

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for ISOFORN\_50T

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

Equivalent concentration x path-length of composite spectrum:  $5.6901 \times 10^{-6}$  grams/liter-meter

### Sample Conditions-

- Chemical name and CAS number: Isophorone, 1,1,3-trimethyl-3-cyclohexene-5-one, 1,5,5-trimethyl-1-cyclohexen-3-one, isoacetophorone, isoforon,  $C_9H_{14}O$  : [78-59-1]
- Physical properties: MW=138.209 g/mole, mp=-8° C, bp=213.5° C, Density (20 C) 09229 g/cm<sup>3</sup>
- Supplier and stated purity: Aldrich, 97%
- Sample class: I (PNNL scale).
- Temperature of White cell (796.0 cm optical path length)  $50 \pm 2$  C
- Diluent (high purity nitrogen) flowed at 24.2 liter/min (21.1° C), ambient atmospheric pressure  $760 \pm 5$  Torr.
- Samples flowed at 2.000, 4.000, 3.000, 1.000, 5.000, 7.000, 12.000, 15.000, 20.000, 25.000 and 30.000 microliters/minute
- Individual samples at equivalent pressures of 0.010018, 0.020030, 0.015023, 0.005007, 0.025028, 0.035034, 0.060050, 0.075053, 0.100044, 0.125039 and 0.150026 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 11 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 = 0.40%, 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 ( $\text{cm}^{-1}$ ), Y=Absorbance (base-10)
- Trace water vapor and  $\text{CO}_2$  features removed by spectral subtraction
- Baseline correction via 7<sup>th</sup> order polynomial subtraction