All data taken at Pacific Northwest National Laboratory (PNNL)
Operators: Steven W. Sharpe, Timothy J. Johnson and Robert L. Sams : sw.sharpe@pnl.gov
Version 1.0, August, 05

Composite spectrum for TDI24_25T
Effective burden of composite spectrum: 1 part-per-million-meter (ppm-meter) at 296 K
Equivalent concentration x path-length of composite spectrum: 7.1702×10^{-6} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: 2,4-Diisocyanatetoluene, 2,4-toluene diisocyanate, 2,4-TDI, $CH_3C_6H_3(NCO)_2$: [584-84-9]
- Physical properties: MW=174.1586 g/mole, mp=20° C, bp=251° C, Density (20 C) 1.214 g/cm^3
- Supplier and stated purity: Aldrich, 96%
- 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 1.500, 0.500, 0.300, 0.800, 0.600, 1.000, 0.200, 1.200, 0.350, 1.100, 0.450, 0.900, 0.700, 0.400 and 1.300 microliters/minute
- Individual samples at equivalent pressures of 0.007889, 0.002628, 0.001577, 0.004203, 0.003152, 0.005251, 0.001050, 0.006300, 0.001837, 0.005774, 0.002361, 0.004723, 0.003673, 0.002098 and 0.006820 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 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 ≥ 1.6 are given zero weight
- Calculated and estimated errors: Type A = 1.04%, Type B ≤ 7%
- Frequency correction (already applied): V(corrected)=V(instrument)*0.99999959-3.45278×10^{-4}

- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Baseline correction via 6^{th} order polynomial subtraction