

Regardless of particle composition there is an upper limit to integrated extinction:

$$\int_0^\infty C_{\text{ext}}(\lambda) d\lambda \leq 4\pi^3 a^3$$

- pg 117

For a spherical particle

$$C_{\text{sca}} = \frac{2\pi}{K^2} \sum_{n=1}^{\infty} (2n+1)(|a_n|^2 + |b_n|^2)$$

$$C_{\text{ext}} = \frac{2\pi}{K^2} \sum_{n=1}^{\infty} (2n+1) \Re(a_n b_n)$$

a_n and b_n are scattering coefficients

AKARI spectra from Jenny's paper:

20/10/17

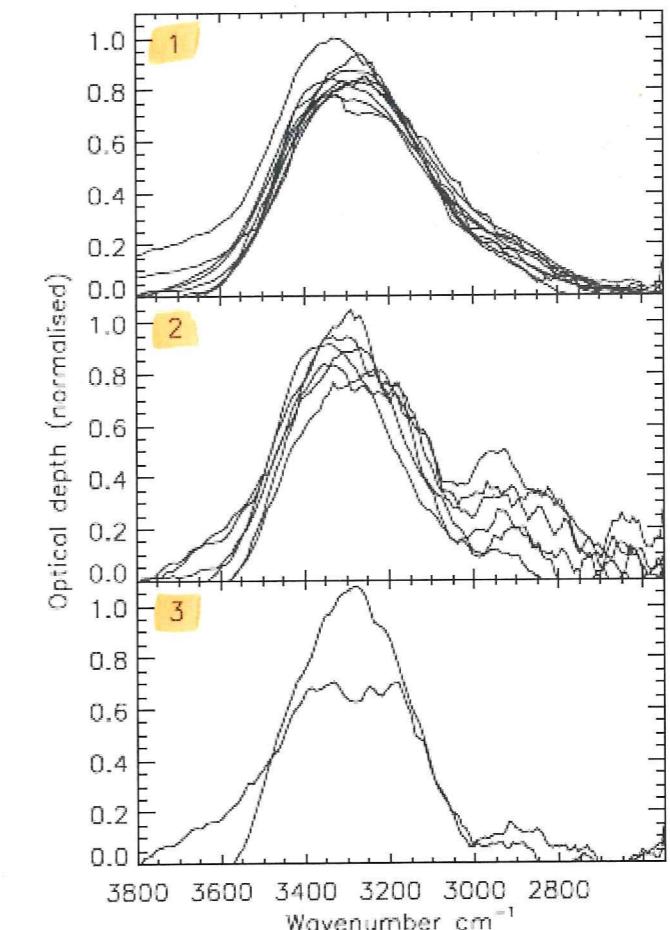


Figure 7. H₂O absorption band profiles for Types 1, 2, and 3. These data have been smoothed, normalized, and plotted without errors, to aid comparison. It is particularly evident in this figure, from the flattened peak of the band profile, that the H₂O band is almost always saturated.

← Type 1:
Include YSOs
→ grain growth
& accretion

← Type 2:
BG stars, more
evolved regions
of molecular cores

← Type 3:
BG stars with
low spectral flux

These are the same spectra as Aleksi used with Omnitfit fits to snow-ice data.

30/10/17

Back from school half term.

Fellowship application event for postdocs.

↳ highlighted strengths of Leverhulme proposal.

Remember:

① Independence - trap progress stopped during career break.

② Novelty - New technique to answer a scientific question.

KEY QUESTION:

"How does grain shape/size/composition affect the physical/chemical structure of ices in space"

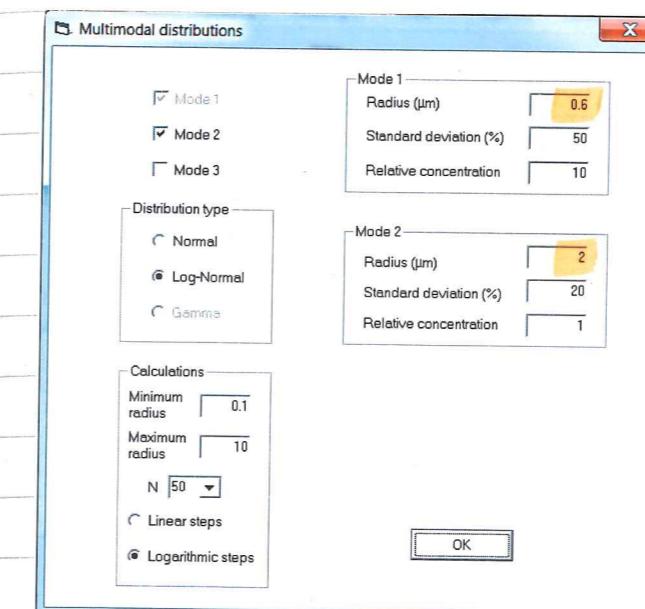
31/10/17

Writing Leverhulme Annual report

↳ include pics & spectra from the trap.

Playing around with miePlot (using "warren" data)

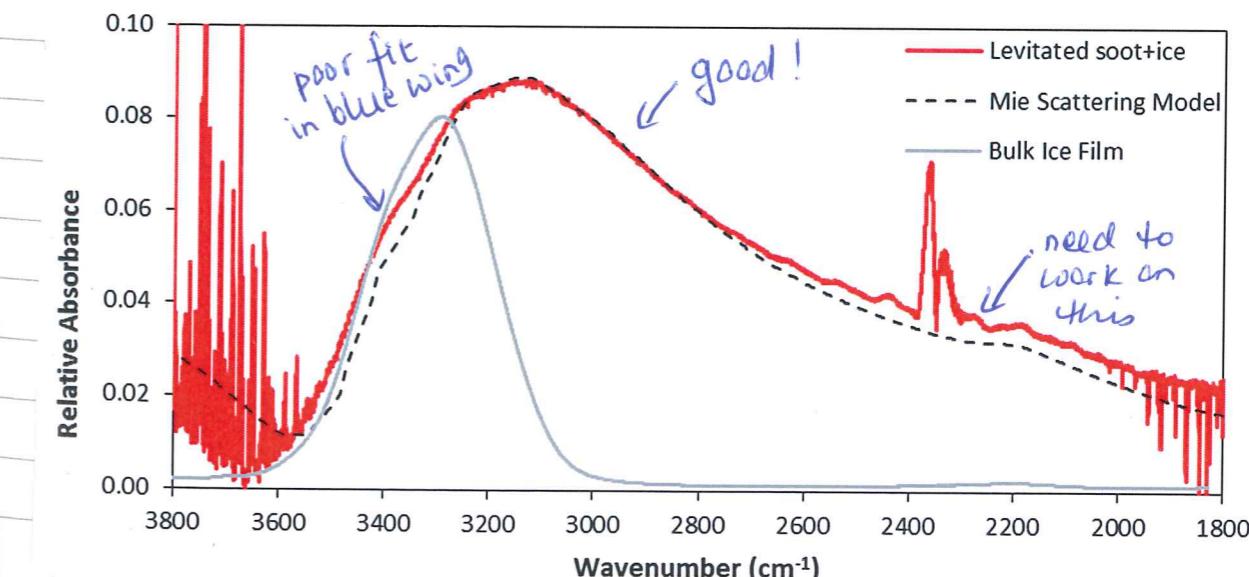
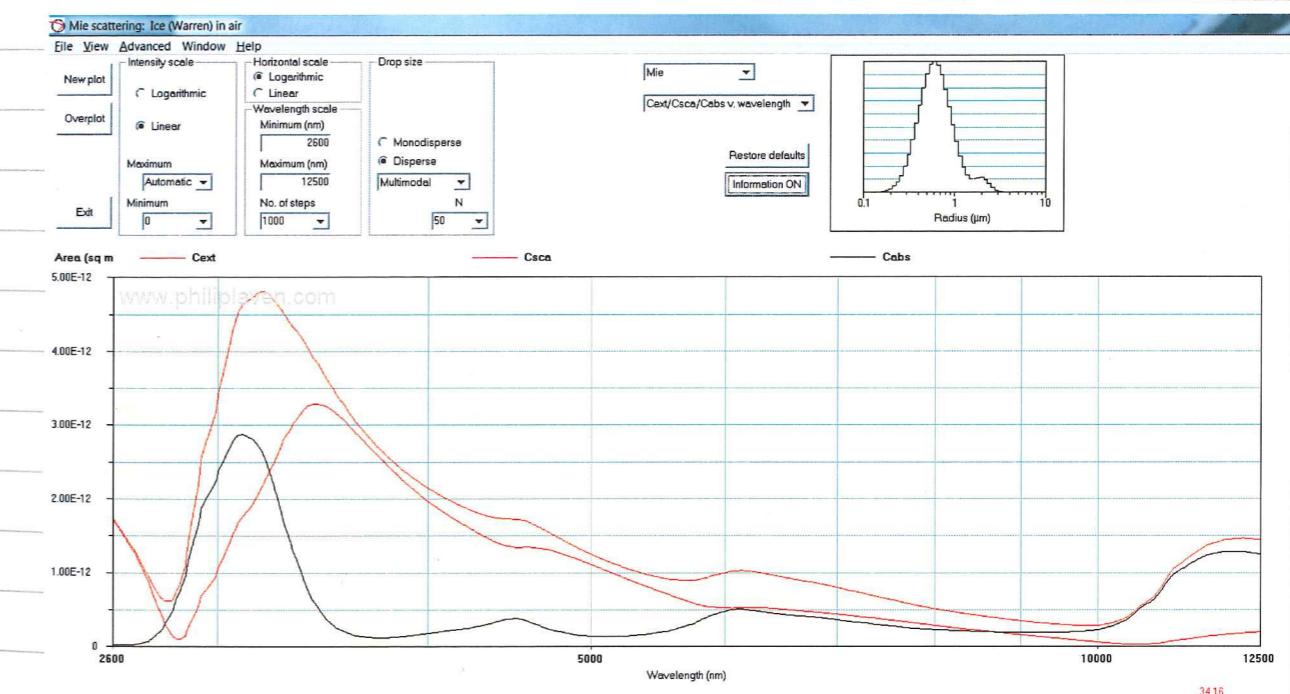
01/11/17



Using a bimodal distribution

0.6 μm + 2 μm particles
1 : 0.1

miePlot_Warren_2-2



Multimodal distributions

<input checked="" type="checkbox"/> Mode 1	Median radius	0.6
<input checked="" type="checkbox"/> Mode 2	Standard deviation	40
<input checked="" type="checkbox"/> Mode 3	Relative concentration	10
Distribution type		
<input type="radio"/> Normal		
<input checked="" type="radio"/> Log-Normal		
<input type="radio"/> Gamma		
Calculations		
Minimum radius	0.01	
Maximum radius	10	
N	50	
<input type="radio"/> Linear steps		
<input checked="" type="radio"/> Logarithmic steps		
OK		

Tri-modal

0.6, 2 and 10 μm
1 : 0.1 : 0.01

MiePlot_Warren_2-2_9

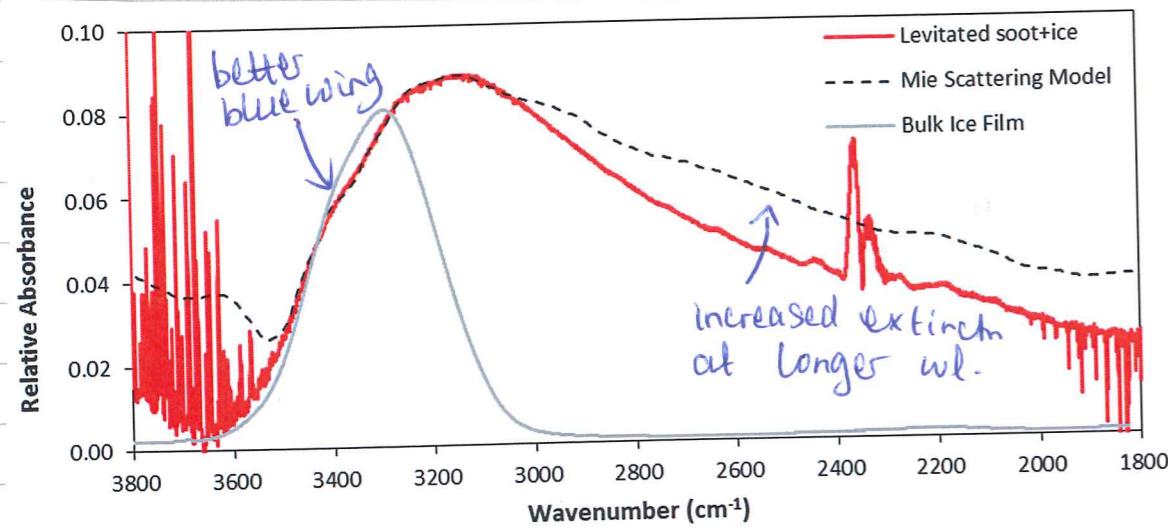
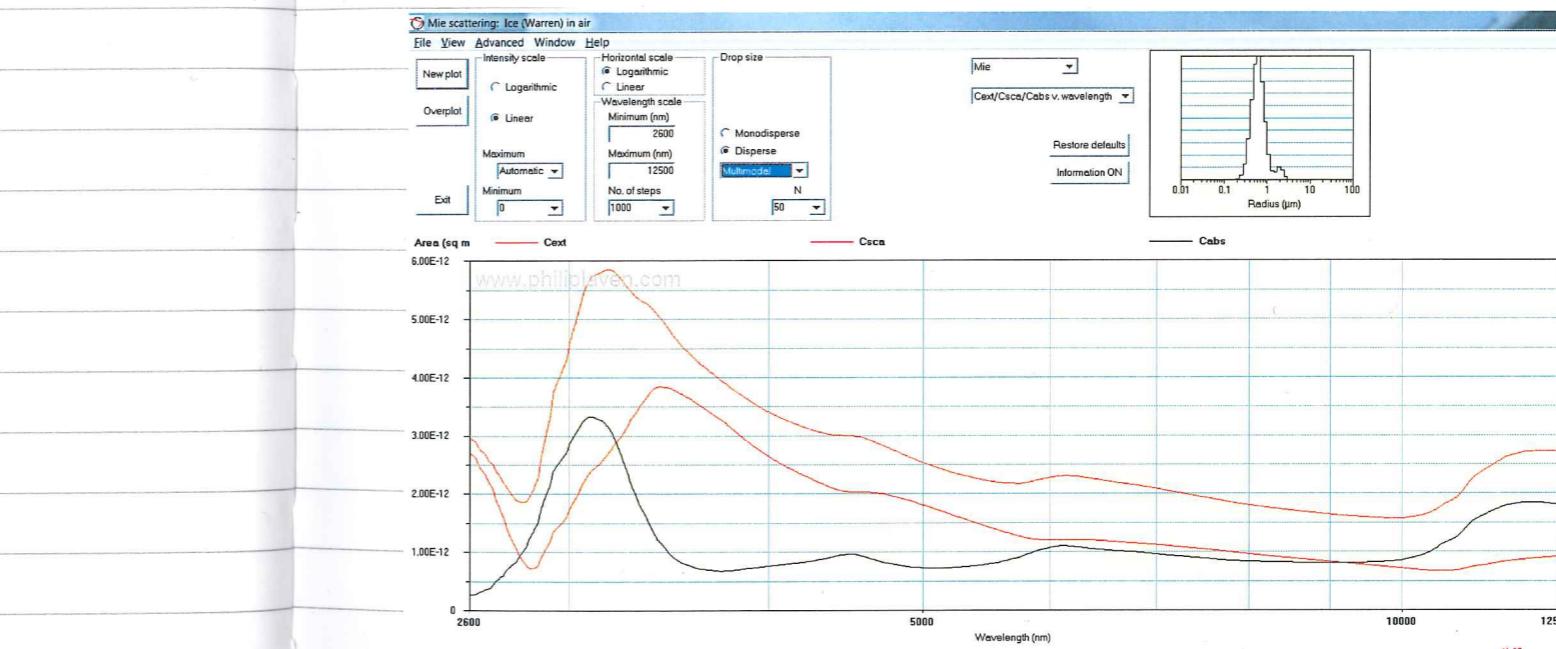
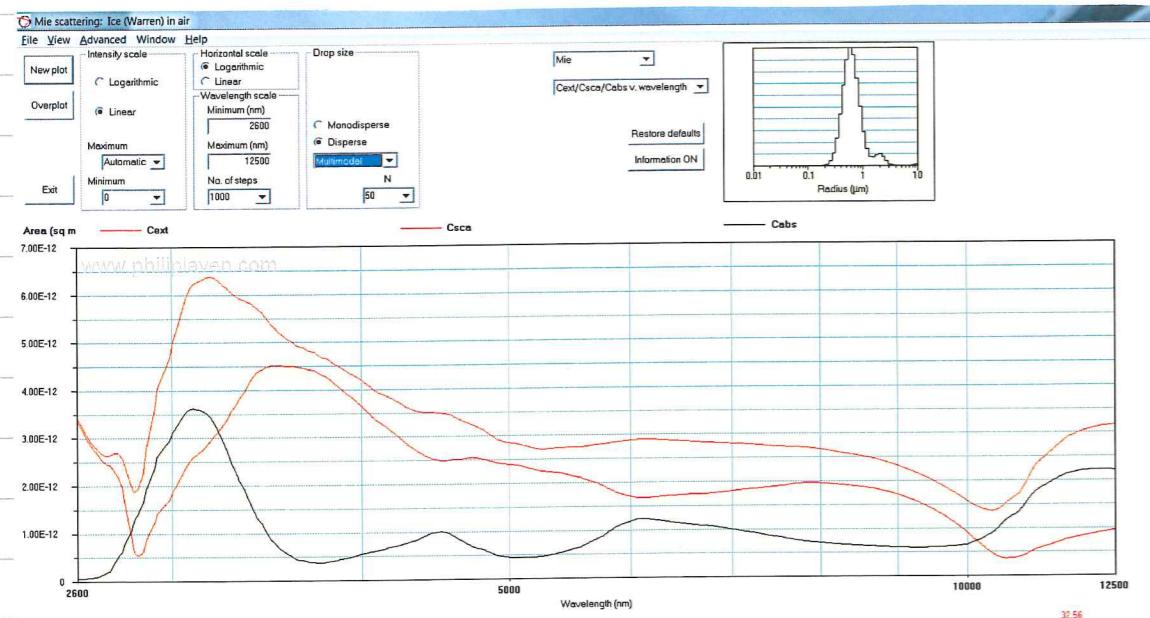
Multimodal distributions

<input checked="" type="checkbox"/> Mode 1	Median radius	0.6
<input checked="" type="checkbox"/> Mode 2	Standard deviation	40
<input checked="" type="checkbox"/> Mode 3	Relative concentration	10
Distribution type		
<input type="radio"/> Normal		
<input checked="" type="radio"/> Log-Normal		
<input type="radio"/> Gamma		
Calculations		
Minimum radius	0.01	
Maximum radius	100	
N	50	
<input type="radio"/> Linear steps		
<input checked="" type="radio"/> Logarithmic steps		
OK		

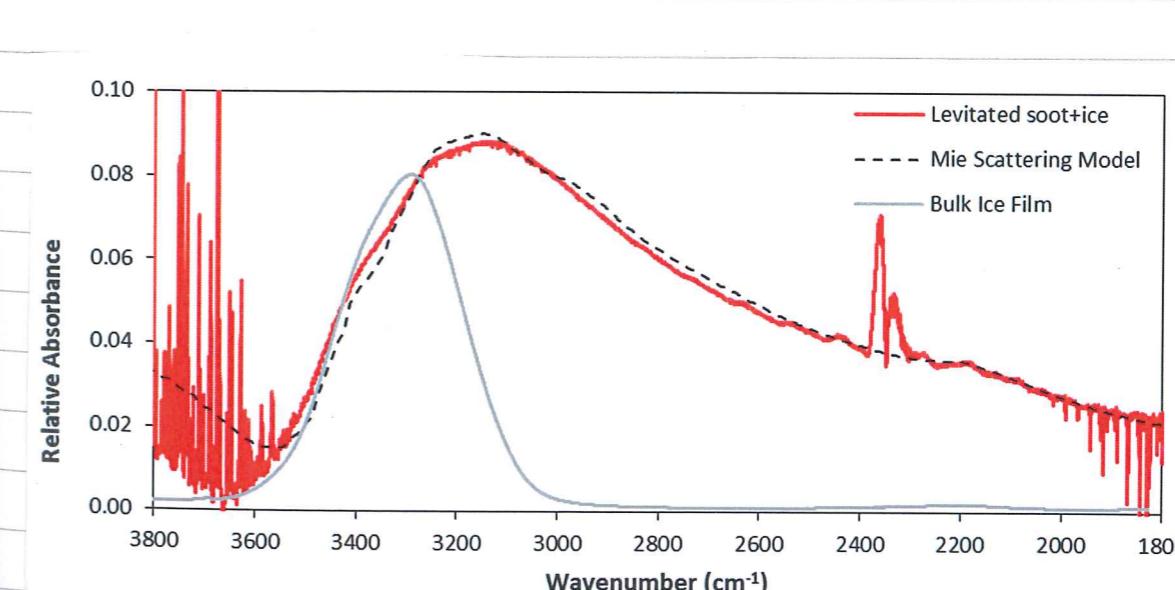
Trimodal

0.6 μm , 2 μm , 100 μm
1 : 0.1 : 0.0001

MiePlot_Warren_2-2_10



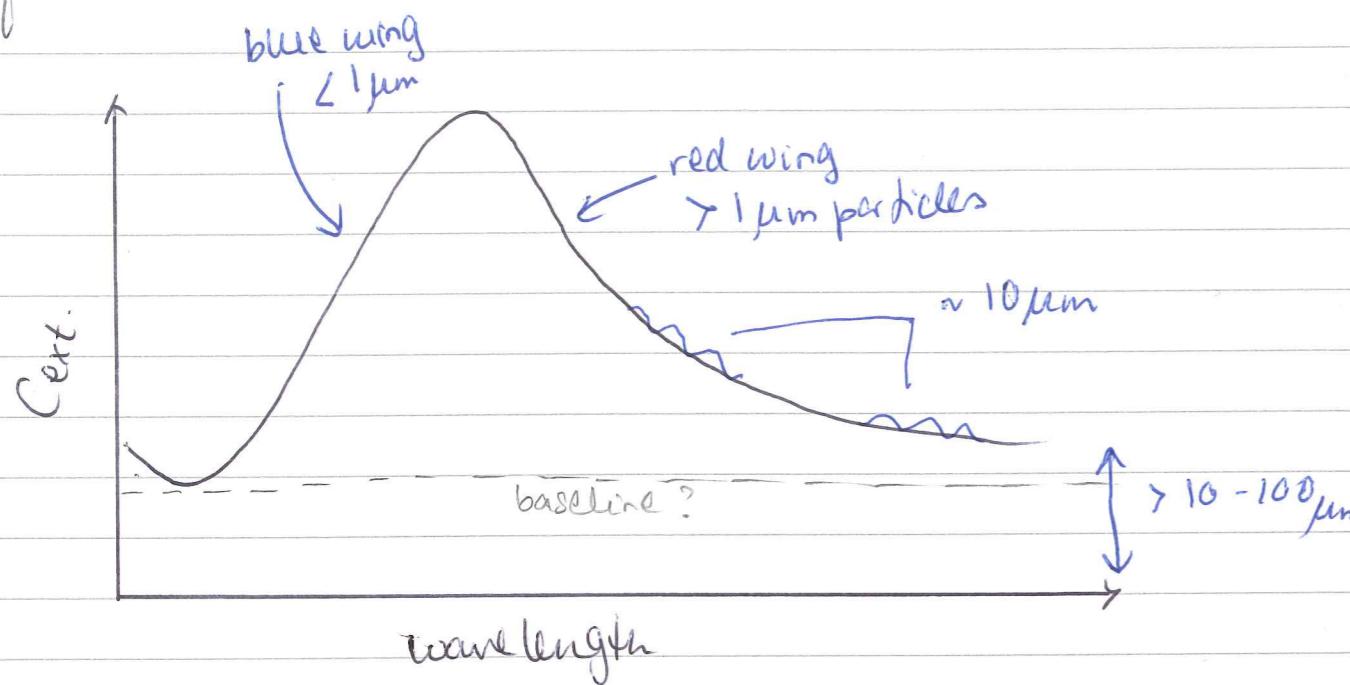
Refining...



Thoughts on data so far:

So it seems that a tri-modal distribution fits best.

By trying out different size, distribution and concentration parameters it looks like your spectra are affected as follows:



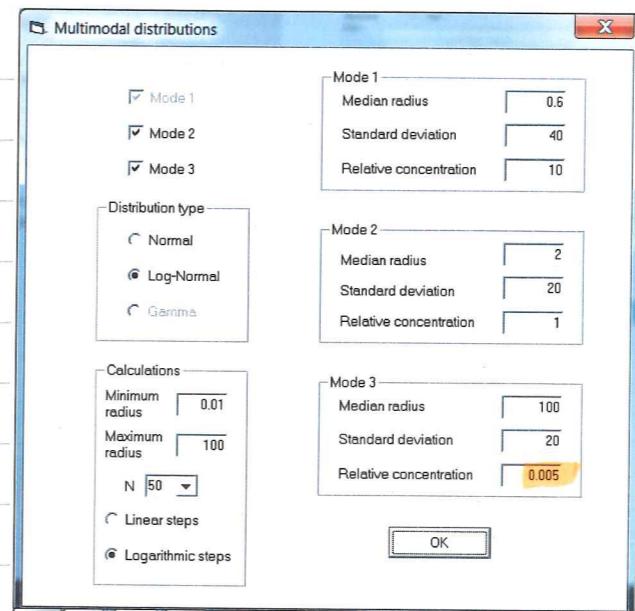
Baseline concerns!

It seems that the apparent Spectral "baseline" is affected by larger particles and so a non-zero baseline is REAL.

So far in plots ~~on~~ on pgs 63-65 I corrected the baseline (linear subtraction to bring whole spectrum to zero) for the lab data.

But looking at the miePlot data — the "baselines" are non-zero and "opacity" increases with larger sizes of particles.

... Refining some more...



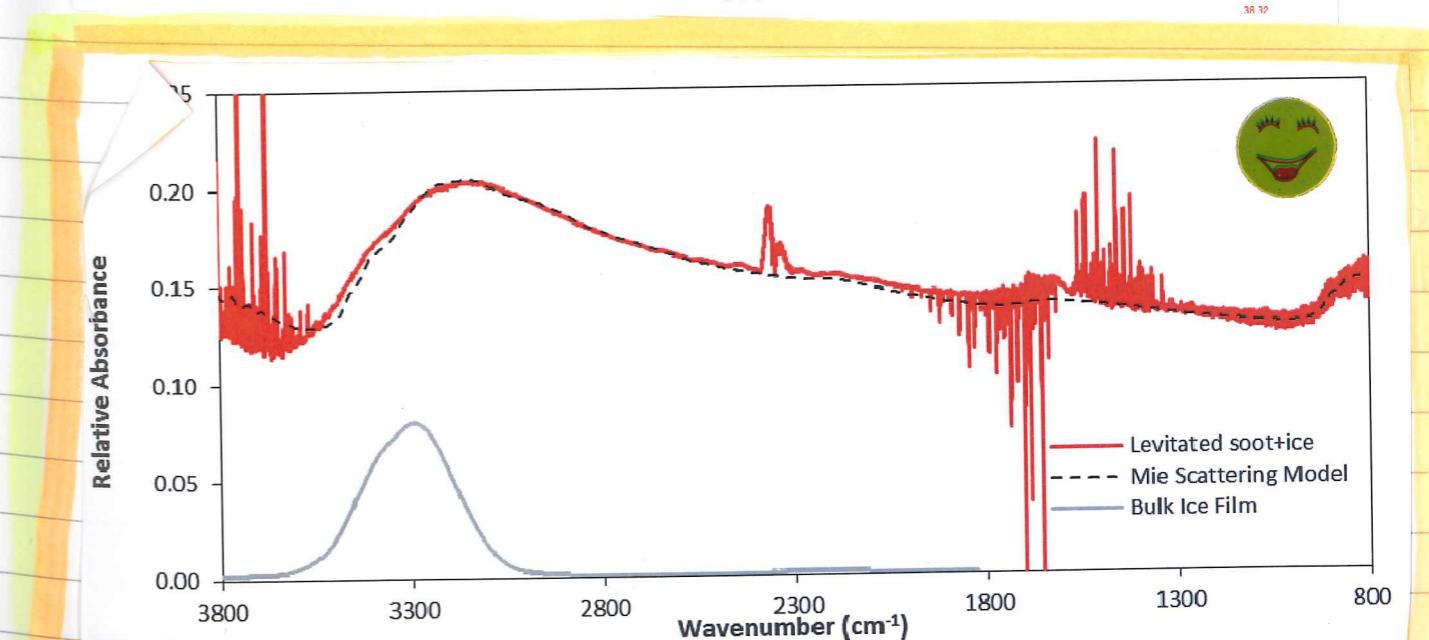
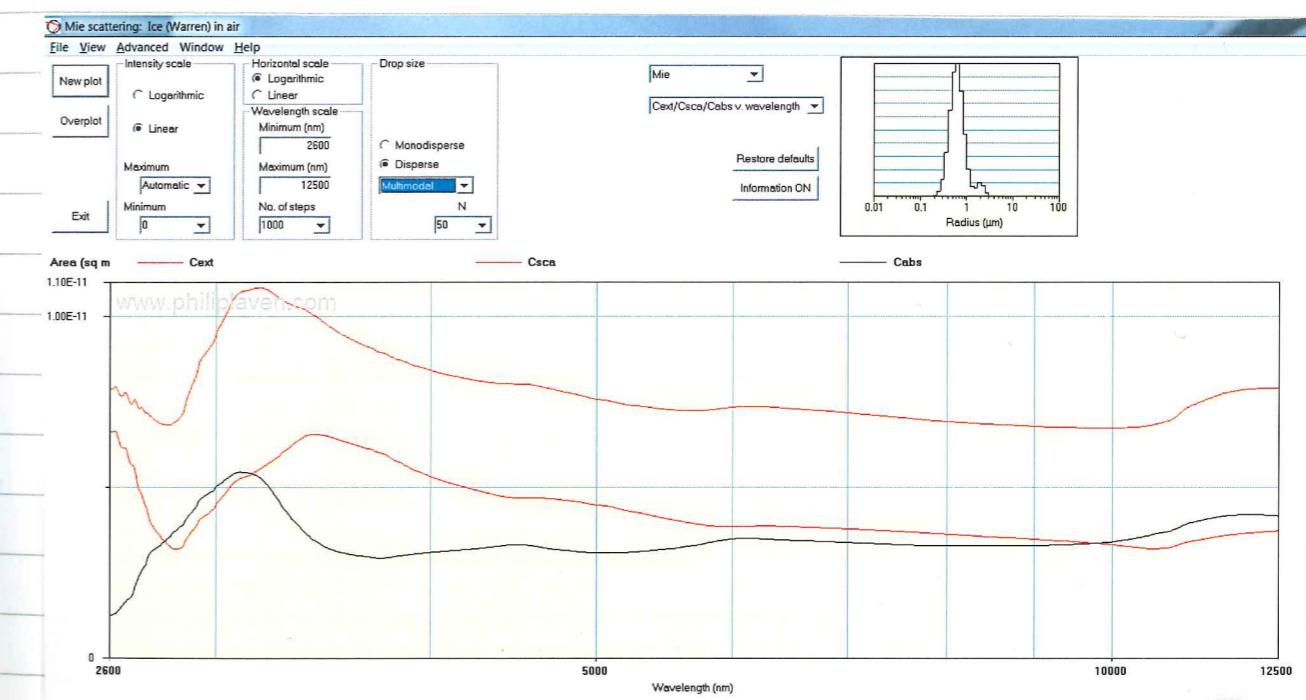
Trimodal

0.6 μm, 2 μm, 100 μm

1 : 0.1 : 0.0005

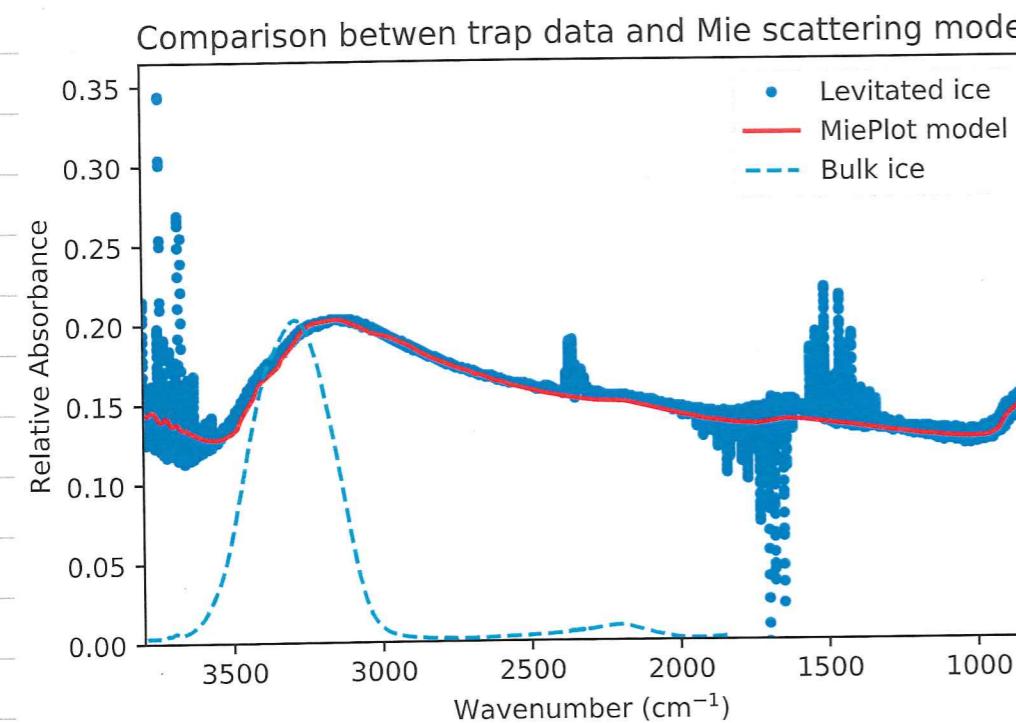
this time lab spectrum is raw — with no baseline correction!

MiePlot_Warren_2-2_11



02/11/17

After lab meeting & Python Club I tried playing around with Python some more to see if I could write a program to plot the miePlot data with lab data. I would eventually like to be able to automate testing parameters in mie Plot and fit it to the lab spectrum.



There is a problem with finding the maximum in the lab data due to the atmospheric water peaks. The workaround is to use a truncated section of lab data around the water peak
 $\sim 3500 - 2800 \text{ cm}^{-1}$

Code →

```
"""
Created on Thu Nov 2 13:26:56 2017
@author: ad3298
"""

import numpy as np
import matplotlib.pyplot as plt

#User input of data files
#lab_filename=input("Enter Lab Data filename")
#mie_filename=input("Enter MiePlot filename")

#read soot+ice data and MiePlot data
#Lab data
lab_wn, lab_abs = np.loadtxt('soot_20170831_0003_raw.txt', dtype=float, \
usecols=(0,1), unpack=1, skiprows=0)

# lab data with no water features
lab_wn_clean, lab_abs_clean = np.loadtxt('soot_20170831_0003_raw_clean.txt',\ 
dtype=float, usecols=(0,1), unpack=1, skiprows=0)

#MiePlot data
mie_wl, mie_cext = np.loadtxt('MiePlot_Warren_2-2_11.txt', dtype=float, \
usecols=(0,3), unpack=1, skiprows=82)

#Water ice data
h2o_wn, h2o_abs = np.loadtxt('bulk_lab_data.txt', dtype=float, \
usecols=(0,2), unpack=1, skiprows=82)

#convert MiePlot wavelength in nm to wavenumber
mie_wn = 10000000/mie_wl

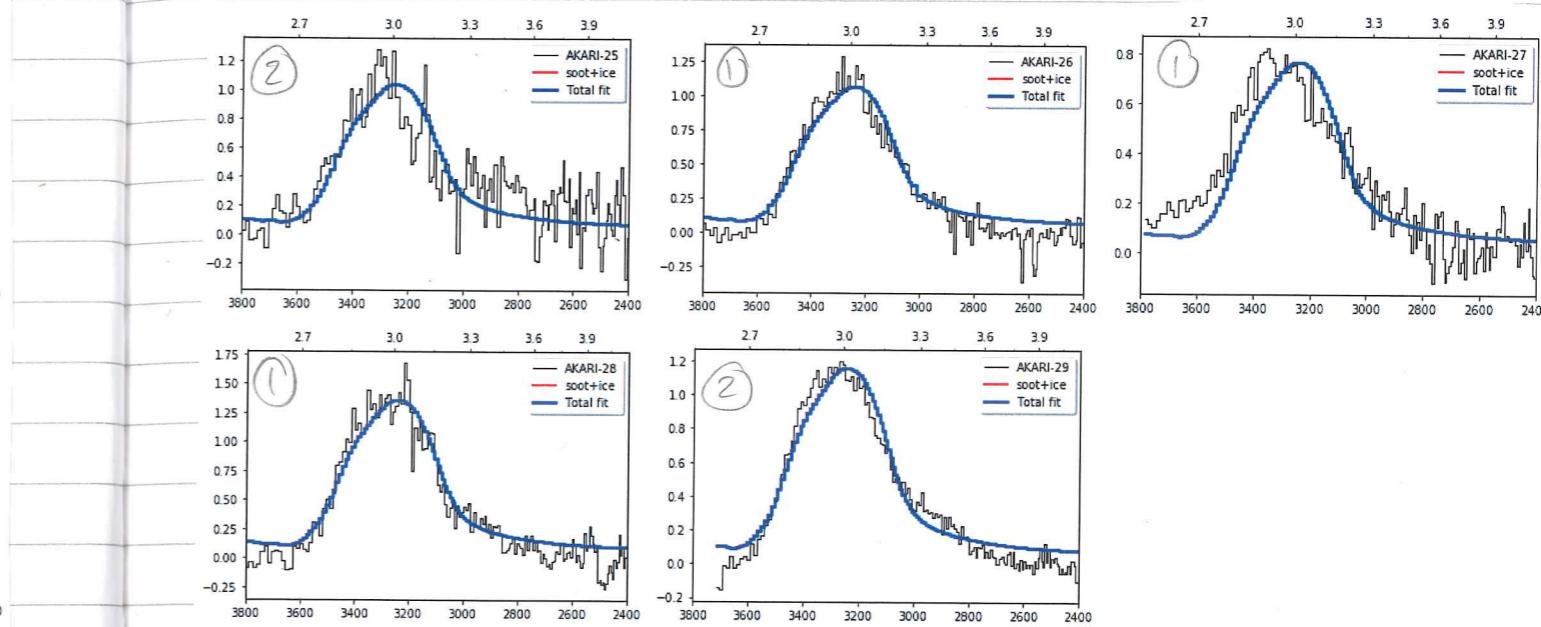
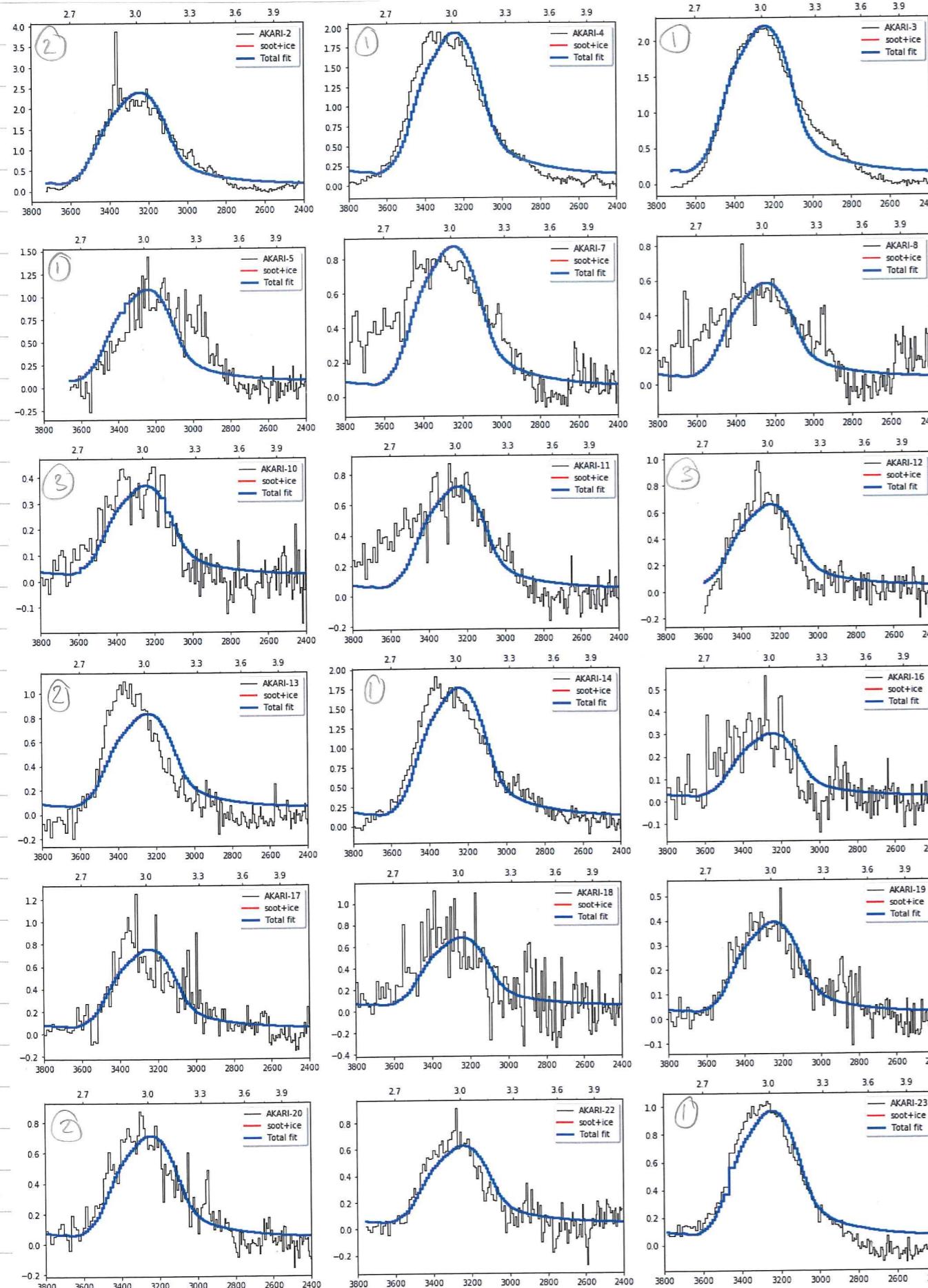
#find peak maxima
lab_max = npamax(lab_abs_clean)
mie_max = npamax(mie_cext)
h2o_max = npamax(h2o_abs)

#normalise data to lab data peak maximum
mie_norm = mie_cext/mie_max*lab_max
h2o_norm = h2o_abs/h2o_max*lab_max

#plots...
plt.plot(lab_wn, lab_abs, '.', label='Levitated ice')
plt.plot(mie_wn, mie_norm, 'r-', label='MiePlot model')
plt.plot(h2o_wn, h2o_norm, 'c--', label='Bulk ice')
plt.xlim(3800,800)
plt.ylim(0, )
plt.xlabel('Wavenumber ( $\text{cm}^{-1}$ )')
plt.ylabel('Relative Absorbance')
plt.title('Comparison between trap data and Mie scattering model')
plt.legend(loc='upper right')
plt.savefig('Lab_Model_Fit.pdf')#name of the figure to save
plt.show()
plt.close()
```

can be jpg or png etc..

03/11/17



Using Mie model data MiePlotData_20171012_Omni_Xscn_0-6

I'm trying to fit some miePlot data to the AKARI data using Omnidfit → the same program that Aleks wrote for fitting the soot-ice data. "anita-soot.py"

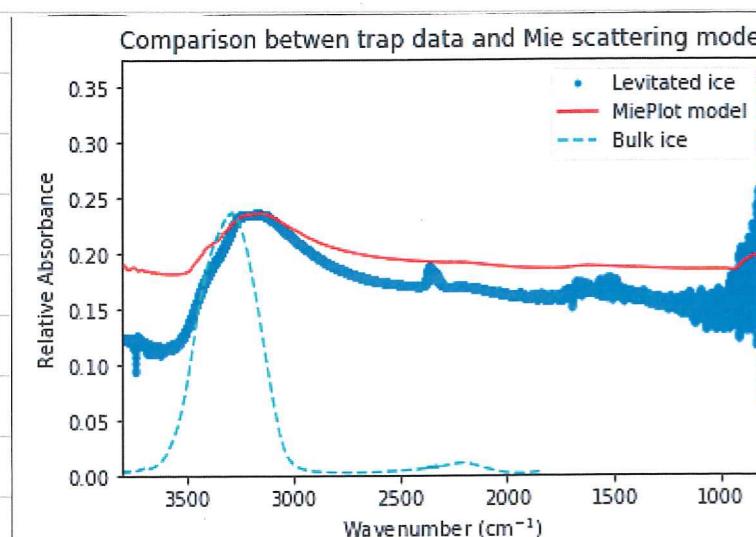
The choice of parameters was purely visual, looking at the miePlot data so far. I used 0.6 μm particles as per Smith et al (1988) (see pg 42 lab book).

Data file used was MiePlot Data - 20171012_Omni_Xscn_0-6
- see pg 54

I prepared the data in a mie.txt file

- ↳ converting wavelength (nm) to wavenumber (cm^{-1})
- ↳ scaling (ext) cross section values to absorbance (approximate) with a factor 5×10^{-14}

c Fitting lab soot/ice spectrum *soot_20170831_0005*



MiePlot_Warren_2-2_19

Mode 1

Nominal radius (um): 0.6

Standard deviation (%) 50

Particle concentration: 5

Mode 2

Nominal radius (um): 2

Standard deviation (%) 20

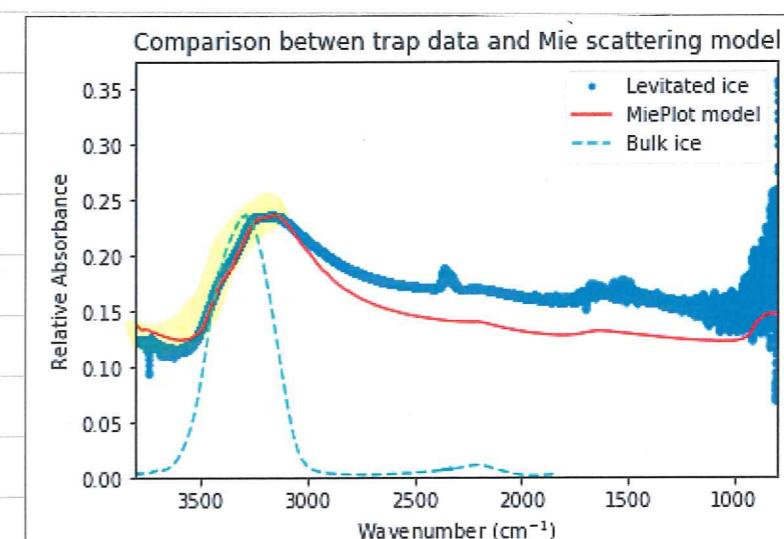
Particle concentration: 0.1

Mode 3

Nominal radius (um): 100

Standard deviation (%) 20

Particle concentration: 0.005



MiePlot_Warren_2-2_22

Mode 1

Nominal radius (um): 0.6

Standard deviation (%) 50

Particle concentration: 10

Mode 2

Nominal radius (um): 2

Standard deviation (%) 20

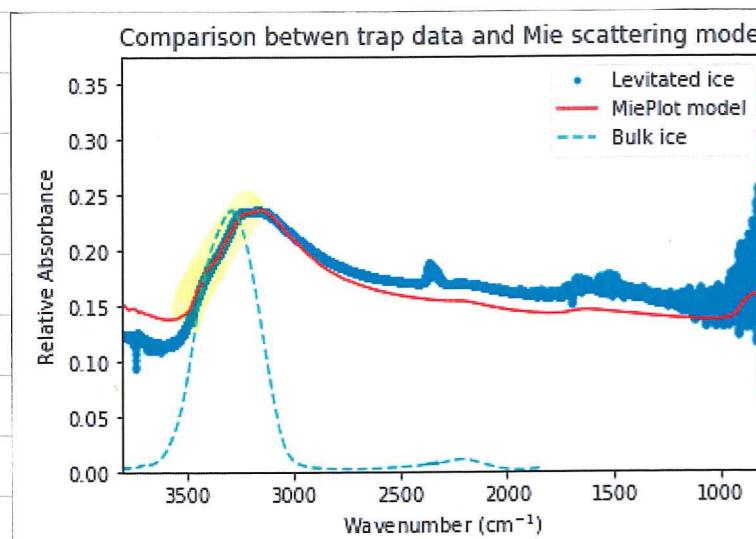
Particle concentration: 0.1

Mode 3

Nominal radius (um): 100

Standard deviation (%) 20

Particle concentration: 0.003



MiePlot_Warren_2-2_20

Mode 1

Nominal radius (um): 0.6

Standard deviation (%) 50

Particle concentration: 5

Mode 2

Nominal radius (um): 2

Standard deviation (%) 20

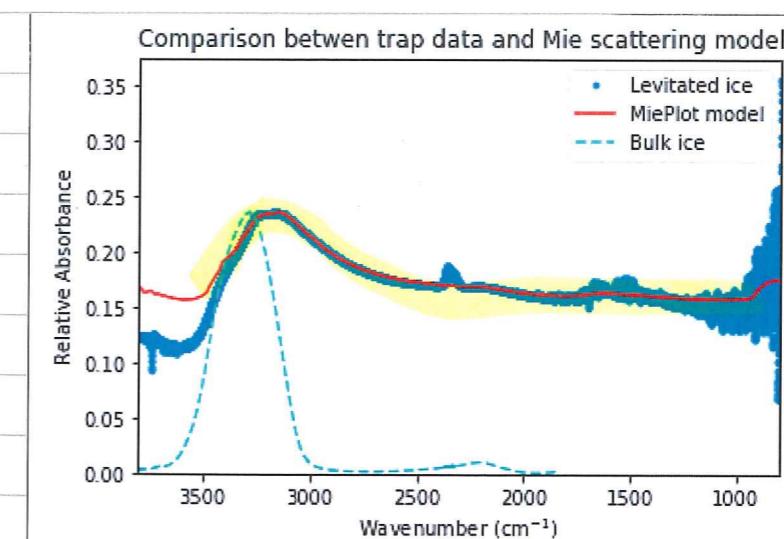
Particle concentration: 0.1

Mode 3

Nominal radius (um): 100

Standard deviation (%) 20

Particle concentration: 0.002



MiePlot_Warren_2-2_23

Mode 1

Nominal radius (um): 0.6

Standard deviation (%) 50

Particle concentration: 7

Mode 2

Nominal radius (um): 2

Standard deviation (%) 20

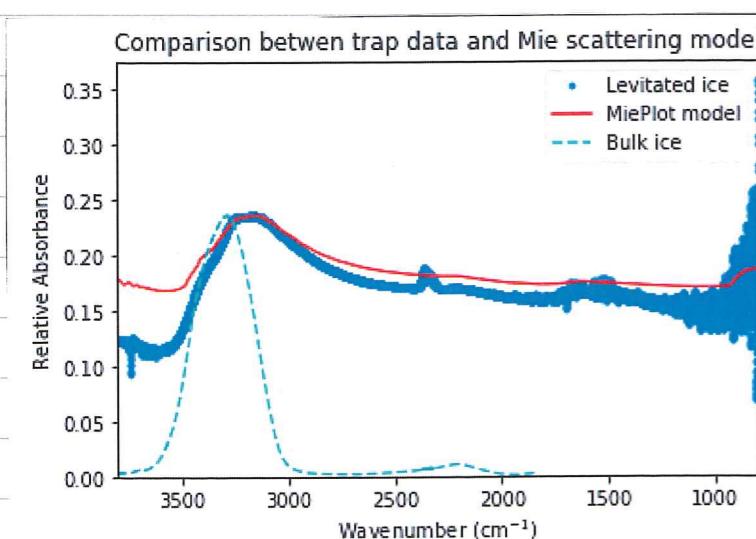
Particle concentration: 0.1

Mode 3

Nominal radius (um): 100

Standard deviation (%) 20

Particle concentration: 0.004



MiePlot_Warren_2-2_21

Mode 1

Nominal radius (um): 0.6

Standard deviation (%) 50

Particle concentration: 4

Mode 2

Nominal radius (um): 2

Standard deviation (%) 20

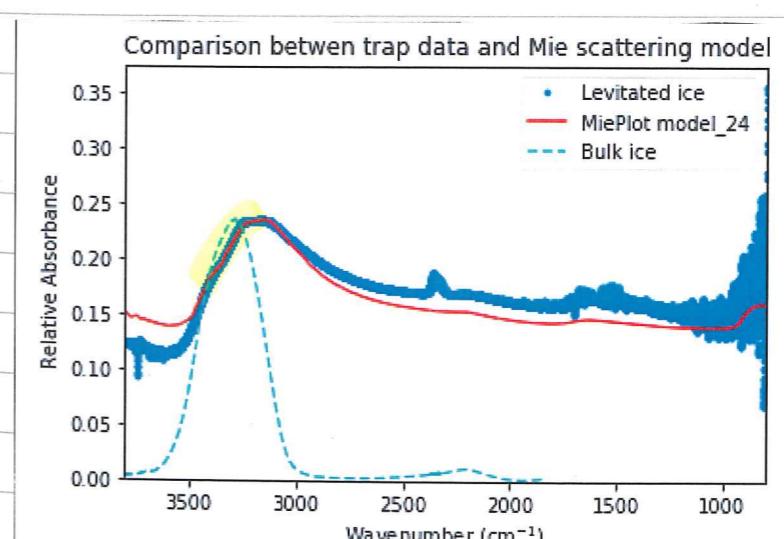
Particle concentration: 0.1

Mode 3

Nominal radius (um): 100

Standard deviation (%) 20

Particle concentration: 0.003



MiePlot_Warren_2-2_24

Mode 1

Nominal radius (um): 0.6

Standard deviation (%) 50

Particle concentration: 10

Mode 2

Nominal radius (um): 2

Standard deviation (%) 20

Particle concentration: 0.1

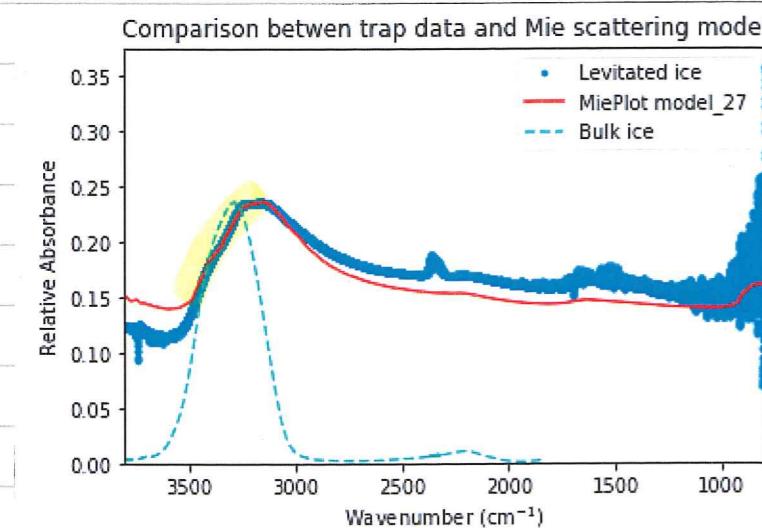
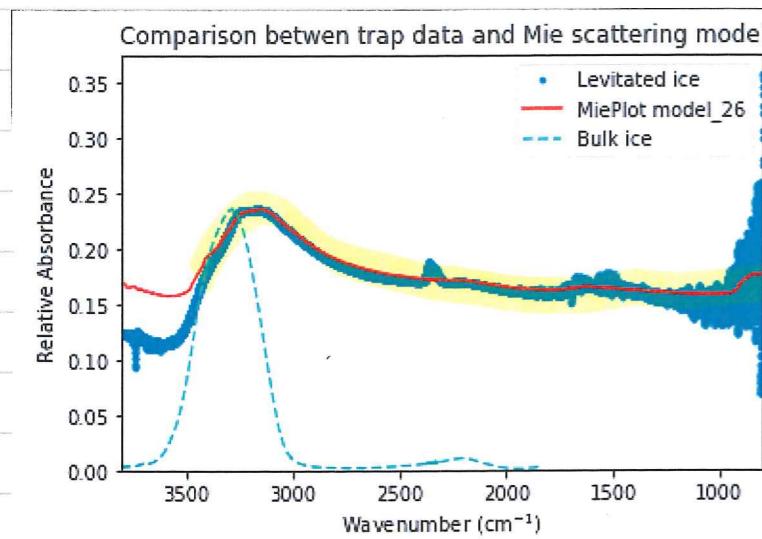
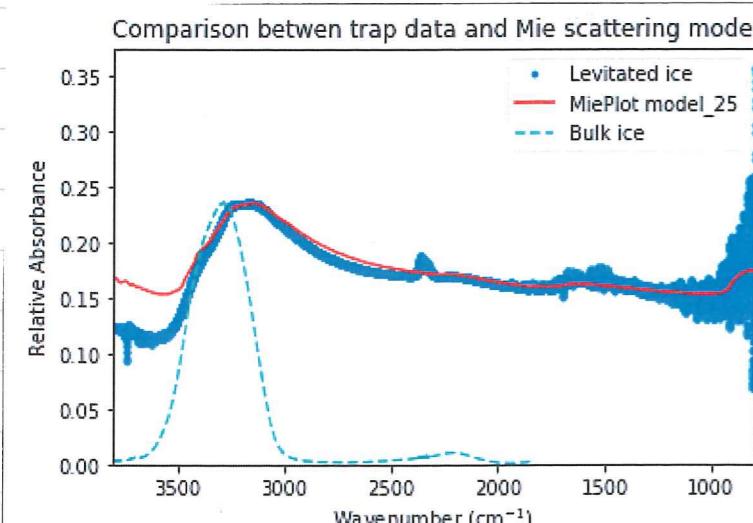
Mode 3

Nominal radius (um): 100

Standard deviation (%) 20

Particle concentration: 0.004

06/11/17



following group meeting - Tim's Talk

- ↳ Look up the "Dust Emissivity parameter" β
 - Characterises the physical properties of interstellar dust - optical properties, grain size, temp
 - Typically β is close to 2
 - ↳ - Grain growth can cause β to decrease ($\rightarrow 0$)
 - Ice mantles increase β ($\rightarrow 3$)
- ↳ Competing grain growth & aggregation
 - keeping $\beta \approx 2$

Dust

Pristine

$$\beta = 1.5 - 2$$

Transitional

$$\beta = 2 - 3$$

Evolved

$$\beta = 0 - 1.5$$

Look up Chen et.al. (2016)

 β dependence on:

- ↳ Grain size $a_{\max} \Rightarrow$ Power Law
- Grain size distribution $n(a) \propto a^{-q}$

- ↳ 3D mapping of local ISM with composite data
Capitanio et.al. arXiv 1706.07711

07/11/17 Trip to Reading to see Ultrasonic Trap.

Today I travelled to Reading Uni to see the ultrasonic trap - Christian Prangs group

Saw levitated water droplets in a very stable trap.

Ultrasound frequency ~ 100 kHz.

Tools for chamber:

- ↳ Small cylinder, with air seal.
- ↳ Can vary humidity
- ↳ droplets / aerosol introduced via syringe
- ↳ Raman spectroscopy + laser + camera
- ↳ x y z manipulation of trap.

Aerosol Society Course

The Fundamentals of Aerosol Science 2017

Programme



10:00 – 10:30 Registration and Refreshments

10:30 – 10:35 Welcome

Professor Benjamin J. Murray – University of Leeds

10:35 – 11:30 Introduction and Fundamentals

Professor Ian Colbeck – University of Essex

11:30 – 12:15 Environmental Sampling

Dr Simon Parker – Defence Science & Technology Laboratory

12:15 – 13:00 Lunch, networking and exhibitor interactions.

13:00 – 13:45 Electrical Properties of Aerosol

Dr Keri Nicoll – University of Reading

13:45 – 14:30 Optical Properties of Aerosol

Professor Jonathan P. Reid – University of Bristol

very interesting
- have slides

14:30 – 14:45 Refreshment Break

14:45 – 15:30 Aerosol Composition

Professor Markus Kalberer – University of Cambridge

15:30 – 16:15 Aerosol Thermodynamics and Kinetics

Professor Benjamin J. Murray – University of Leeds

16:15 – 16:30 Refreshment Break

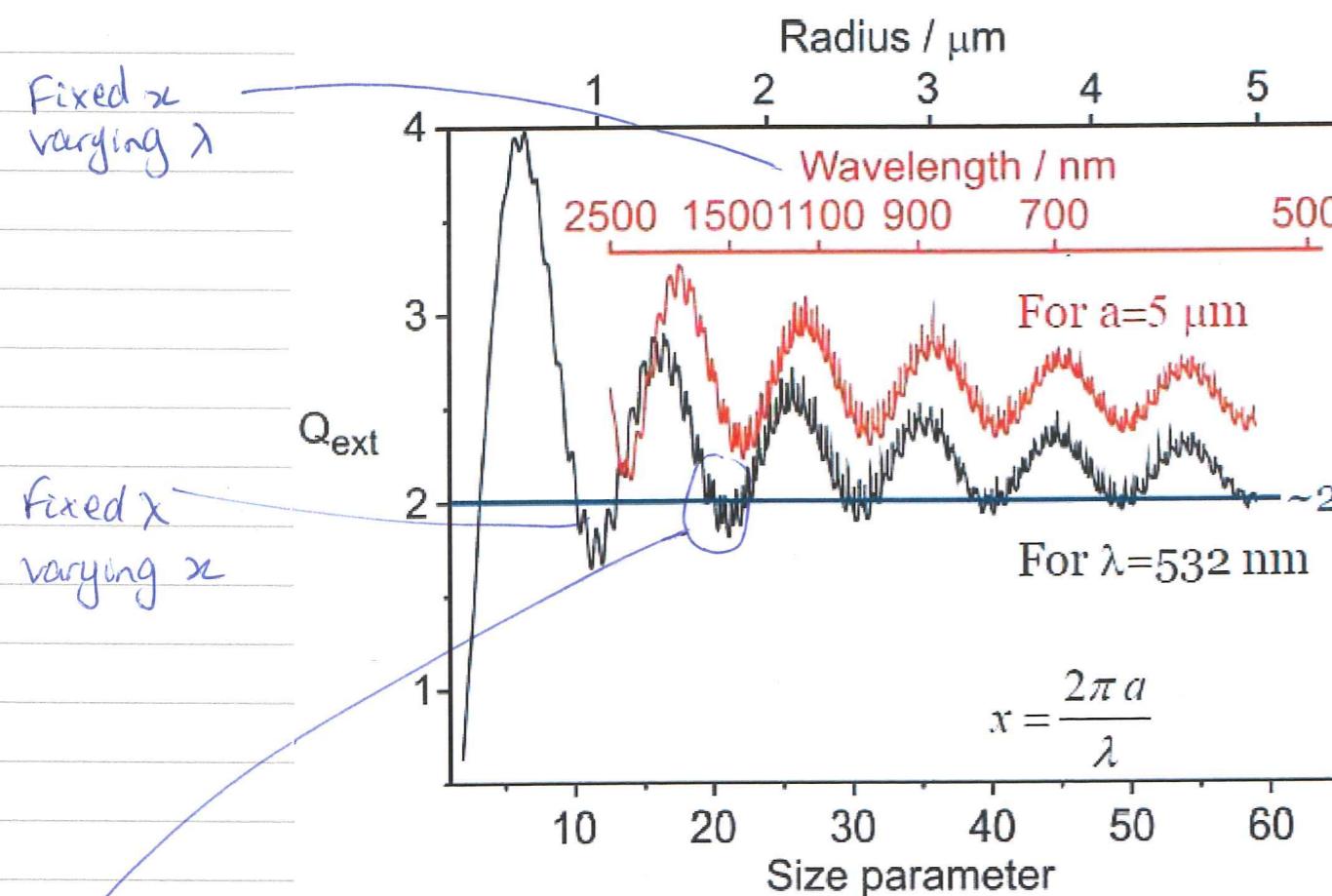
16:30 – 17:15 Aerosol Regulation and Metrology

Dr Paul Quincey – National Physical Laboratory

17:15 – 18:00 Networking Drinks Reception

Join the Aerosol Society committee, event speakers and exhibitors for our pre Annual Aerosol Science Conference drinks reception – an excellent networking opportunity for all.

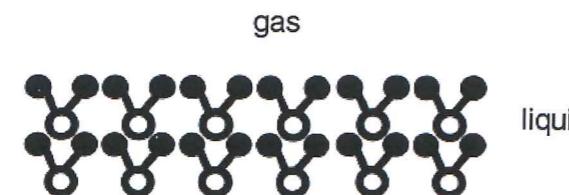
Interesting from Jonathan Reid's Talk:



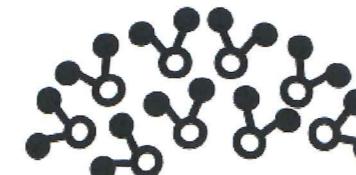
"Ripple structure occurs at discrete size parameters, where combination of wavelength and radius lead to standing wave in droplet" ← could this be the "noise" in my data? pg 23?



Flat surface (~large droplet)



Small droplet



- Small droplets have a greater vapour pressure than a flat surface.
- This is related to the curvature at the surface and intermolecular bonds

Absorbance to n and k converter
Kramers-Kronig analysis.



09/11/17

Today I found it! A Python program with a windows interface where you can convert lab absorbance data to n and k values as a function of wavelength!

Paper: Determination of optical constants n and k of thin films from absorbance data using Kramers-Kronig relationship

Rocha and Pilling
Spectrochimica Acta A 123, pp 436-446 (2014)

Program is downloadable from:

NKABS code.

<https://www1.univap.br/gaa/nkabs-database/data.htm>

Instructions:

- Place a `.txt` file called `Abs.dat` containing waveno. & absorbance data into the same directory as `nkabs.exe` file.
- Run `nkabs.exe`
- Inputs required are
 - thickness of (e.g. 0.4) — in microns
 - no standard refractive index in the visible range
 - n_2 refractive index of substrate (e.g. $MgF_2 = 2.54$)
 - MAPE = mean Absolute Percentage error (%)

Interesting!

Could this be true for desorption of ices too?

Ben Murray's Talk

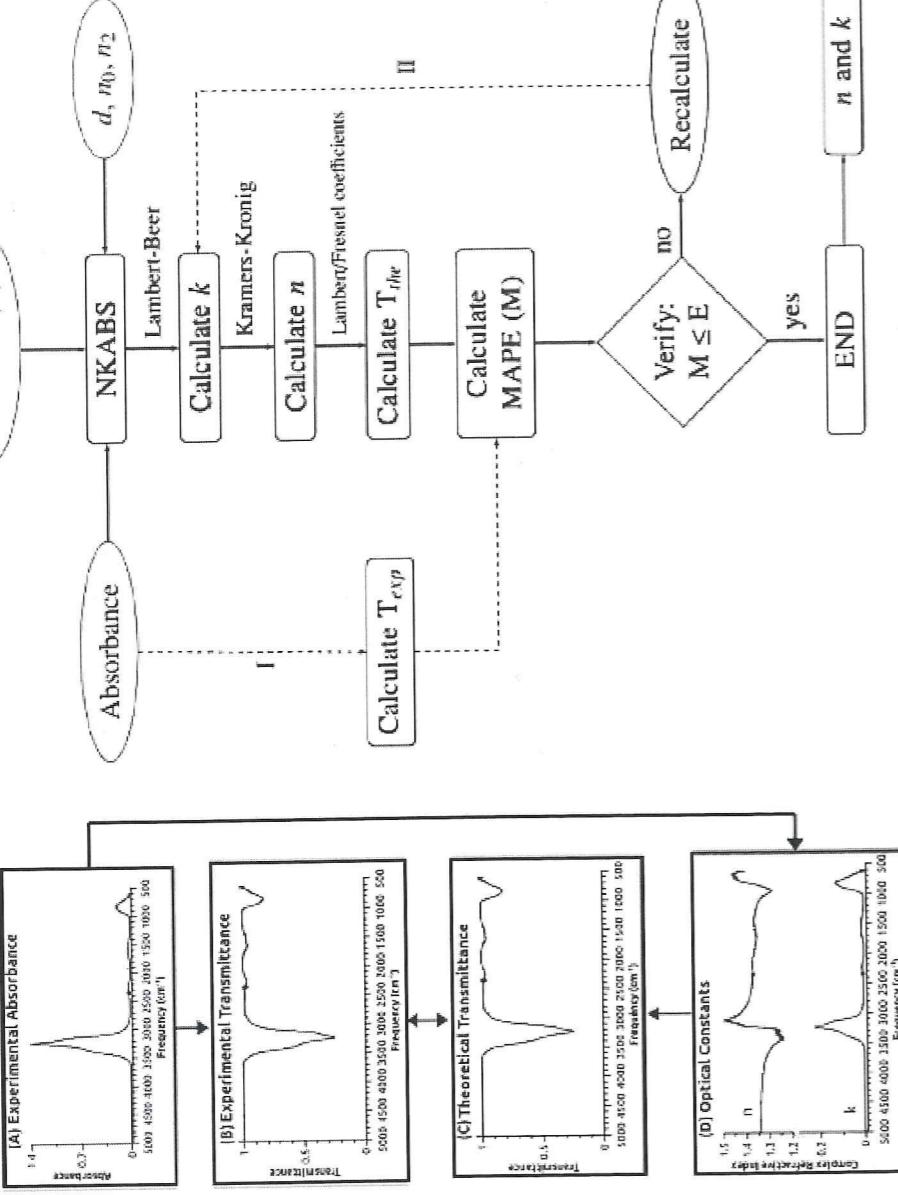
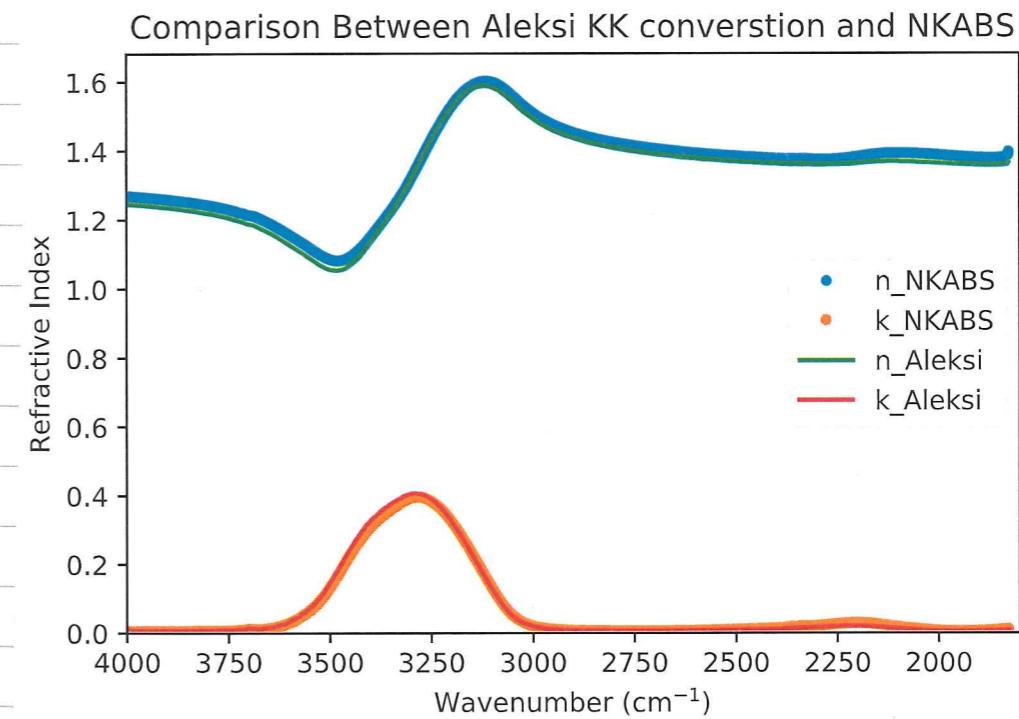


Fig. 4. Left: Illustration of computational procedure of the NKABS code. In block A is shown the absorbance data of the crystalline water at 165 K. The B and C blocks shows the experimental and theoretical transmittance, respectively. In D, is shown the optical constants for crystalline water. The arrows indicates the path executed by code for calculate the optical constants. Right: Execution flowchart of NKABS code. The input parameters are absorbance data, d , n_0 , n_2 and error. When these parameters are informed, the code begins the procedure for obtain the optical constants, using Lambert-Beer law, Kramers-Kronig relationship and also Fresnel and Lambert coefficients. The code evaluate the error and decides if stop or remakes the procedure.

I then ran NKABS on the same lab data that Aleksi used to determine n and k for pure water ice and compared the two.

I was not sure what the ice thickness of the lab data he used was so I ran it a few times to make it match.

Input: Thickness $d = 0.25 \mu\text{m}$
 $n_0 = 1.33$
 $n_2 = 2.54$
 $\text{MAPE} = 5\%$



N.B. This was plotted using Python 😊 — starting to love it

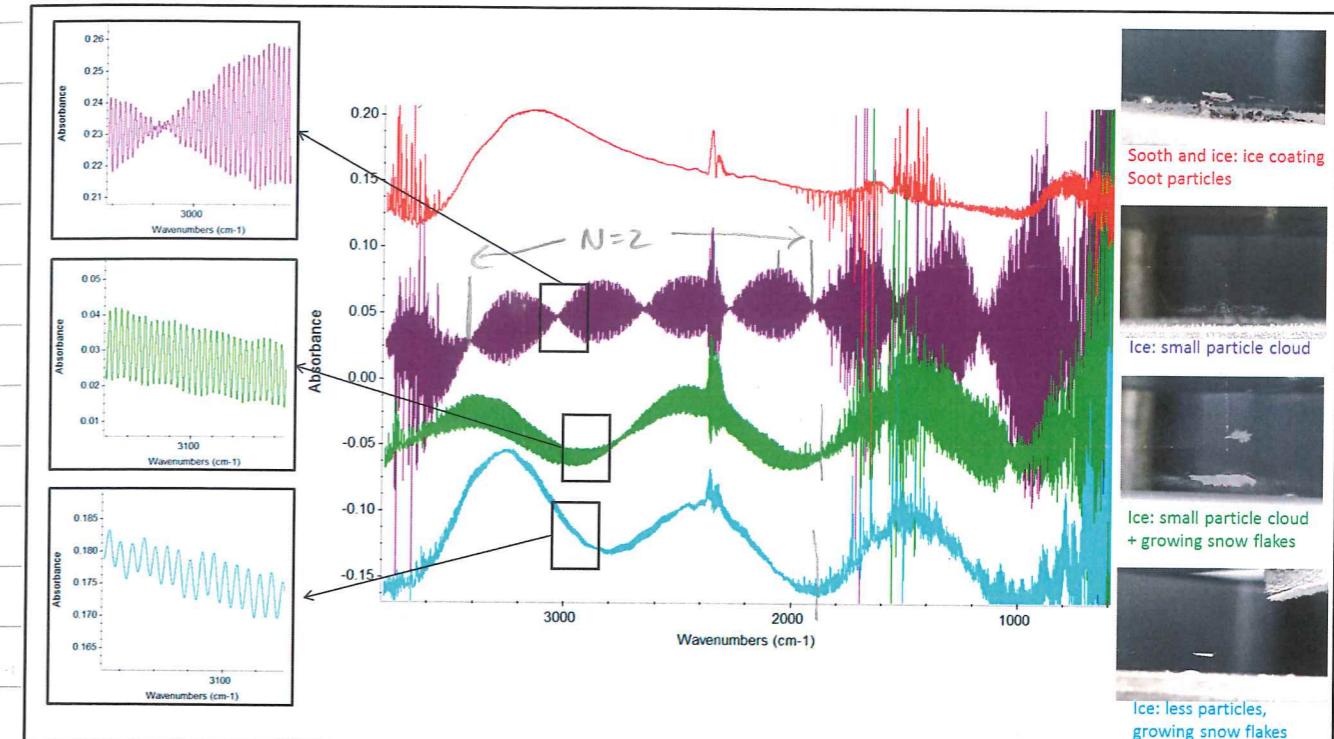
Results: Time to process = 145s
Iterations = 1
 χ^2 = 8.98
MAPE = 2.40

20/11/17 → 26/11/17 Leave (School hole)

- Submitted EWASS Abstract to talk about the ultrasonic trap and comparison with AKARI data + lab data of bulk ices.

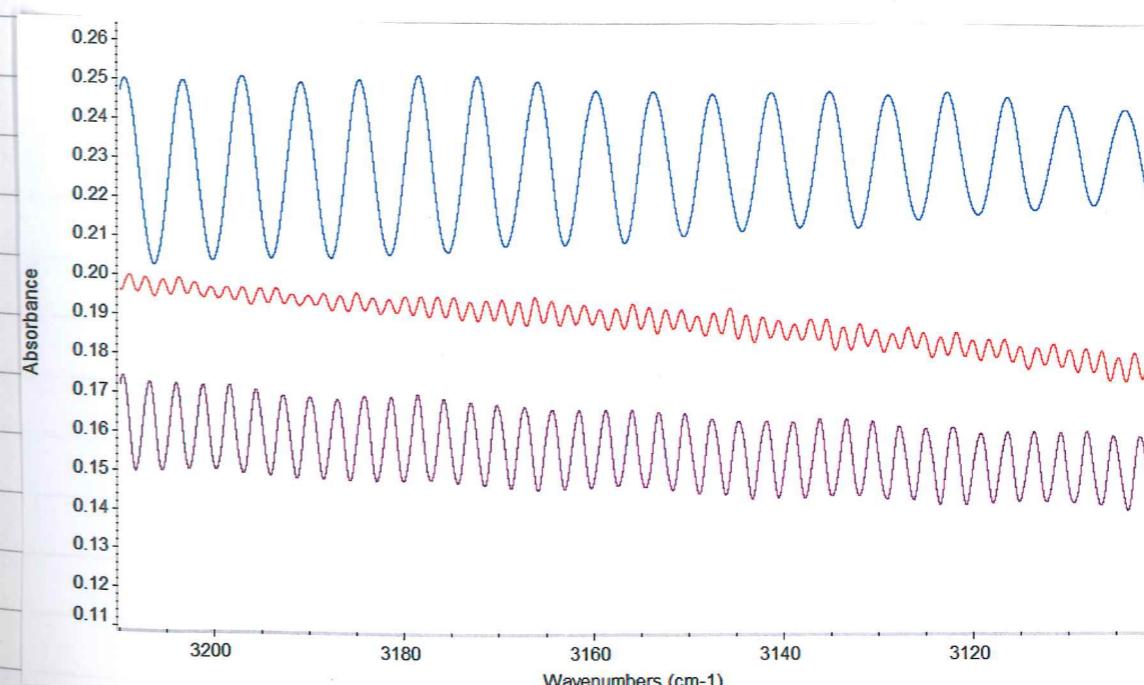
27/11/17 Trip to Belfast to dismantle and pack the atom source.

Taking a closer look at the fine structure in the IR trap data of pure ices



Looking at the spectra on pg 23, there is fine interference structure superimposed on the spectra.

Using this structure, I believe to be caused by interference of light within due to total internal reflection within the particles, it may be possible to calculate the particle size in the same way as thin film interference.



Zoom into the fringe pattern for the three ice spectra above.

N.B. The soot-ice spectra do not exhibit fine structure!

I found a formula in a Perkin-Elmer UV-vis/NIR spectrometer handbook to calculate film thickness of ~~use~~ a film with known refractive index. This formula looks similar to the one Natalia and I found when we were seeing interference patterns in thin substrates. (SEE lab book 2, pg 82)

$$t = \frac{N \lambda_1 \lambda_2}{2n(\lambda_1 - \lambda_2)(n^2 - \sin^2 \theta)^{1/2}}$$

t = thickness

λ_1, λ_2 = min. and max wavelength in range (nm)

N = no. of fringes in range

n = refractive index

θ = angle of incidence

Preciously used formula (that gave an accurate thickness for the ZnSe substrate) was

$$t = \frac{N}{2n(v_1 - v_2)}$$

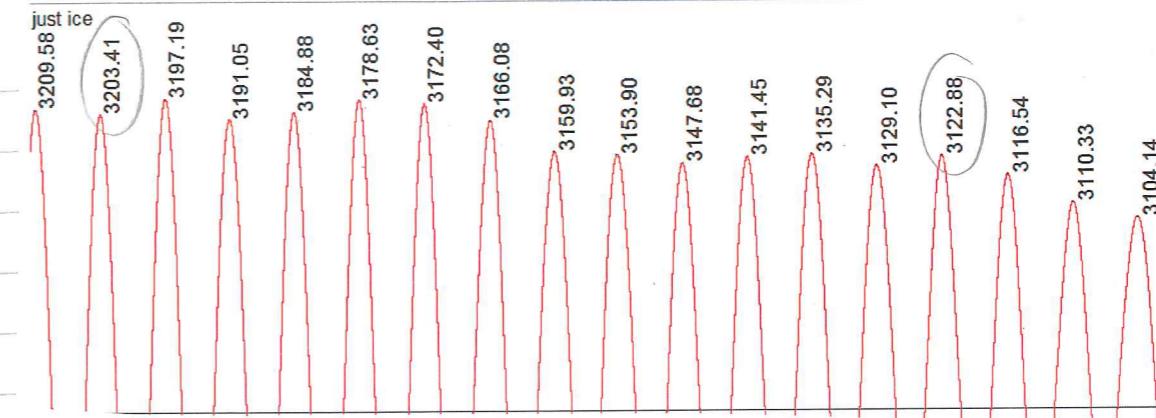
N = no. of fringes

n = refractive index

v_1, v_2 = wavenumber range (cm⁻¹)

NB The second formula was in an IR handbook
 ↳ need to find the source.

www.piketech.com/skin/fashion-mosaic_blue/application-pdfs/CalculatingThickness-FreeStandingFilms-byFTIR.pdf



Application Note - 0502

Calculating the Thickness of Free-Standing Films by FTIR

Qualitative and quantitative analysis of polymer materials is frequently done by preparing a relatively thin film of the material for infrared spectroscopy. These prepared sample materials generally have parallel sides and smooth surfaces and typically produce a well known "fringing effect"^{1,2}, which originates from constructive and destructive interference of the IR beam from these parallel surfaces of the sample. This effect is clearly seen in the FTIR spectrum of a 1.5 mil thickness polystyrene sample shown in Figure 1.

In the spectrum shown in Figure 1, we selected starting and ending points in the spectrum of 2776.51 and 2036.60 cm⁻¹ and counted the number of fringes within this spectral region as 9. To count the number of fringes, select starting and ending points both as minima or maxima of the spectrum and then count the number of opposing minima or maxima. In other words if we select minima values for starting and ending points in the spectrum, then select maxima points to count the number of fringes.

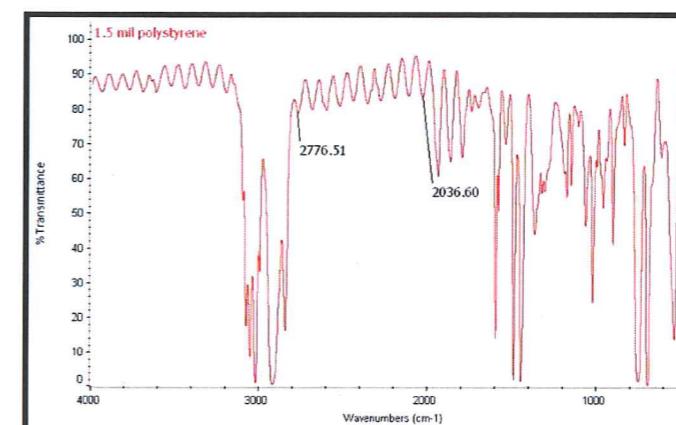


Figure 1. FTIR spectrum of 1.5 mil polystyrene film showing "fringing effect".

From this fringing effect we can calculate the thickness of the film using the following equation;

$$b = 1/2n \times N / (v_1 - v_2)$$

where;

b = film thickness

n = refractive index of sample

N = number of fringes within a given spectral region

v_1, v_2 = start and end point in the spectrum in cm⁻¹

$$= 5 \times 10^{-7} \text{ cm}$$

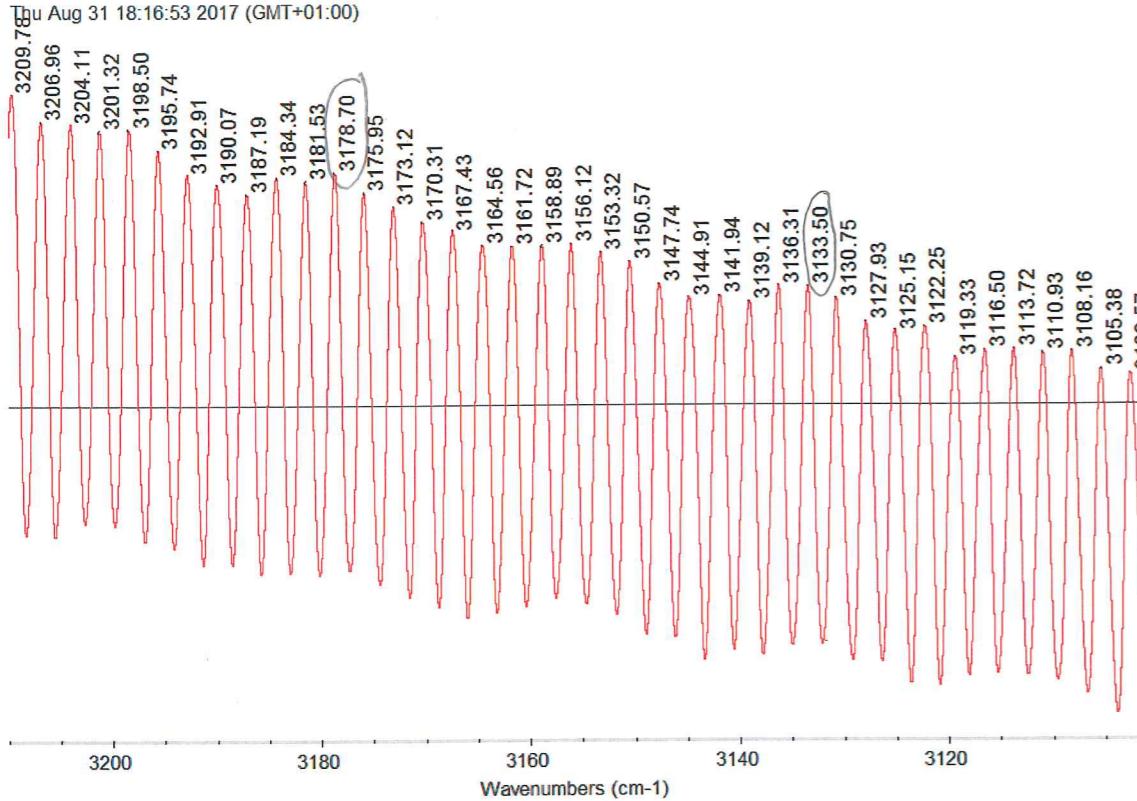
$$= 5 \mu\text{m}$$

Using these values in our equation, we calculate a thickness of 0.003825 cm or 38.25 microns for the polystyrene film. This calculated value compares favorably with the expected thickness of the 1.5 mil film (38 micrometer); however, is more precise.

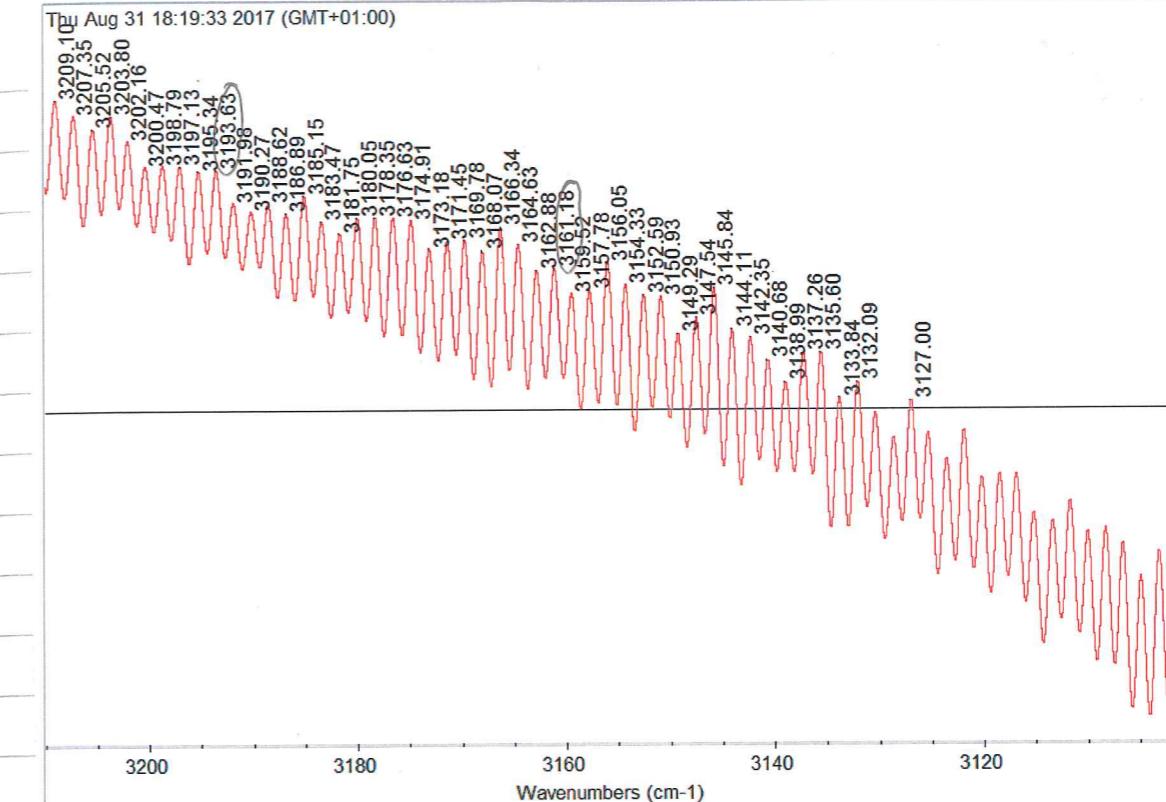
A convenient way to perform the above calculations is by using PIKECalc software (PIKE Technologies part number; 007-0300). With this software package you can enter the values for n , N , v_1 , and v_2 and the thickness of the free-standing film is calculated immediately.

References:

- Griffiths, P. R., de Haseth, J. A., *Fourier Transform Infrared Spectrometry* (John Wiley & Sons, 1986).
- Stuart, B., George, B., McIntyre P., *Modern Infrared Spectroscopy* (John Wiley & Sons, 1998).



(2)



(3)

$$t = \frac{N}{2n(\nu_1 - \nu_2)}$$

$$= \frac{16}{2 \times 1.31 (3178.70 - 3133.50)}$$

$$= 0.135 \text{ cm}$$

$$\nu_1 = 3178.70$$

$$\nu_2 = 3133.50$$

$$N = 16$$

$$n = 1.31$$

$$t = \frac{N}{2n(\nu_1 - \nu_2)}$$

$$= \frac{20}{2 \times 1.31 (3193.63 - 3161.18)}$$

$$= 0.235 \text{ cm}$$

$$\nu_1 = 3193.63$$

$$\nu_2 = 3161.18$$

$$N = 20$$

$$n = 1.31$$

for large sinusoidal pattern:

$$t = \frac{2}{2 \times 1.31 (3800 - 1890)}$$

$$= 3.9966 \times 10^{-4} \text{ cm}$$

$$= 4 \mu\text{m}$$

$$\nu_1 = 3800$$

$$\nu_2 = 1890$$

$$N = 2$$

for Large sinusoidal signal (see pg 89):

$$\nu_1 = 3741$$

$$\nu_2 = 1890$$

$$N = 2$$

$$t = \frac{2}{2 \times 1.31 (3741 - 1890)}$$

$$= 4.12 \times 10^{-4} \text{ cm}$$

$$= 4 \mu\text{m}$$

IR assignments to benzene bands:

Assignment	Pure C ₆ H ₆	C ₆ H ₆ :H ₂ O 1:1	C ₆ H ₆ :H ₂ O 1:10	Pure H ₂ O	(a) 13 K	(b) 30 K	(c) In Ar
H₂O bands							
dOH				3723	3718		
				3694	3696		
dOH-C ₆ H ₆ ^(a)		3616	3585	3584		3585	
OH stretch asym. sym.	v ₁ , v ₃ ^(e) v ₃ v ₁		3288	3279	3270		
		3352			3734		
		3215			3638		
OH bend	v ₂ ^(e)		1631	1650	1653	1655	1589
C₆H₆ bands							
C-H stretch	v ₁₂ + v ₁₆ ^(b) (v ₂ + v ₁₆ + v ₈) v ₁ + v ₈ + v ₆ * v ₁₂ ^{(c)*}	3088 3069 3032 3004	3089 3070 3033 3006	3092 weak 3038 weak	3095	3042	
		3032	3033	3038		3040	
C-H bend	v ₅ + v ₁₇ ^{(c)*} v ₁₀ + v ₁₇ ^{(c)*}	1967 1823	1974 1832	1977 1836	weak weak	1964 1821	
	v ₁₂ ^{(c*, b)*}	1477	1478	1479	1480	1480	
	?	1178	1176	weak			
C-C stretch	v ₁₅ ^(d)	1147	1147			1048	
	bend						
C-C stretch	v ₁₄ ^{(c)*}	1035	1035	1036	weak	1036	

- (a) Silva and Devlin, J Phys Chem (1994) – 3:97 C₆H₆:H₂O at 13 K
- (b) Zhou et al, ApJ (2010) – Benzene formed during irradiation of acetylene ices at 30 K
- (c) Engdahl et al, J Phys Chem (1985); * These assignments were translated from the Herzberg notation (See Bernhardsson et al, J Chem Phys (2000)), now replaced with a modern numbering system – C₆H₆-H₂O matrix isolated in Ar at 17 K
- (d) Bernstein, JCP (1968)
- (e) Hagen et al, A&A (1983)

(f) Bahr et al (2007)

The above table shows a compiled set of bands I see in my spectra and the assignments I found in the literature.

Normal vibrational modes of benzene

06/12/17

I keep going back to 2-3 papers to look up the modes and frequencies of benzene vibration. Here is a compiled list to make my life easier.

Modes, symmetry, vibration energy for all normal modes of benzene

Modes Wilson (Herzberg)	Symmetry	Calculated frequency (cm ⁻¹)	Gas phase frequency (cm ⁻¹)	Description
v ₁ (v ₂)	1a _{1g}	1042	993	Breathing
v ₂ (v ₁)	2a _{1g}	3385	3074	C-H breathing
v ₃ (v ₃)	1a _{2g}	1501	1350	C-H twist
v ₄ (v ₈)	1b _{2g}	724	707	Chair
v ₅ (v ₇)	2a _{2g}	1037	990	Antisymmetric C-H bend
v ₆ (v ₁₈)	1e _{2g}	715	608	Quinoid
v ₇ (v ₁₅)	4e _{2g}	3355	3057	C-H breathing
v ₈ (v ₁₆)	3e _{2g}	1740	1601	Antisymmetric C-H bend
v ₉ (v ₁₇)	2e _{2g}	1276	1178	Symmetric C-H bend
v ₁₀ (v ₁₁)	1e _{1g}	876	847	Antisymmetric C-H bend
v ₁₁ (v ₄)	1a _{2u}	654	674	C-H bend
v ₁₂ (v ₆)	1b _{1u}	1099	1010	Antisymmetric twist
v ₁₃ (v ₅)	2b _{1u}	3345	3057	C-H breathing
v ₁₄ (v ₉)	2b _{2u}	1340	1309	C-C stretch
v ₁₅ (v ₁₀)	1b _{2u}	1185	1150	C-C stretch
v ₁₆ (v ₂₀)	1e _{2u}	431	398	Boat
v ₁₇ (v ₁₉)	2e _{2u}	993	967	Out of plane C-H bend
v ₁₈ (v ₁₄)	1e _{1u}	1115	1038	Twist
v ₁₉ (v ₁₃)	2e _{1u}	1630	1484	C-H antisymmetric twist
v ₂₀ (v ₁₂)	3e _{1u}	3373	3064	C-H breathing

References:

- Penfold et al, J Chem Phys (2009)
- Bernhardsson et al, J Chem Phys (2000)