

All data taken at Pacific Northwest National Laboratory (PNNL)

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Composite spectrum for NOCL\_5T

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

Equivalent concentration x path-length of composite spectrum:  $2.695 \times 10^{-6}$  grams/liter-meter

Corrected for contamination of NO [0.43%], NO<sub>2</sub>[0.25%] and HCl [0.1%].

### Sample Conditions-

- Chemical name and CAS number: Nitrosyl chloride, NOCl : [2696-92-6]
- Physical properties: fw=65.4591 g/mole, fp=-61.5° C, bp=-5.5° C
- Supplier and stated purity: Atomergic Chemicals Corp., 98%
- Sample class: II (PNNL scale). Extremely reactive. In equilibrium with NO + Cl<sub>2</sub>
- Temperature of sample:  $4.93 \pm 0.02$  C
- Diluent: Sample back filled with ultra high purity nitrogen to 760±5 Torr
- Individual samples at 0.45400, 1.09600, 0.38570, 5.5740, 12.73 and 6.2815 Torr. Path length = 19.96 cm. Final data is a composite spectrum.
- Preparation: Multiple freeze-thaw cycles at -100 C to contaminants.

### Instrument Parameters-

- Bruker-66V FTIR, temperature controlled environment, evacuated optics bench
- Modified to include second aperture, between interferometer output and sample cell. This substantially reduces both “ghosting” and warm aperture effects.
- Spectral range: 6,500 to 545 cm<sup>-1</sup> (1.534 to 18.349 microns)
- Instrumental resolution based on maximum interferometer displacement is 0.112 cm<sup>-1</sup>
- Spectral interval after 2X zero-filling interferogram and FFT: 0.06 cm<sup>-1</sup>
- 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<sup>-1</sup>

### Post Processing and Related Parameters-

- Non-linearity detector correction (Bruker proprietary) applied to interferogram (  $\alpha=0.85$ ,  $\beta=530$ )
- Composite spectrum created from 6 individual absorbance (base-10) spectra via classical least squares fit: Intercept=0, slope is fitted, individual absorbance values weighted by T<sup>2</sup> (transmission squared), all absorbance values  $> 1.6$  are given zero weight
- Calculated and estimated errors: Type A = 0.70%, Type B = 5%
- Frequency correction (already applied):  $V(\text{corrected}) = V(\text{instrument}) * 0.99999896 + 8.812 \times 10^{-4}$
- Axis units: X=wavenumbers (cm<sup>-1</sup>), Y=Absorbance (base-10)
- Trace NO, NO<sub>2</sub>, HCl and CO<sub>2</sub> features removed via spectral subtraction
- Baseline correction via 7<sup>th</sup> order polynomial subtraction