# Instructions for using the *icenk* program

Note that all ASCII files are assumed to be whitespace-delimited, plain-text format, unless the file extension is given as *.CSV* (or *.csv*).

**Basic procedure:**

I. Prepare a laboratory infrared spectrum of a film with known thickness and visible-wavelength refractive index. Measure the infrared spectrum and the thickness of a thin film in transmission mode on a substrate with known optical constants (or refractive index). The refractive index of the film material at visible energies must be known. Flatten the baseline to remove channel fringes and set the baseline to zero absorption (or to a transmittance of 1). Store the spectrum in a 2-column ASCII file (wavenumber, spectrum). See example1-spectrum.txt for an example.

II. Prepare the optical constants of the substrate. Store the optical constants of the substrate in a 3-column ASCII file (wavenumber, n, k). See kbr-nk.txt and csi-nk.txt for examples for two commonly used IR-transparent substrates (KBr and CsI).

III. Prepare the input file. Create an ASCII file with all input parameters and their values. See the description of example1-inputfile.txt below. The default name for the input file is icenk-inputfile.txt, but can be specified if the code is run from the command line.

IV. Run the code.
   - In Windows 10: double-click on icenk.exe to run the code.
   - In Linux or other operating system where python3 is installed: from a command prompt, enter the directory where the code is found and type *python icenk.py*. The name of the input file can be added as a command-line argument, otherwise the default input filename icenk-inputfile.txt will be assumed.

   By default, a window will open to display iteration progress in several plots. All messages written to the text window will be appended to the file icenk.log.

V. Check the output. If the algorithm converges on a solution, a 4-column plain ASCII file (wavenumber, calculated absorbance, n, k) is written with the results. See example1-output.txt for an example.

**Format of the input file:**

example1-inputfile.txt

```
## Example input file with minimal input parameters
comment             Amorphous CH3OH at 10K, n=1.314, 4 fringes, measured on a KBr substrate
file_output         example1-output.txt
file_spectrum       example1-spectrum.txt
file_substrate      kbr-nk.txt
thickness_cm        1.02E-04
visible_index       1.314
goal                1.00E-05
```

General format of each line: Column 1 contains the name of a parameter, and column 2 contains a value for that parameter. The names and values used in example1-inputfile.txt are described below. The file README-inputfiles.txt contains the complete list.

- **##**: any line that begins with "##" is ignored by the program
- **comment**: the string in column 2 will be copied to the output file
- **file_output**: the name of an ASCII file for output.
- **file_spectrum**: the name of an ASCII file containing the laboratory absorbance or transmittance spectrum from which the optical constants are to be derived.
- **file_substrate**: the name of an ASCII file containing the optical constants of the substrate material.
- **thickness_cm**: the thickness of the ice film, in units of centimeters (cm).
- **visible_index**: the value of *n* at a higher energy than is present in the spectrum, usually at a wavelength of a visible-light laser.
- **goal**: the desired maximum fractional deviation between the laboratory input spectrum and the spectrum that is calculated by the final values of *n* and *k*.