

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for DES_50T

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

Equivalent concentration x path-length of composite spectrum: 6.3477×10^{-6} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: Diethyl sulfate, diethyl monosulfate, DS, ethyl sulfate, $(C_2H_5O)_2SO_2$: [64-67-5]
- Physical properties: M.W. 154.1806 amu, F.P. $-24^\circ C$, B.P. $208^\circ C$, Density (20 C) 1.177 g/cm^3
- Supplier and stated purity: Aldrich, 98+%
- Sample class: I (PNNL scale).
- Temperature of White cell (815.76 cm optical path length) $49.99 \pm 2 C$
- Diluent (high purity nitrogen) flowed at 25.20 liter/min ($21.1^\circ C$), ambient atmospheric pressure 760 ± 5 Torr.
- Samples flowed at 2.000, 4.000, 1.000, 8.000, 12.000, 3.000, 1.500, 10.000, 6.000, 0.800, 24.000, 5.000, 7.000 and 32.000 microliters/minute
- Individual samples at equivalent pressures of 0.010956, 0.021914, 0.005479, 0.043811, 0.065725, 0.016438, 0.008220, 0.054807, 0.032875, 0.004385, 0.131555, 0.027418, 0.038396 and 0.175523 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 520 cm^{-1} (1.538 to 19.231 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 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 $\leq 7\%$
- Frequency correction (already applied): $V(\text{corrected}) = V(\text{instrument}) * 0.9999965 + 2.87506e-3$

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