

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

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

Equivalent concentration x path-length of composite spectrum:  $5.1108 \times 10^{-6}$  grams/liter-meter

#### Sample Conditions-

- Chemical name and CAS number: 3-Methoxyphenol; Phenol, 3-methoxy-; m-Guaiacol; Phenol, m-methoxy-; m-Hydroxyanisole; m-Methoxyphenol; Resorcinol methyl ether; Resorcinol monomethyl ether; 1-Hydroxy-3-methoxybenzene; 3-Hydroxyanisole  $C_7H_8O_2$ : [150-19-6]
- Physical properties: MW=124.1372 g/mole, mp=-18 °C, bp=244 °C, Density (25 C) = 1.131 g/cm<sup>3</sup>
- Supplier and stated purity: Sigma Aldrich; 96%
- 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 2.000, 1.000, 0.500, 1.300, 0.800, 1.500, 0.600, 0.900, 0.400, 0.700, 0.700 and 1.800
- Individual samples at equivalent pressures of: 0.014536, 0.007267, 0.003633, 0.009445, 0.005811, 0.010895, 0.004360, 0.006540, 0.002906, 0.005086, 0.005088 and 0.013084 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: 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  $cm^{-1}$

#### 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 =3.98%, Type B  $\leq 7\%$
- Frequency correction (already applied):  $V(\text{corrected})=V(\text{instrument}) * 1.00000160 + 3.5903 \times 10^{-4}$
- Axis units: X=wavenumbers ( $\text{cm}^{-1}$ ), Y=Absorbance (base-10)
- 4.0 % water was removed by spectral subtraction and the composite spectrum was rescaled by multiplying by 1.04166
- Baseline correction via 7<sup>th</sup> order polynomial subtraction