

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for SEXTONE_50T

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

Equivalent concentration x path-length of composite spectrum: 4.0407×10^{-6} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: Cyclohexanone, sextone, cyclohexyl ketone, anone, ketocyclohexane, nadone, pimelic ketone, oxocyclohexane, $C_6H_{10}(=O)$: [108-94-1]
- Physical properties: M.W. 98.144 amu, F.P. $-47^\circ C$, B.P. $165^\circ C$, Density (20 C) 0.947 g/cm^3
- Supplier and stated purity: Aldrich, 99+%
- Sample class: I (PNNL scale).
- Temperature of White cell (815.76 cm optical path length) $50 \pm 2 C$
- Diluent (high purity nitrogen) flowed at 25.20 liter/min ($21.1^\circ C$), ambient atmospheric pressure 760 ± 5 Torr.
- Samples flowed at 2.000, 0.500, 7.000, 15.000, 3.000, 6.000, 22.000, 1.500, 10.000, 4.000, 0.700, 5.000, 8.000 and 33.000 microliters/minute
- Individual samples at equivalent pressures of 0.014032, 0.003508, 0.049088, 0.105202, 0.021040, 0.042081, 0.154275, 0.010517, 0.070107, 0.028039, 0.004907, 0.035053, 0.056108 and 0.231413 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 550 cm^{-1} (1.538 to 18.182 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 = 0.57%, Type B $\leq 7\%$
- Frequency correction (already applied): $V(\text{corrected})=V(\text{instrument}) * 0.9999987 - 4.24224 \times 10^{-4}$

- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Baseline correction via 5th order polynomial subtraction
- Trace water vapor features removed via spectral subtraction