

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for NBUTCNO\_25T

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

Equivalent concentration x path-length of composite spectrum:  $4.0813 \times 10^{-6}$  grams/liter-meter

### Sample Conditions-

- Chemical name and CAS number: n-Butyl isocyanate, 1-isocyanatebutane,  $C_5H_9NO$  : [111-36-4]
- Physical properties: fw=99.1322 g/mole, mp=-75° C, bp=115° C
- Supplier and stated purity: Aldrich, 98%
- Sample class: I (PNNL scale).
- Temperature of sample:  $25.02 \pm 0.02$  C
- Diluent: Sample back filled with ultra high purity nitrogen to  $760 \pm 5$  Torr
- Individual samples at 0.56956, 1.13222, 0.73036, 0.30174, 1.2380, 8.4820, 4.0875, 2.2330, 11.0325 and 15.62 Torr. Path length = 19.96 cm. Final data is a composite spectrum.
- Preparation: Multiple freeze-thaw cycles at 77 K 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  $550$   $cm^{-1}$  (1.534 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 ( $\alpha=0.85$ ,  $\epsilon=530$ )
- Composite spectrum created from 10 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 = 1.23%, Type B  $\leq 3\%$
- 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)
- Trace  $CO_2$  vapor features removed via spectral subtraction
- Baseline correction via 6<sup>th</sup> order polynomial subtraction