

All data taken at Pacific Northwest National Laboratory (PNNL)
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Composite spectrum for DMSO_25T

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

Equivalent concentration x path-length of composite spectrum: 3.127×10^{-6} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: Dimethyl sulfoxide, Methyl sulfoxide, DMSO, $(\text{CH}_3)_2\text{SO}$: [67-68-5]
- Physical properties: M.W. 78 amu, F.P. -18.5C , B.P. -189C
- Supplier and stated purity: Aldrich, 99.9%
- Sample class: III (PNNL scale), low vapor pressure sample.
- Temperature of sample: $24.95 \pm 0.02\text{ C}$
- Diluent: Sample back filled with ultra high purity nitrogen to 760 ± 5 Torr
- Individual samples at 0.27000, 0.30400, 0.20800, 0.16563, 0.27300, 0.22700, 0.18600 and 0.24100 Torr. Path length = 20.04 cm. Final data is a composite spectrum.
- Preparation: Multiple freeze-thaw cycles at 77K to remove air. Pump on sample at room temperature to remove CO_2 and other volatile components.

Instrument Parameters-

- Bruker-66V FTIR, temperature controlled environment, evacuated optics bench
- Spectral range: $6,500$ to 600 cm^{-1} (1.534 to 16.667 microns)
- Instrumental resolution (interferogram): 0.112 cm^{-1}
- Spectral intervals after 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 ($\alpha = 0.85$, $\beta = 530$)
- Composite spectrum created from 8 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 = 2.6%, Type B = 10%
- Frequency correction: $V(\text{corrected}) = V(\text{instrument}) * 0.9999984669 + 0.005187$
- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Trace water vapor features removed by spectral subtraction. Baseline correction via 7th-order polynomial subtraction.