

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for ICUMENE_25T

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

Equivalent concentration x path-length of composite spectrum: 4.9485×10^{-6} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: Isocumene, n-propylbenzene, propylbenzene, 1-phenylbenzene, $C_6H_5C_3H_7$: [103-65-1]
- Physical properties: MW=120.1938 g/mole, mp=-101.6° C, bp=159° C, Density (20 C) 0.862 g/cm³
- Supplier and stated purity: Aldrich, 98+%
- Sample class: I (PNNL scale).
- Temperature of White cell (796.0 cm optical path length) 25 ± 2 C
- Diluent (high purity nitrogen) flowed at 24.2 liter/min (21.1° C), ambient atmospheric pressure 760 ± 5 Torr.
- Samples flowed at 2.000, 5.000, 3.500, 7.000, 12.000, 24.000, 48.000, 60.000, 36.000, 18.000, 30.000 and 10.000 microliters/minute
- Individual samples at equivalent pressures of 0.010808, 0.027019, 0.018914, 0.037817, 0.064804, 0.129573, 0.259112, 0.323847, 0.194257, 0.097103, 0.161816 and 0.053932 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 12 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 = 0.14%, 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 from composite spectrum by spectral subtraction
- Baseline correction via 9th order polynomial subtraction