

All data taken at Pacific Northwest National Laboratory (PNNL)
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Composite spectrum for MOPHENOL_60T

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

Equivalent concentration x path-length of composite spectrum: 5.1108×10^{-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/cm³
- Supplier and stated purity: Sigma Aldrich; 96%
- Sample class: I (PNNL scale).
- Temperature of White cell (805.0 cm optical path length) 60 ± 2 °C
- Diluent (high purity nitrogen) flowed at 22.77 liter/min (21.1° C), ambient atmospheric pressure 760 ± 5 Torr.
- Samples flowed at microliters/minute 2.000, 1.000, 3.000, 0.500, 1.200, 0.800, 0.600 and 0.700.
- Individual samples at equivalent pressures of: 0.014585, 0.007289, 0.021851, 0.003640, 0.008731, 0.005815, 0.004360 and 0.005083 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 8 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 =2.60%, 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 (cm^{-1}), Y=Absorbance (base-10)
- 4.46 % water was removed by spectral subtraction and the composite spectrum was rescaled by multiplying by 1.0467
- Baseline correction via 7th order polynomial subtraction