

All data taken at Pacific Northwest National Laboratory (PNNL)  
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Version 1.0, September, 1999

Composite spectrum for F114\_50T

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  $50.02 \pm 0.02$  C
- Diluent: Sample back filled with ultra high purity nitrogen to  $760 \pm 5$  Torr
- Individual samples 1.0040, 2.0661, 3.1480, 4.0911, 10.3319, 1.5005, 2.5355 and 3.6585 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:  $5,000$  to  $600$   $\text{cm}^{-1}$  (1.54 to 16.67 microns)
- Instrumental resolution (interferogram):  $0.1$   $\text{cm}^{-1}$
- Spectral intervals after FFT:  $0.06$   $\text{cm}^{-1}$
- 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:  $15798$  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 = 0.24%, Type B = 3%
- Frequency correction:  $V(\text{corrected}) = V(\text{instrument}) * 1 + 0$
- Axis units: X=wavenumbers ( $\text{cm}^{-1}$ ), Y=Absorbance (base-10)
- Trace water features removed from composite spectrum. Baseline straightened between  $5000$  and  $3500$   $\text{cm}^{-1}$ .