

All data taken at Pacific Northwest National Laboratory (PNNL)
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Composite spectrum for F114_5T

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

Sample Conditions-

- Chemical name and CAS number: Freon-114, 1,2-dichlorortetrafluoroethane, sym-dichlorortetrafluoroethane, fluorocarbon-114, tetrafluorodichloroethane, $\text{CClF}_2\text{CClF}_2$: [76-14-2]
- Physical properties: M.W. 121 AMU, F.P. -94 C , B.P. 3.8 C
- Supplier and stated purity: Aldrich, 99+%
- Sample class: I (PNNL scale)
- Temperature of sample $5.03 \pm 0.02\text{ C}$
- Diluent: Sample back filled with ultra high purity nitrogen to $760 \pm 5\text{ Torr}$
- Individual samples 1.0344, 2.0532, 3.0097, 4.0130, 10.0778, 1.5059, 2.6058 and 3.5624 Torr. Path length = 19.96 cm. Final data is a composite spectrum.
- Preparation: Multiple freeze-thaw cycles at 77K followed by multiple pumpings -80 C to remove carbon dioxide.

Instrument Parameters-

- Bruker-120HR FTIR, evacuated optics bench
- Spectral range: $5,000\text{ to }600\text{ cm}^{-1}$ (1.54 to 16.67 microns)
- Instrumental resolution (interferogram): 0.1 cm^{-1}
- Spectral intervals after 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: 9 (Bruker arbitrary)
- Number of interferograms averaged per single channel spectra: 256
- Detector: Mid-band HgCdTe, photoconductive, 77K operation
- Folding limits: $15798\text{ to }0\text{ cm}^{-1}$

Post Processing and Related Parameters-

- Non-linearity detector correction (Bruker proprietary) applied to interferogram ($\alpha=0.85$, $\beta=530$)
- Composite spectrum created from 8 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 = 0.31%, Type B = 3%
- Frequency correction: $V(\text{corrected}) = V(\text{instrument}) * 1 + 0$
- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Trace water features removed from composite spectrum. Baseline straightened between 5000 and 3500 cm^{-1} .