

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for OTOLDINE\_50T

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

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

Contaminated with water [0.78%] and corrected by rescaling and spectral subtraction. Trace reaction products with windows (KCl) observed at  $1218 \text{ cm}^{-1}$ .

### 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/cm<sup>3</sup>
- Supplier and stated purity: Aldrich, 99+%
- Sample class: I (PNNL scale).
- Temperature of White cell (796.0 cm optical path length)  $50 \pm 2$  C
- Diluent (high purity nitrogen) flowed at 24.2 liter/min (21.1° C), ambient atmospheric pressure  $760 \pm 5$  Torr.
- Samples flowed at 1.000, 5.000, 10.000, 7.000, 14.000, 4.000, 18.000, 3.000, 11.000, 12.000, 23.000, 6.000, 35.000, 8.000 and 47.000 microliters/minute
- Individual samples at equivalent pressures of 0.007008, 0.035066, 0.070142, 0.049119, 0.098290, 0.028045, 0.126373, 0.021068, 0.077259, 0.084271, 0.161562, 0.042147, 0.245921, 0.056241 and 0.330501 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  $550 \text{ cm}^{-1}$  (1.370 to 18.182 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 15 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 = 0.62%, 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 ( $\text{cm}^{-1}$ ), Y=Absorbance (base-10)
- Baseline correction via 7<sup>th</sup> order polynomial subtraction