

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for CYCLODEC\_50T

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

Equivalent concentration x path-length of composite spectrum:  $5.7749 \times 10^{-6}$  grams/liter-meter

### Sample Conditions-

- Chemical name and CAS number: Cyclodecane,  $C_{10}H_{20}$  : [293-96-9]
- Physical properties: MW=140.268 g/mole, mp=10° C, bp=202° C, Density (20 C) 0.858 g/cm<sup>3</sup>
- Supplier and stated purity: Aldrich, 95%
- Sample class: I (PNNL scale).
- Temperature of White cell (805.0 cm optical path length)  $50 \pm 2$  C
- Diluent (high purity nitrogen) flowed at 23.3 liter/min (21.1° C), ambient atmospheric pressure  $760 \pm 5$  Torr.
- Samples flowed at 3.000, 6.000, 12.000, 2.000, 8.000, 4.000, 10.000, 15.000, 5.000, 7.000, 11.000, 9.000, 20.000, 17.000 and 3.500 microliters/minute
- Individual samples at equivalent pressures of 0.014358, 0.028716, 0.057424, 0.009559, 0.038227, 0.019111, 0.047777, 0.071657, 0.023886, 0.033431, 0.052527, 0.042971, 0.095466, 0.081136 and 0.016698 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 16.667 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 ( $\alpha=0.90$ ,  $\epsilon=500$ )
- Composite spectrum created from 15 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  $\geq 1.6$  are given zero weight
- Calculated and estimated errors: Type A = 0.58%, Type B  $\leq 7\%$
- Frequency correction (already applied):  $V(\text{corrected})=V(\text{instrument}) * 0.99999959 - 3.45278 \times 10^{-4}$
- Axis units: X=wavenumbers ( $cm^{-1}$ ), Y=Absorbance (base-10)

- Trace water vapor features removed by spectral subtraction
- Baseline correction via 9<sup>th</sup> order polynomial subtraction