

All data taken at Pacific Northwest National Laboratory (PNNL)  
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Composite spectrum for CLBZ\_50T

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

#### **Sample Conditions-**

- Chemical name and CAS number: Chlorobenzene, Monochlorobenzene, Phenyl chloride,  $C_6H_5Cl$  : [108-90-7]
- Physical properties: M.W. 112 amu, F.P.  $-45C$ , B.P. 131.6C
- Supplier and stated purity: Aldrich, 99.9%
- Sample class: I (PNNL scale).
- Temperature of sample:  $50.04 \pm 0.02 C$
- Diluent: Sample back filled with ultra high purity nitrogen to  $760 \pm 5$  Torr
- Individual samples at 1.7455, 1.10158, 3.7200, 0.75632, 5.8325, 0.48672 and 7.5000 Torr. Path length = 19.96 cm. Final data is a composite spectrum.
- Preparation: Multiple freeze-thaw cycles at 77K to remove air. Place over Calcium sulfate to remove water.

#### **Instrument Parameters-**

- Bruker-66V FTIR, temperature controlled environment, evacuated optics bench
- Spectral range: 6,500 to 600  $cm^{-1}$  (1.534 to 16.667 microns)
- Instrumental resolution (interferogram): 0.112  $cm^{-1}$
- Spectral intervals after 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: 9 (Bruker arbitrary)
- 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 7 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 = 0.85%, Type B = 3%
- Frequency correction:  $V(\text{corrected}) = V(\text{instrument}) * 0.9999984669 + 0.005187$
- Axis units: X=wavenumbers ( $cm^{-1}$ ), Y=Absorbance (base-10)
- Trace carbon dioxide removed from composite spectrum via spectral subtraction. Baseline corrected via 5<sup>th</sup>-order polynomial subtraction.