IARPA MORGOTH'S CROWN: Spectroscopic Unit Conversions

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Spectroscopic Unit Conventions

An IR spectra are usually plotted as absorbance or transmittance as a function of wavelength (λ) in microns (µm) or wavenumbers (cm-1). Often wavenumbers and wavelength are used interchangeably and can be converted using the equation below:

$$\lambda(\mu\mathrm{m}) = \frac{10^{-4}}{\mathrm{cm}^{-1}}$$

Region	Wavelength λ (µm)	Wavenumbers (cm-1)
NIR	0.78 - 2.5	12,800 – 4000
MWIR	2.5 - 50	4000 – 200
LWIR	50 - 100	200 – 10

Absorption or transmittance is typically used for liquid and gaseous samples, or samples which an excitation source can pass through. The mathematical relationships between these quantities, where T is Transmittance, %T is Percent Transmittance, P is the optical power that passes through a sample, P0 is the input optical power, and A is the absorbance are:

Transmittance, T = P / P0

% Transmittance, %T = 100 T

Absorbance,

A = log10 P0 / P

A = log10 1 / T

A = log10 100 / %T

A = 2 - log10 %T

The Beer-Lambert Law states that in the low-concentration regime (where absorbance of light by the sample is linear):

A=ebc

Where A is absorbance

e is the molar absorbtivity with units of L mol-1 cm-1

b is the path length of the sample in cm

c is the concentration of the compound in solution, expressed in mol L-1

For optically thick samples, such as bulk material pellets or surfaces, we rely on reflectivity measurements. In reflectance IR, the excitation source interacts with surface molecules and the energy reflected back to the detector and analyzed. A plot of reflectance versus wavelength or wavenumber resembles the transmission spectrum. Reflectance intensity is often labelled as a percentage (Reflectance %) as a function the ratio of the reflected intensity of sample to a nonabsorbing standard.