

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for TCE\_25T

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

Equivalent concentration x path-length of composite spectrum:  $5.0409 \times 10^{-6}$  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,  $\text{ClHC}=\text{CCl}_2$  : [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:  $25.00 \pm 0.02$  C
- Diluent: Sample back filled with ultra high purity nitrogen to  $760 \pm 5$  Torr
- Individual samples at 1.13065, 2.0170, 16.45, 8.6875, 32.12, 4.2298, 3.1440, 24.58, 12.20 and 6.2456 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  $600 \text{ cm}^{-1}$  (1.534 to 16.667 microns)
- Instrumental resolution based on maximum interferometer displacement is  $0.112 \text{ cm}^{-1}$
- Spectral interval after 2X zero-filling interferogram and 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: 60KHz (HeNe crossing frequency)
- Number of interferograms averaged per single channel spectra: 256
- Detector: Mid-band HgCdTe, photoconductive, 77K operation
- Folding limits:  $15798$  to  $0 \text{ cm}^{-1}$

### Post Processing and Related Parameters-

- Non-linearity detector correction (Bruker proprietary) applied to interferogram (  $\alpha=0.85$ ,  $\beta=530$ )

- Composite spectrum created from 10 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 = 0.40%, Type B = 3%
- Frequency correction (already applied):  $V(\text{corrected}) = V(\text{instrument}) * 0.999997 + 5.18 \times 10^{-4}$
- Axis units: X=wavenumbers ( $\text{cm}^{-1}$ ), Y=Absorbance (base-10)
- Trace carbon dioxide vapor features removed via spectral subtraction
- Baseline correction via 7<sup>th</sup> order polynomial subtraction