

Procedure for Calculating Optical Constants

This file describes how to compute optical constants (wavenumber, n , k) of an ice at near- and mid-infrared wavenumbers from a thin-film sample. The procedure requires laboratory spectra of a sample and a background in **reflectance geometry**. The procedure uses a modification of the Gerakines and Hudson (2020) Python code. See the Gerakines and Hudson procedures for computing optical constants for laboratory spectra in transmission geometry.

1. Obtain a laboratory spectrum of an ice sample in **reflectance geometry** with a known thickness and index of refraction at a visible wavelength. Obtain a reference (background) spectrum. Compute the absorbance spectrum using

$$absorbance = -\log_{10} \left(\frac{sample}{reference} \right)$$

and store the result in a two-column ASCII file (wavenumber absorbance). If necessary, adjust the baseline to zero. See our example file <abs_CH4_30K_Fig5a.txt>.

2. Store the optical constants of the substrate in a three-column ASCII file (wavenumber, n , k). See our example file for a gold substrate <au_nk.txt>.
3. Create an ASCII parameter file with the name <icenk-inputfile.txt>. See our examples in <icenk-inputfile.txt>. The file ReadMe_Parameters gives an alphabetical list of all the input parameters. Not all of these parameters are necessary to compute optical constants.
4. Run icenk.py on a computer with Python3. A window will open displaying the values of experimental absorbance, computed absorbance, n , k , and fractional difference between experiment and computed absorbance as the iteration proceeds.
5. Examine the ASCII output file (wavenumber, computed absorbance, n , k).