

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for DEETHER\_25T

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

Equivalent concentration x path-length of composite spectrum:  $3.052 \times 10^{-6}$  grams/liter-meter

### Sample Conditions-

- Chemical name and CAS number: Diethyl ether, ethyl ether, ether, ethyl oxide, diethyl oxide, sulfuric ether,  $(C_2H_5)_2O$  : [60-29-7]
- Physical properties: F.W 74.12 amu, F.P.  $-116.2$  C, B.P.  $34.5$  C
- Supplier and stated purity: Aldrich, 99+%
- Sample class: I (PNNL scale).
- Temperature of sample:  $25.00 \pm 0.02$  C
- Diluent: Sample back filled with ultra high purity nitrogen to  $760 \pm 5$  Torr
- Individual samples at 1.08131, 2.1817, 4.2948, 17.20, 34.78, 3.0739, 8.1262, 57.01, 4.9101 and 25.67 Torr. Path length = 19.94 cm. Final data is a composite spectrum.
- Preparation: Multiple freeze-thaw cycles at 77 K to remove air. Sample placed over  $CaSO_4$  to remove water.

### 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  $600$   $cm^{-1}$  (1.534 to 16.667 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 ( $\alpha = 0.85$ ,  $\beta = 530$ )
- Composite spectrum created from 10 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 = 0.14%, Type B = 3%
- Frequency correction (already applied):  $V(\text{corrected}) = V(\text{instrument}) * 0.999997 + 5.18 \times 10^{-4}$
- Axis units: X=wavenumbers ( $cm^{-1}$ ), Y=Absorbance (base-10)
- Trace  $CO_2$  vapor features removed via spectral subtraction
- Baseline correction via 7<sup>th</sup> order polynomial subtraction