due: 15/12/14

Polycyclic Aromatic Hydrocarbons in Environmental and Space Science – Project Plan

Progression

	14 Week Project												
Task Description	**1** - (26/1/15)	**2** - (2/2/15)	**3** - (9/2/15)	**4** - (16/2/15)	**5** - (23/2/15)	**6** - (2/3/15)	**7** - (9/3/15)	**8** - (16/3/15)	**9/10/11** (23/3/15 -19/4/15)	**12** - (13/4/15)	**13** - (20/4/15)	**14** - (27/4/15)
Chemical Preparation												
Obtain spectrum Athracene/cylone & meth/eth												
Obtain spectrum Perylene/SDS & diclmeth												
Re-run with alternaing temperatures												
Re-run with alternating concentration of solution												
Compare results to data of materials in plastic												
Obtain spectrum Pyrene/Ethyle Acetate & cylone/diclmeth												
Obtain spectrum Phenanthrene/cyclone & toluene												
Re-run with alternaing temperatures												
Re-run with alternating concentration of solution												
Compare results to data of materials in plastic												
Compare results and discuss problems												
Allow time to repeat/change any investigations if required												
Discussion - why temp, dilute solution and band gap change												
Compare all spectral data; any improvements?												

Required Resources

Equipment

- Spectrometer (USB 2000)
- White and UV light source
- Quartz cells, pipettes and spatulas
- All safety equipment (gloves, mask, glasses)

Materials

- Anthracene (powder form)
- Anthracene (plastic form)
- Perylene (powder form)
- Perylene (plastic form)
- Ethanol (solution)
- Methanol (solution)
- Cyclohexanone (solution)
- SDS (Micellar solution)
- Dichloromethane (solution)
- Pyrene (powder form)
- Phenanthrene (powder form)
- Ethyl Acetate (solution)
- Toluene (solution)
- Sulphuric acid (solution)

Should work proceed faster than expected

Repetition of the investigations should be completed as well as any alterations that are deemed appropriate. Also, analysis of the PAH molecules as solids suspended in oil could be considered. For example using Polysorbate-80 (Tween-80).

Should work proceed slower than expected

If experiments take longer than first anticipated, Anthracene and Perylene should be concentrated on as these are the most interesting of the substances. The other PAHs should be re-introduced to investigations, if time becomes available.

Milestones

At the end of each week (numbered points below), the tasks that must be completed are as follows;

1. Chemical preparation of all mixes of substances and solution completed in order to begin.
2. Finishing chemical preparation and gathering first set of spectra obtained for Anthracene powder and Perylene in solutions.
3. Results next obtained for differing temperatures and alternating concentration of solutions for Anthracene and Perylene. How the concentration of the solution varies the data and why.
4. Compare all of the data from the previous two points as well with Anthracene and Perylene in plastic. Spectra obtained for Pyrene in solution.
5. Spectra obtained for Phenanthrene in solution. Re-running Pyrene and Phenanthrene with alternative temperatures.
6. Re-running Pyrene and Phenanthrene with different concentrations of solutions.
7. Compare Pyrene and Phenanthrene to in plastic.
8. Compare results of all data gathered discussing any problems that can be rectified.
9. Problems are discussed and confirmation gathered of which if any, results need to be changed/repeated.
10. Conclude with discussion. Why has there been a change in the spectra for different temperatures, a different concentration of the solutions. Comment on energy band gaps and why these are different.
11. Compare all spectra and suggest improvements for repetition if possible. A discussion into what other experiments would be useful to complete if more time on the equipment was available.
12. Start of results that have been altered/repeated. Both this week and week 13 are also run-over times; taking into consideration time that may be used if not all of the objectives are completed before Easter.
13. Completion of results which have been altered/repeated.
14. Compare all spectral data gathered from investigation, and completion of report and presentation.

All substance analysis is to be completed with UV and White light sources for both emission and absorption experiments. Also consideration of some of the problems with using solvents as opposed to plastics and why we wish to change the concentration and the temperatures are accounted for. Weeks 9/10/11 is the Easter period. It has been accommodated for and therefore analysis of results with possible repeat of experiments can be completed then.
Experiments show that anthracene is easily dissolvable in cyclohexane. However, this is too toxic for us to deal with so it is possible to use methanol and ethanol. Experiments show that phenanthene may also be dissolved in cyclohexane too, but as this is a toxic solution it may be possible to use cyclohexanone. The initial concentrations of solvents will be 200mg/L. These concentrations will be changed throughout the investigation. It should also be noted that the concentration of the solutions must be below 1600mg/L in order to ensure reabsorption is negligible. This example is based off anthracene from source; *(http://pubs.acs.org/doi/pdf/10.1021/j150619a022).* In order to purify, clean and sterilise the pipettes, quartz cells and spatulas, sulphuric acid will be used.