

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for QUINOLINE\_50T

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

Equivalent concentration x path-length of composite spectrum:  $5.3176 \times 10^{-6}$  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)  $1.093 \text{ g/cm}^3$
- Supplier and stated purity: Aldrich, 98%
- Sample class: I (PNNL scale).
- Temperature of White cell (815.76 cm optical path length)  $50 \pm 2 C$
- Diluent (high purity nitrogen) flowed at 25.20 liter/min ( $21.1^\circ C$ ), ambient atmospheric pressure  $760 \pm 5$  Torr.
- Samples flowed at 2.000, 4.000, 5.000, 2.500, 7.500, 1.500, 15.000, 3.000, 6.000, 1.000, 10.000, 8.000, 12.000 and 22.000 microliters/minute
- Individual samples at equivalent pressures of 0.012316, 0.024636, 0.030803, 0.015406, 0.046217, 0.009243, 0.092433, 0.018487, 0.036978, 0.006165, 0.061646, 0.049311, 0.073985 and 0.135693 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  $570 \text{ cm}^{-1}$  (1.538 to 17.544 microns)
- Instrumental resolution based on maximum interferometer displacement is  $0.112 \text{ cm}^{-1}$
- Spectral interval after 2X zero-filling interferogram and FFT:  $0.06 \text{ cm}^{-1}$
- 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  $0 \text{ cm}^{-1}$

#### **Post Processing and Related Parameters-**

- Non-linearity detector correction (Bruker proprietary) applied to interferogram ( $\alpha=0.90$ ,  $\epsilon=500$ )
- Composite spectrum created from 14 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  $\geq 1.6$  are given zero weight
- Calculated and estimated errors: Type A = 1.12%, Type B  $\leq 7\%$
- Frequency correction (already applied):  $V(\text{corrected}) = V(\text{instrument}) * 0.9999965 + 2.87506e-3$

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