

All data taken at Pacific Northwest National Laboratory (PNNL)
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Version 1.0, April 5, 2010.

Composite spectrum for MEACAC_25T

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

Equivalent concentration x path-length of composite spectrum: 4.7805×10^{-6} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: Methyl acetoacetate; Butanoic acid, 3-oxo-Methyl ester; Acetoacetic acid, methyl ester; Methyl acetylacetate; Methyl 3-oxobutyrate; Acetoacetic methyl ester; Methyl acetylacetonate; Methylester kyseliny acetove; 3-Oxobutanoic acid methyl ester; Methyl 3-oxobutanoate $C_5H_8O_3$: [105-45-3]
- Physical properties: MW=116.1152g/mole, mp=-32° C, bp=171° C, Density (25 C) = 1.076 g/cm³
- Supplier and stated purity: Sigma Aldrich, 99%
- Sample class: I (PNNL scale).
- Temperature of White cell (805.0 cm optical path length) 25 ± 2 C
- Diluent (high purity nitrogen) flowed at 23.3 liter/min (21.1° C), ambient atmospheric pressure 760 ± 5 Torr.
- Samples flowed at microliters/minute 2.000, 5.000, 9.000, 2.000, 7.000, 3.500, 13.000, 6.000, 18.000, 25.000, 11.000, 1.500, 15.000, 22.000 and 4.200
- Individual samples at equivalent pressures of 0.014552, 0.036371, 0.065476, 0.014545, 0.050899, 0.025446, 0.094502, 0.043622, 0.130849, 0.181759, 0.079974, 0.010906, 0.109055, 0.159969 and 0.030535 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: 6,500 to 520 cm^{-1} (1.538 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 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 ≥ 1.6 are given zero weight
- Calculated and estimated errors: Type A =0.815%, Type B $\leq 7\%$
- Frequency correction (already applied): $V(\text{corrected})=V(\text{instrument})\cdot 0.9999996+6.17682\times 10^{-4}$
- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Trace water vapor, carbon monoxide and carbon dioxide were removed by spectral subtraction
- Baseline correction via 7th order polynomial subtraction