

All data taken at Pacific Northwest National Laboratory (PNNL)
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Composite spectrum for GUAIACOL_25T

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; Anasil; Guaiastil; Guaiacolina; 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) 25 ± 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 3.650, 1.400, 4.000, 9.200, 6.300, 8.000, 14.800, 11.100, and 16.000
- Individual samples at equivalent pressures of: 0.026521, 0.010175, 0.029071, 0.066837, 0.045763, 0.058096, 0.107450, 0.080566 and 0.116023 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 9 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 =0.89%, 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)
- Trace water vapor was removed by spectral subtraction
- Baseline correction via 7th order polynomial subtraction