

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for BZALDEH\_5T

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

Equivalent concentration x path-length of composite spectrum:  $4.369 \times 10^{-6}$  grams/liter-meter

### Sample Conditions-

- Chemical name and CAS number: Benzaldehyde, benzoic aldehyde, phenylmethanal, artificial bitter almond oil, benzenecarboxaldehyde, benzenemethylal, benzoyl hydride,  $C_6H_5CHO$  : [100-52-7]
- Physical properties: fw=106.124 g/mole, fp=-26° C, bp=179° C
- Supplier and stated purity: Aldrich, 99.5+%
- Sample class: II (PNNL scale). Low vapor pressure at ambient temperatures
- Temperature of sample:  $5.07 \pm 0.02$  C
- Diluent: Sample back filled with ultra high purity nitrogen to  $760 \pm 5$  Torr
- Individual samples at 0.16000, 0.15680, 0.13000, 0.10500 and 0.11900 Torr. Path length = 19.94 cm. Final data is a composite spectrum.
- Preparation: Multiple freeze-thaw cycles at 0 C to remove air.

### Instrument Parameters-

- Bruker-66V FTIR, temperature controlled environment, evacuated optics bench
- Modified to include second aperture, between interferometer output and sample cell. This substantially reduces both “ghosting” and warm aperture effects.
- Spectral range: 6,500 to 600  $cm^{-1}$  (1.534 to 16.667 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 ( $\alpha=0.85$ ,  $\beta=530$ )
- Composite spectrum created from 5 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 = 3.09%, Type B = 5%
- Frequency correction (already applied):  $V(\text{corrected}) = V(\text{instrument}) * 0.99999896 + 8.812 \times 10^{-4}$
- Axis units: X=wavenumbers ( $cm^{-1}$ ), Y=Absorbance (base-10)
- Baseline correction via 7<sup>th</sup> order polynomial subtraction