

All data taken at Pacific Northwest National Laboratory (PNNL)
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Composite spectrum for ButylNitrite_25T

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°C , B.P. 78°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 $25.04 \pm 0.02^\circ\text{C}$
- Diluent: Sample back filled with ultra high purity nitrogen to 760 ± 5 Torr
- Individual samples at 3.5376, 4.1732, 2.4991, 1.4950, 3.3611, 3.0875, 1.5074, 2.1430, 4.2266 and 2.4084 Torr. Path length = 19.96 cm. Final data is a composite spectrum.
- Preparation: Multiple freeze-thaw cycles at 77K followed by multiple pumpings -35°C to remove carbon dioxide and carbon monoxide. Sample used at -35°C to minimize water.

Instrument Parameters-

- Bruker-66V FTIR, temperature controlled environment, evacuated optics bench
- Spectral range: $6,500$ to 600 cm^{-1} (1.54 to 16.67 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 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 > 1.6 are given zero weight
- Calculated and estimated errors: Type A = 1.2%, Type B = 10%
- Frequency correction: $V(\text{corrected}) = V(\text{instrument}) * 0.9999984669 + 0.005187$
- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Binomial smoothing filter used on data with no degradation to spectral features. Water, carbon dioxide and carbon monoxide removed by spectral subtraction. Compound decomposes when exposed to light and/or heat to produce carbon dioxide and carbon monoxide.