

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for DMCC_25T

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

Equivalent concentration x path-length of composite spectrum: 4.4275×10^{-6} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: Dimethylcarbonyl chloride, DMCC, chloroformic acid dimethylamide, N,N-dimethylcarbonyl chloride, TL-389, $(\text{CH}_3)_2\text{N}-\text{C}(\text{O})\text{Cl}$: [79-44-7]
- Physical properties: MW=107.5395 g/mole, mp=-33° C, bp=165° C, Density (20 C) 1.168 g/cm³
- Supplier and stated purity: Aldrich, 98+%
- Sample class: I (PNNL scale).
- Temperature of White cell (815.76 cm optical path length) 25 ± 2 C
- Diluent (high purity nitrogen) flowed at 25.20 liter/min (21.1° C), ambient atmospheric pressure 760 ± 5 Torr.
- Samples flowed at 2.000, 3.000, 0.700, 8.000, 1.200, 7.000, 1.500, 12.00, 1.000, 5.000, 23.00, 10.00, 0.800 and 33.00 microliters/minute
- Individual samples at equivalent pressures of 0.015912, 0.023871, 0.005569, 0.063663, 0.009548, 0.055698, 0.011938, 0.095495, 0.007961, 0.039805, 0.183104, 0.079621, 0.006370 and 0.26281 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 540 cm^{-1} (1.538 to 18.519 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 = 0.91%, Type B $\leq 7\%$

- Frequency correction (already applied): $V(\text{corrected})=V(\text{instrument})\cdot 0.9999987-4.24224\times 10^{-4}$
- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Baseline correction via 7th order polynomial subtraction
- Trace CO_2 and HCl features removed by spectral subtraction