Units and Conversion Between Units for the PNNL/DOE Infrared Spectral Library

The digital spectral files correspond to *Absorbance* for a sample concentration of one part-per-million (ppm) over an optical path length of one meter (m) at a temperature of 296 Kelvin (K). The units of the Y-axis for the PNNL/DOE library are of $ppm^{-1}\ m^{-1}$.

Absorbance is derived by taking the logarithmic ratio of the transmittance and is unitless. Consequently, one must define what base the logarithmic operation is performed in- "base-e" or base-10". The former is know as the "natural" or "Naperian" *ln* while the latter is referred to as decadic or *log10*. Transmittance is defined as follows:

$$\text{Transmittance} = T = \frac{I}{I_0},$$

where I and I_0 correspond to the incident radiation after and before passing through the sample, respectively. Absorbance is defined as follows:

$$\text{Absorbance} = A = -\log_{10}(T)$$

or

$$\text{Absorbance} = A = -\ln(T)$$

Note that the spectral library is in "base-10" absorbance values and needs to be multiplied by *ln(10)* to convert to naperian units. For example, HITRAN values are always taken as "base-e". In contrast, most analytical chemists use "base-10" values of absorbance.

Conversion between $ppm^{-1}\ m^{-1}$ to other common units are follows:

Decadic or *log-10* conversion

To convert to units of	Multiply PNNL/DOE data by
mole μmole^{-1} m^{-1}	1
torr^{-1} cm^{-1}	13.15789
atm^{-1} m^{-1}	10^6
cm^2 molecule^{-1}	4.03328×10^{-16}

Naperian or *ln* conversion

To convert to units of	Multiply PNNL/DOE data by
mole μmole^{-1} m^{-1}	2.30259
torr^{-1} cm^{-1}	30.29716
atm^{-1} m^{-1}	2.30259×10^6
cm^2 molecule^{-1}	9.28697×10^{-16}

The spectral library corresponds to a concentration (ratio of sample to buffer gas) and the actual number of molecules per unit-volume will depend on the temperature. Regardless of the stated temperature (5, 25 or 50 ˚C), all data sets have been re-normalized to 22.84 ˚C (296 K).

Some useful physical constants:
Loschmidt number = $n_0 = 2.6867773 \times 10^{25}$ molecules m^{-3} (1 atm, 273.15 K)
1 atm = 101.325 KPa
Molar gas constant = R = 8.314 472 J mole^{-1} K^{-1}
Avegadro constant = $N_A = 6.022\ 1415 \times 10^{23}$ molecules mole^{-1}