

All data taken at Pacific Northwest National Laboratory (PNNL)  
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Composite spectrum for AceticAnhy\_25T

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

#### Sample Conditions-

- Chemical name and CAS number: Acetic anhydride, acetyl oxide, acetic oxide,  $(\text{CH}_3\text{CO})_2\text{O}$  : [108-24-7]
- Physical properties: M.W. 102 amu, F.P.  $-73.1\text{C}$ , B.P.  $139.9\text{C}$
- Supplier and stated purity: Aldrich, 99%
- Sample class: II (PNNL scale).
- Temperature of sample:  $25.02 \pm 0.02\text{ C}$
- Diluent: Sample back filled with ultra high purity nitrogen to  $760 \pm 5$  Torr
- Individual samples at 0.84498, 0.99994, 0.50507, 2.1000, 3.0000, 3.1400, 2.0080, 1.5491 and 2.4700 Torr. Path length = 19.96 cm. Final data is a composite spectrum.
- Preparation: Multiple freeze-thaw cycles at 77K to remove air. Sample pumped for 1-hour at  $-20\text{C}$  to minimize acetic acid.

#### 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: 9 (Bruker arbitrary)
- 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 9 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 = 0.32%, Type B = 5%
- Frequency correction:  $V(\text{corrected}) = V(\text{instrument}) * 0.9999984669 + 0.005187$
- Axis units: X=wavenumbers ( $\text{cm}^{-1}$ ), Y=Absorbance (base-10)
- Acetic acid (4.44%) removed from and composite spectrum corrected by spectral subtraction and re-scaling.