

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for HCB_D_25T

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

Equivalent concentration x path-length of composite spectrum: 1.0736×10^{-5} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: Hexachloro-1,3-butadiene, 1,1,2,3,4,4-hexachloro-1,3-butadiene, HCDB, perchlorobutadiene, dolen-pur, gp-40-66, Cl₂C=CClCCl=CCl₂ : [87-68-3]
- Physical properties: MW=260.762 g/mole, mp=-22° C, bp= 215° C, Density (20 C) 1.665 g/cm³
- Supplier and stated purity: Aldrich, 97%
- 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, 0.500, 4.000, 7.000, 3.000, 0.700, 12.000, 1.500, 5.000, 22.000, 1.000, 8.000, 31.000 and 10.000 microliters/minute
- Individual samples at equivalent pressures of 0.009123, 0.002280, 0.018246, 0.031935, 0.013686, 0.003193, 0.055465, 0.006840, 0.022802, 0.100313, 0.004560, 0.036478, 0.141350 and 0.045603 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 530 cm⁻¹ (1.538 to 18.868 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 =1.23%, 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 7th order polynomial subtraction
- Trace carbon dioxide features removed via spectral subtraction