

All data taken at Pacific Northwest National Laboratory (PNNL)
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Composite spectrum for PROCAR_25T

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

Equivalent concentration x path-length of composite spectrum: 4.203×10^{-6} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: Propylene carbonate; 1,3-Dioxolan-2-one, 4-methyl-; Carbonic acid, cyclic propylene ester; Cyclic methylethylene carbonate; Cyclic propylene carbonate; Cyclic 1,2-propylene carbonate; Propylene glycol cyclic carbonate; 1-Methylethylene carbonate; 1,2-Propanediol carbonate; 1,2-Propanediol cyclic carbonate; 1,2-Propanediyl carbonate; 1,2-Propylene carbonate; 4-Methyl-1,3-dioxolan-2-one; 1,2-Propylene glycol carbonate; 4-Methyl-1,3-dioxol-2-one; Dipropylene carbonate; 4-Methyldioxalone-2; 4-Methyl-2-oxo-1,3-dioxolane; 1,2-PDC; Propylenester kyseliny uhlicite; Arconate propylene carbonate; $C_4H_6O_3$: [108-32-7]
- Physical properties: MW=102.0886 g/mole, mp=-50.2° C, bp=240° C, Density (25 C) = 1.205 g/cm³
- Supplier and stated purity: Sigma Aldrich, 99%
- Sample class: I (PNNL scale).
- Temperature of White cell (805.0 cm optical path length) 25 ± 2 C
- Diluent (high purity nitrogen) flowed at 23.3 liter/min (21.1° C), ambient atmospheric pressure 760 ± 5 Torr.
- Samples flowed at microliters/minute 2.000, 4.000, 5.000, 1.000, 2.500, 0.500, 1.500, 3.000, 3.500, 4.500, 1.250, 2.250, 1.750 and 2.750.
- Individual samples at equivalent pressures of 0.018661, 0.037322, 0.046652, 0.009329, 0.023326, 0.004665, 0.013990, 0.027980, 0.032652, 0.041992, 0.011665 0.020999, 0.016332 and 0.025659 Torr. Final data is a composite spectrum.
- Preparation: None

Instrument Parameters-

- Bruker-66V FTIR, evacuated optics bench.
- Modified to include second aperture, between interferometer output and White cell. This substantially reduces both “ghosting” and warm aperture effects.
- Spectral range: 6,500 to 600 cm⁻¹ (1.538 to 16,67 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 ($\alpha=0.90$, $\epsilon=500$)
- Composite spectrum created from 14 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 =2.63%, Type B $\leq 7\%$
- Frequency correction (already applied): $V(\text{corrected})=V(\text{instrument})\cdot 0.9999991-3.45278\times 10^{-4}$
- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Trace carbon dioxide and carbon monoxide were removed by spectral subtraction and several small impurity features were detected through the deviation vector at 1791.5, 1177.6, 1050.9, 774.3 and 729.4 cm^{-1} . The feature at 1791.5 was removed.
- Baseline correction via 7th order polynomial subtraction