

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for C6F6\_50T

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

Equivalent concentration x path-length of composite spectrum:  $7.6601 \times 10^{-6}$  grams/liter-meter

### Sample Conditions-

- Chemical name and CAS number: Hexafluorobenzene, perfluorobenzene, C<sub>6</sub>F<sub>6</sub> : [392-56-3]
- Physical properties: M.W. 186.0564 amu, F.P. 4° C, B.P. 80.5° C, Density (20 C) 1.612 g/cm<sup>3</sup>
- Supplier and stated purity: Aldrich, 99.9+%
- Sample class: I (PNNL scale).
- Temperature of White cell (815.76 cm optical path length)  $50 \pm 2$  C
- Diluent (high purity nitrogen) flowed at 25.20 liter/min (21.1° C), ambient atmospheric pressure  $760 \pm 5$  Torr.
- Samples flowed at 2.000, 1.000, 4.000, 0.400, 10.000, 1.200, 15.000, 2.400, 6.000, 3.000, 1.500, 20.000 and 60.000 microliters/minute
- Individual samples at equivalent pressures of 0.012638, 0.006320, 0.025280, 0.002528, 0.063216, 0.007587, 0.094836, 0.015176, 0.037949, 0.018977, 0.009491, 0.126547 and 0.379692 Torr. Final data is a composite spectrum.
- Preparation: None

### Instrument Parameters-

- Bruker-66V FTIR, evacuated optics bench.
- Modified to include second aperture, between interferometer output and White cell. This substantially reduces both “ghosting” and warm aperture effects.
- Spectral range: 6,500 to 580 cm<sup>-1</sup> (1.538 to 17.241 microns)
- Instrumental resolution based on maximum interferometer displacement is 0.112 cm<sup>-1</sup>
- Spectral interval after 2X zero-filling interferogram and 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 ( $\alpha=0.90$ ,  $\epsilon=500$ )
- 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<sup>2</sup> (transmission squared), all absorbance values  $\geq 1.6$  are given zero weight
- Calculated and estimated errors: Type A = 0.55%, Type B  $\leq 7\%$
- Frequency correction (already applied):  $V(\text{corrected})=V(\text{instrument}) * 0.9999987 - 4.24224 \times 10^{-4}$
- Axis units: X=wavenumbers (cm<sup>-1</sup>), Y=Absorbance (base-10)

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