

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for DIMES_50T

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

Equivalent concentration x path-length of composite spectrum: 5.1927×10^{-6} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: Dimethyl sulfate, DMS, methyl sulfate, sulfuric acid dimethyl ester, $(\text{CH}_3\text{O})_2\text{SO}_2$: [77-78-1]
- Physical properties: M.W. 126.127 amu, M.P. -32°C , B.P. 188°C , Density (20 C) 1.333 g/cm^3
- Supplier and stated purity: Aldrich, 99+%
- Sample class: I (PNNL scale).
- Temperature of White cell (815.76 cm optical path length) $50 \pm 2\text{ C}$
- Diluent (high purity nitrogen) flowed at 25.20 liter/min (21.1°C), ambient atmospheric pressure $760 \pm 5\text{ Torr}$.
- Samples flowed at 3.000, 0.500, 2.000, 5.000, 1.000, 1.500, 10.000, 7.000, 15.000, 30.000, 20.000 and 45.000 microliters/minute
- Individual samples at equivalent pressures of 0.023304, 0.003884, 0.015534, 0.038825, 0.007762, 0.011643, 0.077619, 0.054298, 0.116368, 0.232736, 0.155157 and 0.349195 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 525 cm^{-1} (1.538 to 19.048 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 12 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 = 0.24%, Type B $\leq 7\%$
- Frequency correction (already applied): $V(\text{corrected})=V(\text{instrument}) * 0.9999987 - 4.24224 \times 10^{-4}$

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