

All data taken at Pacific Northwest National Laboratory (PNNL)
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Composite spectrum for DIACETONE_50T

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

Equivalent concentration x path-length of composite spectrum: 4.7823×10^{-6} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: Diacetone alcohol; 2-Pentanone, 4-hydroxy-4-methyl-; Acetylalcohol; Diketone alcohol; 4-Hydroxy-4-methylpentanone; $(\text{CH}_3)_2\text{C}(\text{OH})\text{CH}_2\text{C}(\text{O})\text{CH}_3$; 4-Hydroxy-4-methyl-2-pentanone; 2-Methyl-2-pentanol-4-one; 4-Methyl-2-pentanone-4-ol; Diacetonol; Diacetonol; Diacetone-alcohol; 4-Hydroxy-2-keto-4-methylpentane; 4-Hydroxy-4-methyl-pentan-2-on; 4-Hydroxy-4-methyl-pentan-2-one; Diacetone; 4-Hydroxy-4-methylpentanone-2; 2-Hydroxy-2-methyl-4-pentanone; 2-Methyl-3-pentanol-4-one; 4-Methyl-4-hydroxy-2-pentanone; Hydroxy-4-methyl-2-pentanone; $\text{C}_6\text{H}_{12}\text{O}_2$: [123-42-2]
- Physical properties: MW=116.1583 g/mole, mp=-42.8° C, bp=168° C, Density (25 C) = 0.9306 g/cm³
- Supplier and stated purity: Sigma Aldrich, 99%
- 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 1.500, 9.000, 6.000, 15.000, 11.000, 18.000, 13.000, 24.000, 21.000, 32.000, 28.000, 40.000 and 52.000
- Individual samples at equivalent pressures of: 0.009648, 0.057872, 0.038571, 0.096414, 0.070695, 0.115621, 0.083493, 0.154120, 0.134837, 0.205467, 0.179783, 0.256833 and 0.333839 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: 7,000 to 520 cm^{-1} (1.429 to 19.23 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 13 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 =0.93%, 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 water vapor and carbon dioxide were removed by spectral subtraction
- Baseline correction via 7th order polynomial subtraction