

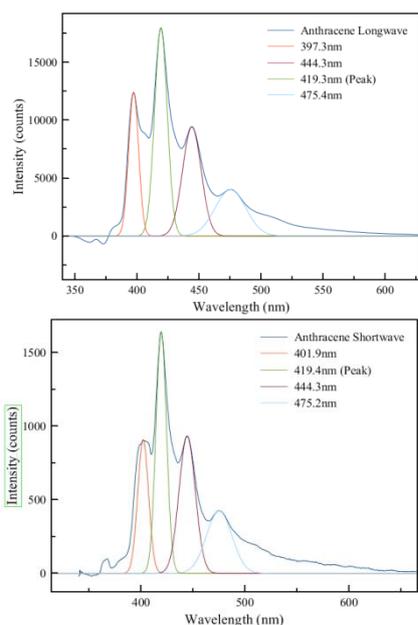
## Preliminary Results

### Long/Short Band Waves

The first investigation used long wave and short wave UV light with the USB 2000, to determine whether the substance responded better to longer or shorter wavelength ranges. Short waves have higher energy, meaning more of the higher energy photons are released. This means less of the lower energy/higher wavelengths are emitted.

The PAH Polymer blocks that were analysed were;

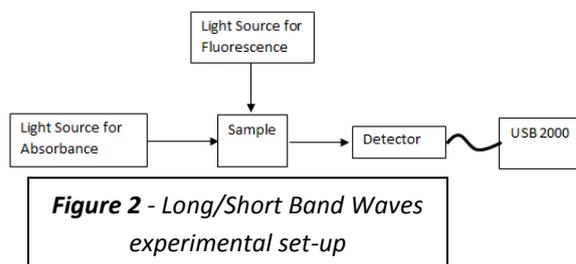
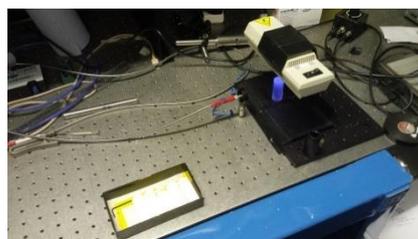
- Anthracene
- Chrysene
- 1,2,5,6 Dibenzanthracene
- Coronene
- Picene
- Phenazine



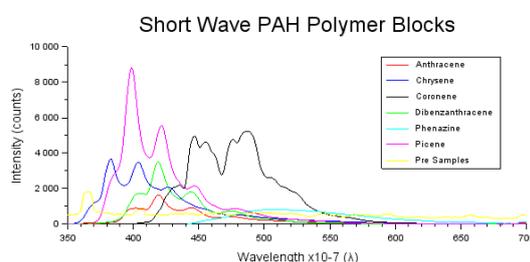
**Figure 1** – ‘Magic Plot’ graphs indicating the peaks in the Anthracene spectrum

### Emission Spectra

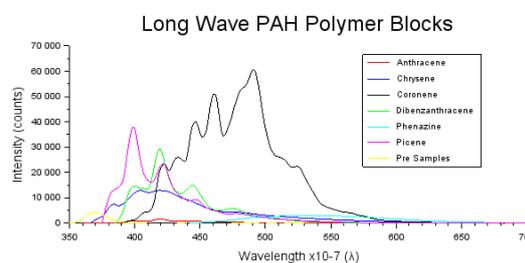
Emission spectra were initially taken using a lamp with a long wave and short wave mode. The long wave mode emitted light over a wide range of 300-350nm, while short wave produced a peak below the range of the detector. The manufacturer notes the peak of the short wavelength mode to be 257nm. The results that were recorded are shown in (**Figure 3a and 3b**).



**Figure 2** – Long/Short Band Waves experimental set-up



**Figure 3a** – Short wave light source emission spectra



**Figure 3b** – Long wave light source emission spectra

Long and short band wave measurements were taken for all PAH samples.

Conclusions revealed that the shorter wavelength excited the substance more. However, long wave emissions were of higher intensity than the short wave. This could be due to the intensity of the light being applied, which cannot be measured for the short wavelength due to being unable to detect the emitted light. *Magic Plot* was used to plot the PAHs which enabled further analysis of the individual peaks of the spectra. For a small area of the investigation, it is necessary that these peaks may be compared with online sources in

order to determine the chemical compound structure of the material.

Phenazine was the one PAH polymer block that had a very broad emission peak, unlike any of the other polymers. It was concluded this arose from the sum of smaller, indistinguishable peaks in the spectrum.

Why did the results seem to be shifted by 20nm?

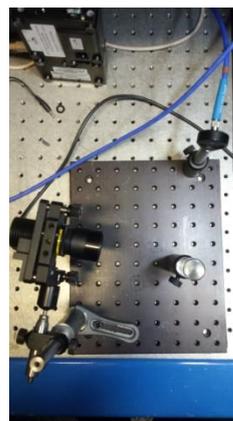
All of the spectra gained using the long/short band wave technique appeared to be, on average, 20nm shifted from the reference spectra. This occurred due to a number of reasons; It was believed broadening played a large part in the error as the sample was excited by a large range source. The shortwave UV light however, was too low for the spectrometer to analyse. It was unable to accurately detect its low wavelength of 257nm. A more precise source of light was needed.

Another reason for the shifting was due to the reference spectra being in solution. The polymer blocks that were analysed are in a matrix form. I.e. A differently arranged polymer structure.

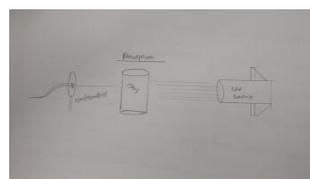
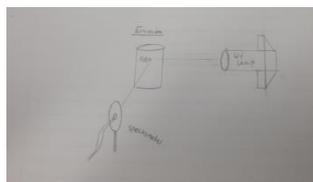
Changing Intensity, Calculating Distance

Other investigations have involved the analysis of the PAHs with UV emission and absorption using a UV lamp of varying intensity having a broad wavelength peaking at 365nm. It was possible to determine the maximum separation distance between the spectrometer and the PAH polymer block using emission and absorption spectroscopy (**Figure 4a and 4b respectively**). This has been achieved by obtaining a spectrum of the sample at maximum intensity and then decreasing the intensity of the UV light on the object until the minimum intensity spectrum is gained, before the substance becomes indistinguishable.

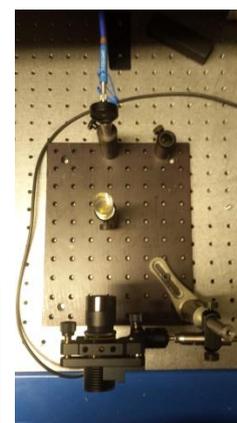
The change in intensity of light applied to the substance simulates the increased distance between the sample and the spectrometer.



**Figure 4a** – UV light Emission spectroscopy experimental set-up



**Figure 4b** – UV light Absorption spectroscopy experimental set-up



To calculate the maximum distance between the sample and the spectrometer, the inverse square law was used (**Equation 1.0**), and results (**figure 5**) were obtained for the maximum separation distance;

**Equation 1.0**      
$$X = \sqrt{\frac{I_{max}}{I_{min}}} * D$$

**X** = Maximum distance achieved before results become indistinguishable.  
**D** = Distance of set up (from spectrometer to sample). *Emission = 12.5cm, Absorption = 9.5cm*  
**I<sub>max</sub>** = Maximum intensity before saturation.  
**I<sub>min</sub>** = Minimum intensity before results become indistinguishable.

<u>Emission</u>	
Sample	Distance (cm)
Anthracene	115.1
Chrysene	122.1
1,2,5,6 Dibenanthracene	188.8
Coronene	131.4
Picene	46.6
Phenazine	41.2

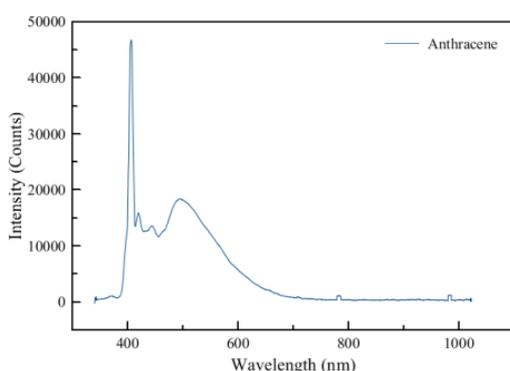
<u>Absorption</u>	
Sample	Distance (cm)
Anthracene	12.40
Chrysene	11.09
1,2,5,6 Dibenanthracene	10.94
Coronene	10.79
Picene	10.14
Phenazine	10.11

**Figure 5** – Maximum distance achieved before results become indistinguishable

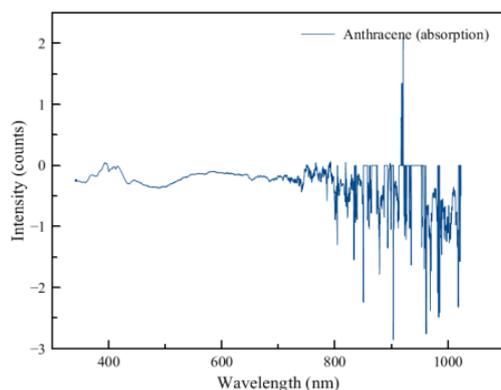
Observing Polymer Blocks with a Blue Laser

A blue laser was used, emitting a steady wavelength of 405nm, with a higher precision than the longwave/shortwave UV lamp. The set up was identical to the previous investigation for the UV lamp.

The results produced by this contained a large peak at 405nm due to reflection. The general spectrum consisted of higher wavelength emissions than the UV lamp. The reason for this is that the lower energy of applied light is more likely to give low energy emissions than when high energy light is applied to a sample.



**Figure 6a** – Anthracene UV laser emission spectrum



**Figure 6b** – Anthracene UV laser absorption spectrum

These initial results provided reference spectra for the samples that will be made use of in solution during future experiments, allowing us to quickly identify the affect solvents have on PAHs. Ignoring the background noise, the negative absorbance on **Figure 6b** results from light being heavily scattered

around the PAH polymer block, and in fact a higher concentration of light hitting the spectrometer than initially.

What next?

**Band Gap**

From all of the spectra gathered it is possible to determine the energy band gap of the material by considering the main emission peak, assuming the PAH is excited by its optimum wavelength. The energy band gap can then be obtained from **Equation 2.0**;

**Equation 2.0**      **Band Gap (eV) =  $\frac{1240}{\lambda}$**

**Alternating Concentrations of PAHs in solution**

Further investigations will be using PAH powder substances in solution and determining how changing the concentration of the substance affects its spectrum. For example, Anthracene dissolved in Cyclohexane. This will be completed by beginning with a known concentration of PAH in solution and increasing the sample–solution ratio. The concentration of the solution will be recorded at the point where the spectrum becomes indistinguishable from the reference spectrum (with the reference being the spectra of PAH polymer blocks). This technique will begin with the analysis of Anthracene. If this proves a success, the other PAHs (that were examined as PAH polymer blocks), will be identified in solution at a later date.

**Alternating Temperatures of PAHs in solution**

Mixing the substances into water and then freezing the solution rapidly using liquid nitrogen, is another step to take. This will enable spectra to be gained for when PAH particles are cooled to extremely low temperatures and behave as particles in ice – simulating the environments of interstellar space and comets. Compressing the hydrocarbons into frozen carbon dioxide could be another area to consider, which simulates the frozen poles of Mars.

**Please Note:**

**The results shown in this document are only a small fraction of the work that has been completed to date.**