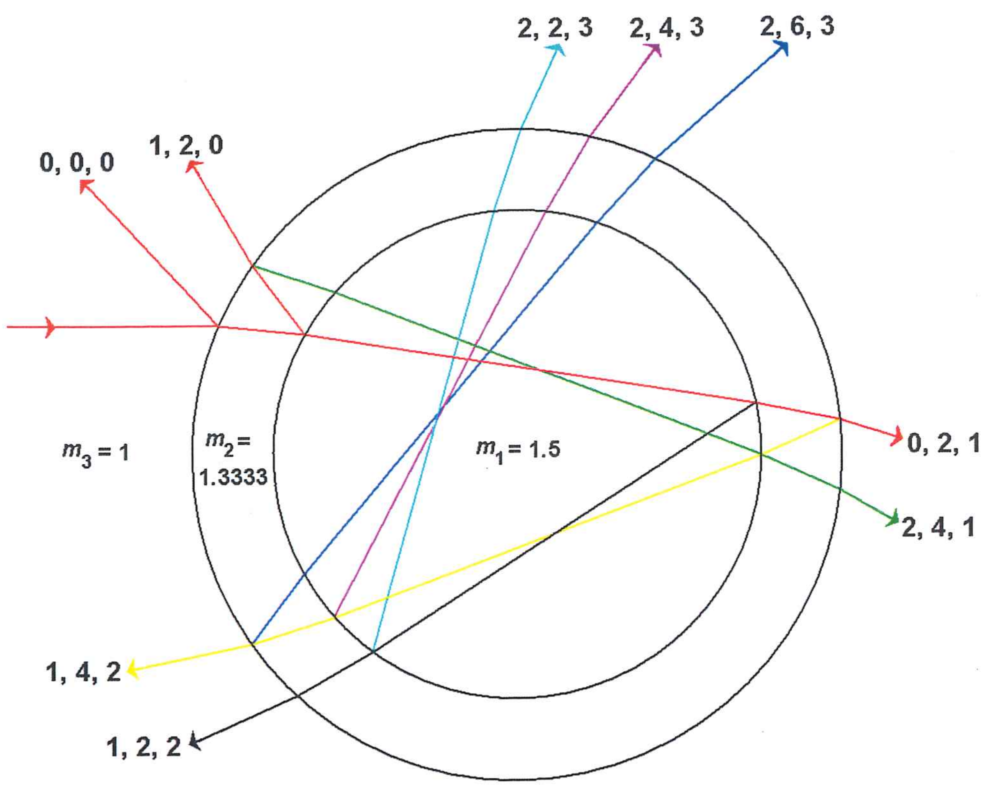
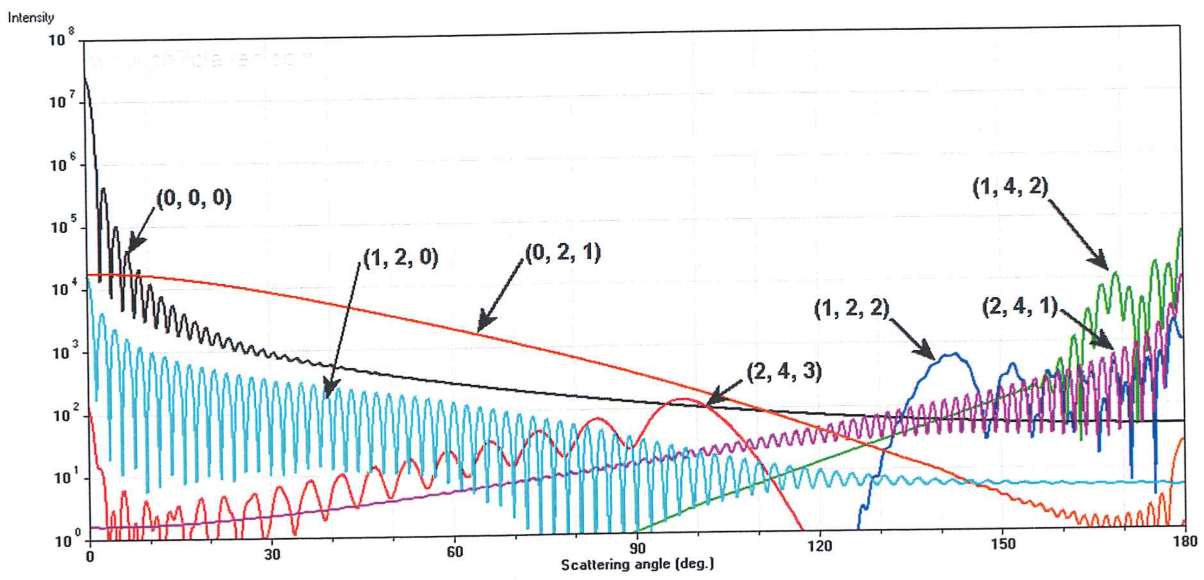
Coated particles



Some geometric ray paths occurring within the coated sphere.
The ray paths are designated by (N, A, B) - see below for further explanation.

Scattering of light by a coated sphere which consists of a spherical core surrounded by a concentric shell or mantle.

N = no. of internal reflections
A = no. of chords in shell A
B = no. of chords in shell B.



Intensity as a function of scattering angle θ calculated using the Aden-Kerker solution for scattering of red light (λ = 0.65 µm = 650 nm) by a coated sphere with a spherical core with refractive index m1 = 1.5, surrounded by a shell with refractive index m2 = 1.3333 immersed in a medium of refractive index m3 = 1. The radius of the core a12 = 7.5 µm and the shell has a thickness of 2.5 µm, giving a total radius of a23 = 10 µm.... Fig isolates the Debye series contributions corresponding to specific ray trajectories (for perpendicular polarisation).

www.philiplaven.com/p8K1.html

05/10/17

In order to use Omnifit I need to get familiar with Python. The Python files I had on the old MAC do not work.

Downloaded & installed Anaconda (Python 2.7) which contains all the required packs.

Edited Natalia's python code for thickness measurement to include Sin fit to the T-file:

sin_fit_thickness.py

```
# -*- coding: utf-8 -*-
"""
Created on Fri Oct 06 11:44:33 2017

@author: ad3298
"""

from scipy.optimize import curve_fit
import numpy as np
import matplotlib.pyplot as plt

print'Enter data file include full filename and extension e.g. T44026.dat'
filename=raw_input()
#load files:data with peaks removed and full set of data. skiprows for the begining.
#Make sure to chop the data to include only the deposition data in the T-file
x,y = np.loadtxt(filename, dtype=float ,usecols=(0,1), unpack=1, skiprows=2)

if np.any(y < 0):
    y = -1*y

#defines the function, p values are the guesses. Attention: np.log is ln, np.log10 is log
#sin function used y0+sin(2pi(x-xc)/w)
#with y0=y-offset, xc=x-offset/phase, w=period, A=amplitude
def intento(x,*p):
        y0, xc, w, A=p
        return y0+A*np.sin(2*np.pi*(x-xc)/w)
guess =[-10, 100, 1800, -1]

#fits the funtion and returns coeff[as many guesses as you have]
coeff, var_mat = curve_fit(intento, x, y, p0=guess, maxfev=1000)
fit = curve_fit(intento, x, y, p0=guess)

#chi squared calculation
chi_squared = np.sum(((y-intento(x,*coeff))**2)/(intento(x,*coeff)) )

#plots:
plt.plot(x, y, '.', label='data' )
plt.plot(x, intento(x,*coeff),'r-', label='Fit')
plt.xlabel('Time (s)')
plt.ylabel(r'Diode Current ($\mu$A)')
plt.show()

print'Chi-sq = %s'%(chi_squared)
print'\ny0 = %s \n xc = %s \n w = %s \n A = %s'%(coeff[0],coeff[1],coeff[2], coeff[3])
```

```
#Refractive index ice layer

y0=coeff[0]
xc=coeff[1]
w=coeff[2]
A=coeff[3]

n2=(y0+A)/(y0-A)

print "\nRefractive index = %s at 632.8 nm"%(n2)

#HeNe laser incident angle is 20 deg at vacuum/ice interface. Require angle at ice/substrate
#Use n1*sin(theta1)=n2*sin(theta2)
#So theta2=arcsin(sin(20deg)/n2). Attention, python numpy works in radians
theta=np.radians(20)

theta2=np.arcsin(theta/n2)
theta2_deg=np.rad2deg(theta2)

print "\ntheta2 = %s rad = %s degrees"%(theta2,theta2_deg)

#time per fringe = 2*w (N.B. w in the fit corresponds to half a fringe)
#thickness per fringe, d = lambda(632.8)/2*n2*cos(theta2)
d=632.8/(2*n2*np.cos(theta2))
print "\nd = %s nm"%(d)

#rate = thickness/fringe / time/fringe
rate=d/w

print "\nDeposition rate = %s nm/s"%(rate)

t= float(input('Enter deposition time in seconds: '))

thickness=rate*t

print "\nThickness = %s nm\n\nNow get out of the lab and have some fun!\n"%(thickness)
```

I tested the code on data from 2014 - T44026.dat for deposition of benzene.

See Lab Book 2 pg 161

Input : filename.dat
Input : Deposition time in (s)

Output →

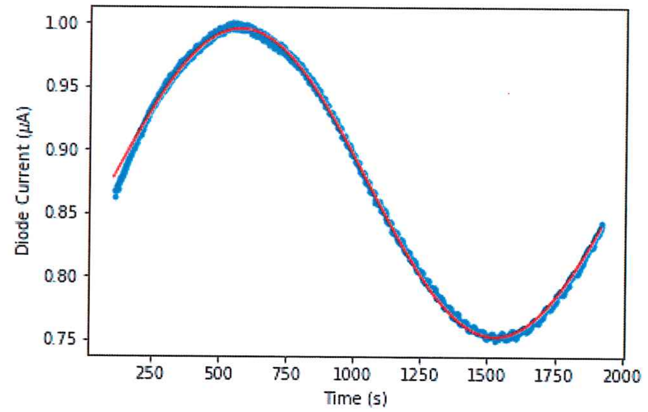

```
Python 2.7.13 |Anaconda, Inc.| (default, Sep 20 2017, 13:50:34) [MSC v.1500 32 bit
(Intel)]
Type "copyright", "credits" or "license" for more information.

IPython 5.4.1 -- An enhanced Interactive Python.
?         -> Introduction and overview of IPython's features.
%quickref -> Quick reference.
help      -> Python's own help system.
object?   -> Details about 'object', use 'object??' for extra details.

In [1]:

In [1]: runfile('Y:/Thickness Calculations/sin_fit_thickness.py', wdir='Y:/Thickness
Calculations')
Enter data file include full filename and extension e.g. T44026.dat

T44026_edited.dat
```




```
Chi-sq = 0.00835653792005

y0 = 0.874114166435
 xc = 100.182100525
 w = 1906.87919391
 A = 0.121370080102

Refractive index = 1.32247368609 at 632.8 nm

theta2 = 0.267114308054 rad = 15.3045224991 degrees

d = 248.045143997 nm

Deposition rate = 0.130079107679 nm/s

Enter deposition time in seconds: 1809

Thickness = 235.313105792 nm

Now get out of the lab and have some fun!
```

Output of the python fit to laser diode signal and thickness calculation.

06/10/17

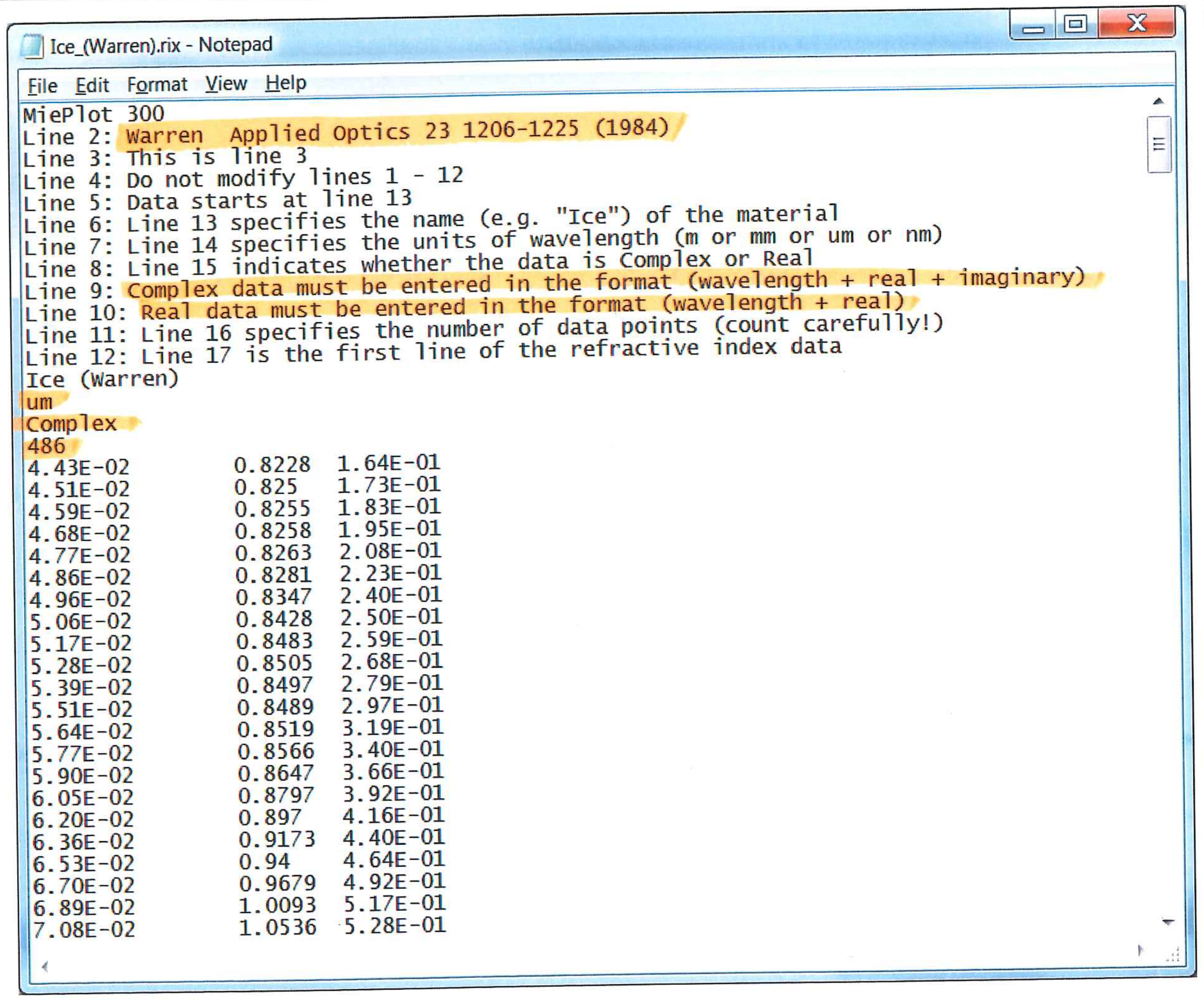
MiePlot — I have been using data from built in library for water ice: Ice (Warren) in air for the test spectra on pgs 32 - 34.

(Temp ~ 0°C)

Warren, Appl Optics 23(8) pp 1206 — 1225 (1984)

Looking at the possibility of loading our own data so that we can look at amorphous ice (10 - 25K) or crystalline ice (160 - 200K)

File format used is:



Ice_(Warren).rix - Notepad

File Edit Format View Help

```
MiePlot 300
Line 2: Warren  Applied Optics 23 1206-1225 (1984)
Line 3: This is line 3
Line 4: Do not modify lines 1 - 12
Line 5: Data starts at line 13
Line 6: Line 13 specifies the name (e.g. "Ice") of the material
Line 7: Line 14 specifies the units of wavelength (m or mm or um or nm)
Line 8: Line 15 indicates whether the data is Complex or Real
Line 9: Complex data must be entered in the format (wavelength + real + imaginary)
Line 10: Real data must be entered in the format (wavelength + real)
Line 11: Line 16 specifies the number of data points (count carefully!)
Line 12: Line 17 is the first line of the refractive index data
Ice (Warren)
um
Complex
486
4.43E-02        0.8228  1.64E-01
4.51E-02        0.825   1.73E-01
4.59E-02        0.8255  1.83E-01
4.68E-02        0.8258  1.95E-01
4.77E-02        0.8263  2.08E-01
4.86E-02        0.8281  2.23E-01
4.96E-02        0.8347  2.40E-01
5.06E-02        0.8428  2.50E-01
5.17E-02        0.8483  2.59E-01
5.28E-02        0.8505  2.68E-01
5.39E-02        0.8497  2.79E-01
5.51E-02        0.8489  2.97E-01
5.64E-02        0.8519  3.19E-01
5.77E-02        0.8566  3.40E-01
5.90E-02        0.8647  3.66E-01
6.05E-02        0.8797  3.92E-01
6.20E-02        0.897   4.16E-01
6.36E-02        0.9173  4.40E-01
6.53E-02        0.94    4.64E-01
6.70E-02        0.9679  4.92E-01
6.89E-02        1.0093  5.17E-01
7.08E-02        1.0536  5.28E-01
```

N.B. Require n and k values of the refractive index

$m = n + ik$

Papers: A study of H_2O ice in the 3 micron spectrum of OH 231.8 + 42 (OH 0739 - 14) 09/10/14

Smith et. al. ApJ. 334, 209 - 219 (1988)

- Source OH 231.8 - 4.2 (OH 0739 - 14) observed with IRTF
  - ↳ at 1μm appears as a red bipolar reflection nebula ~ 30" long.
  - ↳ > 4μm it appears as a compact IR source < 5" diameter.
  - ↳ Near-IR shows O-rich late-type star either M6 I or M9 III.
  - ↳ Deep abs. features ~ 3.1 and 11.5 μm → H_2O
    ~ 9.8 μm → silicates

- Authors compared spectra to models of scattering cross sections of ice-coated grains. — Mie Theory
  "... Since the scattered light spectrum has a significantly different signature compared with the absorption spectrum".

- Continuum — two factors to consider:
  - ↳ (1) Stellar continuum (CO & H_2O abs — gas) "photospheric"
  - ↳ (2) Thermal emission from circumstellar shell ~ 3μm.

- Assumption ∴ H_2O is the dominant absorber in this wl. region.
  - ↳ Extinction in 2.8 - 3.8 μm region is due to grains composed of a small silicate core surrounded by a mantle of H_2O ice.

- Optical constants ("dirty" silicate grains)

Ref: Jones & Merrill, ApJ 209 (1976)

$n = 1.55$ $K = 0.05$

Hagen et. al. Chem Phys 56 (1981)

Smith et. al. (1988)

- Grain Size & Shape:

↳ model based on spherical particles, leaving grain size as the main variable.

↳ Examined two grain size distributions to account for grain growth due to accretion.

↳ Distribution based on a theory of grain growth & formation developed by Oort & Van de Hulst (1946) with the form ("model 1"):

(grain accretion)

$$n(a) \propto \exp\left[-5\left(\frac{a-a_c}{a_+}\right)^3\right] \quad \text{for } a_c < a \leq a_+$$

where a_c = core radius

a_+ = upper limit of total grain radius, a

a = core + mantle radius

↳ Another distribution determined by Mathis, Ruml & Nordsieck (1977) of the form ("model 2"):

(grain collision)

$$n(a) \propto a^{-3.5} \quad \text{for } a_c < a < a_+$$

↳ model 1: $a_+ = 0.6 \pm 0.1\,\mu m$
model 2: $a_+ = 0.7 \pm 0.1\,\mu m$ } grain mantles

Models 1 & 2: $a_c = 0.05 - 0.15\,\mu m$ core
$= 0.1\,\mu m$ selected.

↳ models 1 & 2 – fixed core, varying mantle
model 3 – fixed mantle, varying core.
$0 < a \leq (a_+ - a_m)$
a_m = fixed mantle thickness.
$a_m = 0.2\,\mu m$, $a_+ = 0.7\,\mu m$

↳ models 2 & 3 gave essentially the same results as model 1 ⟹ Spectra not sensitive to size distributions. (See Fig 2c)

Smith et. al. (1988)

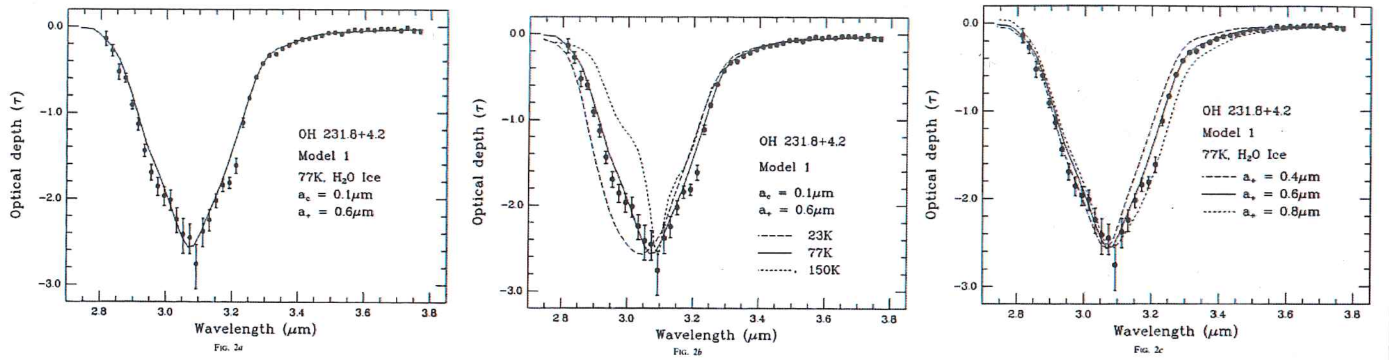
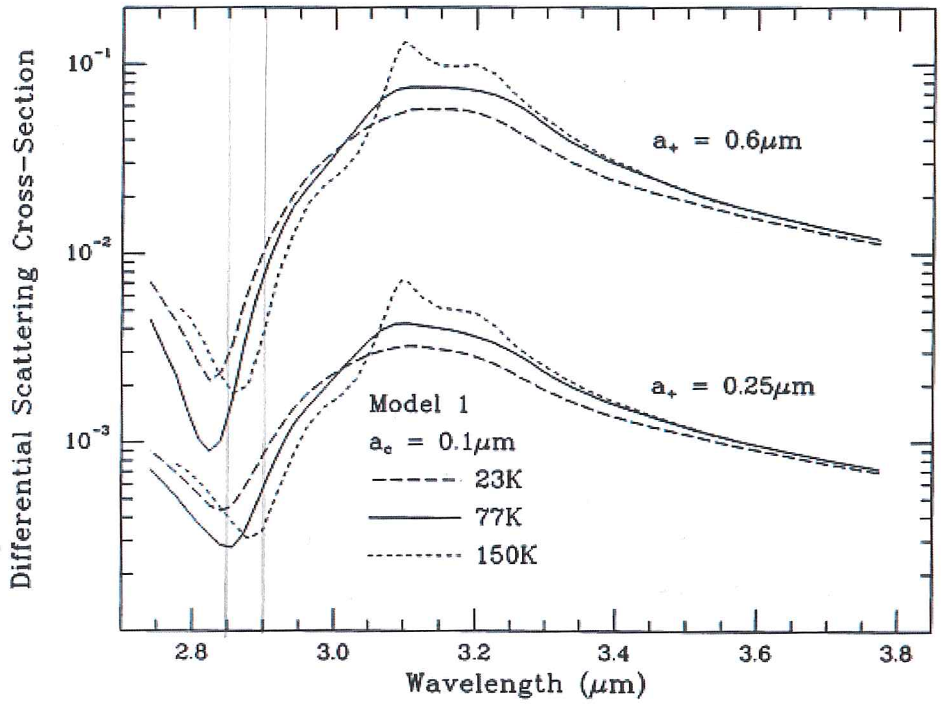


FIG. 2.—Absorption between 2.8 and 3.8 μm relative to the estimated OH 231.8+4.2 continuum, plotted in terms of optical depth (*filled circles*). (a) The solid line shows the extinction produced by small spherical silicate grains coated with amorphous H_2O ice at 77 K, calculated using Mie theory (Model 1, $a_c = 0.1$ μm, $a_+ = 0.6$ μm). (b) The solid and broken lines show the extinction produced by small H_2O ice-coated silicate grains using Model 1 ($a_c = 0.1$ μm, $a_+ = 0.6$ μm), for three different temperatures, 23, 77, and 150 K. (c) The solid and broken lines show the extinction produced by 77 K H_2O ice-coated silicate grains using Model 1 ($a_c = 0.1$ μm) for three different upper limits to the grain mantle size distribution, a_+ = 0.4, 0.6, and 0.8 μm.

- Grain Temperature – See Fig 2b
↳ Best temp ~ 77K.

- Scattering:

these are upside down?



?

FIG. 4.—Differential scattering cross sections (see text for definition) for small silicate grains coated with pure amorphous H_2O ice at 23 and 77 K, and with pure crystalline H_2O ice at 150 K (Model 1, $a_c = 0.1$ μm). The scattering angle in all cases is 90°; the different lines represent different upper limits (a_+) to the grain mantle size distribution.

Differential scattering cross section = the amount of light, for unit incident irradience, scattered into a unit solid angle about a given direction.

When integrated over all angles = Total Scattering X section

↳ Authors say that "the most easily distinguished effects (i.e. where the diff. X sectn. reaches minimum) occurs near 2.85 μm for amorphous (23 & 77K) and near 2.9 μm for crystalline (150K) ice. Clearly no hint of spectral features attributed to scattering can be seen near these wl. in OH231.8+4.2 spectrum"

Smith et. al. (1988)

- Additional absorbers:
  ↳ Authors considered NH_3 — but unlikely.

- New spectra obtained by double sampling — i.e. moving the grating a distance equivalent to half resolution element.
  ↳ Data shows two broad abs. features at 2.95 and 3.2 μm.

- models rely on
  ↳ (1) Accuracy of choice of continuum
  (2) Effect of possible distribution in grain temperature.

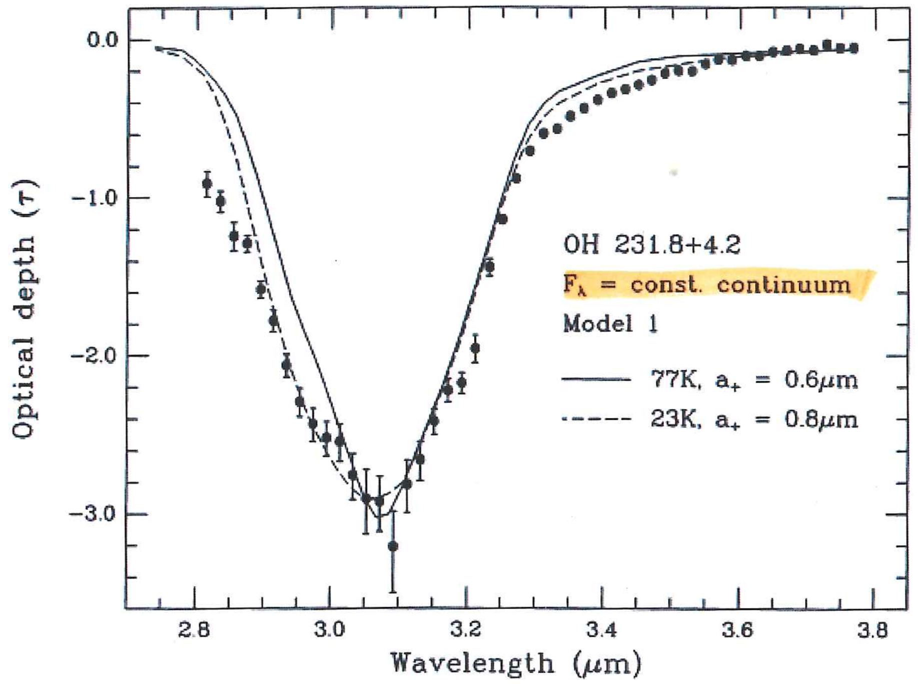


FIG. 6.—Spectrum of OH 231.8+4.2 relative to a F_λ = constant continuum, plotted in terms of optical depth (*filled circles*). The solid line shows the extinction resulting from small amorphous H_2O ice-coated silicate grains at 77 K (Model 1, a_c = 0.1 μm, a_+ = 0.6 μm), while the broken line shows results from ice-coated silicate grains at 23 K (Model 1, a_c = 0.1 μm, a_+ = 0.8 μm).

Model 1 (a_c = 0.1 μm, a_+ = 0.6 μm) at 77 in Fig. 2a no longer provides a good fit. — after continuum changed.

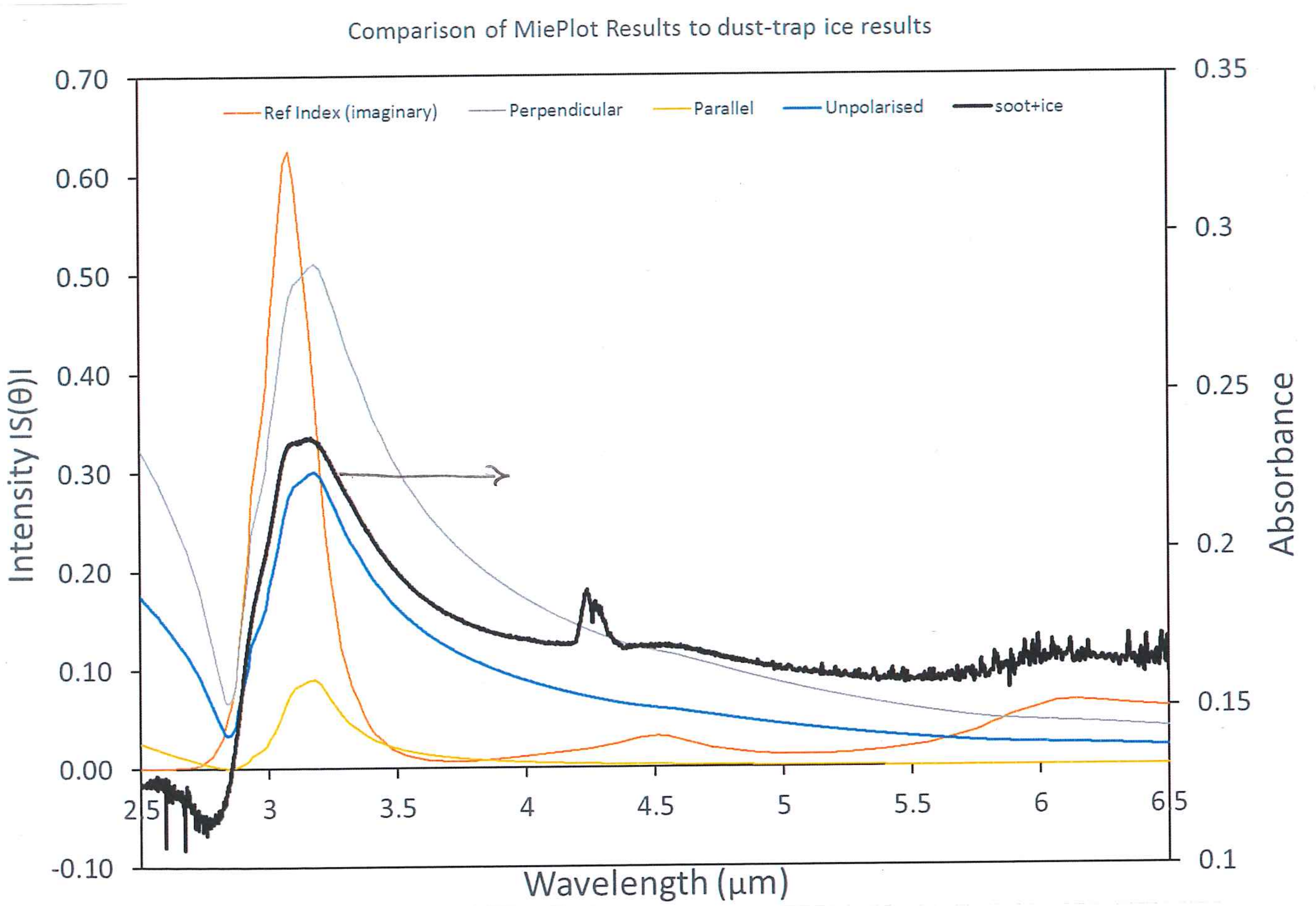
Now model 1 @ 23K is a better fit.

But F_λ = const. continuum is not considered to be an acceptable continuum for this source.

Playing around with MiePlot again 10/10/17

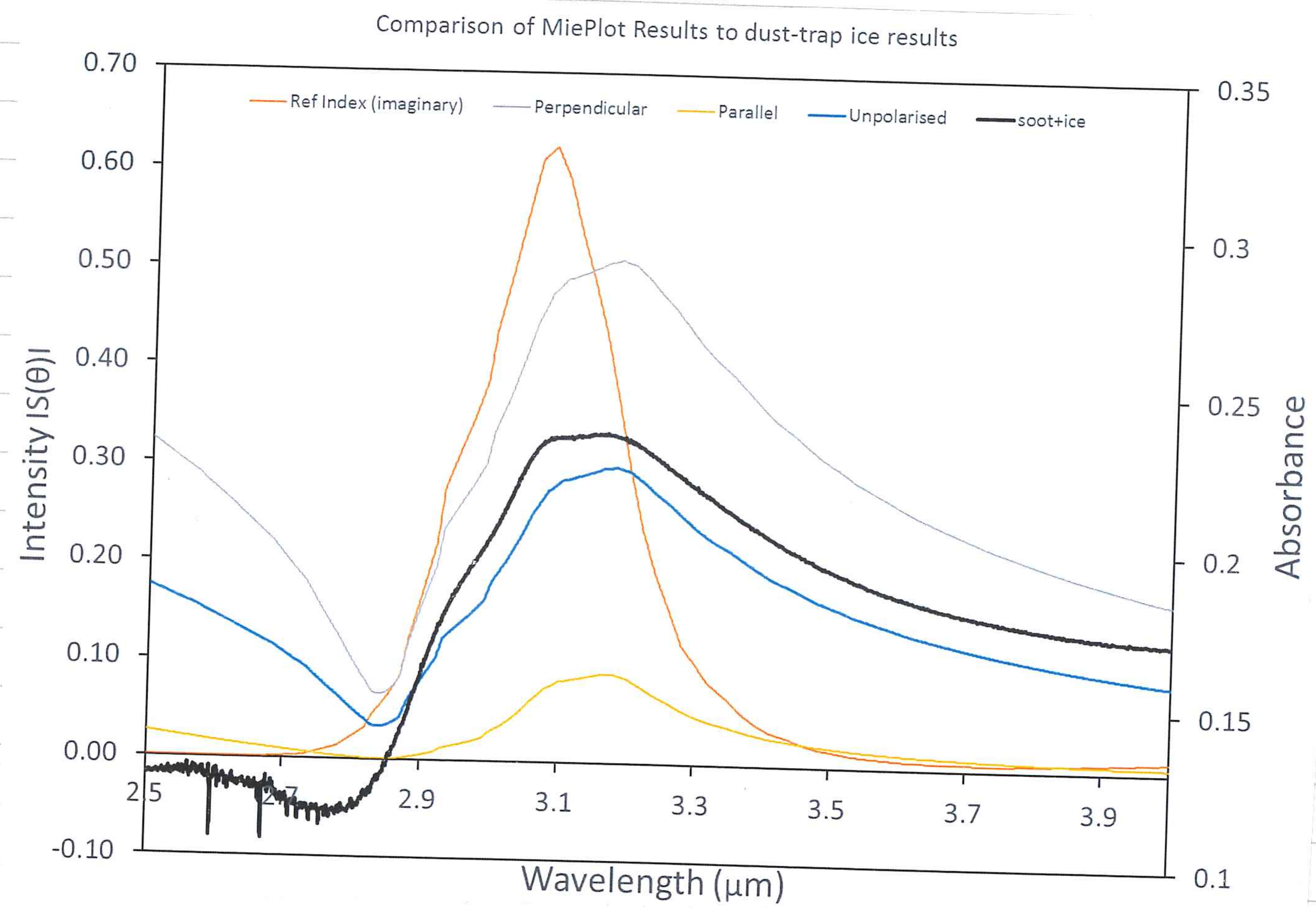
Using a grain size of 0.6 μm from Smith et al. (1988)

Calculation method: Mie (plane wave)
Radius: 0.6 μm
Distribution: normal, 1% standard deviation.
no of samples: 50



Soot + ice data used is Soot_20170831_0005
↳ no baseline correction
↳ BUT note the y-axis (right)

Close up of the O-H stretch 3µm region shows that the shapes of the spectra are very similar.



11/10/17

I found a file from Aleksi that contains data on the n and k values of amorphous water ice measured in the laboratory.

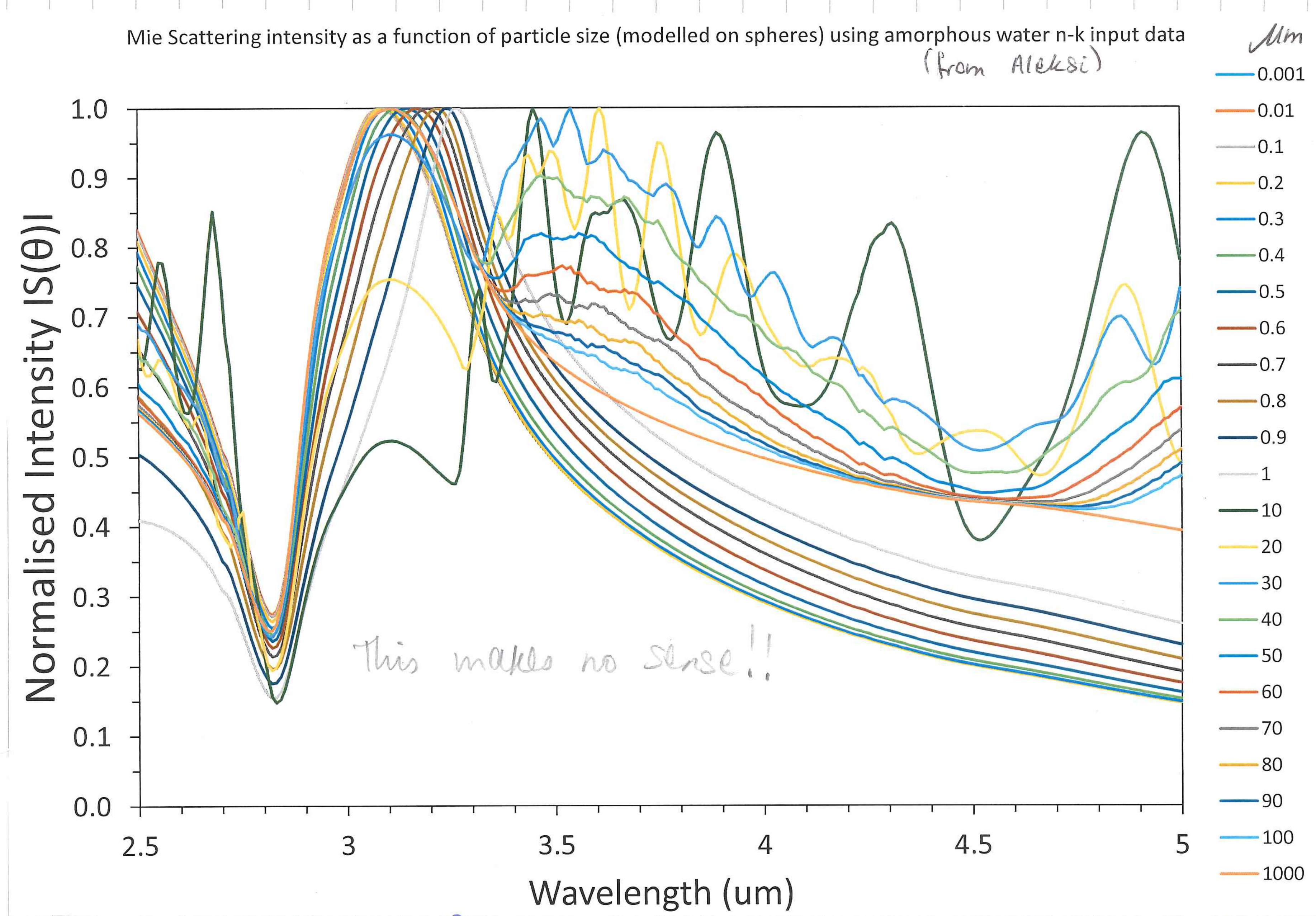
By setting up a text file in the format required by MiePlot (see pg 40) I managed to load it into MiePlot.

See MiePlotData_20171011_Omni.xls

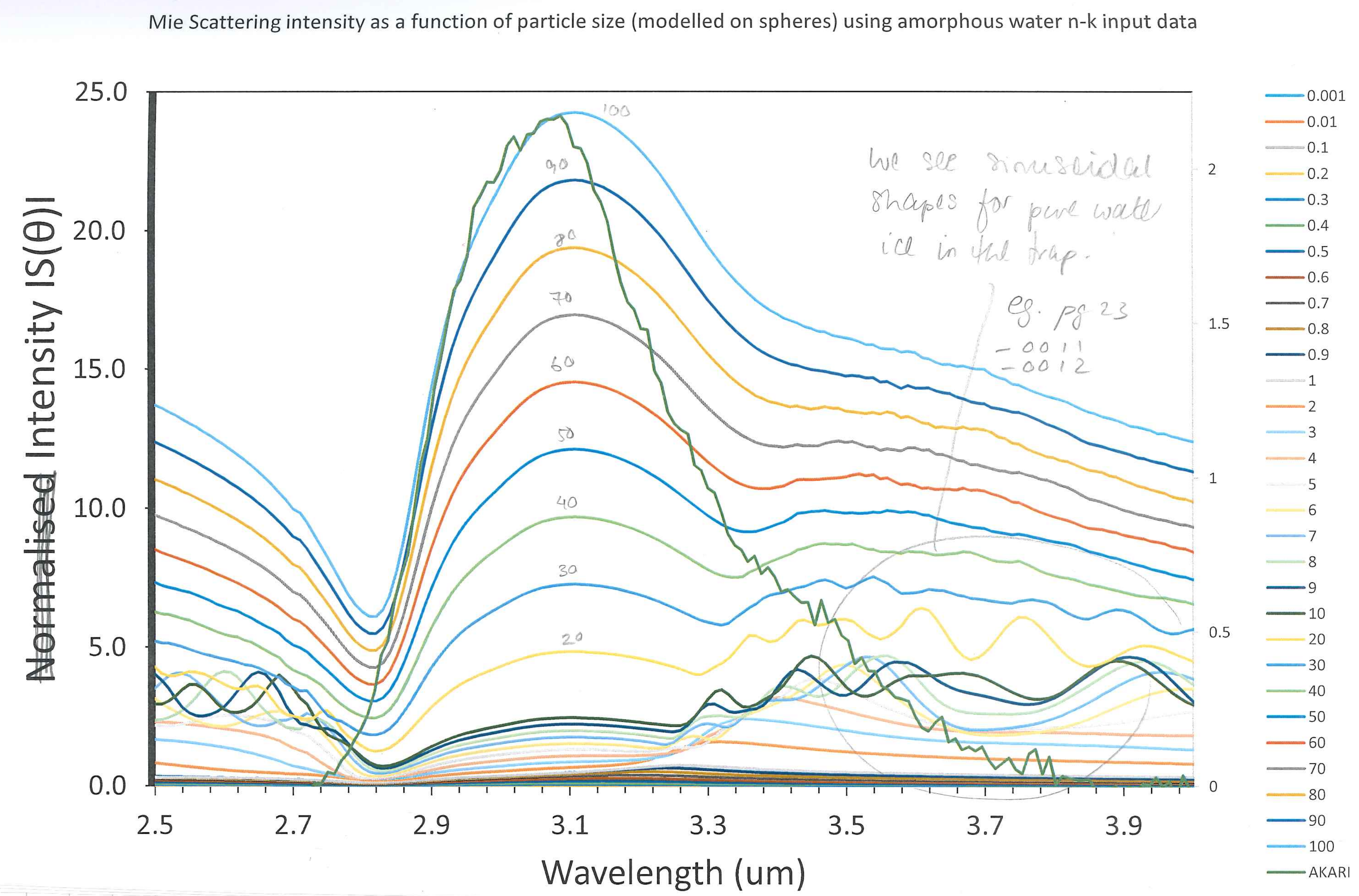
Data file Ice_(Aleksi-omnic).txt

↳ N.B. This file needs to be on a local directory – doesn't seem to like being on the network

1 MiePlot 300
2 Line 2 : Aleksi_omnic_ice_data
3 Line 3 : This is line 3
4 Line 4 : Do not modify lines 1–12   NB. I modified Line 2.
5 Line 5 : Data starts at line 13
6 Line 6 : Line 13 specifies the name (e.g. ""Ice"") of the material
7 Line 7 : Line 14 specifies the units of wavelength (m or mm or um or nm)
8 Line 8 : Line 15 indicates whether the data is Complex or Real
9 Line 9 : Complex data must be entered in the format (wavelength + real + imaginary)
10 Line 10 : Real data must be entered in the format (wavelength + real)
11 Line 11 : Line 16 specifies the number of data points (count carefully!)
12 Line 12 : Line 17 is the first line of the refractive index data
13 Ice (Aleksi_omnifit)
14 um   Edited data highlighted
15 Complex
16 9501
17 Data.   wavelength   real   imaginary   (3 columns! tab delimited)



Calculation : Mie (plane wave)
Radius : variable (see legend)
Distribution : Normal 1% standard deviation
No. of samples : 50 (max allowed by MiePlot)
NB. Data normalised to max peak value in the y-axis.



Same as above but un-normalised. Clearly the contribution to scattering intensity from larger particles is the greatest (>10 μm). But the shape of the scattering peak seems to show that particles < 1 μm contribute to the scattering tail.

12/10/17 Working on Aleksi's Data fitting using Omnifit.
It runs! Yay!

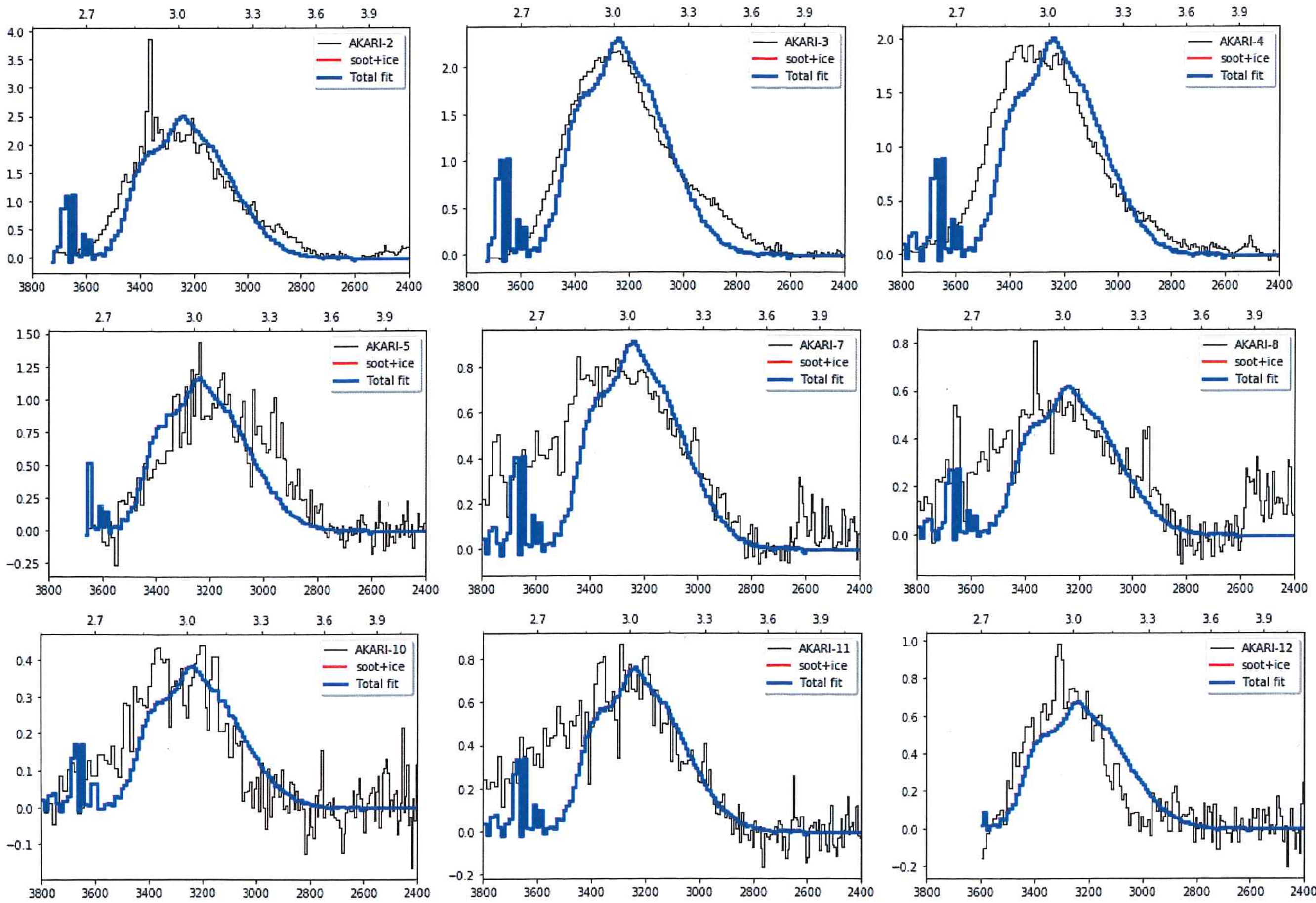
In the folder \omnifit-master
I added the files: AKARI_spectral_data.fits — contains 30 AKARI sources
anita_soot.py — Python routine to fit lab to obs
Soot_ice.txt — Soot & ice lab data to fit.

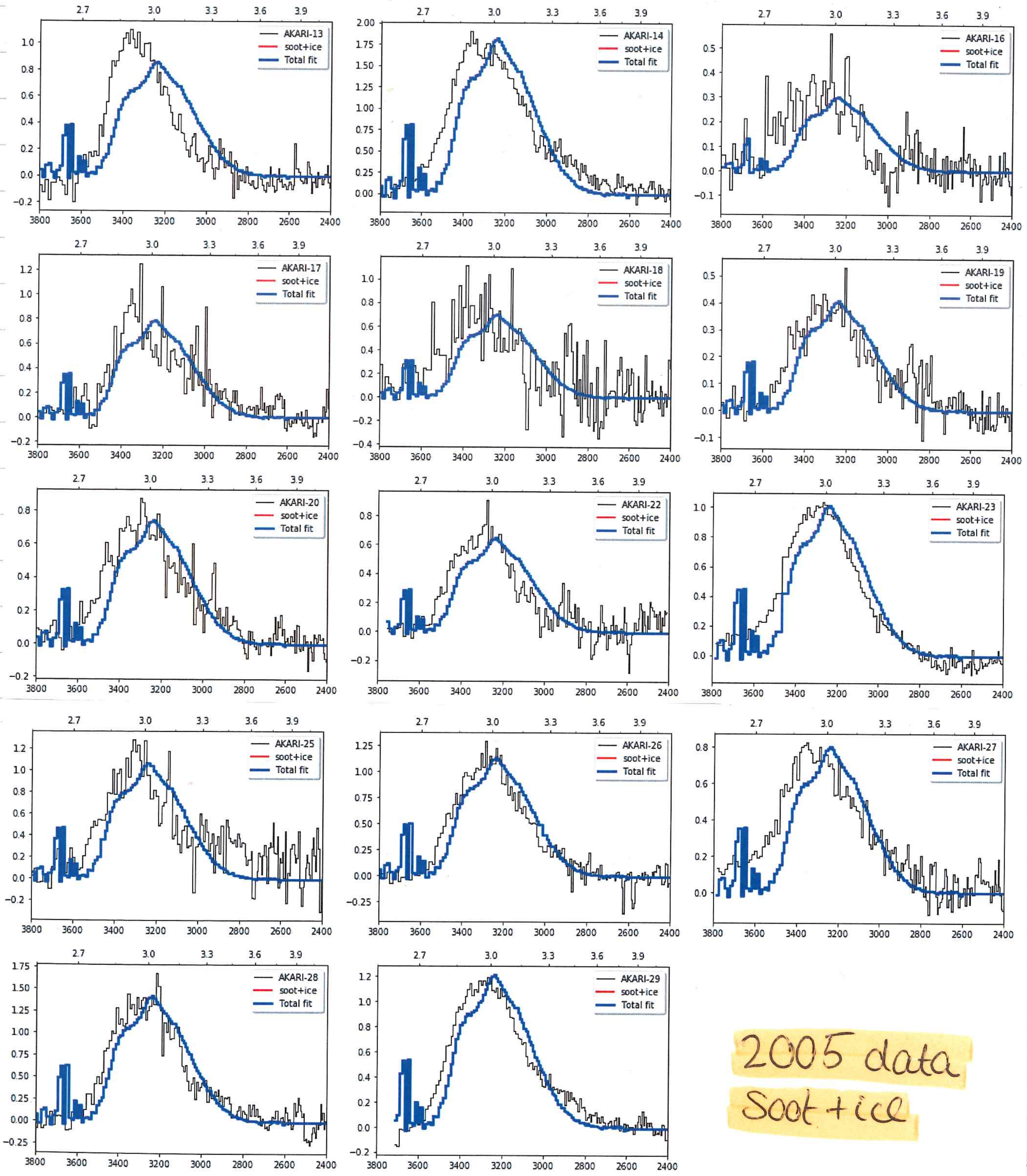
Download python packages lmfit and astropy using Anaconda prompt. Then use eg.

conda install -c conda-forge astropy

Anaconda
usr: zcapp40
pswd: "rus-sun"

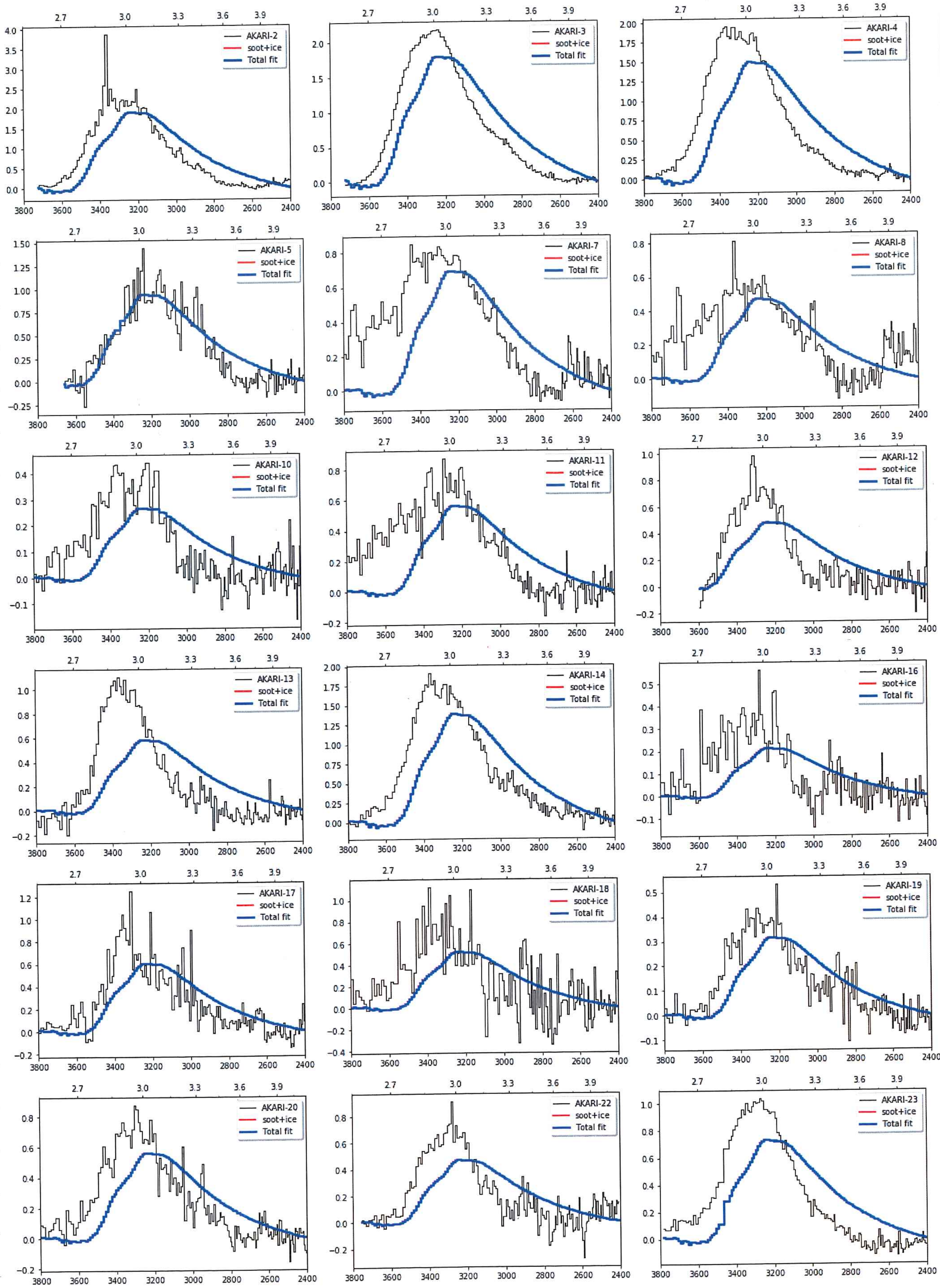
Then run anita_soot.py

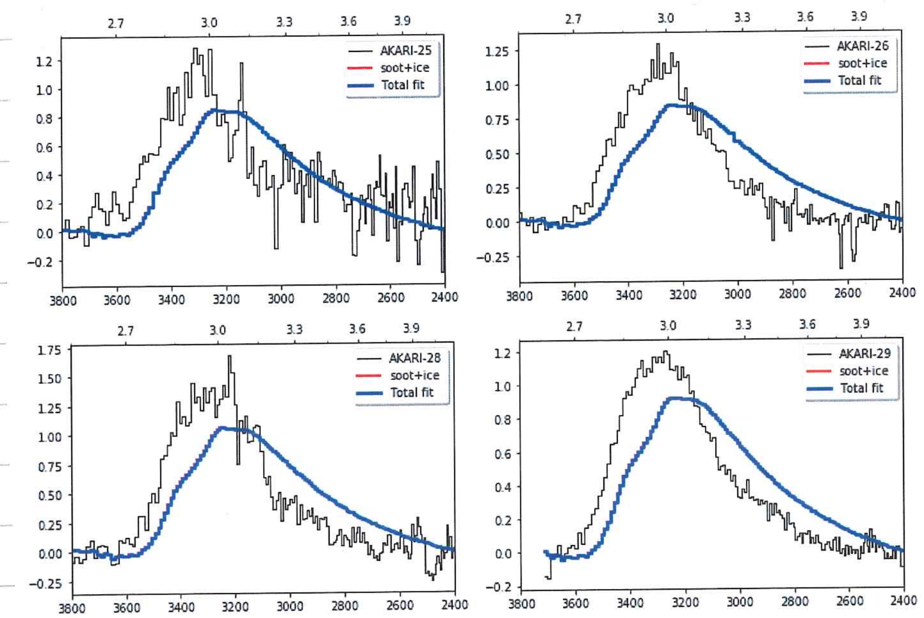




AKARI_fits_soot_ice_2005data

2005 data
Soot + ice





AKARI_fits_soot_20170831_005_bsl-corr

Notably here the blue wing does not fit. This could be because our ice is crystalline (see the shape of the peak).

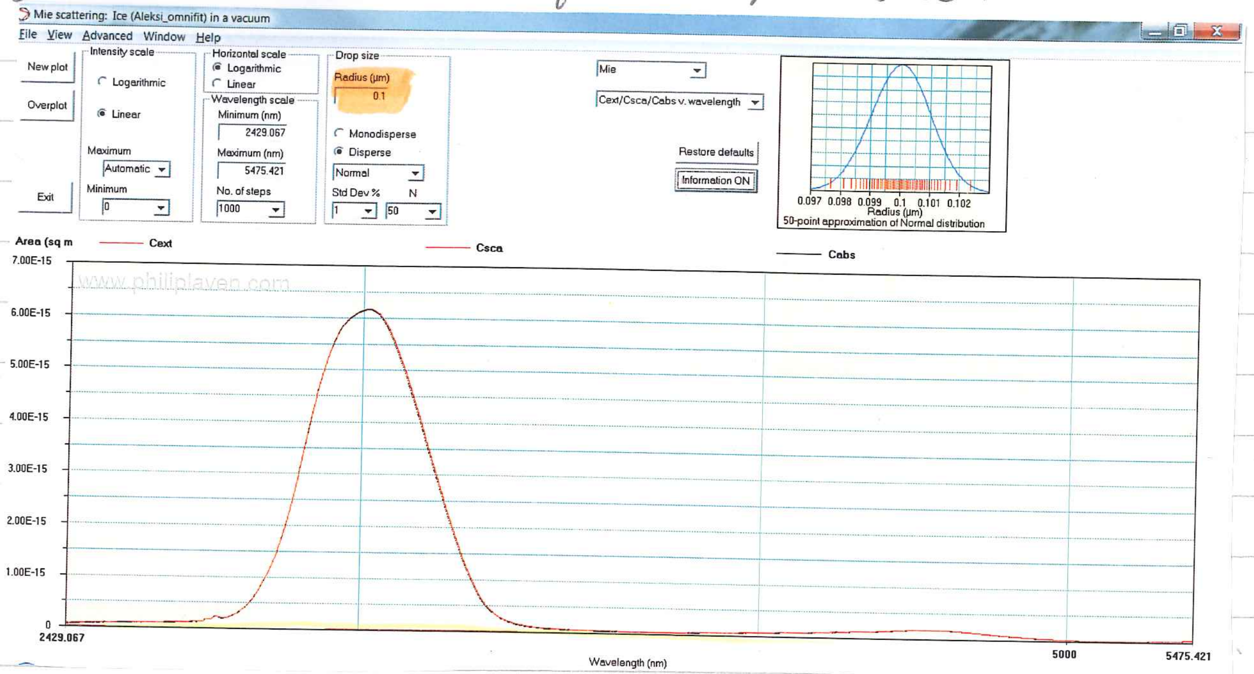
Looking back at Smith et.al — see pg 43, Fig4:
↳ I am not sure if I am looking at the scattering data correctly.
↳ The scattering X-sections shown in their paper appear to be upside down? As if they are interpreting the 'dip' in the spectrum as the absence of light.

Looking back at miePlot:
↳ I found that rather than scattering intensity $|S(\theta)|$ or $|S(\theta)|^2$, I can ask for a plot of cross sections.

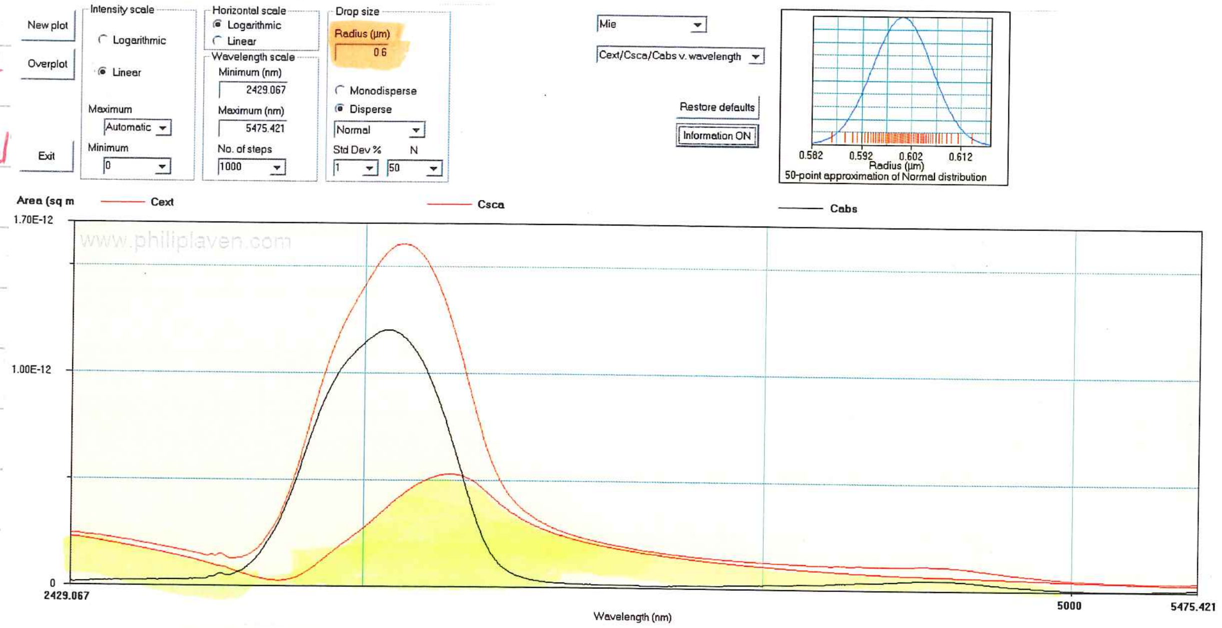
C_{ext} / C_{sca} / C_{abs}

Total? Scat X-scn Absorption X-section

Using Aleksi's n & k data for amorphous ice:

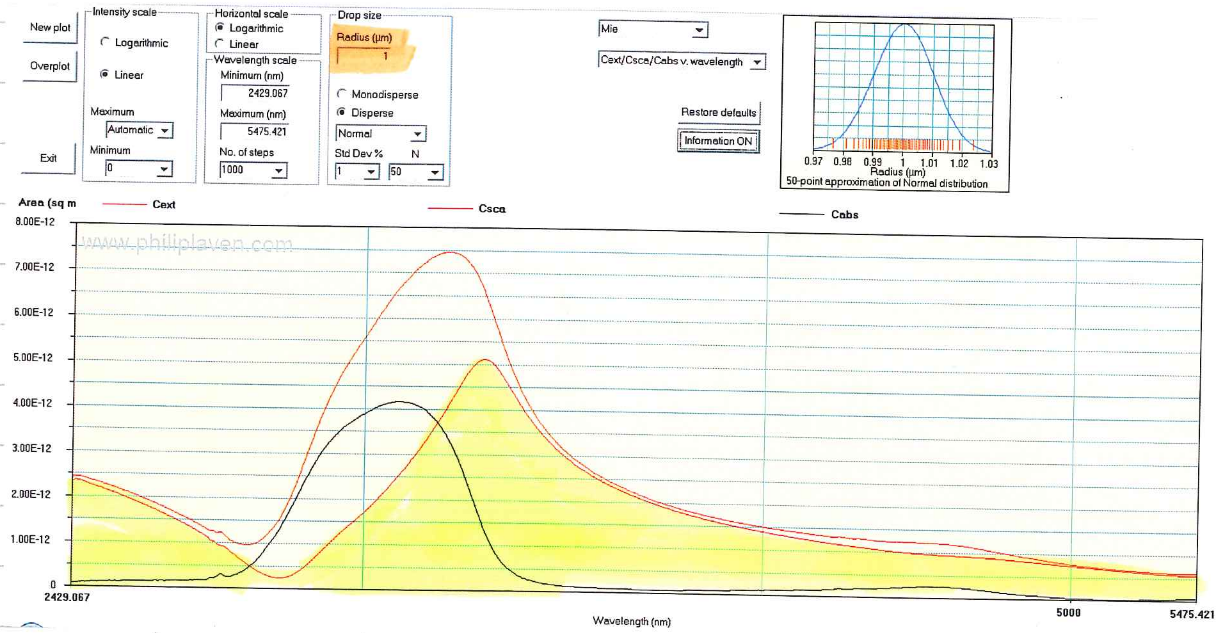


negligible scat tail



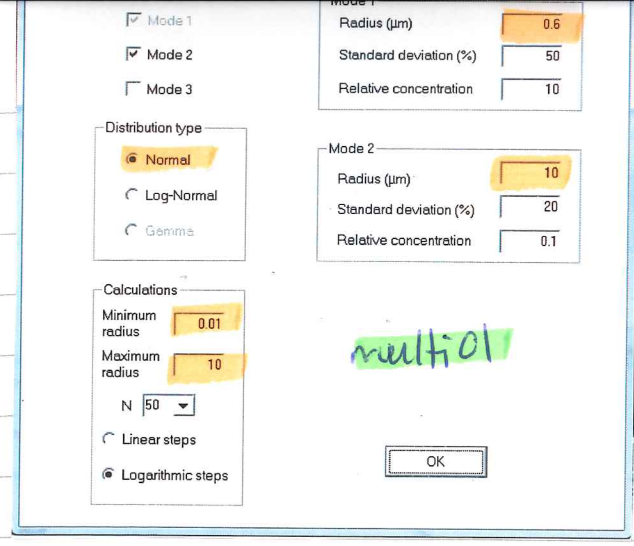
comparable radius to Smith et al (1988)

Scat. tail.

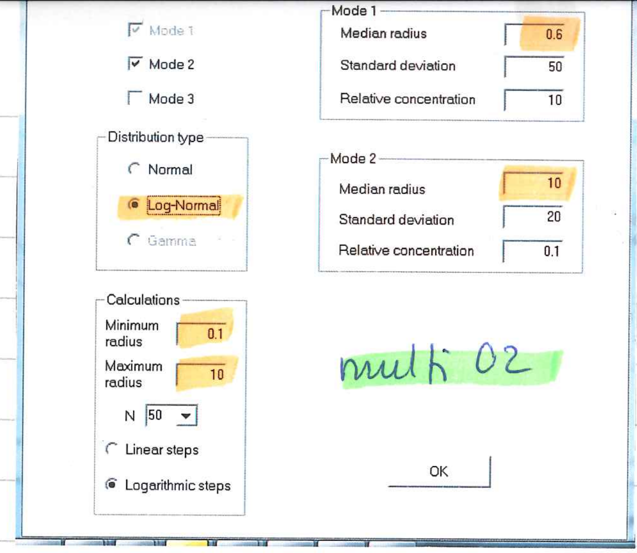


Large Scat. tail

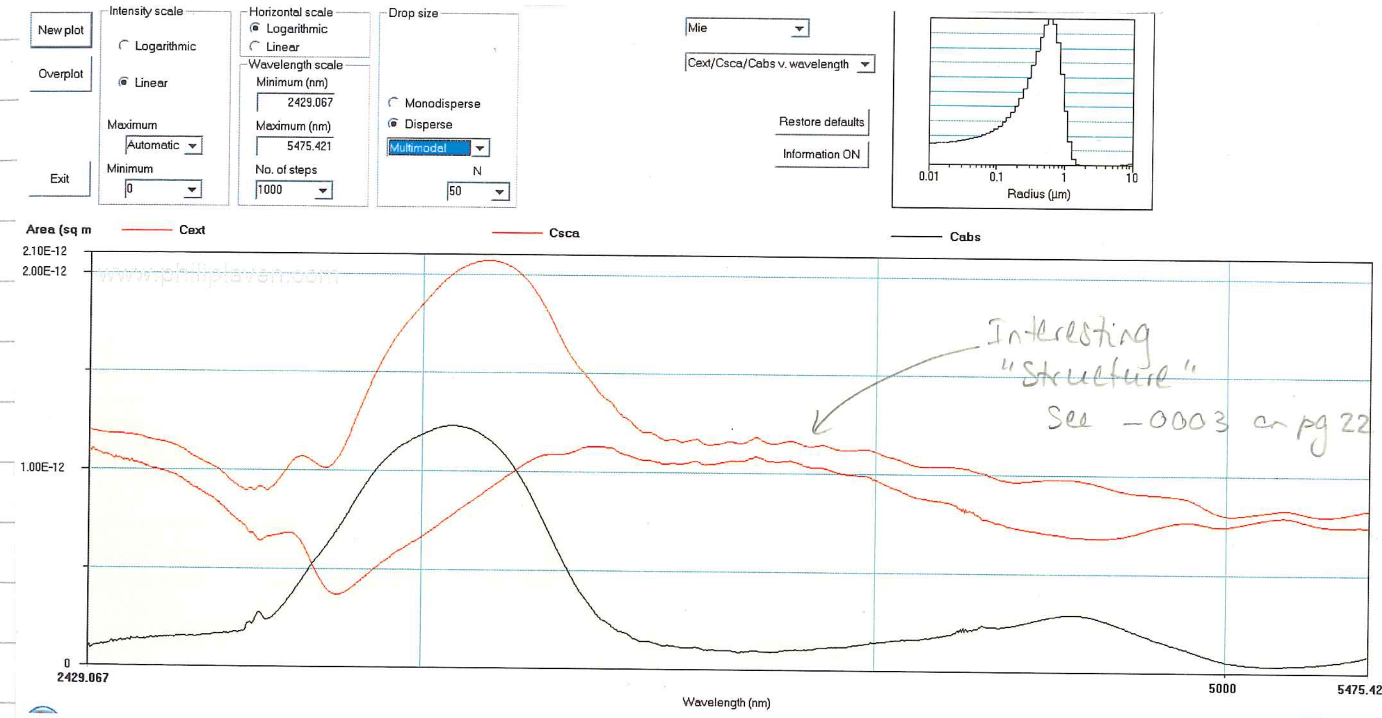
Dispersed, Single normal distribution 1% std N=50



multi01

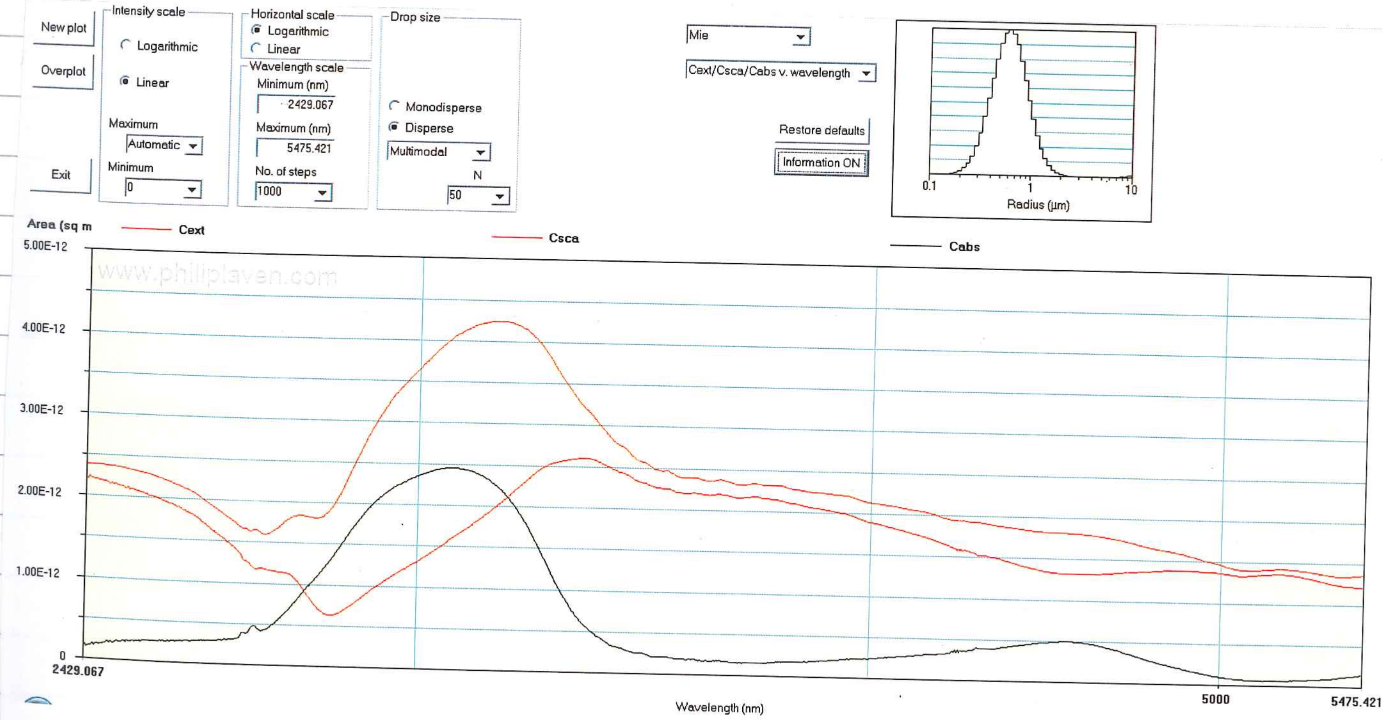


multi 02

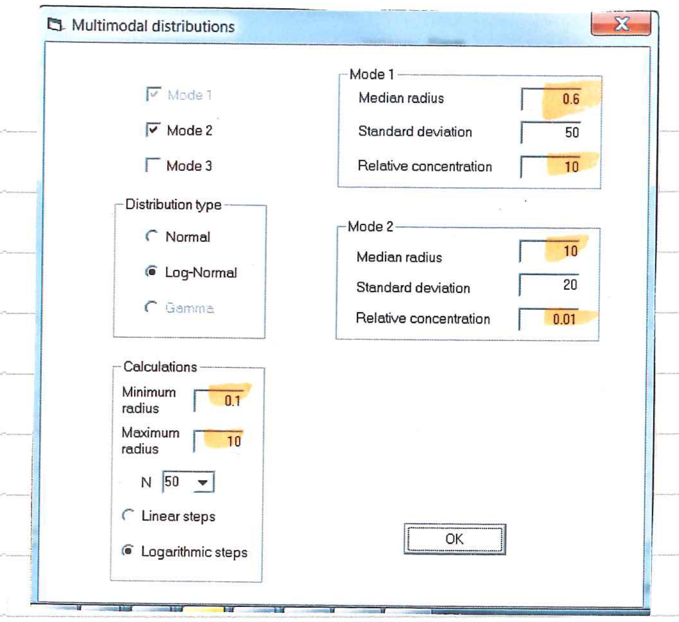


Interesting "Structure" See -0003 on pg 22

MiePlotData_20171012_Omni_Xscn_multi01

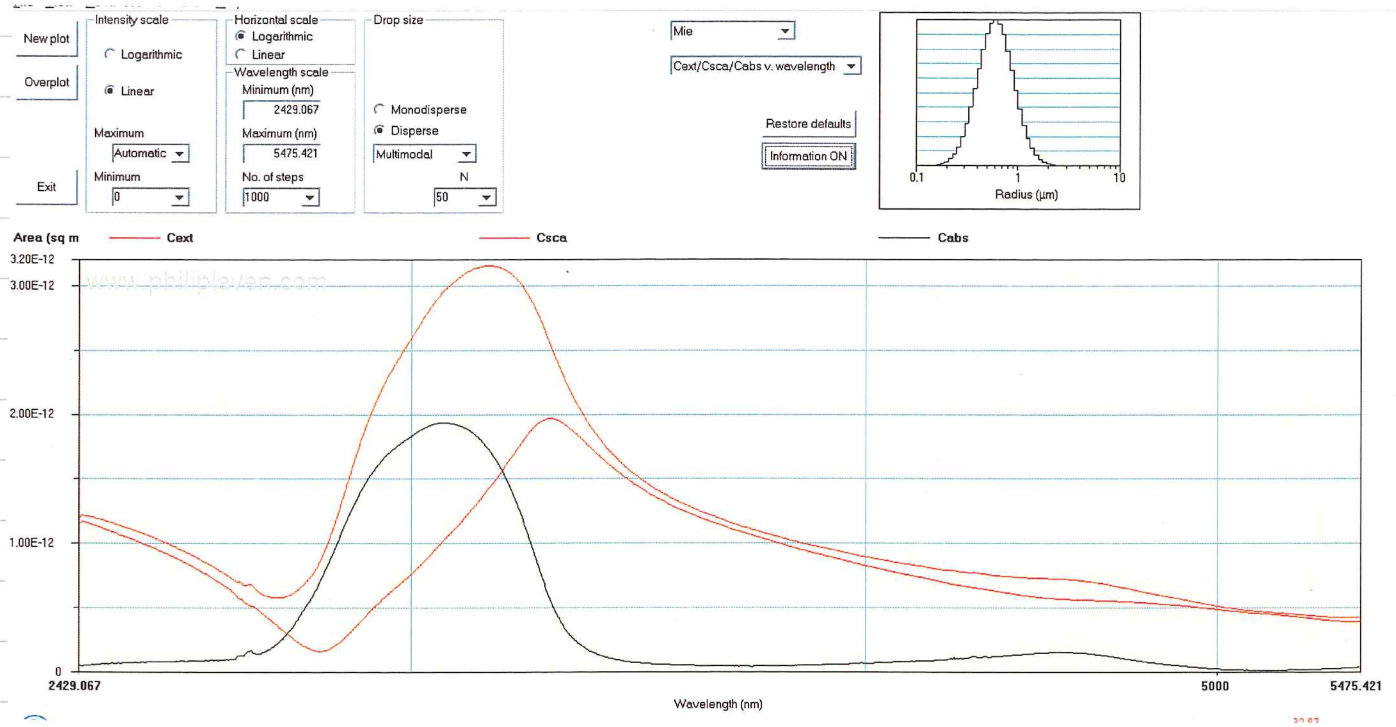


MiePlotData_20171012_Omni_Xscn_multi02



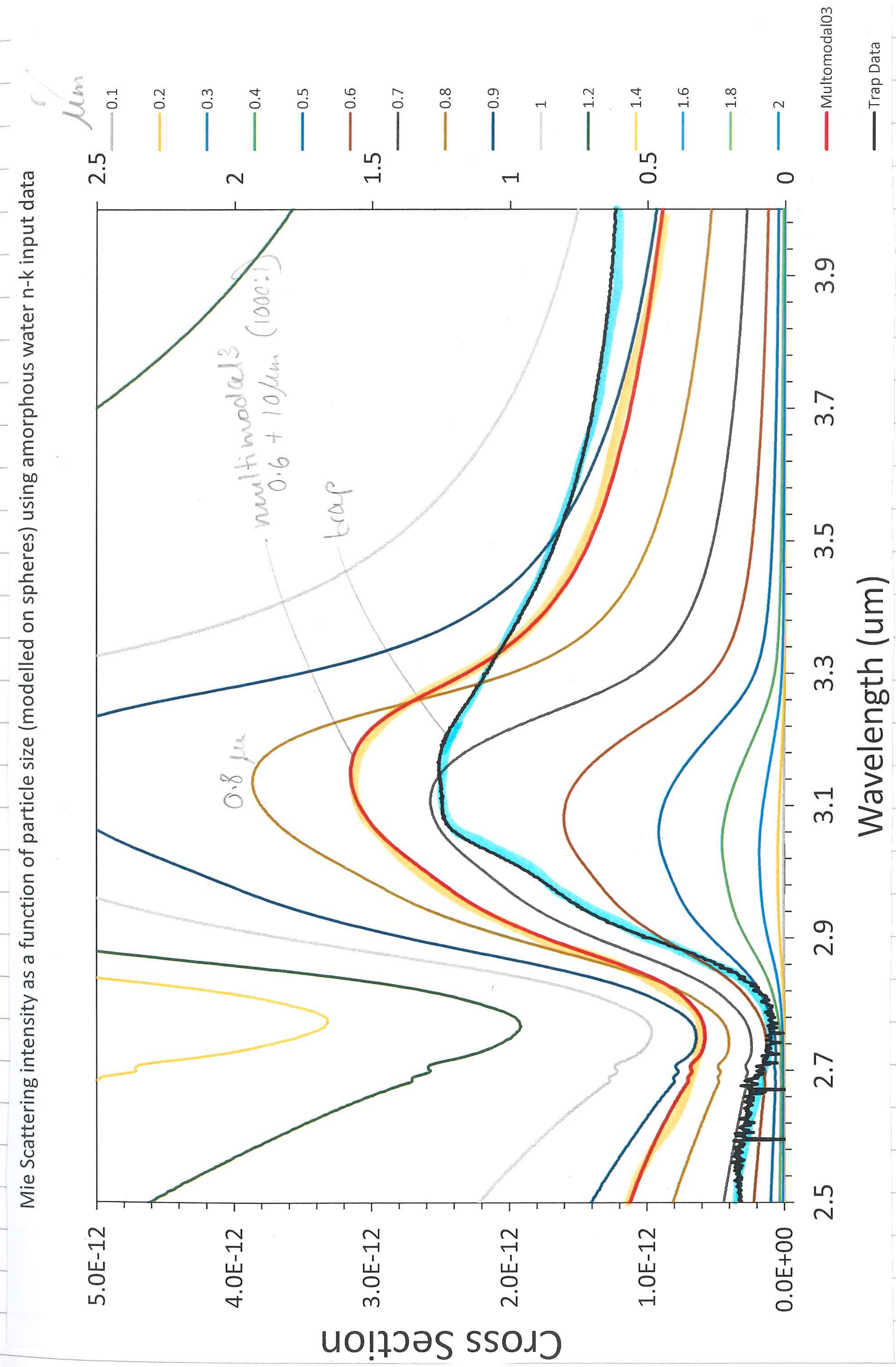
This is the level of scattering that we are seeing in the trap.

This is a distribution of two sizes — 0.6 µm and 10 µm



* It would be interesting to iterate these (automatically) varying size only and find the best fit to the trap data

* Repeat above fits with crystaline ice. → use "Warren" data



18/10/17

Paper: Astrochemistry: Overview and Challenges
Astrochemistry VII – IAU, 2017

van Dishoeck

vanDishoeck 2017 Astrochemistry Challenges:

Challenge 1: To secure new facilities for Astrochemistry in the 2030–2040 timeframe.

Challenge 2: To continue to bring chemists, physicists and astronomers together to characterize and quantify molecular processes that are at the heart of Astrochemistry, to have open lines of communication to prioritize needs, and to convince funding agencies to continue supporting this interdisciplinary research.

Challenge 3: To build realistic gas-grain models from microscopic to macroscopic scales, including translation of laboratory ice chemistry experiments into parameters that can be adopted in models.

Challenge 4: To obtain a full inventory of the chemical constituents of diffuse and translucent clouds, and explain – at the same time – their chemical simplicity and complexity.

Challenge 5: To quantify the importance of top-down versus bottom-up chemistry in the production of carbon-bearing molecules.

Challenge 6: To nail down the dust formation and destruction processes and their efficiencies in the envelopes of evolved low- and high-mass stars, for different metallicities.

Challenge 7: To bridge the gap between subpc galactic and kpc extragalactic astrochemical studies as functions of metallicity out to the highest redshifts, and to use molecular observations of calibrated tracers to unveil a new understanding of star formation in the early Universe.

Challenge 8: To identify and quantify the mechanisms by which molecules, including the more complex ones, are desorbed (intact) from the grain surface in cold clouds.

Challenge 9: To use chemical signatures to constrain physical structure, evolutionary stage and the amount of time spent in certain cloud phases.

Challenge 10: To characterize the chemical and physical structure of outflows, especially near the launching point of the jets and (disk) winds that drive them.

Challenge 11: To identify the main formation routes of complex molecules in dense clouds, to push detections to even higher levels of complexity including prebiotic species like amino acids, and to assess how dynamics and geometry during star formation can affect their abundances.

Challenge 12: To make a chemical inventory of disks (from inner to outer, surface to midplane, and young to old) and relate observed molecular structures to underlying gas and dust structures.

Challenge 13: To determine the (bulk) chemical composition and origin of planet-forming material (inheritance or reset) and relate that to what is found for icy bodies in our own Solar System.

Challenge 14: To determine exoplanetary atmosphere compositions and to characterize the chemical changes along the many steps to planet formation, necessary to relate exoplanetary atmosphere compositions to their birth sites in disks.

Book: Absorption and Scattering of Light by Small particles
Craig Bohren & Donald Huffman

Chapter 4 pg 105

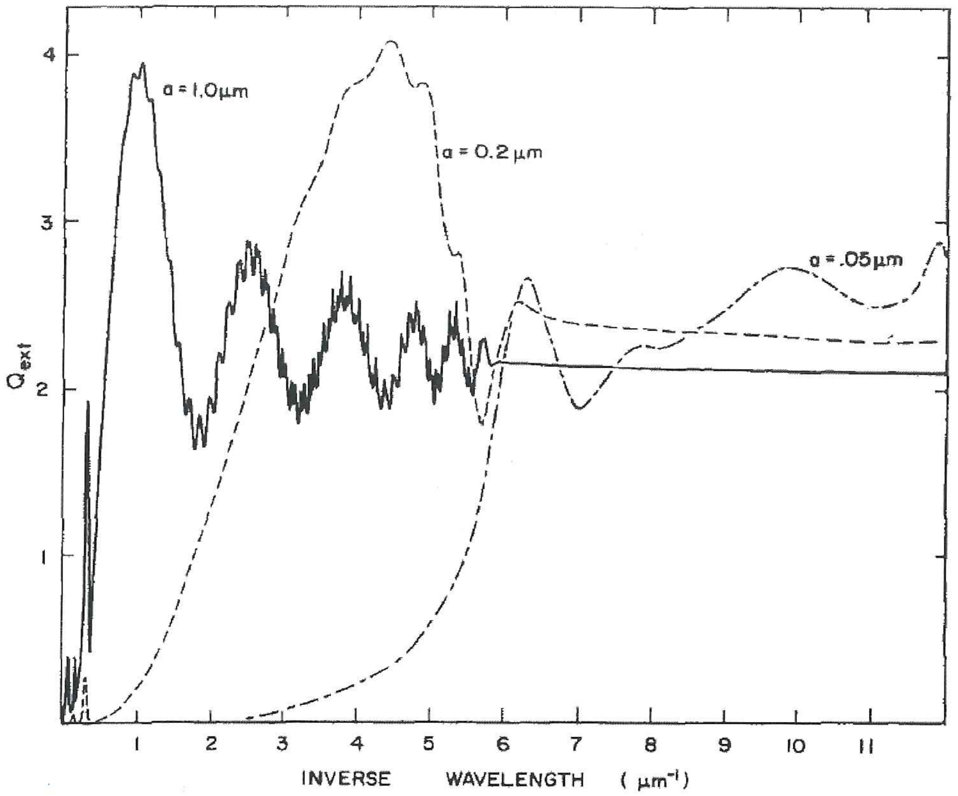


Figure 4.6 Extinction efficiencies for water droplets in air; plotting increment = 0.01 μm^{-1}.

$Q_{ext} = C_{ext} / \pi a^2$ – Extinction efficiency

Note the ripple structure – these look similar to the spectra of pure ice in the lap – See pg 23 Data plots _0011 and _0012

$$\boxed{\underbrace{C_{ext}}_{\text{Extinction X-section}} = \underbrace{C_{abs}}_{\text{Absorption X-section}} + \underbrace{C_{sca}}_{\text{Scattering X-section}}}$$

– eq. 3.25 Ch. 3, p71