

All data taken at Pacific Northwest National Laboratory (PNNL)  
Operator: Steven W. Sharpe and Robert L. Sams, sw.sharpe@pnl.gov  
Version 1.0, June, 2000

Composite spectrum for BnzylCl\_50T

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

#### **Sample Conditions-**

- Chemical name and CAS number: Benzyl chloride, -Chlorotoluene,  $C_6H_5CH_2Cl$  : [100-44-7]
- Physical properties: M.W. 127 amu, F.P.  $-43C$ , B.P.  $179C$
- Supplier and stated purity: Aldrich, 99%
- Sample class: II (PNNL scale). Low vapor pressure sample.
- Temperature of sample  $49.99 \pm 0.02 C$
- Diluent: Sample back filled with ultra high purity nitrogen to  $760 \pm 5$  Torr
- Individual samples at 0.37688, 0.48620, 0.31595, 0.36908, 0.42000 and 0.30666 Torr. Path length = 19.96 cm. Final data is a composite spectrum.
- Preparation: Multiple freeze-thaw cycles at 77K to remove air. Additional pumping at  $-50C$  to remove  $CO_2$  and other volatile impurities.

#### **Instrument Parameters-**

- Bruker-66V FTIR, temperature controlled environment, evacuated optics bench
- Spectral range:  $6,500$  to  $600\text{ cm}^{-1}$  (1.534 to 16.667 microns)
- Instrumental resolution (interferogram):  $0.112\text{ cm}^{-1}$
- Spectral intervals after FFT:  $0.06\text{ cm}^{-1}$
- 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  $0\text{ cm}^{-1}$

#### **Post Processing and Related Parameters-**

- Non-linearity detector correction (Bruker proprietary) applied to interferogram ( $\alpha=0.85$ ,  $\beta=530$ )
- Composite spectrum created from 6 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=0.78%, Type B 5%
- Frequency correction:  $V(\text{corrected}) = V(\text{instrument}) * 0.9999984669 + 0.005187$
- Axis units: X=wavenumbers ( $\text{cm}^{-1}$ ), Y=Absorbance (base-10)
- Trace water vapor features removed by spectral subtraction. Baseline zeroing via 7<sup>th</sup>-order polynomial correction. Small impurity peak observed at  $1352\text{ cm}^{-1}$  and removed by spectral subtraction.