

All data taken at Pacific Northwest National Laboratory (PNNL)  
Operator: Steven W. Sharpe and Robert L. Sams, sw.sharpe@pnl.gov  
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Composite spectrum for PH3\_5T

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

Equivalent concentration x path-length of composite spectrum:  $1.400 \times 10^{-6}$  grams/liter-meter

#### **Sample Conditions-**

- Chemical name and CAS number: Phosphine, Hydrogen phosphide, PH<sub>3</sub> : [7803-51-2]
- Physical properties: M.W. 34 amu, F.P. -133.5 C, B.P. -85 C
- Supplier and stated purity: Aldrich, 99.9995+% (electronic grade)
- Sample class: I (PNNL scale).
- Temperature of sample:  $5.11 \pm 0.02$  C
- Diluent: Sample back filled with ultra high purity nitrogen to  $760 \pm 5$  Torr
- Individual samples at 1.4401, 5.9041, 10.7649, 16.23, 7.8933, 5.0664 and 2.0595 Torr. Path length = 19.94 cm. Final data is a composite spectrum.
- Preparation: Multiple freeze-thaw cycles at 77K 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 cm<sup>-1</sup> (1.534 to 16.667 microns)
- Instrumental resolution based on maximum interferometer displacement is 0.112 cm<sup>-1</sup>
- Spectral intervals after FFT: 0.06 cm<sup>-1</sup>
- 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<sup>-1</sup>

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

- Non-linearity detector correction (Bruker proprietary) applied to interferogram ( $\alpha = 0.85$ ,  $\beta = 530$ )
- Composite spectrum created from 7 individual absorbance (base-10) spectra via classical least squares fit: Intercept=0, slope is fitted, individual absorbance values weighted by T<sup>2</sup> (transmission squared), all absorbance values  $> 1.6$  are given zero weight
- Calculated and estimated errors: Type A = 0.52%, Type B = 3%
- Frequency correction (already applied):  $V(\text{corrected}) = V(\text{instrument}) * 0.999998 + 2.164 \times 10^{-5}$
- Axis units: X=wavenumbers (cm<sup>-1</sup>), Y=Absorbance (base-10)
- Baseline correction via 7<sup>th</sup> order polynomial