

All data taken at Pacific Northwest National Laboratory (PNNL)

Operators: Steven W. Sharpe, Timothy J. Johnson and Robert L. Sams : sw.sharpe@pnl.gov

Version 1.0, November, 04

Composite spectrum for C6F6_25T

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

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

Sample Conditions-

- Chemical name and CAS number: Hexafluorobenzene, perfluorobenzene, C₆F₆ : [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/cm³
- Supplier and stated purity: Aldrich, 99.9+%
- Sample class: I (PNNL scale).
- Temperature of White cell (815.76 cm optical path length) 25 ± 2 C
- Diluent (high purity nitrogen) flowed at 25.20 liter/min (21.1° C), ambient atmospheric pressure 760 ± 5 Torr.
- Samples flowed at 2.000, 5.000, 1.000, 4.000, 0.600, 15.000, 1.200, 10.000, 2.500, 7.000, 3.000, 20.000, 0.800 and 55.000 microliters/minute
- Individual samples at equivalent pressures of 0.012515, 0.031280, 0.006254, 0.025007, 0.003750, 0.093703, 0.007495, 0.062427, 0.015601, 0.043676, 0.018713, 0.124721, 0.004988 and 0.34275 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⁻¹ (1.538 to 17.241 microns)
- Instrumental resolution based on maximum interferometer displacement is 0.112 cm⁻¹
- Spectral interval after 2X zero-filling interferogram and 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: 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⁻¹

Post Processing and Related Parameters-

- Non-linearity detector correction (Bruker proprietary) applied to interferogram ($\alpha=0.90$, $\epsilon=500$)
- Composite spectrum created from 14 individual absorbance (base-10) spectra via classical least squares fit: Intercept=0, slope is fitted, individual absorbance values weighted by T² (transmission squared), all absorbance values ≥ 1.6 are given zero weight
- Calculated and estimated errors: Type A = 0.41%, 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⁻¹), Y=Absorbance (base-10)

- Baseline correction via 9th order polynomial subtraction