample Conditions-

- Chemical name and CAS number: 2,6-Dimethoxyphenol; Pyrogallol 1,3-dimethyl ether; Syringol; 1,3-Dimethoxy-2-hydroxybenzene; 2-Hydroxy-1,3-dimethoxybenzene; 2,6-Dimethoxyphenol; 2,6-Dimethoxyphenyl; 1,3-Dimethyl pyrogallate; 2,6-Dwumetoksyfenol; Pyrogallol dimethylether; Dimethoxyphenol  $C_8H_{10}O_3$  : [91-10-1]
- Physical properties: MW=154.1632 g/mole, mp=56.5 °C, bp=261 °C, Density (25 C) = 1.074 g/cm<sup>3</sup>
- Supplier and stated purity: Sigma Aldrich, 99%
- Sample class: I (PNNL scale).
- Temperature of White cell (805.0 cm optical path length)  $50 \pm 2$  °C
- Diluent (high purity nitrogen) flowed at 22.77 liter/min (21.1 °C), ambient atmospheric pressure  $760 \pm 5$  Torr.
- Samples flowed at microliters/minute 20.000, 10.000, 15.000, 25.000, 18.000, 7.000, 30.000, 12.000, 22.000, 17.000, 40.000 and 34.000 in carbon tetrachloride and 14.000, 22.000, 10.000, 26.000, 18.000, 20.000, 15.000, 17.000 24.000, 16.000, 9.000, 12.000 and 30.000 in carbon disulfide.
- Individual samples at equivalent pressures of: 0.166432, 0.083172, 0.124709, 0.207765, 0.149492, 0.058113, 0.248890, 0.099516, 0.182374, 0.140888, 0.331018 and 0.281216 in carbon tetrachloride and 0.185971, 0.292086, 0.132749, 0.344963, 0.238725, 0.265180, 0.198832, 0.225253, 0.317962, 0.211862, 0.119061, 0.158537 and 0.396183 in carbon disulfide. Final data is a composite spectrum.
- Preparation: The menthol solid was dissolved in carbon tetrachloride at 4.716 mole percent and in carbon disulfide at 2.607 mole percent. Two sets of spectra were taken and carbon disulfide spectrum was not needed for the final composite spectrum.

### 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: 6,500 to 580  $cm^{-1}$  (1.538 to 17.24 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  $\text{cm}^{-1}$

**Post Processing and Related Parameters-**

- Non-linearity detector correction (Bruker proprietary) applied to interferogram ( $\alpha=0.90$ ,  $\epsilon=500$ )
- Composite spectrum created from 12 (dissolved in carbon tetrachloride) and 13 (dissolved in carbon disulfide) 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 =0.38 %, Type B  $\leq 7\%$
- Frequency correction (already applied):  $V(\text{corrected})=V(\text{instrument})\cdot 1.00000160+3.5903\times 10^{-4}$
- Axis units: X=wavenumbers ( $\text{cm}^{-1}$ ), Y=Absorbance (base-10)
- Carbon tetrachloride and carbon disulfide features were removed by spectral subtraction and the composite spectrum was corrected by rescaling.
- Baseline correction via 7<sup>th</sup> order polynomial subtraction