

All data taken at Pacific Northwest National Laboratory (PNNL)
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Composite spectrum for PHENOL_25T

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

Equivalent concentration x path-length of composite spectrum: 3.8746×10^{-6} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: Phenol; Carboic acid; Baker's P and S Liquid and Ointment; Benzenol; Hydroxybenzene; Izal; Monohydroxybenzene; Monophenol; Oxybenzene; Phenic acid; Phenyl alcohol; Phenyl hydrate; Phenyl hydroxide; Phenylic acid; Phenylic alcohol; PhOH; Benzene, hydroxy-; Benzophenol; Acide carbolique; Baker's P & S liquid & Ointment; Fenol; Fenolo; Paoscle; Phenole; Carbolsaure; Phenol alcohol; Phenol, molten; component of Anbesol; component of Campho-phenique cold sore gel; component of Campho-phenique gel; component of Campho-phenique liquid; Phenic alcohol C_6H_6O : [108-95-2]
- Physical properties: MW=94.1112 g/mole, mp=41° C, bp=182° C, Density (25 C) = 1.071 g/cm³
- Supplier and stated purity: Sigma Aldrich, 99%
- Sample class: I (PNNL scale).
- Temperature of White cell (805.0 cm optical path length) 25 ± 2 C
- Diluent (high purity nitrogen) flowed at 23.3 liter/min (21.1° C), ambient atmospheric pressure 760 ± 5 Torr.
- Samples flowed at microliters/minute 5.000, 10.000, 4.000, 2.000, 15.000, 22.000, 3.000, 17.000, 44.000, 13.000, 8.000, 20.000, 49.000, 31.000, 16.000 and 39.000 in carbon tetrachloride and 2.000, 4.000, 10.000, 1.000, 12.000, 7.000, 5.000, 15.000, 6.000, 22.000, 11.000, 33.000, 44.000, 27.000, 17.000 and 47.000 in carbon disulfide.
- Individual samples at equivalent pressures of: 0.040115, 0.080208, 0.032075, 0.016033, 0.120183, 0.176292, 0.024017, 0.136061, 0.352206, 0.104019, 0.064020, 0.160051, 0.392124, 0.247978, 0.127989 and 0.312224 Torr in carbon tetrachloride and 0.026332, 0.052643, 0.131573, 0.013154, 0.157763, 0.092004, 0.065717, 0.197100, 0.078820, 0.289005, 0.144502, 0.433450, 0.577858, 0.354548, 0.223205 and 0.617095 in carbon disulfide. Final data is a composite spectrum.
- Preparation: The phenol solid was dissolved in carbon tetrachloride at 10.059 mole percent and in carbon disulfide at 6.971 mole percent. Two sets of spectra were taken and combined in 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: $7,300$ to 550 cm⁻¹ (1.370 to 18.18 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 16 (dissolved in carbon tetrachloride) and 16 (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 ≥ 1.6 are given zero weight
- Calculated and estimated errors: Type A =2.13%, Type B $\leq 7\%$
- Frequency correction (already applied): $V(\text{corrected})=V(\text{instrument})\cdot 0.9999996+6.17682\times 10^{-4}$
- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Carbon tetrachloride and carbon disulfide and trace water features was removed by spectral subtraction and the composite spectrum was corrected by rescaling.
- Baseline correction via 7th order polynomial subtraction