

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

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

Equivalent concentration x path-length of composite spectrum:  $3.0499 \times 10^{-6}$  grams/liter-meter

### Sample Conditions-

- Chemical name and CAS number: Acetol; 2-Propanone, 1-hydroxy-; CH3C(O)CH2OH; Hydroxyacetone; Acetone alcohol; Acetylcarbinol; Hydroxypropanone; Methanol, acetyl-; 1-Hydroxy-2-propanone; 1-Hydroxyacetone; 1-hydroxypropan-2-one; hydroxyacetone (acetol); hydroxypropan-2-one C3H6O2: [116-09-6]
- Physical properties: MW=74.0785 g/mole, mp=-17° C, bp=145.6° C, Density (25 C) = 1.08 g/cm<sup>3</sup>
- Supplier and stated purity: Alfa Aesar; 95%
- Sample class: I (PNNL scale).
- Temperature of White cell (805.0 cm optical path length)  $25 \pm 2$  C
- Diluent (high purity nitrogen) flowed at 22.77 liter/min (21.1° C), ambient atmospheric pressure  $760 \pm 5$  Torr.
- Samples flowed at microliters/minute 2.000, 9.000, 5.000, 13.000, 7.000, 18.000, 15.000, 11.000, 21.000, 23.000, 34.000, 28.000, 39.000, 26.000 and 31.000
- Individual samples at equivalent pressures of: 0.023140, 0.104103, 0.057812, 0.150291, 0.080904, 0.207983, 0.173273, 0.126914, 0.242160, 0.265152, 0.391964, 0.322707, 0.449365, 0.299456 and 0.356996 Torr. Final data is a composite spectrum.
- Preparation: None

### Instrument Parameters-

- Bruker-66V FTIR, evacuated optics bench.
- Modified to include second aperture, between interferometer output and White cell. This substantially reduces both “ghosting” and warm aperture effects.
- Spectral range: 7,200 to 510 cm<sup>-1</sup> (1.389 to 19.608 microns)
- Instrumental resolution based on maximum interferometer displacement is 0.112 cm<sup>-1</sup>
- Spectral interval after 2X zero-filling interferogram and 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 ( $\alpha=0.90$ ,  $\epsilon=500$ )

- Composite spectrum created from 15 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  $\geq 1.6$  are given zero weight
- Calculated and estimated errors: Type A =0.96%, Type B  $\leq 7\%$
- Frequency correction (already applied):  $V(\text{corrected})=V(\text{instrument}) * 1.00000160 + 3.5903 \times 10^{-4}$
- Axis units: X=wavenumbers ( $\text{cm}^{-1}$ ), Y=Absorbance (base-10)
- Trace carbon dioxide and 9.42% water were removed by spectral subtraction and the composite spectrum was rescaled by multiplying by 1.10400.
- Baseline correction via 7<sup>th</sup> order polynomial subtraction