

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for OTOLDINE_25T

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

Equivalent concentration x path-length of composite spectrum: 4.411×10^{-6} grams/liter-meter

Contaminated with water [0.83%] and corrected by rescaling and spectral subtraction. Trace reaction products with windows (KCl) observed at 1218 cm^{-1} .

Sample Conditions-

- Chemical name and CAS number: o-Toluidine, 1-amino-2-methylbenzene, 1-methyl-2-aminobenzene, 2-aminotoluene, 2-methylaniline, o-tolyamine, $\text{C}_6\text{H}_4\text{CH}_3\text{NH}_2$: [95-53-4]
- Physical properties: MW=107.1548 g/mole, mp=-14.7° C, bp=200.2° C, Density (20 C) 1.004 g/cm³
- Supplier and stated purity: Aldrich, 99+%
- Sample class: I (PNNL scale).
- Temperature of White cell (796.0 cm optical path length) 25 ± 2 C
- Diluent (high purity nitrogen) flowed at 24.2 liter/min (21.1° C), ambient atmospheric pressure 760 ± 5 Torr.
- Samples flowed at 5.000, 7.000, 0.700, 2.000, 11.000, 1.000, 15.000, 4.000, 8.000, 2.500, 9.000, 23.000 and 6.00 microliters/minute
- Individual samples at equivalent pressures of 0.035220, 0.049302, 0.004930, 0.014081, 0.077413, 0.007036, 0.105395, 0.028094, 0.056173, 0.017552, 0.063153, 0.161326 and 0.042063 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: $7,300$ to 550 cm^{-1} (1.370 to 18.182 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 = 0.74%, Type B $\leq 7\%$
- Frequency correction (already applied): $V(\text{corrected})=V(\text{instrument})*0.99999959-3.45278 \times 10^{-4}$
- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Baseline correction via 7th order polynomial subtraction