

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for CLETHOH_25T

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

Equivalent concentration x path-length of composite spectrum: 3.315×10^{-6} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: 2-Chloroethanol, ethylene chlorohydrin, 2-chloroethyl alcohol, glycol chlorohydrin, $\text{ClCH}_2\text{CH}_2\text{OH}$: [107-07-3]
- Physical properties: fw=80.51 g/mole, fp=-62.6° C, bp=128.7° C
- Supplier and stated purity: Aldrich, 99%. Unknown contaminant feature at 1368 cm^{-1} .
- Sample class: II (PNNL scale). Sample soluble in Viton O-rings and difficult to handle.
- Temperature of sample: 25.03 ± 0.02 C
- Diluent: Sample back filled with ultra high purity nitrogen to 760 ± 5 Torr
- Individual samples at 1.01750, 1.09950, 2.1025, 4.3000, 3.1868, 1.5340, 3.5303 and 2.6680 Torr. Path length = 19.94 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: 7,150 to 600 cm^{-1} (1.399 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 ($\alpha = 0.85$, $\beta = 530$)
- 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 = 1.40%, Type B = 5%
- Frequency correction (already applied): $V(\text{corrected}) = V(\text{instrument}) * 0.999997 + 5.18 \times 10^{-4}$
- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Trace water vapor (0.49%) and carbon dioxide (0.17%) corrected for and removed via spectral subtraction. Residual CO_2 features still observable due to pressure effects.
- Baseline correction via 7th order polynomial subtraction