

Description of Parameters

The table below lists the possible parameters for <icenk-inputfile.txt> to run icenk.py. Except for <approx_terms> and <input_angle>, the parameters are the same as in Gerakines and Hudson (2020, Astrophysical Journal, Volume 901, Issue 1, id52, 10pp). The parameters <approx_terms> and <input_angle> must be specified in <icenk-input.txt>.

Parameter	Allowed Values	Default Value	Description
approx_terms	real number ≤ 0.01	none	Necessary for numerical diffraction of $d\ln R/dk$. Must be included in the input file
bak_interval	integer > 0	10	Number of iteration steps between saving a backup of the current iteration data
comment	string	none	Comment to be written at the top of the output file
file_bak	string	icenk-bak.tmp	Name of file where the current iteration data are stored
file_output	string	icenk.out	Name of output file
file_spectrum	string	spectrum.dat	Name of file containing input spectrum
file_start	string	none	Name of the file from which to load the initial values of n and k . Ignored unless value is other than an empty string
file_substrate	string	substrate.dat	Name of the file containing the substrate's n and k values
goal	real number > 0	1.0E-3	The calculation stops when the maximum fractional deviation falls below this value
input_angle	real number > 0	none	The incident angle of the beam upon the ice sample in degrees. Must be included in the input file
iteration_max	integer > 0	10000	Allowed maximum number of iterations
lorentz_hgt	real number > 0	0.01	Lorentzian height as a fraction of $ n_{\text{limit}} - n $. Ignored unless n_{fix} is True
lorentz_wid	real number	20 x resolution	Lorentzian width in units of wavenumbers. Default uses value of the resolution parameter. Ignored unless n_{fix} is True

n_fix	True, False	False	If True, attempt to compensate for values of n below n_limit
n_limit	real number	0.0	Minimum value of n allowed before a correction is applied. Ignored unless n_fix is True
plot_interval	integer > 0	1	Number of iteration steps between updates to the plots
plot_size	real number > 0	10	Size of plot window in inches
resolution	real number > 0	2 x wavenumber spacing	Resolution (in cm ⁻¹) of the input absorbance spectrum. Default is taken from the wavenumber spacing in spectrum
step	real number > 0	0.95	Initial fraction of the k-correction to be applied at each iteration step
step_adapt	True, False	False	If True, attempt to modify step according to current performance
step_dnrate	real number > 0	0.02	Scaling factor to determine how quickly the step size is decreased. Ignored unless step_adapt is True
step_interval	integer > 0	2	Number of iteration steps between attempts to modify the step. Ignored unless step_adapt is True
step_max	real number > 0	0.95	Maximum value allowed for the step parameter
step_min	real number > 0	1.0E-3	Minimum value allowed for the step parameter
step_uprate	real number > 0	0.01	Scaling factor to determine how quickly the step size is increased. Ignored unless step_adapt is True
thickness_cm	real number > 0	1.0E-4	Thickness of the ice sample in cm.
visible_index	real number > 0	1.0	Known refractive index of the ice at visible wavelengths
xrange1	real number => 0	max wavenumber	Start of wavenumber range to plot. Default is maximum value from spectrum.
xrange2	real number => 0	min wavenumber	End of wavenumber range to plot. Default is minimum value from spectrum.