

All data taken at Pacific Northwest National Laboratory (PNNL)
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Composite spectrum for ACETOL_50T

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

Equivalent concentration x path-length of composite spectrum: 3.0499×10^{-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/cm³
- Supplier and stated purity: Alfa Aesar; 95%
- Sample class: I (PNNL scale).
- Temperature of White cell (805.0 cm optical path length) 50 ± 2 C
- Diluent (high purity nitrogen) flowed at 22.77 liter/min (21.1° C), ambient atmospheric pressure 760 ± 5 Torr.
- Samples flowed at microliters/minute 5.000, 12.000, 7.000, 16.000, 10.000, 14.000, 22.000, 19.000, 27.000, 25.000, 30.000, 37.000, 33.000 and 40.000
- Individual samples at equivalent pressures of: 0.057796, 0.138711, 0.080926, 0.185072, 0.115701, 0.161916, 0.254848, 0.220126, 0.312893, 0.289793, 0.347845, 0.429123, 0.382834 and 0.464041 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⁻¹ (1.389 to 19.608 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 ($\alpha=0.90$, $\epsilon=500$)

- Composite spectrum created from 14 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 =1.34%, 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 (cm^{-1}), Y=Absorbance (base-10)
- Trace carbon dioxide and 8.13% water were removed by spectral subtraction and the composite spectrum was rescaled by multiplying by 1.0885
- Baseline correction via 7th order polynomial subtraction