

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for MBENZOATE\_25T

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

Equivalent concentration x path-length of composite spectrum:  $5.6054 \times 10^{-6}$  grams/liter-meter

### Sample Conditions-

- Chemical name and CAS number: Methyl benzoate, benzoic acid methyl ester, clorius, essence of niobe, methyl benzenecarboxylate,  $C_6H_5CO_2CH_3$  : [93-58-3]
- Physical properties: M.W. 136.15 amu, F.P.  $-12^\circ C$ , B.P.  $198.5^\circ C$ , Density (20 C)  $1.094 g/cm^3$
- Supplier and stated purity: Aldrich, 99%
- Sample class: I (PNNL scale).
- Temperature of White cell (815.76 cm optical path length)  $25 \pm 2 C$
- Diluent (high purity nitrogen) flowed at 25.20 liter/min ( $21.1^\circ C$ ), ambient atmospheric pressure  $760 \pm 5$  Torr.
- Samples flowed at 1.000, 2.000, 5.000, 0.600, 1.200, 8.000, 0.500, 7.500, 0.400, 4.000, 3.000, 11.000, 6.000 and 14.000 microliters/minute
- Individual samples at equivalent pressures of 0.005880, 0.011756, 0.029383, 0.003526, 0.007051, 0.046988, 0.002936, 0.044029, 0.002348, 0.023473, 0.017607, 0.064541, 0.035204 and 0.082144 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  $550 cm^{-1}$  (1.538 to 18.182 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  $\geq 1.6$  are given zero weight
- Calculated and estimated errors: Type A = 0.19%, Type B  $\leq 7\%$
- Frequency correction (already applied):  $V(\text{corrected})=V(\text{instrument}) * 0.9999987 - 4.24224 \times 10^{-4}$

- Axis units: X=wavenumbers ( $\text{cm}^{-1}$ ), Y=Absorbance (base-10)
- Baseline correction via 7<sup>th</sup> order polynomial subtraction
- Trace water vapor features removed via spectral subtraction