Conversion of photostable Zn-MA crystals to photoreactive

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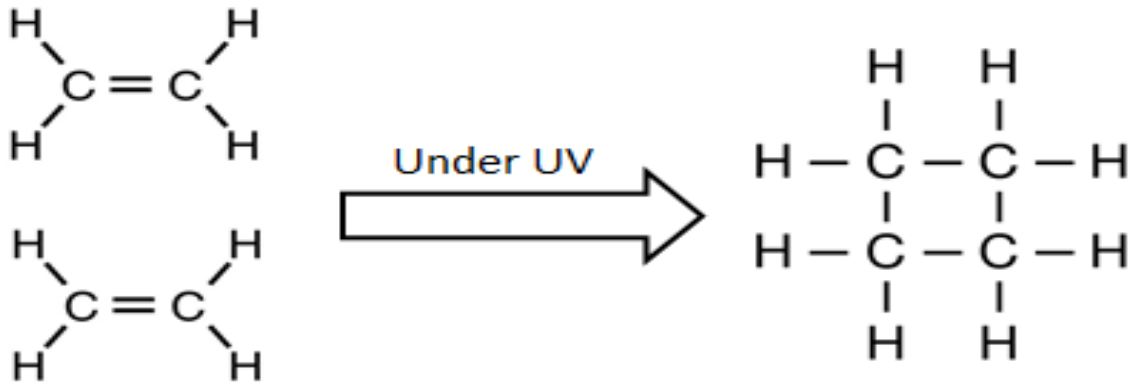
Background Information

What is photodimerization?



Two pairs of C=C double bonds form a cyclobutane structure

Schmidt's criterion for photodimerization to occur:

1. Potentially reactive C=C double bonds need to be aligned parallel
2. Distance between the C=C double bonds need to be 4.2Å or less

What is Crystal Engineering?

- Using one's understanding of structures at a molecular level
- To synthesize solid state structures with particular characteristics to serve different purposes.

Purpose of Research

Problem

- Skin cancer caused by overexposure to UV radiation is increasingly plaguing the world

- Kills over 2,500 people in the United Kingdom (UK) every year

Solution

How to reduce number of skin cancer cases?

- Raise the awareness of people's exposure to UV rays
- Synthesize photoreactive Zn-MA crystals which can be placed in accessories (ie. watches or phone covers)
- These crystals turn from transparent to opaque under exposure of UV light, which alerts the users

Methodology

Synthesis of Zn-MA crystals

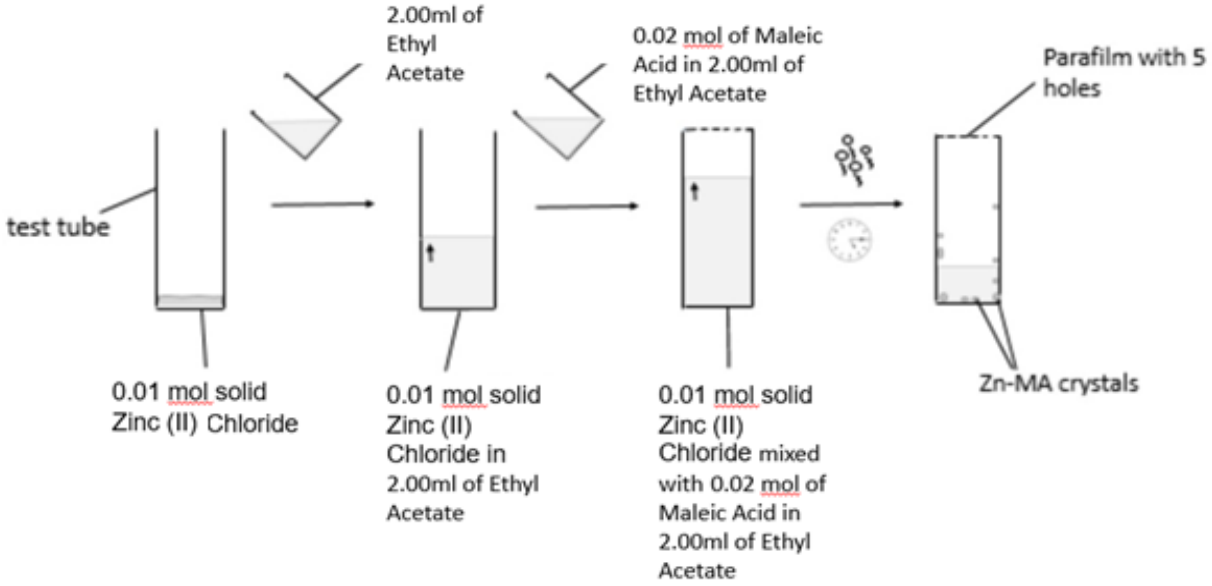
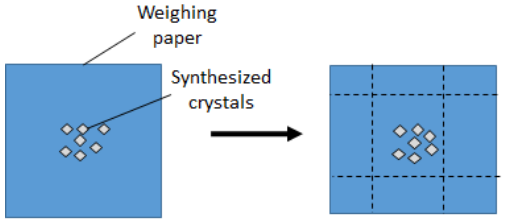


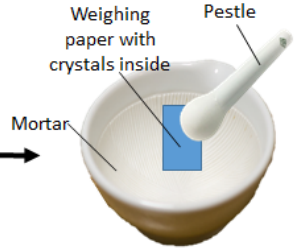
Figure 2. Slow Evaporation Method

Methods to convert photostable Zn-MA crystals to photoreactive

Grinding



Fold weighing paper along dotted lines to secure crystals inside



Grind crystals at room temperature using mortar and pestle for 10 minutes, until crystals are powdery.

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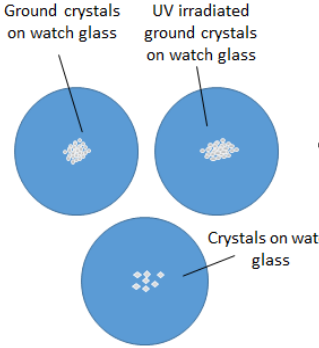
Heating



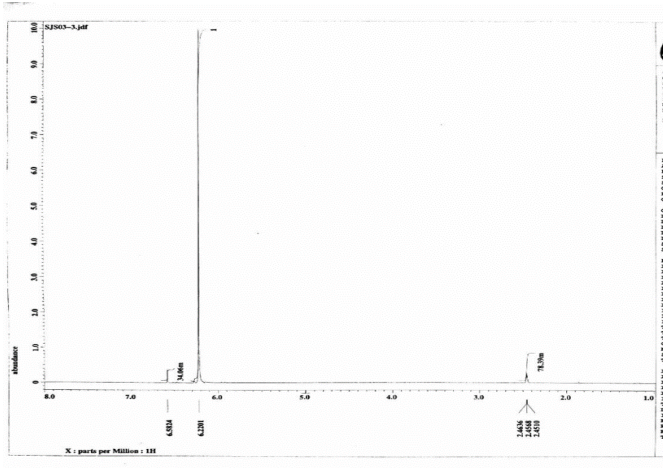
Crystals heated on a heating plate for 20 minutes in total. Temperature was 80°C at first, then was increased by 10°C every 5 minutes.

Helps to realign the C=C bonds within the crystal such that it fulfil Schmidt Criterion and can be converted to a photoreactive crystal

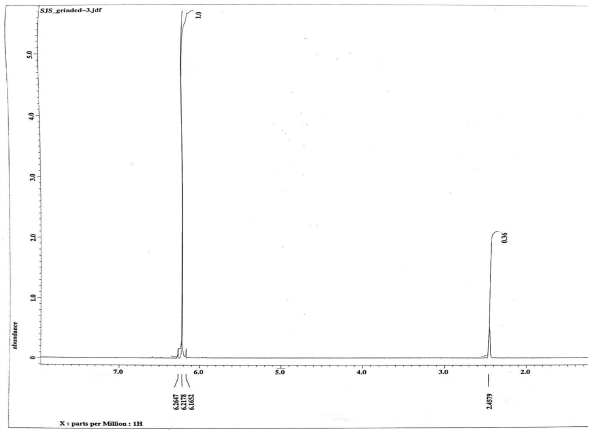
Analysis: NMR spectroscopy was performed on the synthesized crystals

Results and Discussion

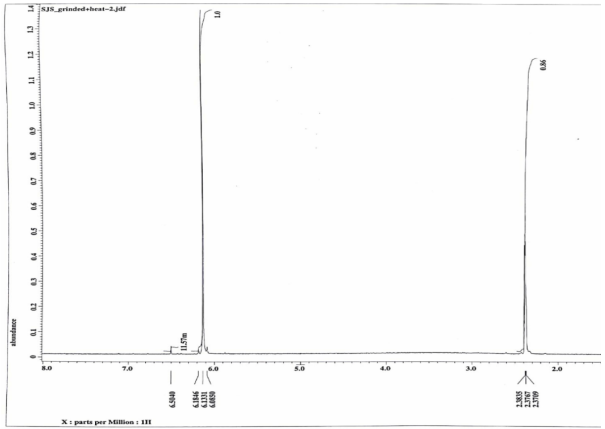
NMR Spectrums



Spectrum 1.1: NMR Spectrum of Synthesized Crystals



Spectrum 1.2: NMR Spectrum of Ground Crystals



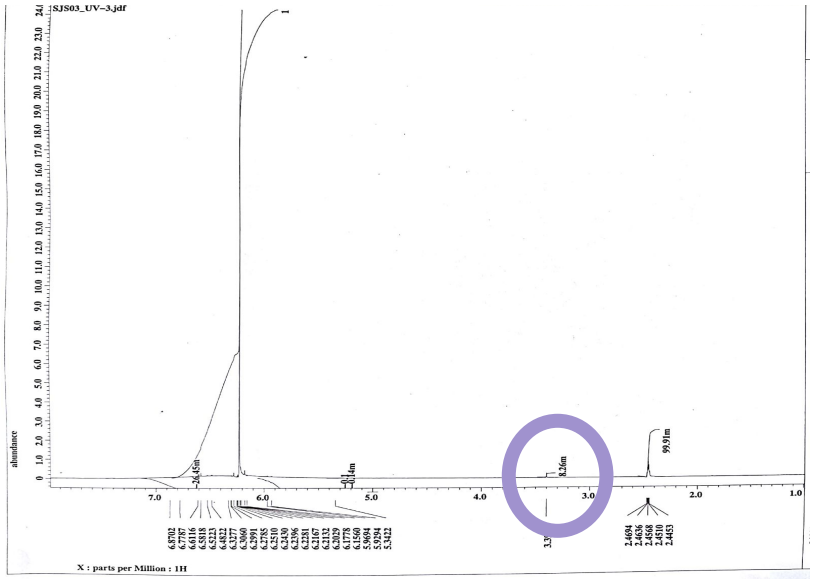
Spectrum 1.4: NMR Spectrum of Heated and Ground Crystals

Characteristics peaks are present at both 6.1ppm and 2.5ppm (see Spectrum 1.1)

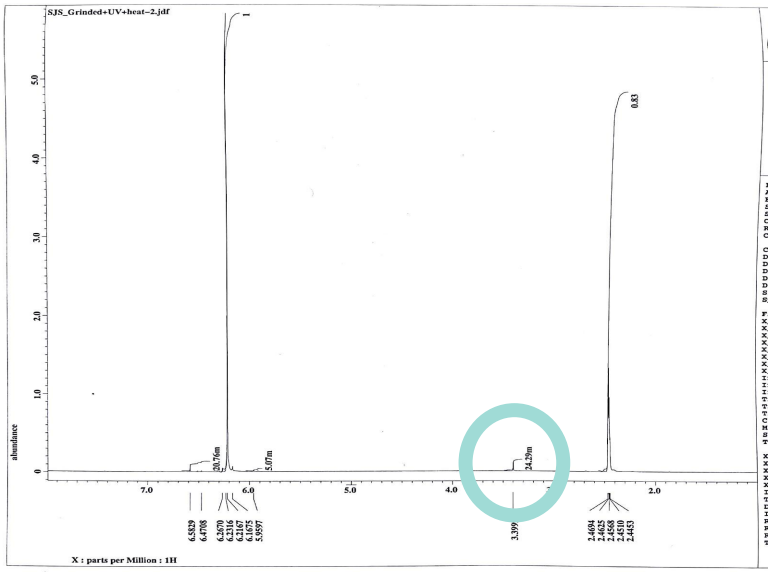
Similar characteristics peaks are present in both Spectrum 1.1, 1.2 and 1.4

Shows that these crystals are photostable

NMR Spectrums



Spectrum 1.3: NMR Spectrum of UV Irradiated Ground Crystals



Spectrum 1.5: NMR Spectrum of UV Irradiated, heated and ground crystals

New characteristic peak corresponding to cyclobutane protons at 3.4ppm

New characteristic peak corresponding to cyclobutane protons at 3.4ppm in Spectrum 1.5.

Underwent **small extent of photodimerization**

Conclusion

- Ground crystals, and ground and heated crystals are photostable, while the UV-irradiated crystals are photoreactive. It is possible that carbon-carbon double bonds were realigned through heating and grinding, but did not undergo photodimerization without UV-irradiation.
- Since the crystal was ground to powder form, visible change from transparent to opaque cannot be observed, making it unsuitable for everyday use.
- The combined effects of heating and grinding also help in increasing possibility of crystals undergoing photodimerization.

Future Work

- Crystals that underwent a small extent photodimerization only did so after 48 hours of UV irradiation. This shows that more needs to be done, such as grinding more or heating longer, to synthesize more photo-sensitive crystals that can photodimerize under sunlight which is very much less intense than UV irradiation.
- Increase the number of times and duration the crystal is ground for
- Heat crystals at a higher temperature.

Thank You :)