Conversion of photostable Zn-MA crystals to photoreactive

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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 4.2 Å 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 & Heating

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
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
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 :)