

All data taken at Pacific Northwest National Laboratory (PNNL)  
Operator: Steven W. Sharpe, sw.sharpe@pnl.gov  
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Composite spectrum for ButylNitrite\_5T

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

### Sample Conditions-

- Chemical name and CAS number: n-Butyl nitrite, Butyl nitrite, 1-Butyl nitrite, Butyric nitrite, nitrous acid n-butyl ester,  $\text{CH}_3(\text{CH}_2)_3\text{ONO}$  : [544-16-1]
- Physical properties: M.W. 103 amu, F.P.  $-13^\circ\text{C}$ , B.P.  $78^\circ\text{C}$ , Decomposes upon heating to form oxides of carbon and nitrogen
- Supplier and stated purity: Aldrich, 95%
- Sample class: III (PNNL scale), sample undergoes photo- and thermal-decomposition
- Temperature of sample  $5.03 \pm 0.02^\circ\text{C}$
- Diluent: Sample back filled with ultra high purity nitrogen to  $760 \pm 5$  Torr
- Individual samples 3.4900, 2.0717, 2.9947, 4.2362, 1.7186 and 2.3973 Torr. Path length = 19.96 cm. Final data is a composite spectrum.
- Preparation: Multiple freeze-thaw cycles at 77K followed by multiple pumpings  $-35^\circ\text{C}$  to remove carbon dioxide and carbon monoxide. Sample used at  $-35^\circ\text{C}$  to minimize water.

### Instrument Parameters-

- Bruker-66V FTIR, temperature controlled environment, evacuated optics bench
- Spectral range:  $6,500$  to  $600 \text{ cm}^{-1}$  (1.54 to 16.67 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 = 1.5%, Type B = 10%
- Frequency correction:  $V(\text{corrected}) = V(\text{instrument}) * 0.9999984669 + 0.005187$
- Axis units: X=wavenumbers ( $\text{cm}^{-1}$ ), Y=Absorbance (base-10)
- Binomial smoothing filter used on data with no degradation to spectral features. Water and carbon dioxide removed by spectral subtraction. Compound decomposes when exposed to light and/or heat to produce carbon dioxide and carbon monoxide.