

All data taken at Pacific Northwest National Laboratory (PNNL)
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Composite spectrum for GUAIACOL_50T

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

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

Sample Conditions-

- Chemical name and CAS number: Guaiacol; Phenol, o-methoxy-; o-Guaiacol; o-Hydroxyanisole; o-Methoxyphenol; Anastil; Guaiastil; Guaicolina; Guajol; Guasol; O-Methyl catechol; Pyrocatechol monomethyl ether; Pyroguaiac acid; 1-Hydroxy-2-methoxybenzene; 2-Hydroxyanisole; 2-Methoxyphenol; Guaicol; Guajakol; Methylcatechol; Methylcatachol; 2-methoxyphenol (guaiacol); 2-Methoxy phenol (guiacol); o-Guaiacol; guiacol; ortho-Guaiacol; Catechol monomethyl ether; guaiacol (2-methoxyphenol) $C_7H_8O_2$: [90-05-1]
- Physical properties: MW=124.1372 g/mole, mp=28° C, bp=205° C, Density (25 C) = 1.112 g/cm³
- Supplier and stated purity: Sigma Aldrich, 100%
- Sample class: I (PNNL scale).
- Temperature of White cell (805.0 cm optical path length) 50 ± 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 3.000, 2.750, 7.500, 4.300, 8.800, 6.000, 10.700, 12.200, 16.400, 13.100, 18.000, 15.000 and 22.900
- Individual samples at equivalent pressures of: 0.021318, 0.019513, 0.053218, 0.030507, 0.062434, 0.042557, 0.075883, 0.086521, 0.116214, 0.092817, 0.127517, 0.106264 and 0.162187 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 520 cm^{-1} (1.379 to 19.23 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 13 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 =0.61%, 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 (cm^{-1}), Y=Absorbance (base-10)
- Trace water vapor was removed by spectral subtraction
- Baseline correction via 7th order polynomial subtraction