All data taken at Pacific Northwest National Laboratory (PNNL)
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Composite spectrum for TCE_5T
Effective burden of composite spectrum: 1 part-per-million-meter (ppm-meter) at 296 K
Equivalent concentration x path-length of composite spectrum: 5.0409×10^{-6} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: Trichloroethylene, TCE, Ethinyl trichloride, Acetylene trichloride, ethylene trichloride, triciene, 1,1,2-Trichloroethylene, Tri, trichloroethene, Tri-Clene, Trielene, Trilene, Trichloran, Trichloren, Algylen, Trimar, Triline, Trethylene, Westrosol, Chlorylen, Gemalgene, Germalgene, 1,1,2-trichloroethene, 1-chloro-2,2-dichloroethylene, 1,1-dichloro-2-chloroethylene, 1,2,2-trichloroethylene, anamenth, benzinol, blacosolv, blancosolv, cecolene, chlorilen, chlorylea, chorylen, circosolv, crawhaspol, densinfluat, dow-tri, dukeron, fleck-flip, flock flip, fluate, lanadin, lethurin, narcogen, narkogen, narkosoid, Nialk, perm-a-chlor, perm-a-clor, petzinol, philex, threthylene, Triad, Trial, triasol, triklone, Triol, tri-plus, tri-plus m, vestrol, vitran, trieline, Trichlorathane, $ClHC=CCl_2$: [79-01-6]
- Physical properties: fw=131.3889 g/mole, fp=–84.8° C, bp=8.67° C
- Supplier and stated purity: Aldrich, 99.5+%
- Sample class: I (PNNL scale).
- Temperature of sample: 5.07 ± 0.02 C
- Diluent: Sample back filled with ultra high purity nitrogen to 760±5 Torr
- Individual samples at 1.10835, 4.2810, 2.2215, 23.72, 12.54 and 7.9065 Torr. Path length = 19.94 cm. Final data is a composite spectrum.
- Preparation: Multiple freeze-thaw cycles at -100 C 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 600 cm^{-1} (1.534 to 16.667 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 (α=0.85, ε=530)

- Composite spectrum created from 6 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 = 0.42%, Type B ≤ 3%
- Frequency correction (already applied): V(corrected) = V(instrument)*0.999997+5.18x10^{-4}
- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Trace carbon dioxide features removed from composite spectrum via spectral subtraction
- Baseline correction via 7^{th} order polynomial subtraction