

All data taken at Pacific Northwest National Laboratory (PNNL)  
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Composite spectrum for DMSO\_50T

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

Equivalent concentration x path-length of composite spectrum:  $3.127 \times 10^{-6}$  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.  $-18.5\text{C}$ , B.P.  $-189\text{C}$
- Supplier and stated purity: Aldrich, 99.9%
- Sample class: III (PNNL scale), low vapor pressure sample.
- Temperature of sample:  $49.98 \pm 0.02\text{ C}$
- Diluent: Sample back filled with ultra high purity nitrogen to  $760 \pm 5$  Torr
- Individual samples at 0.23750, 0.27570, 0.22900, 0.17900, 0.33877 and 0.18200 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  $\text{CO}_2$  and other volatile components.

### Instrument Parameters-

- Bruker-66V FTIR, temperature controlled environment, evacuated optics bench
- Spectral range: 6,500 to 600  $\text{cm}^{-1}$  (1.534 to 16.667 microns)
- Instrumental resolution (interferogram): 0.112  $\text{cm}^{-1}$
- Spectral intervals after FFT: 0.06  $\text{cm}^{-1}$
- 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  $\text{cm}^{-1}$

### Post Processing and Related Parameters-

- Non-linearity detector correction (Bruker proprietary) applied to interferogram ( $\alpha = 0.85$ ,  $\beta = 530$ )
- Composite spectrum created from 6 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 = 6.4%, Type B = 10%
- Frequency correction (already applied):  $V(\text{corrected}) = V(\text{instrument}) * 0.9999984669 + 0.005187$
- Axis units: X=wavenumbers ( $\text{cm}^{-1}$ ), Y=Absorbance (base-10)
- Baseline correction via 7<sup>th</sup>-order polynomial subtraction.