All data taken at Pacific Northwest National Laboratory (PNNL)
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Composite spectrum for DMA_50T
Effective burden of composite spectrum: 1 part-per-million-meter (ppm-meter) at 296 K
Equivalent concentration x path-length of composite spectrum: 4.98917×10^{-6} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: 2,6-Dimethylaniline, 2,6-xylidine, o-xylidine, 1-amino-2,6-dimethylbenzene, $H_2NC_6H_3(CH_3)_2$: [87-62-7]
- Physical properties: MW=121.1816 g/mole, mp=11° C, bp=214° C, Density (20 C) 0.984 g/cm^3
- Supplier and stated purity: Aldrich, 99+%
- Sample class: I (PNNL scale).
- Temperature of White cell (815.76 cm optical path length) 50 ± 2 C
- Diluent (high purity nitrogen) flowed at 25.20 liter/min (21.1° C), ambient atmospheric pressure 760 ± 5 Torr.
- Samples flowed at 2.000, 3.000, 5.000, 1.000, 12.000, 6.000, 3.500, 2.500, 7.000, 15.000, 10.000, 4.000, 20.00 and 23.000 microliters/minute
- Individual samples at equivalent pressures of 0.011779, 0.017665, 0.029439, 0.005886, 0.070615, 0.035303, 0.020585, 0.014704, 0.041160, 0.088211, 0.058792, 0.023514, 0.117536 and 0.135149 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 540 cm^{-1} (1.538 to 18.519 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 (α=0.90, ε=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 ≥ 1.6 are given zero weight
- Calculated and estimated errors: Type A = 0.56%, Type B ≤ 7%
- Frequency correction (already applied): V(corrected)=V(instrument)*0.9999994+4.8215×10^{-4}

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