

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for ETBZATE\_50T

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

Equivalent concentration x path-length of composite spectrum:  $6.1828 \times 10^{-6}$  grams/liter-meter

### Sample Conditions-

- Chemical name and CAS number: Ethyl benzoate; Ethyl benzenecarboxylate; Benzoic ether; Essence of niobe; 2-methoxy-1-phenyl-ethanone; Benzoic acid, ethyl ester C<sub>9</sub>H<sub>10</sub>O<sub>2</sub> : [93-89-0]
- Physical properties: MW=150.1745 g/mole, mp= -34° C, bp=212° C, Density (25 C) = 1.045g/cm<sup>3</sup>
- Supplier and stated purity: 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 23.3 liter/min (21.1° C), ambient atmospheric pressure 760 ± 5 Torr.
- Samples flowed at microliters/minute 2.000, 1.000, 3.000, 6.000, 4.000, 8.000, 5.000, 7.000, 16.000, 12.000, 10.000 and 14.000.
- Individual samples at equivalent pressures of 0.010758, 0.005383, 0.016156, 0.032339, 0.021562, 0.043136, 0.026971, 0.037769, 0.086341, 0.064781, 0.053985 and 0.075609 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 600 cm<sup>-1</sup> (1.5385 to 16.67 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 12 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 =0.79%, Type B  $\leq 7\%$
- Frequency correction (already applied):  $V(\text{corrected})=V(\text{instrument}) * 1.0000016 + 3.59033 \times 10^{-4}$
- Axis units: X=wavenumbers ( $\text{cm}^{-1}$ ), Y=Absorbance (base-10)
- No features were removed via spectral subtraction
- Baseline correction via 7<sup>th</sup> order polynomial subtraction