

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for QUINOLINE_25T

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

Equivalent concentration x path-length of composite spectrum: 5.3176×10^{-6} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: Quinoline, 1-azanaphthalene, 1-benzazine, 1-benzine, B-500, benzopyridine, chinoleine, leucol, C_9H_7N : [91-22-5]
- Physical properties: M.W. 129.161 amu, F.P. $-16^\circ C$, B.P. $238^\circ C$, Density (20 C) 1.093 g/cm^3
- Supplier and stated purity: Aldrich, 98%
- Sample class: I (PNNL scale).
- Temperature of White cell (815.76 cm optical path length) $25 \pm 2 C$
- Diluent (high purity nitrogen) flowed at 25.20 liter/min ($21.1^\circ C$), ambient atmospheric pressure 760 ± 5 Torr.
- Samples flowed at 2.000, 1.000, 0.700, 4.000, 6.000, 3.000, 2.500, 1.500, 5.000 and 3.500 microliters/minute
- Individual samples at equivalent pressures of 0.012185, 0.006095, 0.004266, 0.024328, 0.036492, 0.018248, 0.015207, 0.009110, 0.030398 and 0.021270 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 570 cm^{-1} (1.538 to 17.544 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 10 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 = 2.34%, Type B $\leq 7\%$
- Frequency correction (already applied): $V(\text{corrected}) = V(\text{instrument}) * 0.9999965 + 2.87506e-3$

- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Trace water vapor features removed via spectral subtraction
- Baseline correction via 7th order polynomial subtraction