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August 12, 2010

Solvent Effects on the Absorption Spectrum of 9-Nitroanthracene

PERSONAL EXPEREINCE

The ACS SEED Program was a great opportunity as a high school student who has taken chemistry. I had the opportunity to work with a group of college graduates and help them to complete part of their research work. Since this an internship, I was able to learn concepts and techniques used in a chemistry laboratory setting and still have a summer job. As part of this internship I prepared a poster about what I learned and some details about the research I was working.

Photophysics of 9-Nitroanthracene

In taking part of Dr. Carlos Crespo research team, my assignment was to obtain the absorption spectra of 9-nitroanthracene in acetonitrile and cyclohexane. 9-nitroanthracene is a polycyclic aromatic compound found in the environment, which is produced from incomplete combustion processes and atmospheric nitration reactions (Figure 1). We prepared solutions of 9-nitroanthracene to record its absorption spectrum in two different solvents of different polarity using a UV-Vis spectrometer. Before taking the absorption spectra in these solvents, the purity of 9-nitroanthracene was verified by injecting the solutions in a HPLC system.

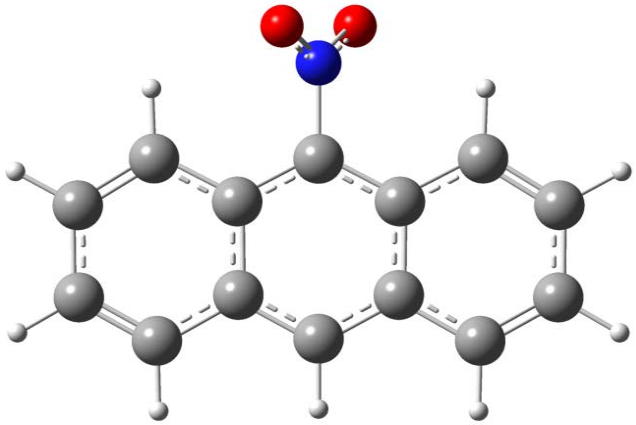

Figure 1. Molecular structure of 9-nitroanthracene. The 9-nitroanthracene is a polycyclic molecule is composed of 14 carbon atoms (in gray), 9 hydrogen atoms (in white), two oxygen atoms (in red) and 1 nitrogen (in blue).

INSTRUMENTATION

HPLC: High Performance Liquid Chromatography

This is a machine allows solvents to be pumped through a column in order to separate chemical compounds based on elution times due to their characteristic affinities to the stationary versus the mobile phases. The solvent that is pumped through the column is called the mobile phase. The column contains the stationary phase. The solution containing 9-nitroanthracene was injected into the injection port and was directed into the column by the mobile phase. A photodiode array detector is used to obtain the absorption spectra of the chemical compounds that elutes from the column with different retention times.

Ultra Violet-Visible Absorbance Spectrometer

This machine tells us how much light is being absorbed or transmitted by the solution. It plots the amount of light absorbed by the solution versus the wavelength of the light source. The absorption spectrum is a physical property that uniquely identifies a given chemical compound.

RESULTS AND DISCUSSION

Figure 2 shows the absorption spectra of 9-nitroanthracene in acetonitrile and in cyclohexane from 270 nm to 500 nm. The y-axis represents how much light of a particular wavelength is being absorbed by the solution. The x-axis represents the wavelengths of the light source used to simulate the sunlight. Figure 2 shows that 9-nitroanthracene absorbs light in the spectral region between 300 to 450 nm. This is

important because the sunlight reaching the earth's surface occurs at wavelengths above ~290 nm. Thus, 9-nitroanthracene is able to absorb sunlight and is prone to degradation and formation of new chemical compounds in the environment. Figure 2 shows that the absorption spectrum of 9-nitroanthracene in acetonitrile is shifted to longer wavelengths relative to that in cyclohexane. In addition, the absorption spectrum of 9-nitroanthracene shows more structure in cyclohexane than in acetonitrile. These results shows that different solvents have different interactions with 9-nitroanthracne.

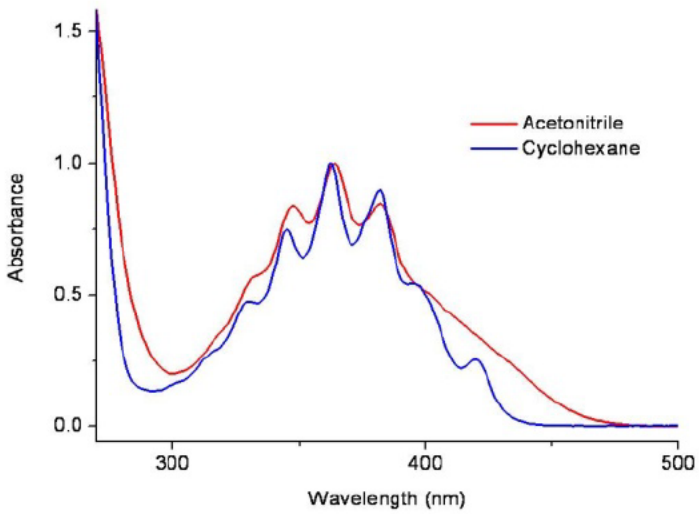

Figure 2. Comparison of the absorption spectrum of 9-nitroanthracene in acetonitrile and cyclohexane.

Absorption spectrum of 9-NA in cyclohexane: Dependence on Concentration

Concentrations of 9-nitroanthracene in cyclohexane used are $1.67*10^{-4}$ M, $3.33*10^{-4}$ M, $5.00*10^{-4}$ M, $6.67*10^{-4}$ M, $8.33*10^{-4}$ M and $1*10^{-3}$ M. The absorption spectra of 9-nitroanthracene at different concentration is shown in Fig. 3. As Fig. 3 show, no changes in the absorption bands are observed with an increase in concentration shown that aggregates are not been formed at concentrations as high as 10^{-3} M in cyclohexane solutions.

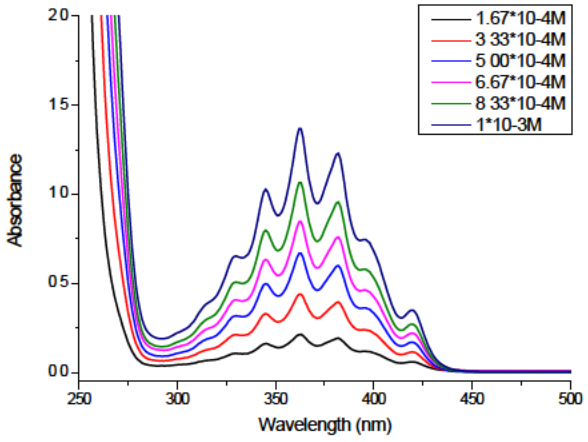

Figure 3. Absorption spectrum of 9-anthracene as a function of concentration.

FUTURE WORK

This work shows that that absorption of sunlight can potentially transform 9-nitroanthracene in the environment. However, how 9-nitroanthracene is chemically transformed by light absorption and what products might be formed as result of this transformation is unknown. As part of the ACS SEED Summer Program we characterized the absorption properties of 9-nitroanthracene in cyclohexane acetonitrile solvents using absorption spectroscopy. Future work will be aimed at quantifying the yield of degradation of 9-nitroanthacene and at characterizing the major products formed after light absorption in different solvents used to mimic the solvent environment in which nitro-PAHs are found in nature.

ACKNOWLEDGEMENTS

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