

Updated python code for benzene, to constrain refractive index

```
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=input()
x,y = np.loadtxt(filename, dtype=float, usecols=(0,1), unpack=1, skiprows=2)
if np.any(y < 0):
    y = -1*y

#sin function used  $y_0 + \sin(2\pi(x-x_c)/w)$ 
#with  $y_0 = y_{\text{offset}} = A(n+1)/(n-1)$ ,  $x_c = x_{\text{offset}}/\text{phase}$ ,  $w = \text{period}$ ,  $A = \text{amplitude}$ 
def intento(x,*p):
    A, xc, w, n=p
    return A*((n+1)/(n-1)+np.sin(2*np.pi*(x-xc)/w))
guess = [0.01, -600, 1000, 1.4]

#parameter bounds
width = 1200
param_bounds=([0,-width/2, -width, 1.4],[0.1, +width/2, width, 1.5])

#fits the function and returns coeff[as many guesses as you have]
coeff, var_mat = curve_fit(intento, x, y, p0=guess, bounds=param_bounds,\
                             maxfev=10000)

#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()

A=coeff[0]; xc=coeff[1]; w=coeff[2]; n=coeff[3]
y0=A*(n+1)/(n-1)

print("Chi-sq =", chi_squared, "\n")
print("y0 =", y0, "\nxc =", xc, "\nw =", w, "\nA =", A)
print("\nRefractive index =", n, "at 632.8 nm")

# $n_1 \sin(\theta_1) = n_2 \sin(\theta_2)$ , So  $\theta_2 = \arcsin(\sin(\theta_1)/n_2)$ 
theta=np.radians(20) #Attention, python numpy works in radians
theta2=np.arcsin(theta/n)
theta2_deg=np.rad2deg(theta2)
print("\ntheta2 =", theta2, "rad \ntheta2 =", theta2_deg, "degrees")

#thickness per fringe,  $d = \lambda / (2n \cos(\theta_2))$ 
d=632.8/(2*n*np.cos(theta2))
print("\nd =", d, "nm")

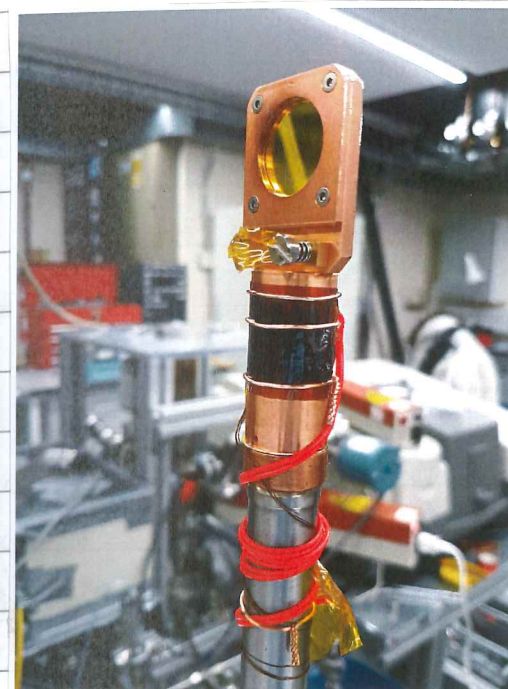
#rate = thickness/fringe / time/fringe
rate=d/w
print("\nDeposition rate =", rate, "nm/s")

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

thickness=rate*t
print("\nThickness =", thickness, "nm")
```

changed the heater today.

12/12/17



Replaced burnt heater & showed Rachel.

Needed to rewire feedthrough as one of the heater wires broke off the pin.

Re-wound the wires for ease of access to feedthrough if we need to get at the pins in the future.

we got ASTRID2 beamtime!

SCHEDULE

PI : ISA-18-115

VUV photoabsorption spectroscopy of benzene and water in argon matrices and astrophysically relevant conditions

Co-I : ISA-18-114 (Andrew)

Investigation into the nature of sponteletrics using VUV abs. spectroscopy

Co-I : ISA-18-116 (Rachel)

Systematic VUV studies of electron-irradiated, condensed molecular films of CO_2/NH_3

April			May			June		
S 01			T 01			F 01		
M 02			W 02			S 02		
T 03			T 03			S 03		
W 04			F 04			M 04		23
T 05			S 05		Sergio's Experiments	T 05		
F 06			S 06			W 06		
S 07			M 07			T 07		
S 08			T 08			F 08		
M 09			W 09			S 09		
T 10			T 10			S 10		
W 11			F 11			M 11		
T 12			S 12			T 12		
F 13			S 13			W 13		
S 14			M 14			T 14		
S 15			T 15			F 15		
M 16			W 16			S 16		
T 17			T 17			S 17		
W 18			F 18			M 18		25
T 19			S 19		Other part of Rachel's Experiments	T 19		
F 20			S 20			W 20		
S 21			M 21			T 21		
S 22			T 22			F 22		
M 23			W 23		Anita's Experiments	S 23		
W 24			T 24			S 24		
W 25			F 25			M 25		26
T 26			S 26			T 26		
F 27			S 27			W 27		
S 28			M 28			T 28		
S 29			T 29			F 29		
M 30			W 30			S 30		
			T 31					
18	work days excl. 4 Sat.		21	work days excl. 4 Sat.		19	work days excl. 5 Sat.	



Anita Dawes

Ice Spectroscopy, Scattering and Levitation: A New Laboratory Perspective

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Microscopic icy dust grains play a crucial role in the chemical evolution of dense molecular clouds and are a vital component in **star and planet formation** in the interstellar medium.

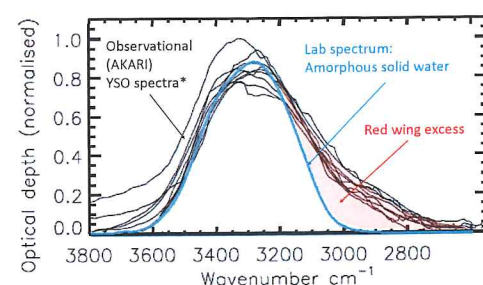
However little is known about how or whether **dust grain size, structure and composition** influence the physical and chemical properties of the ice mantles that accrete upon them.

Since most of what we know about the physical and chemical properties of icy grain mantles in dense molecular clouds comes from direct **observation** and via comparison of infrared absorption features with **laboratory spectra**...

...This raises an important question →

Are
ices grown
in the laboratory
representative of
ices in the
interstellar
medium

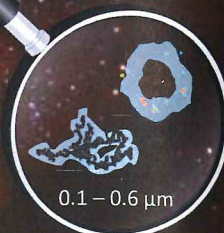
Discrepancies between Lab and Observations: the 3 μm H_2O ice absorption band profile



- The 3 μm (3333 cm^{-1}) interstellar OH stretch band profile exhibits a **red wing excess**
- This has not been reproduced in the laboratory
- Suggested causes are
 - Other molecular species (e.g. methanol)
 - Aromatic and aliphatic carbonaceous grain CH stretches
 - Grain size and shape effects**



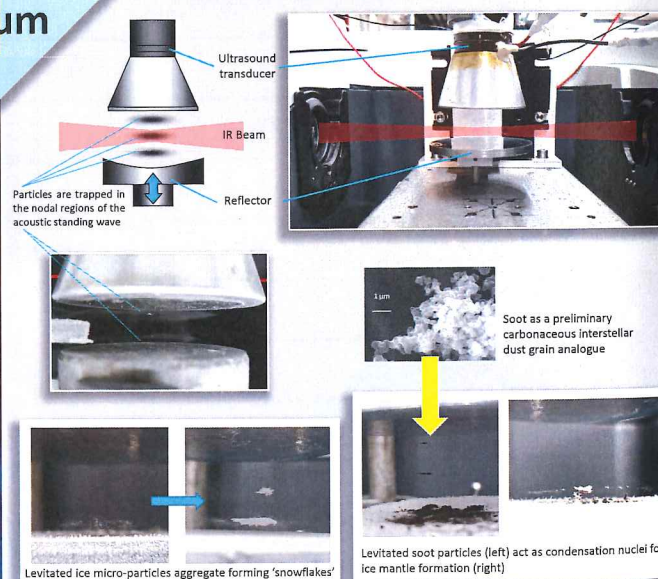
1-2 cm

0.1 - 0.6 μm

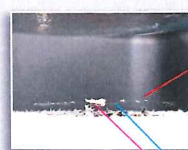
Lab ice analogues VS Icy grains in space

- Typically polished metal/crystal substrate
- Flat cm^2 surfaces
- Carbonaceous/silicate
- Possibly fractal-like
- 0.1 - 0.6 μm

A novel laboratory technique: Acoustic levitation



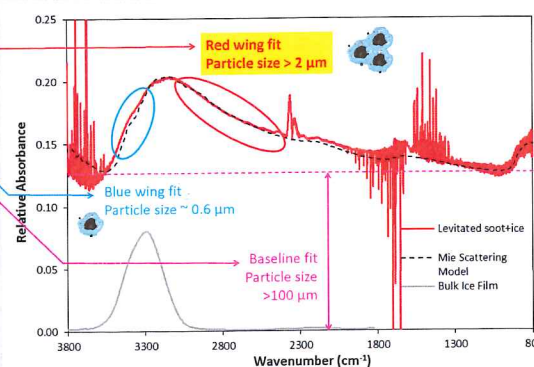
First laboratory results: an answer to the red wing problem?



Icy soot particles levitated in the acoustic trap.

Infrared spectrum of the levitated particles above (red), fitted with a Mie scattering model (dashed black) and compared to a lab spectrum of an ice film on a substrate (grey).

A sub micron sized 'cloud' of particles aggregate to form micron sized particles which in turn aggregate to form the larger mm-sized in the centre



- Mie scattering (spherical particle) model best fit with a tri-modal distribution of crystalline ice particles:

Particle Size (μm)	0.6	2	100
Relative number density	100	10	0.05
Spectral contribution	Blue wing	Red wing	Baseline

Extended red wing:

- Strikingly comparable to observational spectra
- Well fitted with a Mie scattering model
- Indicative of icy grain aggregation (micron sized particles)

Work in progress...

Further development of the acoustic trap to control ice temperature (amorphous vs crystalline) and composition, dust structure and composition (silicate vs carbonaceous) and investigate the factors that govern aggregation

... and compare with observations

ASTRID2 Beamtime!

09/04/18

Dates I was there:

09/04 - 12/04

Set up + start of Spontelectric week
Spontelectric week 11/04 - 18/04

17/04 - 23/04

Rachel's week I 19/04 - 23/04

16/04 - 28/04

Rachel's week II 16/04 - 20/04
My week 21/04 - 28/04

Rachel's week

Pure CO_2 irradiated + unirradiated

Pure NH_3 " "

$\text{NH}_3 + \text{CO}_2$ " "

My week → P.T.O.