

**Title of the project** : **Synthesis and transformations of a few anthracene derivatives – A green perspective**

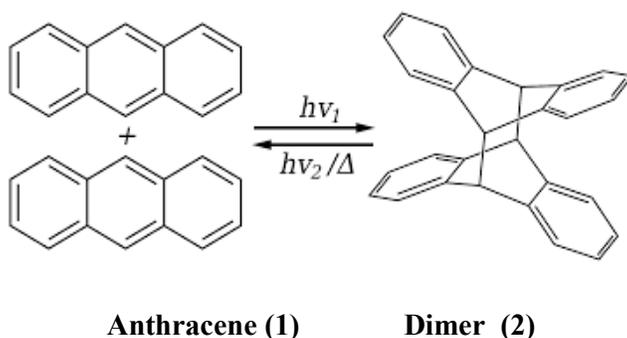
**Amount allocated** : **Rs. 3,30,000/- (UGC Reference No. F. 1553-MRP/14-15/KLCA009/UGC-SWRO dated 04/02/2015)**

**Principal Investigator** : **Dr. V Santhi**  
**Asst. Professor in Chemistry**  
**Govt. Victoria College, Palakkad**

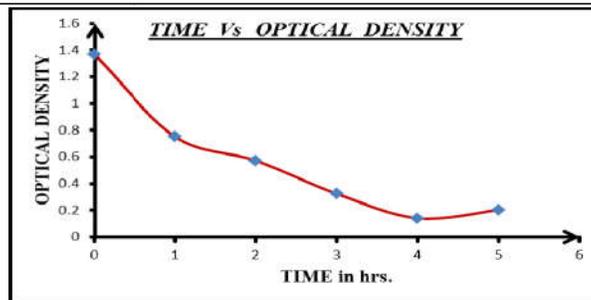
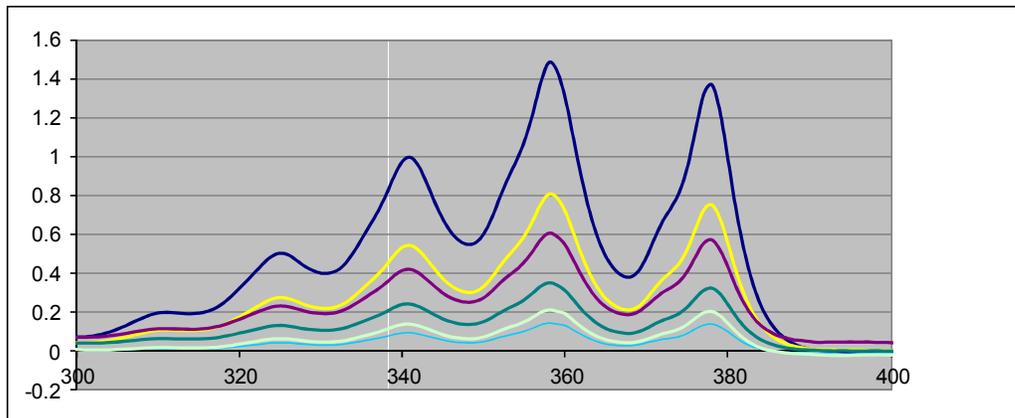
### Summary of the Project

Inspired from the nature, certain photoactive molecules undergo light induced chemical reactions by storing solar energy in the chemical bonds. Here we have used anthracene dimerization process to harvest solar energy.

Anthracene is a solid polycyclic aromatic hydrocarbon consisting of three fused benzene rings derived from coal-tar or other residues of thermal pyrolysis, with molecular formula  $C_{14}H_{10}$  having molar mass of 178.23. Anthracene has the ability to photo dimerise with irradiation by UV light. This results in considerable changes in the physical properties of the material. The dimer is connected by two covalent bonds resulting from the [4+4] cyclo addition. Photo dimerization of anthracene is a reversible reaction so the dimer reverts to anthracene thermally or with UV irradiation below 300 nm.

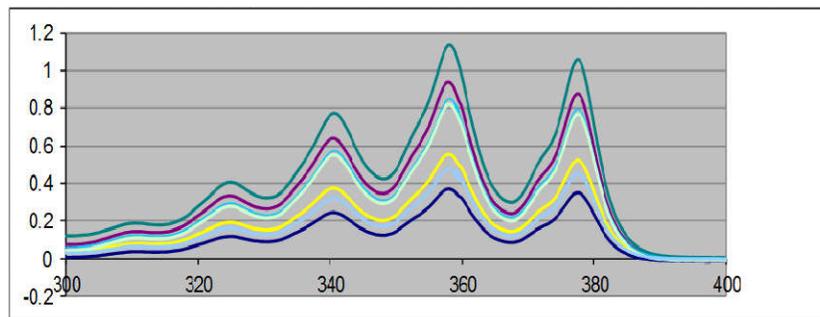


In the context of literature data available on the dimerisation of anthracene, in this project studied the dimerization of anthracene in greener method (using sun light) and to compare its data with that of controlled method (using UV reactor). The reaction was monitored using UV spectra

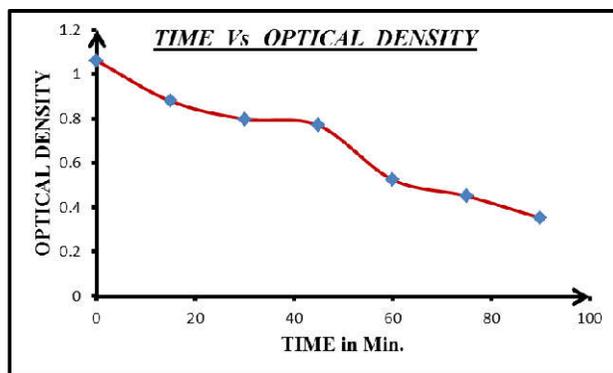


From above data, it can be seen that the absorption / optical density value at 378 nm decreases as time increases i.e., conversion of anthracene into its dimer occurs upto 4<sup>th</sup> hr. and at 5<sup>th</sup> hr., there occurs an increase in the optical density. The 4<sup>th</sup> hr. may be the saturation point of the reaction and beyond that, there may occur the reverse reaction from dimer to anthracene. It may be due to the effect of heat (due to IR radiation) from the sunlight.

Under UV reactor conditions it can be seen that unlike green reaction, there is a decrease in the optical density as the time increases i.e., there occurs a dimerization reaction (forward reaction) and no any reverse reaction. It may be due to the fact that in the UV reactor only UV radiation of particular wavelength is coming and no IR radiations (absence of the heat content), which may be responsible for the reverse reaction.



**The UV absorption spectra of anthracene for each 15 Min. (Conventional method)**

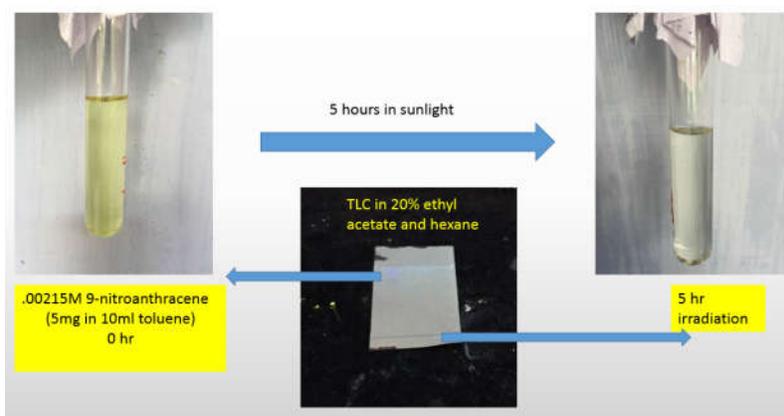


**A plot of TIME ( in minutes.) against O.D at 378 nm**

From the studies it was found that the dimerization reaction under sunlight happening  $1/5^{\text{th}}$  times that of under controlled method with a power of 125 W. It is very interesting to note that the sunlight have the reasonable content of UV radiation and can be used for such solar energy conversions. It can be observed that, as the polarity of the solvent increases % conversion of anthracene decreases. Hence we can say that the rate of anthracene dimerization is inversely proportional to polarity of the solvent and in our observations, toluene is found the best solvent for dimerization reaction.

Further, we thoroughly investigated the various factors like concentration, solvents, and substituents influencing the dimerization process. Since it is a first order reaction the percentage conversion of anthracene increases with increase in the concentration of anthracene. It is interesting to note that nitro anthracene shows a high reactivity towards the dimerization process under sunlight when compared with that of anthracene.

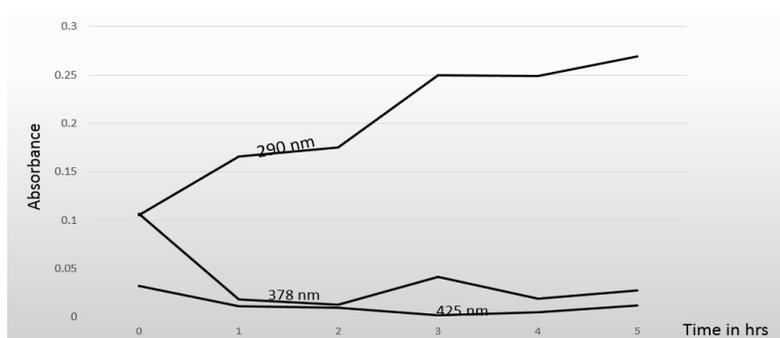
#### Photochemical studies of 9-nitroanthracene



## 9-nitroanthracene in toluene at 0 hr and 5hrs of irradiation

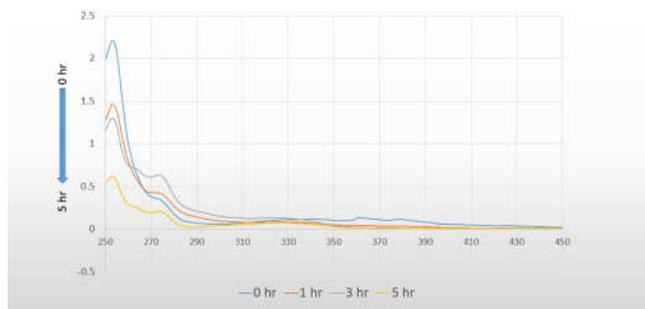


UV-Vis spectra of 9-nitroanthracene in toluene under sunlight at  $t=0$ ,  $t=1$ ,  $t=2$ ,  $t=3$ ,  $t=4$  and  $t=5$

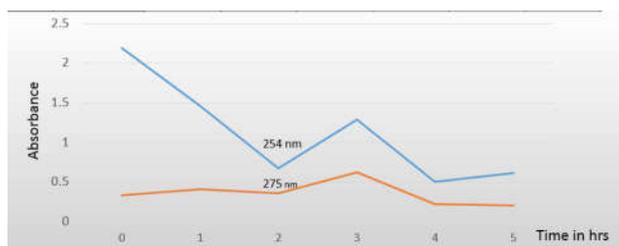


Plot of Time Vs Absorbance of irradiated 9-nitroanthracene in toluene

At 290 nm, it can be observed that the absorbance or optical density is increased as the time of irradiation is increased. It can be explained as 9-nitroanthracene is converted into another compound which has higher absorbance at 290nm. The characteristic peak of anthracene is at 378nm. The absorbance is decreased from zero hour to five hours. So the formed product will be having different absorbance character from that of anthracene. It can be observed from the plot that at 5th hour of irradiation, the peaks of anthracene is almost minimal.



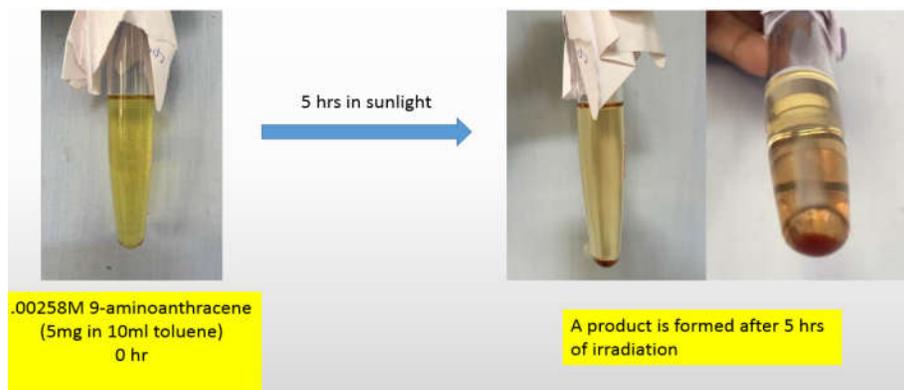
UV-Vis spectra of 9-nitroanthracene in chloroform under sunlight from  $t=0$  to  $t=5$

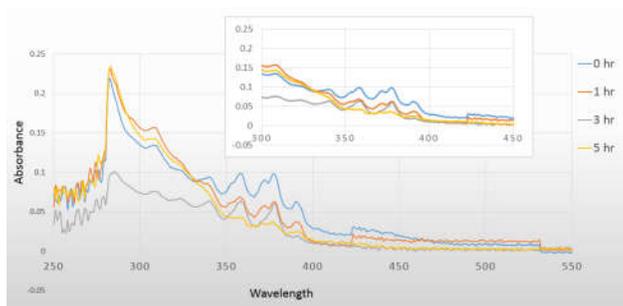


Plot of time Vs absorbance of irradiated 9-nitroanthracene in chloroform

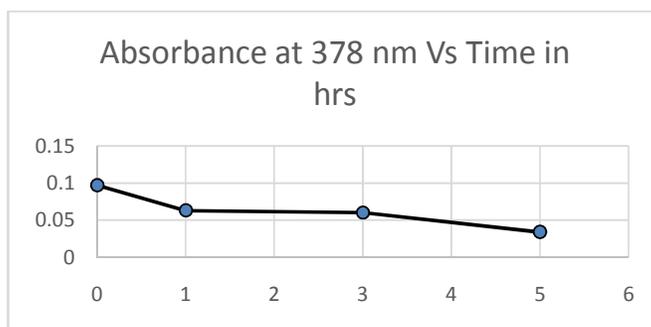
The product formed is anthraquinonemonoxime plus nitric oxide as the IR absorption peaks can be assigned for those. Reasoner suggested the possibility of formation of this compound when 9-nitroanthracene is irradiated under sunlight.

Photochemical studies of 9-amino anthracene





UV-Vis spectra of irradiated 9-nitroanthracene in toluene at t=0, t=1, t=3, t=5



Plot of absorbance at 378nm Vs time of irradiated 9-nitroanthracene in toluene

The spectrum shows that a new product is formed which is entirely different from anthracene and 9-nitroanthracene as their characteristic peaks are absent. From the previous studies and the possibilities from the color of the compound it can be said that the formed product may be azo or nitroso compounds which absorb at these ranges.

Our investigations suggest that the dimerization reaction can be used to harvest and store solar energy. It can also be extended to other industrial chemical reactions for solar energy harvesting process to eliminate the need to burn fossil fuels. Further investigation is required to fabricate energy storing devices based on such kind of photochemical reactions.

## Publications

1. Arifa P.V., Liya T., Revathy S., Shanthil M and Santhi V. study on photochemical dimerization of anthracene., CTRIC Book of abstracts, OP 08, pp 16-17 (Organized by Dept of Applied Chemistry, CUSAT, Kerala India.
2. One paper under preparation.