

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for TCE111_5T

Effective burden of composite spectrum: 1 part-per-million-meter 5.492410^{-6} grams/liter-meter

[Composite spectrum corrected for contamination of 1,1-Dichloroethene \[0.50%\] by rescaling.](#)

Sample Conditions-

- Chemical name and CAS number: 1,1,1-Trichloroethane, 1,1,1-tce, aethane tt, alpha-trichloroethane, solvent 111, methyl chloroform, CH_3CCl_3 ; [71-55-6]
- Physical properties: fw=133.4047 g/mole, fp=-32.6° C, bp=74.1° C
- Supplier and stated purity: Aldrich, 99.5%
- Sample class: I (PNNL scale).
- Temperature of sample: 4.91 ± 0.02 C
- Diluent: Sample back filled with ultra high purity nitrogen to 760 ± 5 Torr
- Individual samples at 1.09865, 2.0894, 0.49385, 8.0748, 4.3218, 17.85, and 31.95 Torr. Path length = 19.96 cm. Final data is a composite spectrum.
- Preparation: Multiple freeze-thaw cycles at 77 K to remove air.

Instrument Parameters-

- Bruker-66V FTIR, temperature controlled environment, evacuated optics bench
- Modified to include second aperture, between interferometer output and sample cell. This substantially reduces both “ghosting” and warm aperture effects.
- Spectral range: 6,500 to 500 cm^{-1} (1.534 to 20.000 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 ($\alpha=0.85$, $\beta=530$)
- Composite spectrum created from 7 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 = 1.74%, Type B $\leq 3\%$
- Frequency correction (already applied): $V(\text{corrected}) = V(\text{instrument}) * 0.99999896 + 8.812 \times 10^{-4}$
- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Trace carbon dioxide and 1,1-dichloroethene features removed via spectral subtraction
- Baseline correction via 7th order polynomial subtraction