

All data taken at Pacific Northwest National Laboratory (PNNL)

Operators: Steven W. Sharpe, Timothy J. Johnson and Robert L. Sams : [sw.sharpe@pnl.gov](mailto:sw.sharpe@pnl.gov)

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Composite spectrum for BBR3\_25T

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

Equivalent concentration x path-length of composite spectrum:  $1.0315 \times 10^{-5}$  grams/liter-meter

At higher burdens of  $\text{BBr}_3$  a broad feature grew in at  $\sim 1400 \text{ cm}^{-1}$  and is suspected to be the dimer of  $\text{BBr}_3$ . See PDF file for detail.

### Sample Conditions-

- Chemical name and CAS number: Boron tribromide, boron bromide,  $\text{BBr}_3$ ; [10294-33-4]
- Physical properties: fw=250.54 g/mole, fp= $-46^\circ \text{ C}$ , bp= $90^\circ \text{ C}$
- Supplier and stated purity: Aldrich, 99.995%
- Sample class: I (PNNL scale).
- Temperature of sample:  $24.97 \pm 0.02 \text{ C}$
- Diluent: Sample back filled with ultra high purity nitrogen to  $760 \pm 5 \text{ Torr}$
- Individual samples at 0.57010, 0.75111, 14.60, 0.36000, 5.1280, 0.27920, 0.17777, 20.58, 0.44777, 9.1566, 0.65720, 0.25250 and 1.4070 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  $600 \text{ cm}^{-1}$  (1.534 to 16.667 microns)
- Instrumental resolution based on maximum interferometer displacement is  $0.112 \text{ cm}^{-1}$
- Spectral interval after 2X zero-filling interferogram and 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: 60KHz (HeNe crossing frequency)
- Number of interferograms averaged per single channel spectra: 256
- Detector: Mid-band HgCdTe, photoconductive, 77K operation
- Folding limits: 15798 to  $0 \text{ cm}^{-1}$

### Post Processing and Related Parameters-

- Non-linearity detector correction (Bruker proprietary) applied to interferogram ( $\tau = 0.90$ ,  $\nu = 500$ )
- Composite spectrum created from 13 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 = 0.77%, Type B = 3%
- Frequency correction (already applied):  $V(\text{corrected}) = V(\text{instrument}) * 0.999998 + 1.287 \times 10^{-4}$
- Axis units: X=wavenumbers ( $\text{cm}^{-1}$ ), Y=Absorbance (base-10)
- Trace hydrogen bromide vapor features removed via spectral subtraction

- Baseline correction via 7<sup>th</sup> order polynomial subtraction