

All data taken at Pacific Northwest National Laboratory (PNNL)  
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Composite spectrum for CS<sub>2</sub>\_25T

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

Equivalent concentration x path-length of composite spectrum:  $3.135 \times 10^{-6}$  grams/liter-meter

#### **Sample Conditions-**

- Chemical name and CAS number: Carbon disulfide, carbon bisulfide, CS<sub>2</sub> : [75-15-0]
- Physical properties: M.W. 76.14 amu, F.P. -111 C, B.P. 46.3 C
- Supplier and stated purity: Aldrich, 99.9+% (HPLC grade)
- Sample class: I (PNNL scale).
- Temperature of sample:  $25.04 \pm 0.02$  C
- Diluent: Sample back filled with ultra high purity nitrogen to  $760 \pm 5$  Torr
- Individual samples 0.29874, 0.62177, 7.1438, 7.0058, 1.00457, 2.3527, 0.45402, 15.01, 32.85, 0.80855 and 0.14334 Torr. Path length = 19.94 cm. Final data is a composite spectrum.
- Preparation: Multiple freeze-thaw cycles at -80 C to remove air.

#### **Instrument Parameters-**

- Bruker-66V FTIR, temperature controlled environment, evacuated optics bench
- Modified to include second aperture, between interferometer output and sample cell. This substantially reduces both “ghosting” and warm aperture effects.
- Spectral range: 6,500 to 600 cm<sup>-1</sup> (1.534 to 16.667 microns)
- Instrumental resolution based on maximum interferometer displacement is 0.112 cm<sup>-1</sup>
- Spectral intervals after FFT: 0.06 cm<sup>-1</sup>
- 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<sup>-1</sup>

#### **Post Processing and Related Parameters-**

- Non-linearity detector correction (Bruker proprietary) applied to interferogram ( $\alpha = 0.85$ ,  $\beta = 530$ )
- Composite spectrum created from 11 individual absorbance (base-10) spectra via classical least squares fit: Intercept=0, slope is fitted, individual absorbance values weighted by T<sup>2</sup> (transmission squared), all absorbance values  $> 1.6$  are given zero weight
- Calculated and estimated errors: Type A = 0.62%, Type B = 3%
- Frequency correction (already applied):  $V(\text{corrected}) = V(\text{instrument}) * 0.999997 + 5.18 \times 10^{-4}$
- Axis units: X=wavenumbers (cm<sup>-1</sup>), Y=Absorbance (base-10)
- Trace water and carbon dioxide vapor features removed via spectral subtraction
- Baseline correction via 7<sup>th</sup> order polynomial subtraction