

All data taken at Pacific Northwest National Laboratory (PNNL)
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Composite spectrum for F134A_50T

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

Sample Conditions-

- Chemical name and CAS number: Freon-134a, 1,1,1,2-Tetrafluoroethane, HFC-134a, FCH_2CF_3 : [811-97-2]
- Physical properties: M.W. 102 AMU, F.P. -101 C, B.P. -26.5 C
- Supplier and stated purity: Aldrich, 99+%
- Sample class: I (PNNL scale)
- Temperature of sample 50.04 ± 0.02 C
- Diluent: Sample back filled with ultra high purity nitrogen to 760 ± 5 Torr
- Individual samples 1.03360, 2.0955, 1.4515, 3.6392 and 9.8010 Torr. Path length = 19.96 cm. Final data is a composite spectrum.
- Preparation: Multiple freeze-thaw cycles at 77K followed by multiple pumpings -35 C to remove carbon dioxide and carbon monoxide. Sample used at -35 C to minimize water.
- **Instrument Parameters-**
- Bruker-120HR FTIR, evacuated optics bench
- Spectral range: 5,000 to 600 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 to 0 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 5 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 = 0.48%, Type B = 3%
- Frequency correction: $V(\text{corrected}) = V(\text{instrument}) * 1 + 0$
- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Water features observed and removed from composite spectrum.