

Parameter	Allowed Values	Default Value	Description
approx_terms	1, 2, or 3	1	Number of terms to use in the approximation of $d\ln T/dk$
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 the output file
file_spectrum	string	spectrum.dat	Name of the file containing the 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
iteration_max	integer > 0	10000	Allowed maximum number of iterations
laser_wavelength	real number > 0	6.7E-5	Wavelength (in cm) of the laser used to measure the thickness of the sample in fringes. Ignored unless thickness_fringes > 0
lorentz_hgt	real number > 0	0.01	Lorentzian height, as a fraction of $ n_{limit}-n $. Ignored unless n_fix is True
lorentz_wid	real number	$20 \times$ 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	10.0	Size of the plot window, in inches
resolution	real number ≥ 0	$2 \times$ wavenumber spacing	Resolution (in cm^{-1}) of the input absorbance spectrum. Default is taken from wavenumber spacing in spectrum

Parameter	Allowed Values	Default Value	Description
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.
thickness_fringes	real number ≥ 0	0.0	Thickness of the ice sample, in number of laser interference fringes. Used with laser_wavelength to calculate the thickness in cm. Overrides any value given by thickness_cm. Ignored if value = 0
visible_index	real number > 0	1.0	Known refractive index of the ice at visible wavelengths
xrange1	real number ≥ 0 , default	max wavenumber	Start of wavenumber range to plot. Default is maximum value from spectrum.
xrange2	real number ≥ 0 , default	min wavenumber	End of wavenumber range to plot. Default is minimum value from spectrum.